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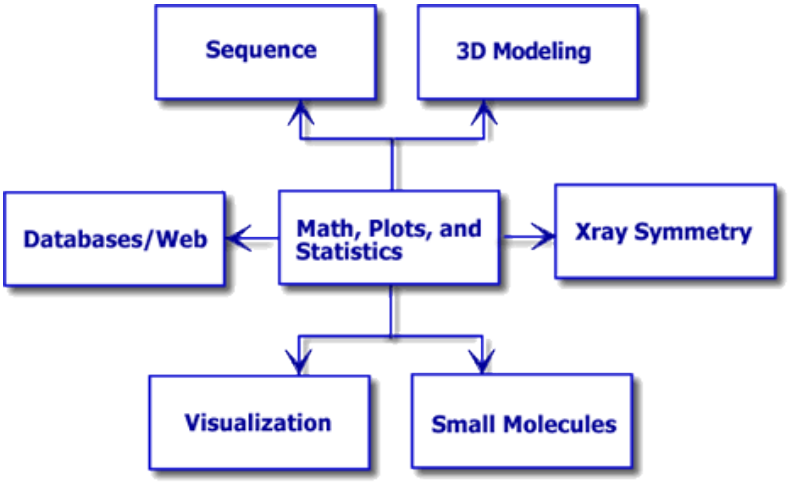
1. Introduction



ICM stands for Internal Coordinate Mechanics and was first designed and built to predict low energy conformations of biomolecules. ICM also is a programming environment for various tasks in computational structural biology, sequence analysis and rational drug design. The original goal was to develop algorithms for energy optimization of several biopolymers with respect to an arbitrary subset of *internal coordinates* such as bond lengths, bond angles torsion angles and phase angles. The efficient and general global optimization method which evolved from the original ICM method is still the central piece of the program. It is this basic algorithm which is used for peptide prediction, homology modeling and loop simulations, flexible macromolecular docking and energy refinement. However the complexity of problems related to structure prediction and analysis, as well as the desire for perfection, compactness and consistency, led to the program's expansion into neighboring areas such as graphics, chemistry, sequence analysis and database searches, mathematics, statistics and plotting.

The original meaning became too narrow, but the name was kept. The current integrated ICM shell contains hundreds of variables, functions, commands, database and web tools, novel algorithms for structure prediction and analysis into a powerful, yet compact program which is still called ICM. The seven principal areas are centered around a general core of shell−language and data analysis and visualization.

1.1. Release notes

Last Updated: Feb 03,2004 .

In this section we keep track of all the latest changes in different modules of ICM.

new table commands: group by table column; split a table column `append` a table by shared column

string //= string operation introduced Jan 27 2003

new topological representation for proteins. ribbonStyle="cylinders" Jan 26, 2003 ICM has a new algorithm to find helical axes, decide where to split a helix and draw adaptive−size cylindrical helices. It shows alpha−helices, 3/10 helices and Pi helices. From GUI display toolbar: see the submenu of the ribbon representation.

Name(ms_ swiss) returns swissprot names or an empty string. Jan 25 2003

PDB table has HETATM names and swisprot sequence IDs. Jan 26, 2003

better hbond display. Jan 23, 2003 Hydrogen bonds are shown with little spheres if they bridge two atoms represented as "balls−and−xsticks".

better skin starting from a ribbon display Jan 21, 2003 a_//DD selection is improved to include C− and N− terminal backbone atoms if ribbon is displayed. Previously, displaying skin starting from a ribbon display in ICM objects generated skin with gaps near C− and N− termini. Now this problem (as well as the skin) is "patched" :−) .

new view preferences: GRAPHICS.hydrogenDisplay . Jan 25, 2003 non−polar or all hydrogens can be hidden, see `GRAPHICS.hydrogenDisplay` . From GUI: see the Presets in the Display toolbar.

inserting rows with add table command. Jan 15, 2003 The `add` *table i_row* [*table_selection*] command will insert or duplicate rows.

Reading a chemical table from a *subset* of mol−file entries. Jan 15, 2003 Large mol/sdf−files can be indexed with the ICM `write index` tool, and a subset of these entries can be loaded into ICM as molecular objects. Now a subset of compounds can also be loaded into a chemical table.

```
read index "Chem04"
read table Chem04[{11,123,444}] # a table: pictures+properties
read mol Chem04[{11,123,444}]   # creates 3 objects
```

Finding ICMversion and the version of binary file. Jan 8, 2003 Now the program version is recorded in the binary file and can be extracted from it.

```
Version( s_binaryFile binary ) # string version of binary file
Version( s_binaryFile gui    ) # version of ICM which saved this file
```

read binary list to make a table of content for a binary file. Dec 29, 2003

```
read binary list "file.icb" name="table_of_obj_names"
```

export to mol2 format improved. Dec 29, 2003 residue names are written in upper case, N−HN bond type is fixed.

Representing PI− and 3/10−helices in alignment and sequence view. Dec 22, 2003 Pi−helices are now wider and 3/10 narrower in alignment views. They also are shown with a different color which can be edited in the icm.clr file (piRibbon and threetenRibbon)

Copying the SITE/FEATURE information upon convertion and copy object. Dec 22, 2003

montecarlo `output` option for shorter output. Dec 22, 2003 The new option in the `montecarlo` command shortens the output by displaying only the **DY** lines, as well as steps which reach any of simulation limits.

Fixed bugs Dec 20, 2003

- alignment of many identical sequences is now correct
- crashes associated with deleting maps are fixed
- selection by 'Pi' helix, code `I,` is enabled (`a_/SI`)

New funcitons for BIOMT transformations. Dec 15, 2003 The following functions can generate all BIOMOLECULES of an object:

- Nof(os_1 "bio") or Nof(symmetry) # the number of BIOMOLECULES in the current
- Select(os_1 "bio" i_biomol) # selects molecules which need to be transformed
- Transform(os_1 "bio" i_biomol) # N*12 vector with transformations.

Name of linked sequence or alignment. Dec 15, 2003

```
Name( a_molsel sequence )
Name( a_molsel alignment )
```

return an array of sequence names, or array of alignment names.

Control light with GRAPHICS.light and display new reflection. Dec 14, 2003 New real array controls the properties of light in molecular graphics. The Display toolbar has four sliders to control the light preferences. See: `GRAPHICS.light` .

Select by chain with a_Cabc . Nov 17, 2003

Fading display images in and out. Nov 17, 2003 display intensity= will dim the picture and merge it with the background.

Deleting sequences from the alingment without deleting them from the shell. Nov 9, 2003 E.g.

```
  delete sh3 only Fyn Spec  # removes sequences Fyn and Spec from alignment sh3
```

Merging grobs into one with the double−slash (//) operator Nov 9, 2003

Displaying Hydrogen Bonds between heavy atoms (X−ray style) Nov 6, 2003

fast findSymNeighbors macro to generate symmetry neighbors Nov 4, 2003

correct recognition and treatment of rhombohedral and hexagonal lattices Oct 30,2003

Selecting table rows by an array of values. Oct 23, 2003 T.number == {3 1 14} will select all rows with the `number` column equal to either 3 1 or 14. Similarly for real arrays.

new symmetry and transformation functions plus some reshuffling. Oct 17, 2003

- transform a_ i_symm_transformation [translate]
- set symmetry obj R_3_6_abcAlphaBetaGamma s_symGroup_or_i_Group
- set symmetry map i_SpaceGroupNumber

- Transform(s_group| iGroup | obj | map)−> R_12N_all_transformations
- Transform(s_group| iGroup | obj | map iTrans)−> R_12_transformation_i
- Transform(s_symbolic_transformation)−> R_12
- Transform(R_6)−> R_12
- Transform(M_4x4 or M_3x3) −> R_12_transformation
- Transform(R_12 inverse)−> R_12_inverse_transformation

- Symgroup(s_group | i_groupNumber | object | map) −> s_uniqueGroupName
- Symgroup(s_group | i_gr | obj | map number) −> i_canonicalNumber1to230

- String(R_12N transform) −> s_symbolic_transformations"

- Xyz([as_| grob]) −> M_xyz
- Xyz(M_xyz, R_3_6cell, [cell|reverse]) −>M_xyz1_to|from_fractional
- Xyz(M_xyz, obj_, [cell|reverse]) −>M_xyz1_to|from_fractional
- Xyz(M_xyz, i_symm_transformation, s_sym_group, R_6_cell [translate]) −>M_xyz_transformed
- Xyz(R_x1y1z1x2y2z3...)−>M_xyz

- Cell(as_ r_margin) −> {a b c 90. 90. 90.} # helps set symmetry

Name family of functions

- Name(os_ | ms_ | rs_ | as_ [atom | residue | molecule | object]) −> array of names
- Sarray(as_ [residue]) −> array of atom or residue strings

color grob as_ Oct 7, 2003 After voting Green for Peter Miguel Camejo, the `color` *g_grob as_selection color* was added. It finds a patch at `GROB.atomSphereRadius` around the atom selection and colors it.

read separate library files Sep 30,2003 the `read library` command has been extended to read or re−read individual library files, e.g.

```
LIBRARY.res = {"icm","/home/jack/jack.res"}
read library residue

read library atom "new.cod"
read library color "new.clr"
read library drestraint "new.cnt"
read library vrestraint "new.rst"
read library charge "new.bci"
```

GRAPHICS.displayMapBox Sep 18,2003 Parameter `GRAPHICS.displayMapBox` controls if the bounding box of a map is displayed.

superimpose by one or two atoms Aug 28,2003 the `superimpose` command has been extended to allow superposition by a single atom (e.g. superimpose a_1./2/ca a_2.//ca) or by a pair of atoms forming an axis (e.g. superimpose a_2./2/ca,cb a_2.//ca,cb).

Selections for molecules with linked sequences (a_Q) and linked alignments (a_C) July 17,2003

version 3.24 released July 9, 2003

read pdb sequence corrected to generate chain IDs consistent with read pdb July 9,2003 Now in both `read pdb` and `read pdb sequence` the numerical chain IDs are changed into literal chain IDs (`0` becomes `a` , `1` becomes `b` etc.). Example:

```
read pdb "1afb"
 a_1afb.b,c,d chains are created
read pdb sequence resolution "1afb"
 1afb_b19 1afb_c19 1afb_c19 sequences are extracted. 1.9A is resolution
```

full het−molecule names in read pdb: parsing HETNAM July 2, 2003 The names of ligands stored in the `HETNAM` records are not parsed and shown. They also are stored in ICM objects.

print bar s_ mxNumIter July 2, 2003 shell command to see progression bar Example:

```
l_commands = no
print bar " Start" 100
for i=1,100
  read pdb "1crn"
  print bar "." 100
endfor
print bar " End\n"
```

Substrings of sarrays and inverted sarrays. July 2, 2003 `Sarray` (S,3,5) extracts substrings from 3 to 5. If the order of boundaries is inverted, the strings will be inverted too.

Chemical arrays. July 2, 2003 (see also Chemical Spreadsheets below). an ICM array of objects is introduced. We called it parray (array of pointers). It will be able to carry a list of objects of different kind. The first object implemented is a *chemical* object (a.k.a. `mol` object) which can be read from an `sdf` file (see `read table mol`). Note that these mol−objects do not exist in ICM shell as individual 3D molecular objects. Function Nof will return the number of occurencies of a smart string in each molecule of an array. This iarray can be added to a table as a descriptor. Other functions to add descriptors of molecules from a `parray` are being added.

The following functions have been added to deal with molecular arrays:

keyword	description	syntax
parray	array of pointers to molecules (P)	ls parray
Parray()	returns parray of molecules	Parray(S|s smiles|mol)−>P
Nof()	returns the number of smarts in mol−array	`Nof` (*P* { `atom` | *s_smart* })
Sarray(P)	returns sarray of mol−files	Sarray(P)−>S
Smiles(P)	returns a sarray of smiles	Smiles(P)−>S
read mol	creates a separate ICM object	read mol input=String(P[i])

Name(s_ simple) function July 2, 2003 removes all non−alpha−numeric simbols from a string and replaces them by underscore. Example:

```
  Name( " %^23 a 2,3 xreno−77−butadien" simple)
```

```
23_a_2_3_xreno_77_butadien
```

improved String(rs_) function July 1, 2003 String(rs_) returns residue ranges selected. Now it breaks the range for residues which are sequential in structures but with the discontinuous numbers. Also, the function is more compact for multiple single−residue molecules. Example:

```
read pdb "1eye"
String( a_/* )
  a_1eye.a/5:50,65:274|a_1eye.2:247  # numbers break between 50 and 65
```

Chemical Spreadsheets: read table mol June 25, 2003

the `read table mol` command reads an sdf file and converts it into an ICM table. The mol−file part of each entry is stored in a separate column which is visualized as a molecular drawing. Other fields are parsed and the type is determined. The resulting table can be manipulated with in ICM−GUI and saved with the `write table mol` command.

Rarray(ali [`simple`]) June 19, 2003 symmetrical average pairwise conservation for each position in a multiple alignment.

Score(rs_ [`simple`]) June 19, 2003 linked−alignment−derived conservation score array for the selected residues. Take a Mean(`Score` (*rs_* `simple`)) to calculate an average measure of conservation.

set randomize i_newRandomSeedValue June 13, 2003 new command to reset and activate the randomSeed value in the middle of a session. It will affect all commands and functions using random values.

Trim(S_sourse, `all`) July 12, 2003 removes white space from both ends of each string in an array.

new Matrix function. June 11, 2003 To make a matrix from the shell directly, you can now provide a rarray and row−length. Example:

```
icm/def> Matrix({1. 2. 3. 4. 5. 6.}, 3)
#>M
1. 2. 3.
4. 5. 6.
icm/def> Matrix({1. 2. 3. 4. 5. 6.}, 4)
 Error>  non−matchind dimension [4] and vector size [6]
```

reading and writing csv and tsv table formats. June 1, 2003

```
read table separator="," "tt.csv"   # will now understand csv/tsv formats
```

ICM also supports extended csv format with line commends under option comment=s (for example: read table separator="," "tt.csv" comment="#"). See `read table separator...`

direct reading of individual stack conformations from compressed files. June 1, 2003 The new stacks now support direct reading of separate conformations, and the write binary method uses the compressed format as well.

read map xplor; write map xplor; read map "ccp4_format" fixed. May 30 2003 read and write in text xplor format has been fixed. Also ICM can now read more versions of the ccp4 binary maps.

Further acceleration of compress stack fast. May 22 2003 an additional step is added to the fast stack compression to speed up compression in stacks where conformations similar in energy has higher changes of being similar according to the `compare` command. Also, the conformations are now not refixed everytime a new conformation is loaded.

Selecting residues and molecules with numerical names. May 21 2003 Sometimes, the names of molecules or residues in the PDB look like an integer. Consequently ICM interprets selections looking like `a_999` or `a_/142` as selection by *number* rather than by *name* . Now to select molecules with numerical names you can use backslash, e.g. `a_\999` or `a_/\142` .

find database name=s_tableName output=s_outputFileNameRoot distance=i_MaxNofMutations . May 7 2003 find database commands was extended and new options added:

1. find database [name=s_tableName] # an option added
2. find database exact [distance=i_MaxNofMutations] [name=s_tableName] # two options added
3. find database now creates a table with results (previously it only saved the search results to a file.

Also the search result table now has a header which allows you to download and display a structure by double−clicking on the table record.

Force field: Correct torsion potential for xi3 of Methionine derived and implemented. May 1 2003 We analyzed the database of high resolution crystallographic structures and derived the new torsion potential for Methioinine. File `icm.tot` has been modified to include the new torsion type.

find database [protein|nucleotide|type] . May 1 2003 the find database command is extended to avoid matching a database sequence of the wrong type. That was necessary since PDB blast files contain both protein and nucleic acid sequences.

read conf i_ "compressedStack.cnf" . May 1 2003 Direct reading of conformations from a compressed stack is now possible. The compressed format becomes the default stack format.

write stack : highly compressed stack files. April 29 2003 Large stack files containing multiple conformations can be now saved in a highly compressed form. New syntax:

```
write stack simple .. # will save stack in old uncompressed format
write stack           # will save stack in new compressed format
```

compress stack fast. April 24 2003 Compression of large stacks speeded up for very large stacks from hours to seconds.

Rmsd(as_tetheredAtoms). April 18 2003 Rmsd function extended to return RMSD AFTER superposition by tethers.

`superimpose` by tethers. April 18 2003 New `superimpose as_atomsByTethers` allows to superimpose by equivalences defined via tethers.

version 3.019 released Apr 16, 2003

option `virtual` added to the `strip` command. April 10 2003 the strip command is extended to delete virtual atoms

linked sequences and alignments presented in the workspace. April 5 2003

version 3.018 released Apr 1, 2003

new options of the `Energy` (rs_ [simple | base | s_energyTerms]) Apr 1, 2003 allows to calculate standard normalized energy values for residues (option simple). Also allows to dynamically redefine the terms for which the residue energies are calculated.

read pdb assigns bond types to compounds. March 29 2003 `read pdb` now uses a new file called comp.cif to assign bond types correctly upon reading a pdb entry. (Note: the pdb entries do not contain bond type descriptions). However, the formal charges still need to be edited manually, and only after that the build hydrogen command can be applied to the pdb−heter−compounds.

improvements of `Energy` (rs_) and over 100 fold speed up of the energy strain calculations Mar 28, 2003 surface, entropy and grid energy terms added to the residue energies (see the Feb 24,2003 note). The `calcEnergyStrain` macro switched to the new method for calculating the residue energies which led to a dramatic speed up.

bug in `undisplay skin` fixed. March 25, 2003

Max(grob | macro | sequence | alignment | profile | table | map) March 22 2003 shell limits (to increase modify icm.cfg file).

Matrix(M, rowFrom rowTo colFrom colTo) extracting a sub−matrix March 12 2003 use 0 to skip (meaning all the values).

Rarray(M, i_flag) matrix to array transformations March 11 2003 The `Rarray` (M [i_flag]) function is extended to allow extraction of different groups of elements of the matrix. The possibilities are the following: elements by rows, by columns, the upper and lower triangles, the diagonal elements, the upper and lower triangles without diagonal elements

Matrix(n, R_diagonal), Histogram (R n|R_ruler R_Weights) and Rarray(from to step) March 11 2003

Nof(grob {1|2|3}) March 10 2003 to return the number of dots, lines and triangles respectively

compress grob [*selection] March 8 2003 returns new number of dots in i_out and r_out. Syntax extended to allow all grobs, selections and explicit lists.

coloring pockets by electrostatic potential. March 8 2003 Any grob (or 3D−mesh) can be colored by electrostatic potential. Since for molecular surface the potential is calculated in a direction away from the surface. color grob potential [reverse | simple] now calcualtes the mean and rmsd of the electrostatic potential at the surface. Also, there is option `reverse` to temporarily invert the normals for the electrostatic potential calculation and option `simple` to ignore correction by normals.

Example:

```
read pdb "1est"
delete a_!1
convert
icmPocketFinder a_ 4.6 yes no
display g_pocket1
make boundary
color g_pocket1 potential reverse
```

Distance(as_ [r_default]) : function to return the tether length of for each atom improved (to fit the new Group function) . March 8 2003 Now it is guaranteed to return an element for each selected atom.

Group : new function allowing to project an atomic property to residues. March 8 2003

Group(rarray | iarray , as_atom_selection , "min"|"max"|"avg"|"rms"|"sum"|"first"|"count") (count does not require the first argument). Example:

```
read pdb "2ins"
Group( Mass( a_A//c* ), a_A//c* , "sum" )   # computes residue masses
```

Improvements of the `convert` command. March 6 2003

- oxt C−terminus recognized and recreated by the convert command
- hydrogens for Cd atom or proline are correctly built

New soft van der Waals and soft electrostatics. March 3 2003 Better soft electrostatics functions are implemented to match the soft van der Waals. They work in both distance dependent mode and the Columb mode (see `electroMethod`). It is activated automatically if `vwMethod` is set to `"soft"` and matches the `vwSoftMaxEnergy` parameter.

Recognition of the C−terminus by the IcmSequence function and the convert command. Feb 24 2003 Now you can use IcmSequence(a_/* "nter","@cter") function and the C−terminal residue after the special @ symbol will be added only of atom `oxt` is found in the last residue of a molecule. Without ampersend it will always be added.

The new fast residue energy function: Energy(a_/*). Feb 24 2003 An improved and fast residue energy function helping to compute the energy strain much faster than before. It also covers all energy terms except the grid map terms.

Strength for multiple alignments (a new function) Feb 17 2003 A function to measure the strength of a multiple alignment is introduced. The strength can be computed with either normalized residue comparison matrix or with an `"exact"` un−normalized matrix. In the second case a conserved tryptophan, for example, returns a higher value, than conserved alanine. The function can be called as: `Rarray`(ali_ [*exact])

ICM version 3.016 released. Feb 21 2003

sequenceColorScheme preference introduced for alignment coloring Feb 17 2003

It uses the new CONSENSUSCOLOR table values and allows multiple styles of alignment coloring. sequenceColorScheme = "greyscale" 1 = "no color" 2 = "residue type" 3 = "icm−combo" 4 = "consensus strength" 5 = "greyscale" **option `mute` for the icm `read` command Feb 17 2003**

tethers can apply a constant force to atoms under tzMethod = "function" Feb 2 2003

name= s_ option in the read alignment {fasta|msf} command Jan 29 2003

individual stick radii Jan 28 2003

In order to modify the default values of stick/ball radii from the command line follow this example:

```
set field as_Residue_Selection number=3 r_newStickRadius
```

the ball radius will be changed according to the radio of the **default** parameters (e.g. `GRAPHICS.ballRaduis/GRAPHICS.stickRadius`)

Next(as_ tree) Jan 24 2003

The tree option allow to select icm−obj−atoms next in the tree.

better atom labels (displaying formal charges and chirality with atomLabelStyle=6) Jan 24 2003 also new option type= for `display atom label` command

selection for phase angles of chiral centers V_//FC Jan 24 2003 e.g.

```
set chiral a_//ca 3
unfix V_//FC
display atom label type=6
```

recognizing up/down prolines in IcmSequence (better regularization). Jan 20 2003

new display option: displaying transparent skins, ribbons and sticks. Jan 13 2003 display a_2 ribbon transparent display skin transparent display stick transparent

read from http extended to all platforms (Windows, LINUX, Unix). Jan 13 2003

compress grob [r_minEdgeLength=0.5] Jan 8 2003 a new algorithm to drastically reduce the complexity of 3D meshes/grobs. For example, if you want to simplify the skin surface, do the following read pdb "1crn" make grob skin smooth compress g_1crn 1. # 1A minimal size

write sequence select Dec 21 2002

separater width parameters for different graphics representations Dec 20 2002 `GRAPHICS.clashWidth` , `GRAPHICS.grobLineWidth` , `GRAPHICS.hbondWidth` , `GRAPHICS.mapLineWidth.`

Sarray(rs [name|residue]) functions Dec 19 2002 to display residue selections

GRAPHICS.displayLineLabels preference Dec 21 2002 to control the appearence of distance labels.

Grob("distance",as,[as]) function Dec 18 2002

evolutionary−tree display Dec 15 2002

read sequence [group [=s_name]] Dec 10 2002 read sequences and group them on the fly

clashThreshold parameter Dec 10 2002 When you display clashes, a clash is defined as an interatomic distance below clashThreshold*(sum of van der Waals radii) Not there is a shell parameter clashThreshold = 0.82 which controls the threshold.

write binary, read binary and list binary command and icm−projects Dec 10 2002 The following objects can now be written in one file as binary objects: table grob integer real string iarray rarray sarray. The default file extension is `.icb` (icm binary) Example:

```
write binary table grob integer real string iarray rarray sarray "file"
quit
..
icm
list binary "file.icb"
read binary "file.icb"
```

mutating terminal residues Dec 10 2002 The `modify` command extended and patched to allow replacement of nucleotides.

mute option in read object Dec 10 2002 Allows to temporarily switch the overwrite mode on

delete option in build and build string Dec 10 2002 Allows to temporarily switch the overwrite mode on

set stereo [on|off] Dec 9, 2002 to toggle the stereo mode from scripts and from the command line.

set table .. [i_size| auto] Dec 6, 2002 set table will extend, align or shorten a table

appending to arrays or table arrays Dec 6, 2002

```
a //= 1   # appends to an iarray or creates a new iarray
b //= 1.1 # appends to an rarray or creates a new rarray
s //= "a" # appends to an sarray or creates a new sarray
#
global group table t Sarray(0) "name" Rarray(0) "value"
t.name  //= "unite"  # adds 1st name element
t.value //= "0."     # adds 1st value element
```

Other new in place operations:

```
i += 1    # or −=
r += 1.1  # or −=
s += "string"
```

creating a global table from inside a macro Dec 6, 2002 declaration

```
global group table ...
```

will create a global table even if you run this command from inside a macro

delete mute .. Dec 5, 2002 temporarily sets `l_confirm` to `no`

new selections for GUI Nov 18, 2002 To assist selection of either GUI−selected or all− displayed atoms/residues we added new function: `Select([residue|molecule|object])` Also, `a_/DD` and `a_//DD` will select residues or atoms, respectively displayed by either atomic or residue representations (previously the same selection was written like this: `a_/D | a_//D`) `i_out` returns the number of selected atoms.

Path(last) and File(last) function No 18, 2002

to return the absolute path of the last icm shell script called. to return the script file name: File(last)

Info(display) function Nov 12, 2002

Info(display) function returns the commands which allow to restore the view. It is used in the writeProject macro.

superimpose in arbitrary order Nov 8, 2002

superimpose os1 os2 I_atomNumbers1 I_atomNumbers2

automated exclusion of virtual atoms from superimpose/Rmsd/Srmsd, the `virtual` option. No 8, 2002

new tzMethod : tethers/distance restraints Oct 28, 2002 new `tzMethod` = "function" applies a upper/lower bound drestraint function to tethers. The parameters of the function are controlled by properties of the object to which the tethers are directed:

- bfactor : local tz weight
- area : upper bound
- charge : lower bound

direct extraction of object comments from multiple object file Oct 18, 2002

`Namex` **(** *s_MultiObjectFile* **)**

Molecular selections by chemical formula Oct 18, 2002

you can now select molecules by chemical formula, with prefix 'F' e.g. a_FSO4,FNO2

new options for read object and read pdb Oct 16, 2002

```
read object s_file [name=s_newObjName] # to redefine obj name
read object s_file [delete]            # to temporarily switch off l_confirm
read pdb s_file [delete]
```

move command extended from one molecule to objects and multiple molecules Oct 16, 2002

box/lasso selection of grobs added Oct 14, 2002

alignments: support for title, graphical mask/boxes and comments added Oct 13, 2002

set area rs_ {r_area|R_areaArray} Oct 8, 2002
the `Date` function to return the current day, month year and time Oct 8, 2002

pdbDirStyle = "PDB website" for easy access to the pdb files. Oct 4, 2002 E.g.

Name(s_root, unique) to get a unique icm−shell object name . Oct 4, 2002

Max(s_root) to get maximal numerical suffix value . Oct 2, 2002

File(s_filename, "length") to get the file length . Oct 1, 2002

File(icm_object) to get the source file name for an object. Sep 28, 2002

Changing alignment coloring and consensus with `CONSENSUS_strength` . Sep 25, 2002

ICM 3.0 version released. Sep 12, 2002

- the master view with multiple molecular objects, 3D meshes, sequences, alignments
- cross−selection via 3D objects, sequences or alignments
- multiple alignment viewer
- dynamic pop−up menus for molecules, residues, sequences, alignment 3D meshes, etc.
- convenient display dialog
- stereo for LINUX
- drag−and−drop

better map coloring Aug 25, 2002 maps are colored in more sensible way now. One can color both by relative values with respect to the mean and the standard deviation (the `auto` option), as well as by absolute map values. Electrostatic maps are colored by default so that the zero potential area is transparent, positive is blue and negative potential is red.

Path(directory) returns current working directory Aug 24, 2002

Saving iarray of atom numbers and selecting atoms by iarray. Aug 24,2002 `Iarray` (*as_*) now returns integer array of relative atom numbers in this object. `Select` (*os_ iarray*) returns selection of specified atom numbers

Selecting atoms and residues by user−defined field values Aug 18,2002

User can define one atom field (see `set field` and `Field` (*selection* [*i_field*])) and three residue fields. Now one can also select atoms or residues using the `Select` function with arguments looking like this: "u>3." for atoms. For residues `"u"`, `"v"` and `"w"` values can be used for three user fields. Example:

```
Select(a_/* "u>3.") # select residues with 1st user field greater than 3.
```

improvement of `split grob` . Limit size of generated grobs 11,2002

Now you can specify the minimal size of a grob generated as a result of the the `split` command, e.g.
`split gg 500.0`

extracting grob vertices with certain color Aug 11,2002

Grob(grob { from_R, to_R, from_G, to_G, from_B, to_B })
function which returns a grob with selection of points of the source grob. The selected points will have colors between the RGB values provided in the 6−dim. array of limits (from 0. to 1.).

set grob label s_Label Aug 10,2002

Assign a string label to a grob.

Name(*object_type* select) August 10, 2002 Returns string array of names of the selected objects.

Nof(*object_type* select) August 10, 2002 Counts the selected objects. Convenient for GUI scripting (see the icm.gui file).

sort objects and sort molecules July 30, 2002 You can now resort objects and molecules by a user field or by molecular mass. See `sort objects` or `sort molecules`.

Access to the warning messages from shell: the `Warning` function July 24, 2002 Example:

```
if Warning() message = Warning(string)
```

Permissions for tables: set property args table1 table2 .. July 24, 2002

tables can now have a number of properties: read only, edit the cells only, etc. See the `set property` command.

Error(string) Text of each error message and its numerical error code July 24, 2002

Now all icm error messages you can extract the full text of the message. Example:

```
if Error errorMessage = Error(string)
print i_out  # the numerical code of the message
```

Remove unwanted characters. Trim(s_sourse, s_listOfOkCharacters) July 18, 2002

Revert order in arrays July 18, 2002

```
  Iarray( {1 2 3} reverse)  # returns {3 2 1}
  Sarray( S reverse)
  Rarray( R reverse)
```

Unique atomic ordering for chemical compounds: the `make unique` command. July 15, 2002

Fast refinement into electron density (the `gcMethod` preference). July 15, 2002

explicit sequence type for the `Sequence`(*s_seq* [`nucleotide` | `protein`]) function. April 22, 2002

option `box` in make grob map April 10, 2002 It controls addition of the surrounding box to the contoured map.

averaging two matching arrays: Mean (R1 R2) April 9, 2002

minimize loop command and making loop optimization movies April 9,2002 The `build model` command may not be able to find a perfectly matching loop. Two sorts of problems may appear: the imperfections of the loop attachments and the clashes of the loop to the body of the model. They are resolved with the `minimize loop` *i_loopNumer* command.

window={minValue,maxValue} range for color mapping April 8, 2002 Now the `display` and `color` commands in which you color a selection by a matching array of values, can be told what range of values the array is clamped to. A single digital value can also be used as a color with the `window` option. Example:

```
color ribbon a_/ Bfactor(a_/ simple) window=-0.5//2.
color ribbon a_/14 0.8 window=-0.5//2. # single value coloring
```

This command will clamp Bfactor(a_/ simple) values which are normally around zero, but may range from large negative values to large values, to the [−0.5,2.] range.

relative B−factor. April 3, 2002 In `read pdb` now the average B−factor for all non−water atoms is calculated for X−ray objects. The normalized B−factor (***(b−b_av)/b_av***) is now returned by the `Bfactor`(as_ `simple`) function. This is much better for coloring ribbons by B−factor since it only depends on ratios to the average. We recommend to use:

```
color ribbon a_/ Trim(Bfactor( a_/ simple ),-0.5,3.)//-0.5//3. # or
color a_// Trim(Bfactor( a_// simple ),-0.5,3.)//-0.5//3.  # for atoms
```

This scheme will give you a full sense of how bad a particular part of the structure is.

save tab− and comma delimited tables. April 3, 2002 `s_fieldDelimiter=","` or `"\t"` will be now affecting write table You can also specify it in the command line like this:

```
write table separator="," # or separator="\t", etc.
write table header separator="," # will save column names
```

Atom chirality April 1, 2002 (not a joke!) Atom chirality flags have been introduced. Each atom can have a chirality flag set to:

- zero − non−chiral center
- 1 − left topoisomer
- 2 − right topoisomer
- 3 − racemic mixture of both isomers

Here is a short summary of new commands and functions associated with chirality:

i/o	chirality flag is read from a mol file or ICM object.
`set chiral` *as_ flag*	set chirality flag to a selection
`a_//X[1230LRB]`	select chiral atoms, e.g. `a_//X1` for left atoms, `a_//X` is equivalent to `a_//X123`
`show` *as_*	shows a new `Xi` field with the chirality value
`l_racemicMC`	this flag allows to switch chirality in icm global optimization

Dot−separated chemical formula for multiple molecules March 30,2002

Use String(dot, selection) to get a dot separated chemical formula (String(all, selection) will give the total formula).

Setting, storing and extracting user−defined properties of atoms, residues, molecules and objects March 22. 2002

User can now store real properties of atoms, residues, molecules and objects directly in the object.

- To set those properties, use the `set field selection [number=i] property` command.
- To extract the property use `Field`(*selection*, *i_fieldNumber*)
- To clear use the `set field clear` *selection* command (or explicitly set it to zero).

Level	Max.Nof_fields	example
Atom	1	`set field a_//c* Mass(a_//c*)`
Residue	3	`set field a_/trp 1. number=2`
Molecule	16	`set field a_W Random(1.,10.,Nof(a_W)) number=12`
Object	16	`set field a_*. Rarray(Count(Nof(a_*.)))`

Version() function to report the license codes. March 12. 2002 The `Version` function now returns one−character license codes (e.g. " H D ").

```
Version()
Version(full)
```

parsing more PDB object types. March 9, 2002 ICM now recognizes more object types as specified by the `EXPDTA` card of a pdb−file, see `Type` (os_ 2):

`"ICM"` ready for energy calculations. Those objects are either built in ICM or `converted` to the ICM−type.
`"X−Ray"` determined by X−ray diffraction
`"NMR"` determined by NMR
`"Model"` theoretical model (watch out!)
`"Electron"` determined by electron diffraction
`"Fiber"` determined by fiber diffraction
`"Fluorescence"` determined by fluorescence transfer
`"Neutron"` determined by neutron diffraction
`"Ca−trace"` upon reading a pdb, ICM determines if an object is just a Ca−trace.
`"Simplified"` special object type for protein folding games.

Passing arguments to an ICM script: `icm −a string` option March 8, 2002 You can initialize s_icmargs string with the `icm −a 'args'` option. Example:

```
% icm −s −a 'a1.sdf a2.sdf'
 s_icmargs
 a1.sdf a2.sdf
 args = Split(s_icmargs)
 for i=1,Nof(args)
   print args[i]
```

```
endfor
```

`String( { as_ | rs_ | ms_ | os_ } i_number ) March 1, 2002` Function String (selection) is further extended to print i−th element of a selection. It is convinient in scripts. For atoms it will also show the full information about an atom, rather than only the ranges of atom numbers.

Detecting if `pmf` parameters (Nof(pmf). Feb 16, 2002 Nof(pmf) function reports the number pmf types.

Converting selections to strings. `String( as_ | rs_ | ms_ | os_ ) function extended. Feb 14, 2002` Now you can make a selection at any level and the String function will return a selection string which can be stored in variables, arrays and tables. Note, that the chemical formula is now returned by the String(all as_) or String(dot as_) function (keyword may be the last arugment as well).

Accumulating numbers of visits in the `compress` stack command. Feb 12, 2002 Now when you compress the conformation stack, the number of visits after the compression will be the total number of visits from all.

"Ca−trace" objects. Feb 9, 2002 Frequently Ca−trace−only objects in PDB create problems in automated database analysis scripts. Now this type is identified upon readin and it can be checked with the Type(a_ 2) command. Also if you try to convert the `"Ca−trace"` object to the ICM type, the `convert` command returns an error. If the object is mixed and contains both all atom models and Ca−traces, the Ca−traces will be skipped.

improvements of the convert command. Feb 6, 2002 Previously when the `convert` command was applied to an object with *missing* atoms in the backbone, the `convert` command had problems and generated ICM objects deviated from their pdb−templates significantly. This problem is now fixed. Also, ICM reports the deviation from the template and it is returned in the `r_out` command.

Unification of the `a_//` and `a_1.//` selections. Feb 12, 2002 There was a discrepancy between short forms of selections of all residues and all atoms. Now for the selections have the same level (e.g. a_// or a_1.// select all atoms in the current or the first object, respectively)

setting number of visits and energy for stack conformations. Jan 29, 2002 You can now specify the number of visits and the energy manually in the `store conf` command.

writing sequence groups into fasta/msf files. Jan 27, 2002 groups of sequences can be now saved or shown to fasta or msf files.

uncompressing bzip2 on the fly. Jan 25, 2002 Seemless treatment of the `.bz2` compressed files is added. E.g.

```
read sequence "aaa.seq.bz2"
364255 sequences loaded:
```

setting b−factors at residue level. Jan 20, 2002 Previously b−factors were always assigned at the atom level. Now, if you have a real array of residue energies (e.g. returned by the Energy(rs_) function, you can assign b−factors at the residue level with a simple command:

`set` *bfactor rs_ R_resBfactors*

reading .sdf .mol files Jan 18, 2002

Features from multiple sdf files are now extracted into the S_out string array upon reading. E.g.

```
read mol "aaa.mol"
logp = Rarray(Field(S_out,"logp",1,"\n")) # rarray of logp values
can_numbers = Trim(Field(S_out,"cas_rn",1,"\n"))
```

selecting water Jan 17, 2002

Selecton a_W selects both water molecules and deuterated waters. This may now replace less rigorous a_w* expressions in macros. E.g. `delete a_W` This selection is equivalant to the longer `Mol( a_/hoh,dod )` expression.

selecting aromatic atoms. Jan 15, 2002

Selection a_//R will select aromatic atoms. It selects all heavy atoms connected by aromatic bonds and hydrogens attached to them.

moving selections from one object to another Jan 11, 2002

Frequently a selection of atoms, residues of molecules need to be tranferred from one object to another. Now there is a function `Select`(selection, os_targetObject). Example :

```
read pdb "2ins"
copy a_  "bb"
aa = a_1.2,4,5//c*
bb = Select(aa,a_bb.)  # moves the selection
```

This is useful in macros.

surface energy Jan 5, 2002

The surface energy can now be calculated using grid potentials.

preference GRID.gcghExteriorPenalty Jan 3, 2002

van der Waals grid energy *outside* van der Waals grids "gc" and "gh" used to be positive to push molecules back to the grid box. Now there is a preference: `GRID.gcghExteriorPenalty` which can be set to `"repulsive"` (the previous mode) or to `"zero"` to have no field outside the box.

zero−size rarrays and iarrays can be created. Jan 1, 2002

Rarray(0) and Iarray(0) now allow to create arrays of zero size.

convertObject macro extended to convert a selected set of molecules Dec 26, 2001

s_skipMessages allows to suppress printing of selected error and warning messages Dec 15, 2001

`s_skipMessages` is new shell string variable which contains a list of error/warning codes which you want to suppress in your icm output. Despite suppression of the message, the error is still generated and can

be returned with the `Error`(string) function in `i_out.` Example:

```
s_skipMessages = "[234][5243]"
```

Macro to write sequences in the alignment order. Nov 28, 2001 Frequently you may want to renumber your object (which may contain omitted loops and ends) according to a full protein sequence. Now you can do it automatically with the

`align number` *ml_ seq_*

command.

Macro to reorder sequences in the alignment in the read order. Nov 26, 2001

The alignment changes the input order of sequences. To keep the order the same in an alignment, you may now use the

`reorderAlignmentSeq(` ali_) macro from the `_bioinfo` file.

See the `Align` function for more details.

Macro to write sequences in the alignment order. Nov 24, 2001

A tiny macro `wrSeqAli` (file `_macro`) allows to write sequences in the alignment order.

Type(seq_ 2) : type of a sequence Nov 22, 2001 find out the sequence type with the Type(seq_ 2) function.

normal distribution : Random(mean std N "gauss") Nov 14, 2001

Generate an array with normally distributed numbers with the Random() function, e.g. Random(0., 1., 10, "gauss")

set grob reverse : inverting normals in grobs, Nov 9, 2001 Permanently change direction of normals of one or all grobs allows to change direction of lighting as well as influence the sign of Volume(grob). Now one can:

```
set grob reverse # all grobs
set g_ reverse   # a specific grob
```

full pairwise alignment with arbitrary positional weights, Nov 8, 2001 We introduced a new command to set custom sequence residue areas (e.g. `set area 1crn_m {0.3,1.,1.3,0.8,..}`). This 'areas' can be used by the `Align(seq1,seq2,area)` function for weighted pairwise alignment. Example:

```
set area 1crn_m 0.
set area 1crn_m Random(0. 2. Length(1crn_m))
```

New macros, Nov 7, 2001

`icmCavityFinder` to find closed cavities
`icmPocketFinder` to find open cavities

potential of mean force , Nov 4, 2001

A new energy term `"mf"` is added. It allows to establish interactions according to pairs of atoms types. This term can be used both for chemical superposition and pharmacophore modeling (e.g. you know several ligands to the same receptor and want to derive the pharmacophore model), or for scoring the docking solutions in virtual ligand screening. Example:

```
read pmf "ident.pmf"
buildpep "his ; ala trp" # two molecules: his and ala-trp
fix v_//omg
montecarlo "mf"
```

read pdb sequence chain case, Nov 2, 2001

Originally PDB was case insensitive. However, in some entries it is used to specify different chains, e.g. A and a in 1fnt . ICM now copes with this misdemeanor of PDB.

~/.icm/user_startup.icm file, Oct 28, 2001

font control in GUI terminal: Oct 25 , 2001

`icm.cfg` file can now be define the **font size** in the terminal window. The specification may look like this:

```
XTermFont *-fixed-medium-*-*-*-24-*
```

gui simple: keep the original terminal window and start gui , Oct 22 , 2001

Previously the `gui` command under Unix/Linux disabled the original terminal window and created a new one inside the GUI window. This new window had problems with font controls. Now you can keep the original window and start GUI.

```
% icmgl
 gui simple
   # or
% icmgl -G
```

Distance(alignment1 alignment2 exact) , Oct 21, 2001

a measure of differences between two alignments (see `Distance`(*ali*,*ali*,*exact*)) to evaluate the influence of alignment parameters on alignments, or to evaluate differences between a trial alignment and a 'golden' standard.

display origin , Oct 19, 2001

allows to display coordinate frame. Also: undisplay origin

set v_ reverse , Oct 18, 2001

modify internal coordinates while keeping the remote part of the molecule unmoved

copy a_ tether , Oct 18, 2001

the copy command is extended to allow simultaneous copying and imposing tethers to the copy. Also, now the default name of the copy−object is `a_copy.`

refineModel macro, Oct 17, 2001

`refineModel` macro from the `_macro` file allows to refine models resulting either from homology model (in this case it is supposed to be tethered to the target object) or any other source. It performs iterative energy refinement with appropriate annealing of the tethers. If you only want to improve the predicted side chains, use `refineModel 0 yes`

a_//Z selection for tether−target atoms, Oct 18, 2001

Previously one could select tethered atoms (`a_//T`) but not the atoms **to which this atoms are tether** . Now it can be done with the `a_//Z` selection.

montecarlo reverse, Oct 16, 2001

a new `reverse` option of the `montecarlo` command allows to make a more intellegent random move of a molecule fragment surrounded by other static molecules. It prevents the movement of the whole molecule if a backbone angle at N−terminus is changed.

Average gradient amplitudes of residues Oct 14, 2001

Gradient(rs_ | as_) now returns not only the array of gradient lengths for atoms (e.g. Gradient(a_//*)) but also returns averaged gradient lengths for each selected residue if the selection is of residue level (e.g. Gradient(a_/*)). This can be used to color the ribbon or to direct a montecarlo procedure.

Easy coloring of 3D models by space averaged alignment strength. Oct 8,2001

see ribbonColorStyle

```
ribbonColorStyle = "reliability"
```

allows to color a ribbon model by alignment strength with 3D gaussian averaging of the conservation signal. `selectSphereRadius` controls the radius of the averaging.

Reading NMR entries with CRYST data .

Some new NMR entries in PDB have illegal CRYST ORIGX etc. data. Previously ICM complained about them. Now, it the experiment is NMR, the crystallographic symmetry fields are skipped.

Sampling with probabilities according to b−factors . Oct 5,2001

Now you can use a new `bfactor` option of the `montecarlo` command to sample 'hot' parts of structure with higher probabilities. The relative frequences are taken from the b−factors of the atoms belonging to the mc−variables. Example:

```
buildpep "ala his trp glu"  # default b-factor=20
set bfactor a_/2  1000.     # make 2nd his hot
montecarlo bfactor
```

To preserve the old bfactors, save them before the simulation and restore after. E.g.

```
b_old = Bfactor(a_//*)   # save
..
set bfactor a_/10:20 200.
montecarlo bfactor
..
set bfactor a_//* b_old  # restore
```

Detection of missing fragments in pdb-files. Oct 3,2001

ICM detects chain missing residues according to the differences between SEQRES sequence and the residues with coordinates and returns the total number of missing residues in the `i_out` system variable. E.g.

```
read pdb "1amo.a/"
make sequence a_1.1  # sequence 1amo_1_a extracted
if(i_out>1) then
  read pdb sequence "1amo"  # sequence 1amo_a read
  a=Align(1amo_a 1amo_1_a)
  build model 1amo_a a_1.1 a   # patch the missing fragments
endif
```

Renumber residues in fragments. Oct 3, 2001 previously only renumbering of the whole protein chain was allowed Example:

```
read pdb "1crn"
align number a_/10:20 101  # renumber a fragment starting from 101
```

Total masses of residues, molecules, objects. Oct 3, 2001

The same extension as the one below was applied to the Mass function (e.g. Mass(a_/*) returns masses of residues.

Total charges of residues, molecules, objects. Sep 14, 2001

`Charge( os_ | ms_ | rs_ | as_ [formal | mmff] )` now returns the array of total charges for each selected unit (e.g. Charge(a_/*) returns an array of total charges of each selected residue)

Numbers of atom arrays in residues, molecules, objects. Sep 13, 2001

```
Nof( a_*.* atom ) # returns an iarray of number of atoms in each molecule
```

Cheminformatics: Modifications of non-ICM objects Aug 10, 2001 Example:

```
read mol "scaffold.mol" # contains r1 atoms
read mol "bblocks.sdf"  # contains blocks with attachment points atoms
modify a_1.//r1 a_2.//a # build a molecule
build hydrogen
```

```
set type mmff
set charge mmff
convert
```

Modeling: tzMethod = "**weighted**" to use b−factors of atoms for weighting tethers. Aug 7, 2001 method of imposing and calculating `tethers`. The three alternatives are the following

1. `"simple"` : equal weight tethers to 3D points (the old one)
2. `"weighted"` : individual weights are calculated from atomic B−factors by dividing $8*PI^2$ by the B−factor value. All the weights additionally are multiplied by the `tzWeight` shell parameter.
3. `"z_only"` : tethers are imposed only in the Z−direction towards the target Z−coordinate. These type of tethers allow to pull a molecule into a z−plane. This may be useful if you are trying to generate a flat projection of a three−dimensional molecule.

Modeling: tzMethod = "**z_only**" to tethers to the `z−plane` of other atoms. Aug 1, 2001

Distance restraints improvements. July 17, 2001.

Target distance allows to have a target not in the middle of upper and lower bounds.

v_//T and v_//F selections

New maps and binding site predictions− Sep. 01.

Two commands have been extended:

- make map potential (no terms) . − calculates new map m_atoms. Can be used on pdb−objects
- make grob map exact r_contourLevel . − allows to specify absolute (exact) contouring level

A new map with gaussian envelope around atoms can be quickly built for ICM and non−ICM objects and used to find *semi−closed* pockets. If contoured at 0.3 it gives

```
buildpep "his arg"
make map potential Box( a_ 3.) solid
make grob m_atoms 0.2 exact  # contours near vw-raduis.
display cpk
display g_atoms
```

To identify pockets: try different contouring levels and split the grobs.

bug fixes:

modify phase branch convert a_ "new name"

1.2. Brief history of ICM

ICM author's heads *in italic*


Ruben Max

The first lines of ICM were born in 1985 out of a desire to design a fast yet general framework for predicting the structure of complex biological macromolecules and their complexes. I formulated a set of requirements for a program for molecular mechanics in a full set of internal coordinates, and started working on the internal coordinate algorithms and the Fortran code of the first program blocks. By 1991 the batch parameter files were replaced by a command language and an interactive shell that looked quite similar to the current version of ICM; the molecules started to follow commands and sample the energy minima.

Max Totrov and I extended or rewrote most parts of ICM from 1991 to 1994. By 1993 several people (Alexey Mazur, Mikhail Petukhov, and Dmitry Kuznetsov) had also contributed to the fortran version of ICM, however their contributions did not survive in the current version of the program. Alexey pursued the development of molecular dynamics in internal coordinates which was first formulated and tested in a series of papers in 1989 and, later, branched out of ICM.

The all−C version of ICM emerged in 1994 as a result of a full rewrite. Some features were lost, but more were gained. **Serge Batalov** joined the development of the program in the fall of 1994, about the time Molsoft was founded.

Max and I together with the new Molsoft developers, namely **Eugene Raush** who is writing the graphics user interface, and Constantin Skorodumov, keep ICM strong, clean, healthy and alive.

1.3. ICM distribution and support

ICM is being developed, distributed and supported by Molsoft, LLC.

If you have any problem with our programs, go to the Molsoft Support Center at

```
https://www.molsoft.com/support
```

or contact Molsoft via e−mail:

```
support@molsoft.com
```

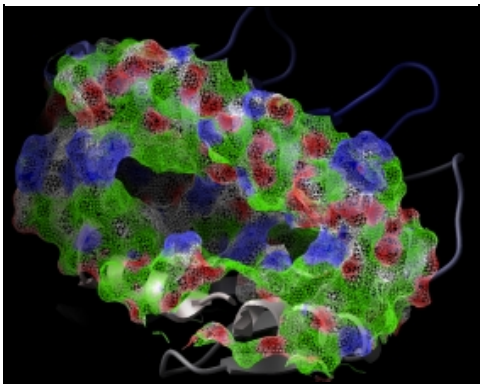
In the support center you can easily post a problem or make a suggestion and monitor its progress. Please indicate the platform, the version of the program, and do not forget all the necessary files to reproduce it. Some of the commands or functions described in this manual belong to specific modules and are not available in the ICM−main program.

1.4. What can you do with ICM? (a program overview)

Let us go through the short overview of ICM applications.

1.4.1. Graphics

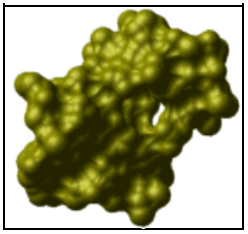
Versatile surface and structure views to elucidate protein function



The views include

- binding and active site surfaces with mapped properties
- automatic identification and views of cavities and open binding pockets
- electrostatic surfaces

Analytical molecular surface (skin)

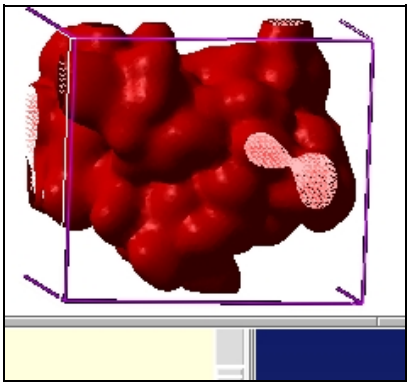


The contour−buildup algorithm calculates the smooth and accurate analytical molecular surface in seconds. This surface can be saved as a geometrical object, saved as a vectorized postscript file.

The skin is used in the REBEL algorithm to solve the Poisson equation, as well as in the molecular surface analysis routines (e.g. a projection of physical properties on the receptor surface).

Also ICM can build and draw a solvent−accessible surface (see `surface`) and

* a gaussian molecular density which can be contoured at different



levels and to generate different smooth molecular envelopes and enclosed pockets and cavities:

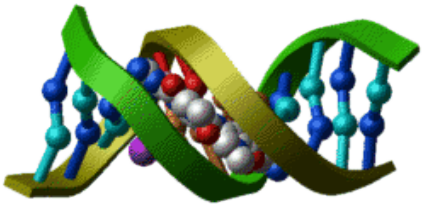
```
make map potential Box( a_ 3.)
make grob m_atoms exact 0.5 solid
display g_atoms smooth
```

Schematic representations of DNA and RNA

PDB entry: `101d`

ICM command:

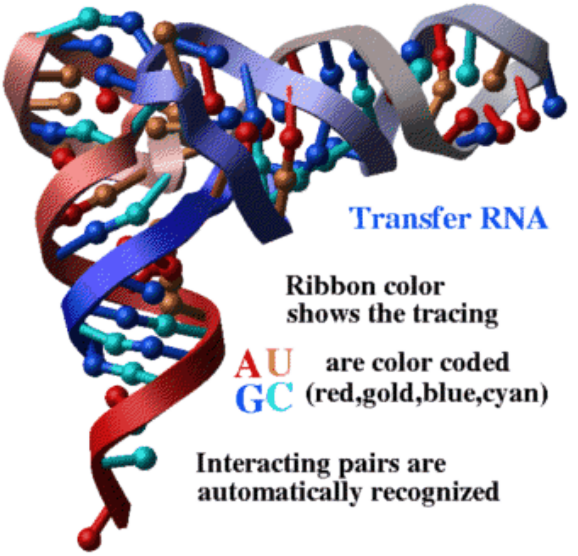
```
nice "101d"
```



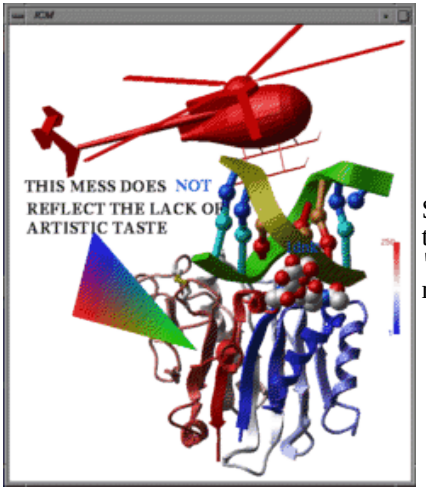
PDB entry: `4tna`

ICM commands:

```
nice "4tna"
color ribbon a_N/* Count(Nof(a_N/*))
```



Complex combined representations

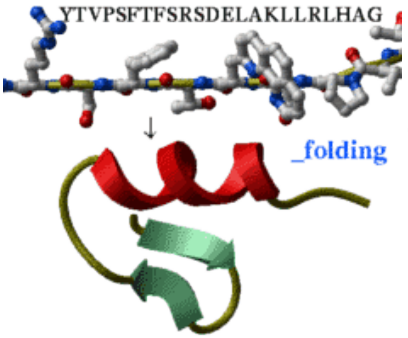


Simplified molecular representations are built automatically (e.g. the protein−dna complex is shown with one command: `nice "1dnk"`). You can combine different types of molecular representations with solid or wire geometrical objects.

Molecular representations include wire models, ball−and−stick models, ribbons, space filling models, and skin representation.

1.4.2. Simulations

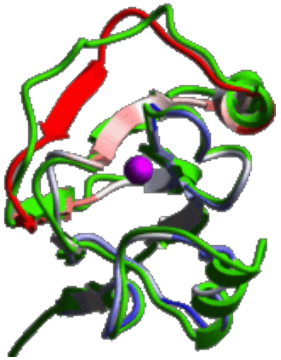
Prediction of peptide structure from sequence



Take a peptide sequence and predict its three−dimensional structure. Of course, success is not guaranteed, especially if the peptide is longer than about 25 residues but some preliminary tests are encouraging.

You will also get a movie of your peptide folding up. Just type the peptide sequence in the `_folding` file and go ahead.

High quality models by homology



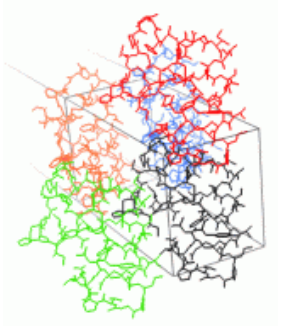
ICM has an excellent record in building accurate models by homology. The procedure will build the framework, shake up the side−chains and loops by global energy optimization. You can also color the model by local reliability to identify the potentially wrong parts of the model.

ICM also offers a fast and completely automated method to build a model by homology and extract the best fitting loops from a database of all known loops (see `build model` and `montecarlo fast`). It just takes a few seconds to build a complete model by homology with loops.

Loop modeling and protein design

ICM was used to design two new 7 residue loops and in both cases the designs were successful. Moreover, the predicted conformations turned out to be exactly right (accuracy of 0.5Å) after the crystallographic structures of the designed proteins were determined in Rik Wierenga's lab. Use the `_loop` script to predict loop conformations and calcEnergyStrain to identify the strained parts of the design.

Crystallographic symmetry



ICM has a full set of commands and functions to generate symmetry related molecules and generate "biological units".

Docking two proteins

Docking two proteins reliably is still an unsolved problem. However, there has been a considerable progress. In some cases (e.g. beta lactamase and its protein inhibitor) the ICM docking procedure predicted the binding geometry correctly based only on the global energy optimization. ICM will generate a number of possible solutions using both the explicit atom model of the receptor and the receptor grid potential and refine them by explicit global optimization of the surface side−chains. Even though success is not guaranteed, the generated solutions can be useful, especially if any additional information about the binding is available.

Finding pockets and docking a flexible ligand to a receptor

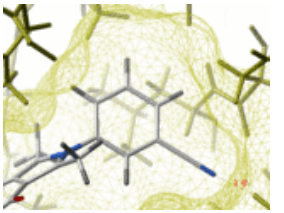
As demonstrated in several recent papers, short flexible peptides can be

successfully docked *ab initio* to their receptors. This method is a blend of the peptide folding with the grid potentials representing the receptor. A similar method can be applied to any chemical. A chemical can be built from a 2D representation and optimized. The "drugable" pockets can be predicted with an algorithm based on the contiguous grid energy densities.

Scanning a database of flexible ligands

In virtual screening the flexible docking is applied to hundreds of thousands of individual ligands. This version of docking is fast and requires an accurate relative binding or ranking function to discriminate between the true ligands and hundreds of thousands of potential false positives. The ligand sampling and docking procedure is a combination of the genuine internal coordinate docking methodology with a sophisticated global optimization scheme.

Accurate and fast potentials and empirically adjusted scoring functions have led to an efficient virtual screening methodology in which ligands are fully and continuously flexible.

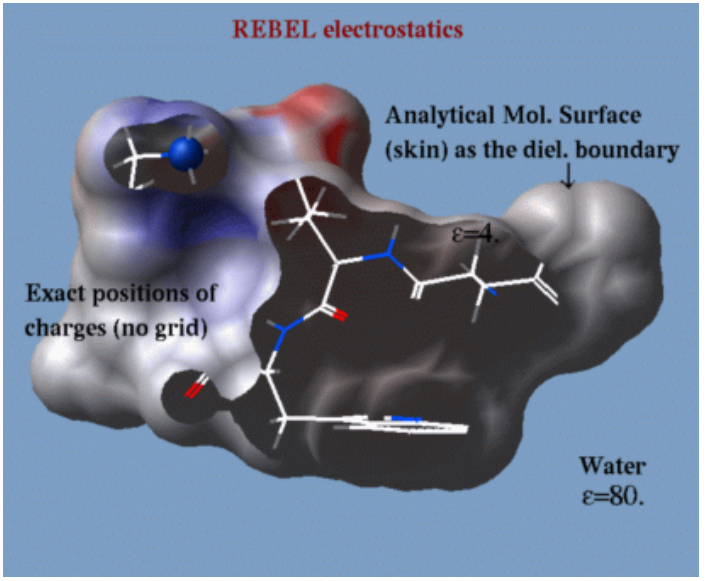


Calculating electrostatic potential

ICM incorporates a very fast and accurate boundary element solution of the Poisson equation to find the electrostatic free energy of a molecule in solution. This algorithm (abbreviated as REBEL) can be used dynamically during conformational search. The components of the electrostatic free energy are used to calculate the binding energy and evaluate the transfer energy between water and organic solvents.

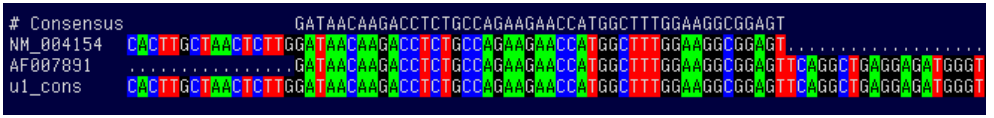
ICM uses generalized Born approximation to calculate the electrostatic solvation energy and its gradient dynamically during local and global conformational searches.

The electrostatic potential can be projected on a molecular surface for the identification of possible binding sites.



1.4.3. Sequence analysis

Genomics



Handling gigabytes of genomic sequence, fast cross−comparison of millions of sequences was another challenge solved in the ICM program. ICM can identify a unique subset of millions of sequences, assemble sequences from Unigene clusters into alignments (`SIM4` program is used a part of the procedure).

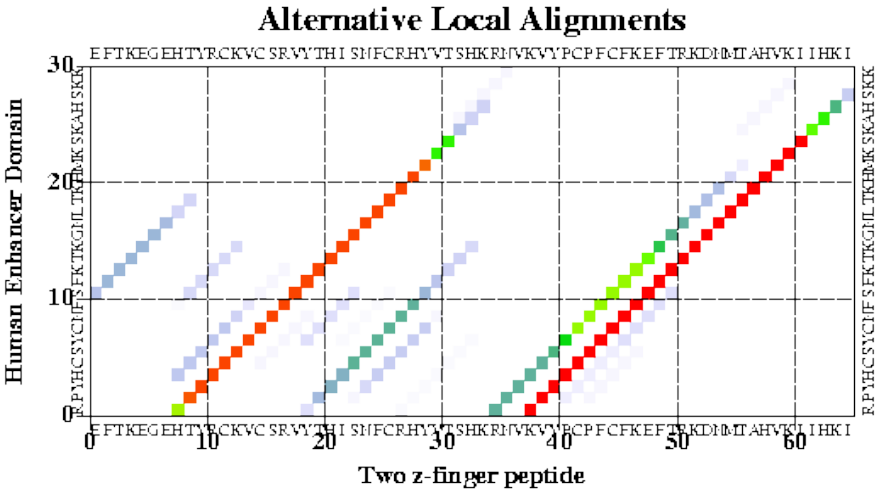
Similarity dotplot: alternative alignments and repetitive subdomains

It looks like this:

Using the `plotSeqDotMatrix` macro:

```
read sequence s_icmhome + "zincFing.seq"
plotSeqDotMatrix 2drp_d 3znf_m \
"Two z−finger peptide" "Human Enhancer Domain" 5 20
```

Here the color shows the local significance of the alignment. You can change the method to calculate probability, color scheme and residue comparison matrices and calculate it interactively or in batch.



Pairwise sequence alignment and its significance

Make a pairwise sequence alignment and evaluate the probability that the two aligned sequences share the same structural fold. The alignment is performed with the Needleman and Wunsch algorithm modified to allow zero gap−end penalties (so called `ZEGA alignment`). The ZEGA probability is a more sensitive indicator of structural significance than the BLAST P−value. The structural statistics was derived by Abagyan and Batalov, 1997:

```
read sequence s_icmhome + "sh3.seq"
show Align(Fyn Spec)   # the probability will be shown
```

You can change residue comparison matrices, gap penalties and do many alignments in batch.

Multiple sequence alignment

Read any number of sequences in fasta or swissprot formats and automatically align the sequences, interactively or in a batch. It will look like this:

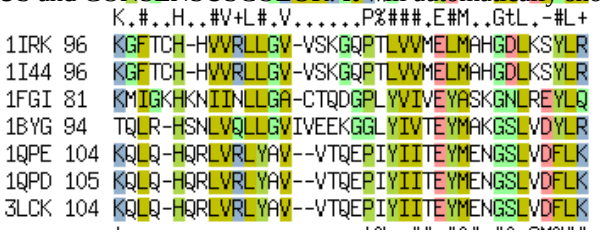
```
# Consensus ...#.^.YD%..+~..−#~# K~−.#~##.~~..~WW.#.   ~~.~G%#P.
Fyn      ----VTLFVALYDYEARTEDDLSFHKGEKFQILNSSEGDWWEARSLTTGETGYIPS
Spec     DETGKELVLALYDYQEKSPREVTMKKGDILTLLNSTNKDWWKVE−−VNDRQGFVP−
Eps8     KTQPKKYAKSKYDFVARNSSELSM−KDDVLELILDDRRQWWKVR−−−NSGDGFVPN

# nID 7 Lmin 56 ID 11.5 %
#MATGAP gonnet 2.4 0.15
```

ICM commands:

```
read sequence s_icmhome + "sh3.seq"
group sequences sh3
align sh3
```

```
show sh3
```

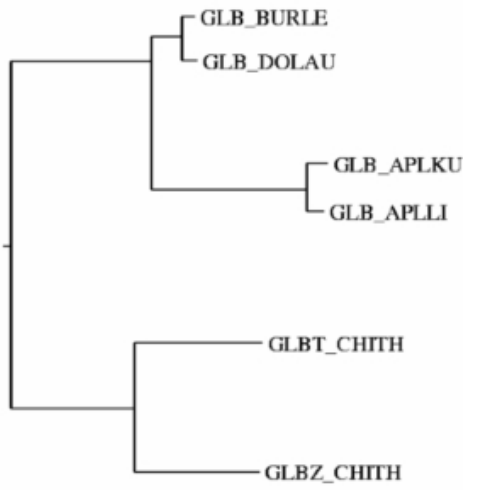
The gui version of ICM also has a multiple alignment viewer with dynamic coloring according to conservation tables CONSENSUS and CONSENSUSCOLOR. It will automatically show secondary structure and other features.



Evolutionary trees, 2d and 3d sequence clustering

Relationships between sequences can be presented in three forms:

- as evolutionary trees (ICM uses the neighbor−joining method for tree construction);
- as 2D distribution of sequences using the two main principal axes (use plot2Dseq macro);
- as 3D distribution. This can be analyzed in stereo using controls of molecular graphics (use ds3D macro: `ds3D Distance(alig) Name(alig)`).



Sensitive Sequence Similarity Search, ZEGA

Search your sequence (interactively or in batch) through any database and generate a list of possible homologues which are sorted and evaluated by probability of structural significance. The ZEGA alignment (full dynamic programming with zero end gaps) is used for each comparison and an empirical probability function described in JMB,1997 is used to assign a P−value to each hit. This search may give you more homologues that a BLAST search! The output may presented in a linked table form:

Table of hits

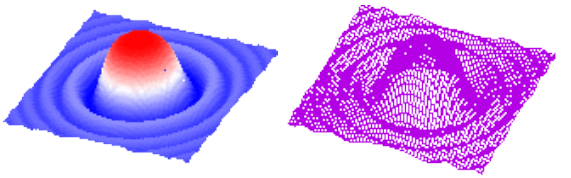
NA1	NA2	ID	SC	pP	DE
Fyn	`1nyf`_mNo	100.	62.81	20.94	fyn
...	*lines skipped*	...	...	...	...

Eps8	1tud_m17	21.	17.04	4.17	alpha−spectrin
Eps8	1fyn_a23	22.6	17.02	4.16	phosphotransferase fyn
Eps8	1efn_a25	22.	16.64	4.11	fyn tyrosine kinase
Eps8	1hsq_mNo	24.2	16.87	4.1	phospholipase c−gamma (sh3 domain)

3D plots of functions

Take a `matrix` and represent it in 3D in a variety of forms. View it in stereo, color, label, transform with the mouse. Example:

```
read matrix s_icmhome + "def"
make grob def solid color
display
```



1.4.4. Modules of ICM

ICM is distributed in the following packages:

- ICM−main
- ICM−bioinfo (sequence analysis)
- ICM−REBEL (electrostatics)
- ICM−docking (includes cheminformatics)
- ICM−pro (includes the above four modules)
- ICM−homology (fast homology building and database loop searches in addition to ICM−pro)
- ICM−VLS (virtual ligand screening, includes ICM−pro)

The modules have the following features:

ICM−main

- shell for molecules, numbers, strings, vectors, matrices, tables, sequences, alignments, profiles, maps
- ICM−language and macros
- graphics, stereo
- imaging and vectorized postscript
- animation and movies
- mathematics, statistics, plotting
- presentation of the results in html format
- user−defined and automated interpretation of web links
- HTML−form−output interpretation
- pairwise and multiple sequence alignments, evolutionary trees, clustering
- secondary structure prediction and assignment, property profiles, pattern searching
- superpositions, structural alignment, Ramachandran plots
- protein quality check
- analytical molecular surface
- calculations of surface areas and volumes
- cavity analysis
- symmetry operations, access to 230 space groups

- database fragment search
- identification of common substructures in PDB
- read pdb, mol2, csd, build from sequence
- energy, solvation, MIMEL, side−chain entropies, soft van der Waals, tethers, distance and angular restraints
- local minimization
- ab initio peptide structure prediction by the Biased Probability Monte Carlo method
- loop simulations
- side−chain placement

ICM−REBEL (electrostatics)

- electrostatic free energy calculated by the boundary element method
- coloring molecular surface by electrostatic potential
- binding energy (electrostatic solvation component)
- maps of electrostatic potential and its isopotential contours

ICM−docking and chemistry

- indexing of chemical databases in SD, mol2 and csd format
- searching and extracting from the indexed databases
- fast grid potentials
- scripts for flexible ligand docking
- scripts for protein−protein docking
- 2D (SMILES) to 3D conversion, type and charge assignment, mmff geometry optimization, low−energy rotamer generation
- refinement in full atom representation

ICM−bioinformatics

- fast comparison and redundancy removal of millions of genomic or protein sequences
- multiple EST clustering, alignment and consensus derivation
- database indexing and manipulations
- functions to evaluate sequence−structure similarity
- scripts to recognize remote similarities in the protein sequence and PDB databases
- search a pattern through a database
- searching profiles and patterns from the Prosite database through a sequence
- HTML representation of the search results with interpretation of links
- interactive editor of sequence−structure alignment
- automated building of models by homology with loop sampling and side−chain placement (fast homology model building combined with the database loop search is a separate module which is ICM Homology).

ICM−Homology

- sequence−structure alignment (threading)
- ultra−fast automated homology model building with a database loop search
- loop modeling and refinement, side−chain placement
- surface analysis

As a method for structure prediction, ICM offers a new efficient way of global energy optimization and versatile modeling operations on arbitrarily fixed multimolecular systems. It is aimed at predicting large structural rearrangements in biopolymers. The ICM−method uses a generalized description of biomolecular structures in which bond lengths, bond angles, torsion and phase angles are considered as independent variables. Any subset of those variables can be fixed. Rigid bodies formed after exclusion of some variables (i.e. all bond lengths, bond angles and phase angles, or all the variables in a protein domain, etc.) can be treated efficiently in energy calculations, since no interactions within a rigid body are calculated. Analytical energy derivatives are calculated to allow fast local minimization. To allow large scale conformational sampling and powerful molecular manipulations ICM employs a family of new **global optimization** techniques such as: Biased Probability Monte Carlo (Abagyan and Totrov, 1994), pseudo−Brownian docking method (Abagyan, Totrov and Kuznetsov, 1994) and local deformation loop movements Abagyan and Mazur, 1989).

A set of ECEPP/3 **energy** terms is complemented with the parameters for rare atoms and atom types, as well as the solvation energy terms, **electrostatic polarization energy** and side−chain **entropic** effects (Abagyan and Totrov, 1994), making the total calculated energy a more realistic approximation of the true free energy. The MMFF94 force field has also been implemented. Powerful molecular graphics, the ICM−command language, and a set of structure manipulation tools and penalty functions (such as multidimensional variable restraints, tethers, distance restraints) allow the user to address a wide variety of problems concerning biomolecular structures.

1.5. Notational conventions

The following notational and typographical conventions are used throughout the manual.

- **Bold.** Command names may appear in bold in syntax descriptions. (e.g. **montecarlo**). Type them as they appear in the text.
- `Typewriter` font is used for command words, examples and ICM−shell prompts. This `text` can also be copied into the shell.
- *Italic* font is used for command or function arguments which should be replaced with actual values. For example, if you see

  /whatever/your/ICM/directory/

  and your ICM directory actually is

  ```
  /usr/pub/icm
  ```

  the latter is what you should actually type.

  Short prefixes shown in parentheses may be used to specify argument type: `integer` (i), `real` (r), `string` (s), `logical` (l), `preference` (p), `iarray` (I), `rarray` (R), `sarray` (S), `matrix` (M), `sequence` (seq), `profile` (prf), `alignment` (ali), `map` (m), graphics object, or grob (g), structure factor (sf), atom selection (as), residue selection (rs), molecule selection (ms), object selection (os), variable selection, e.g. a subset of torsion angles, (vs), and `table` (T). These prefixes are also used to construct formal argument names for macros. For example, *I_Color* would mean an integer array with color information, or *s_ObjName* would mean a string variable or constant (e.g. `"crn"`) specifying the object name.

- Optional arguments appear in square brackets **[ ]**.
- Braces **{ }** are used for mutually exclusive groups or arguments. For example:

  `set charge` *as_* { *r_Charge* | `add` *r_Increment* } means either

  `set charge` *as_ r_Charge* or

  `set charge` *as_* `add` *r_Increment*

- The default values in ICM macros are shown in parenthesis and in typewriter font:

  `icmPocketFinder` *as_receptorMol r_threshold* (`3.`) *l_display* (`yes`)

1.6. Common abbreviations

In addition to the abbreviated ICM−shell−objects prefixes (see above), abbreviations may be used for energy terms, and some other frequently used words.

abbr.	description
as_	atom selection
ali	alignment
conf	conformation
cn	distance restraints
grad	gradient
ey	energy
hb	hydrogen bonds
ls	list
ms_	molecular selection
MC, mc	montecarlo
MB	Mouse Button
mn	maximal number of *items*
n	number of *items*
os_	object selection
re, res	residue
rs_	residue selection
rs	variable restraint
seq	sequence
to	torsion
tz	tether
ty	type
va, var	variable internal coordinate in a molecule (torsions, phase angles, planar angles, bond lengths).
vw	van der Waals
wt	weight

It is convenient to declare these abbreviations as aliases to the corresponding full words in the `_startup` file for fast typing. For example:

```
ls seq
```

instead of

```
list sequence
```

1.7. Getting started

Start the GUI (Graphics User Interface) version of ICM by typing `icm -g` or `icm -G` and hitting `RETURN`. This executable will look the `$ICMHOME` shell variable. The commands of the GUI menu will be taken from `$ICMHOME/icm.gui` file. Feel free to change it. The GUI is meant to be self−explanatory. In this manual we will mostly focus on the shell commands and function, since in many cases the GUI gives you only limited subset of possibilities.

1.7.1. ICM−shell

ICM−shell is a basic interface between a user and the ICM−program. The shell can be used from the GUI version or directly. This is a powerful and flexible environment for a multitude of versatile tasks ranging from mathematics and statistics to very specialized molecular modeling tasks.

Start ICM by typing:

```
icm
```

Make sure that your .cshrc login file contains

```
setenv ICMHOME  /whatever/your/ICM/directory/is/
```

Do not forget the slash at the end. It is also useful to add your $ICMHOME directory to your $path since there are some ICM related shell scripts and utilities which you may want to access.

You will see the ICM−prompt inviting you to type a command. The first thing to know is **how to get help**. You may just type **help** and use **/** *whatever* to find what you want, or use **help commands** or **help functions** to find out about the syntax. Now type:

```
aa=2.4
```

You have just created a new ICM−shell variable `aa` and assigned a value of 2.4 to it. You can create a variable with a name which is not already in use in the ICM−shell, does not contain space or delimiters like ".","," and starts from a letter (e.g. 1aag is an illegal name, except for sequences). Let us go on:

```
bb=2.*aa
```

Now you have created another ICM−shell variable `bb` and its value is probably 4.8. Find it out by typing:

```
print " bb=", bb
```

or any of these commands:

```
list "b*"
list integers
show bb
```

The next step would be to type a conditional expression like:

```
if (bb != 4.8) print "something went wrong"
```

or something even more elaborate:

```
if (bb != 4.8) then
  print "something went wrong"
else
  print "It really works"
endif
```

You can always start a for−loop such as:

```
cc={"sushi","sashimi","negi maki","toro","period."}
for i=1,Nof(cc)
# Nof returns the number of elements.
#  Index i runs from 1 to 5
   print "*** I just like to eat  ",cc[i]
endfor
```

Notice that anything after a pound sign # in ICM scripts is a comment.

We have just played with a real variable `bb` and string array `cc` . They had their unique names and we could create, read, write, delete and rename them.

ICM−shell objects

Furthermore, the ICM−shell can handle many other different types too, namely, it may contain in its memory entities of 16 different types, such as

- `integer` , (e.g. `a=10, b= −3`)
- `real` , (e.g. `c = −3.14`)
- `string` , (e.g. `d = "ICM rules"`)
- `logical` , (e.g. `e = (2 > 43); f = yes`)
- `preference` , (i.e. fixed multiple choices, try `show wireStyle`)
- `iarray` , (i.e. integer arrays, `g={−2,3,−1}`)
- `rarray` , (i.e. real arrays, `h={ −2.3, 3.12, −1.}`)
- `sarray` , (i.e. string arrays, `i={"mek","yerku","erek"}`)
- `matrix` , (read from a disk file, e.g. `read matrix "def.mat"`)
- `sequence` , (i.e. amino acid or nucleotide sequences)
- `alignment` , (i.e. pairwise or multiple sequence alignments, read from a file)
- `profile` , (i.e. protein sequence profiles)
- `map` , (i.e. density functions defined on the 3D grid)
- `grob` (abbreviation for GRaphic OBject, which is different from molecular graphics objects, and contains dots, lines and solid surfaces; it can be a contoured electron density, 3D plot, an arrow,

etc)

- atomic/molecular objects and related selections of atoms (`a_//ca,c,n`) residues (`a_/2:15`) molecules (`a_1.b,c/`) objects (`a_1,2.`) and, finally ..,
- `table` , or spreadsheet. Several arrays are linked together in a table. Table can also have a header with some additional data fields. Tables are essentially simple databases which can be manipulated with, sorted and searched with ICM commands.

The more complicated objects, like arrays, sequences, alignments, maps etc., can be read from a disk file (e.g. `read sequence "a.seq"`) or created by an ICM command or function (e.g. `a=Sequence("ACFASDTRSEEDFFF")` or `make sequence a_1.1`)

Atomic objects are usually specified by an atom, residue, molecule or object selection which are collectively referred to as selections.

All of the listed entities have their unique names in the ICM−shell and can be `read`, renamed (e.g. `rename myFactors bbb`), deleted (e.g. `delete myFactors aaa`), written to a file with a standard type−specific extension (e.g. `write aaa "surf"` will create file `surf.gro` , the extension type depends on the object), shown, often printed and displayed graphically.

A number of ICM−variables have reserved names and are used by the program. For example, the `mncalls` variable always describes the number of molecular energy evaluations during a minimization, `s_pdbDir` is the path to your pdb files, etc. You may customize some of those ICM−shell variables by redefining them in the system−wide `_startup` file, and `$HOME/.icm/user_startup.icm` file. The standard `_startup` file reads `icm.ini` file which contains many standard directory and parameter definitions, e.g. :

```
read all s_icmhome+"icm.ini" # initialize icm variables
```

Important: be careful when negative numbers appear in the command line. If not separated from the previous numeric argument by a **comma,** they will be interpreted by ICM−shell as an expression, i.e. the two arguments will simply be replaced by their difference. For example, the command

```
display string "I like crambin" −0.9 −0.3
```

is **wrong,** a comma is needed, otherwise `−0.9 −0.3` will be substituted by `−1.2`. This command will place the string in a point with screen coordinates `X=−1.2` and `Y=0.0` (the default), not in `X=−0.9` and Y=−0.3 as might be expected. The safest way should be to use commas as separators in the argument list in the command line, like the following:

```
display string "I like crambin" −0.9 , −0.3
```

is correct, the two arguments are separated by comma

Now you can use the mouse to rotate and translate molecules and strings. The left mouse button is associated with rotation, the middle mouse button is translation and the right mouse button clicks are used for drop down menus in GUI and labeling (double click is a residue label). A more detailed list of graphics controls is given below.

As far as the keyboard commands and prompting, try to use the arrow keys for invoking previous commands and TAB for prompting (e.g. atom **TAB**) to see the available commands and functions.

1.7.2. The first steps

You first ICM commands may be the following:

```
read pdb "1crn"
display ribbon
```

or simply

```
nice "1est"
```

You can also:

```
read mol  s_icmhome + "ex_mol"  # or
read mol2 s_icmhome + "ex_mol2" # or
read csd ...
```

The second way to create a molecular object is building the extended chain given the amino−acid sequence. The simplest way to build a short peptide is to use `alias` BS to the `build string` command. Type

```
BS nter ala his leu tyr cooh   # or
buildpep "AHLY;AGGAR" # to build two molecules
```

In a more complex case create a file, say `mymol.se, .se` being the standard extension for the object sequence files. The file should contain the names of molecules (field ml) and their sequence (field se) and may look like this:

```
ml mol1
se nter ala gly his ser trp cooh
ml mol2
se hoh
ml mol3
se hoh
```

Type:

```
build "mymol"
```

to build the object. Now you can display the three molecular objects you have just loaded, i.e. crambin, the two peptides. We will use the `cpk` and the `xstick` graphics representations.

```
display a_2.           # a_2. means 'the second object'
display cpk a_1./2:10  # a_.. means 'residues 2:10 of the first object'
display xstick a_1./16:18
```

You can also replace residues with the `modify` command:

```
modify a_2./his "tyr"
```

Let us clear the scene and start doing some more fun things:

```
delete a_*. # a_*. selects all the objects
build "mymol"
```

```
display     # by default displays everything
set vrestraint a_/*  # this command will increase the efficiency
montecarlo
```

Of course, there is a more elaborate possible setup for a montecarlo run (see `_folding` script) and graphics should not be used for a real run. However, the above example is pretty much what you need to do to run the Biased Probability Monte Carlo Minimization to find the global minimum which models the solution structure of this peptide.

Now let us make a quick tour into multiple sequence alignments. First, get your sequence file (most formats will be accepted). The simplest default file format (then you do not need format type specs like: msf, pir, etc) is the fasta format (angular bracket and sequence name followed by the sequence)

```
> seq1
ASDFREWWDYIEQ
> seq2
SDRTYIEQWWDCVN
```

There are some example multiple sequence files in the ICM−directory. Let us do the following:

```
read sequences s_icmhome+"sh3"   # example sh3.seq file
group sequence "*" sh3ali
show sequences alignments
align sh3ali                     # redo the multiple sequence alignment
unix gs sh3ali.eps               # gs is a PostScript previewer
show Align(Fyn, Eps8)            # make a pairwise alignment
```

If you want to go directly to more elaborate sessions and scripts, or have a "How can I ..." question, you may hop to the User's guide section.

2. Reference Guide

2.1. ICM command line options

Option	Description
−a arg_string	initialize `s_icmargs` string with the arg_string
−b	inhibit Buffered output
−c	clean: do not save _seslog
−e 'commands'	execute semi−colon separated icm commands and quit
−g [menuFile]	start GUI menu bar, using menu file [default=icm.gui]
−G [menuFile]	start GUI menu and keep the original terminal window
−n	do Not execute _startup file
−s	Silent mode (l_warn=no l_commands=no l_info=no l_confirm=no)
−p	set path for ICMHOME, e.g. −p/opt/icm/
−w	web cgi mode: combination of −p and −s, e.g. −w/opt/icm/
−d(or −display) address	sets/redirects the X display (default is $DISPLAY)
−24	enforce high quality 24−bit image mode at the expense of double buffering
−B[max_beeps]	no more than max_beeps on errors (default=300)
−X	report the computer identification number for a node−locked license GUI options:
−style={motif|windows|platinum|cde}	sets the GUI style
−session=session	restores the earlier session
−geometry WxH+X+Y	sets the client geometry of the main widget, e.g. −geomerty 200x200+150+700
−fn or −font font	defines the GUI font
−bg or −background color	sets the default background color
−fg or −foreground color	sets the default foreground color
−btn or −button color	sets the default button color
−name name	sets the GUI name
−title title	sets the title (caption)
−visual TrueColor	forces to use a TrueColor visual on an 8−bit display
−ncols count	limits the number of colors on a 8−bit display
−cmap	causes to install a private color map on an 8−bit display

2.2. Command line editing

(cursor is in the text window).

Operation	Shortcut Key
command word completion/prompting	**TAB**

up−history	**UP** arrow
down−history	**DOWN** arrow
forward−char	**RIGHT** arrow
backward−char	**LEFT** arrow
beginning−of−line	**CTRL**+A
delete−char	**CTRL**+D
end−of−line	**CTRL**+E
backward−delete−char	**Backspase** or **CTRL** F+H
kill−to−line−end	**CTRL**+K
insert−overstrike toggle	**CTRL**+O
paste	**CTRL**+P
delete/copy−whole−line	**CTRL**+U
delete/copy−word	**CTRL**+W
yank (identical to paste)	**CTRL**+Y

Use the **TAB** key when you do not know what to do or to **avoid unnecessary typing** as well as probable typos in long names. This prompting is very convenient and is consistent with the **tcsh** UNIX shell. It will not only prompt you for possible completions, but also prompt you for available files in the `read` command (hit TAB after the double quote mark) and available selection of items in `preference`.

Examples:

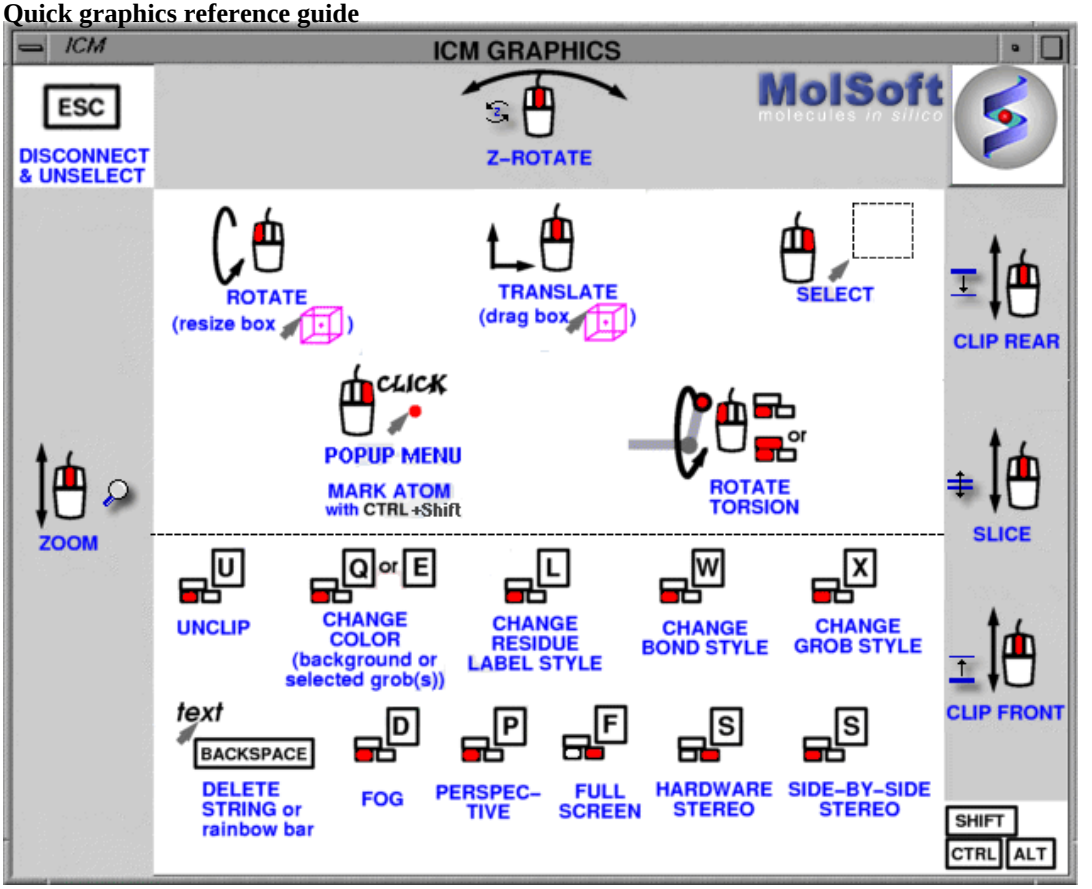
```
show Ic TAB      # completes function name IcmSequence()
read pdb "TAB    # gives you all local *.pdb *.brk files
read sequence "1a TAB  # lists 1a*.seq files
```

2.3. Graphics controls

The rough picture is simple: rotate with the *left* mouse button, translate, drag, crop, and zoom (drag along the left window margin) with the *middle* button, and select/pop with the *right* button. However these are only the defaults which can be customized.

The default shortcut keys are stored in the `icm.clr` file. Thefore, the mapping of keys/mouse buttons to particular graphics operations is *flexible* and can be easily redefined. The `GUI` controls and the **popup** menu are additional to the older shortcut keys listed here. The following shortcut keys to speed up operations in the graphics window (see the quick graphics reference guide) are defined by default. If some of these definitions are not working, check your `icm.clr` file in the `$ICMHOME` directory and modify the key/mouse−operation mapping to your liking.

Quick graphics reference guide



It is necessary to have the cursor in the graphics window. For some operations you may need to move cursor in a specified area (e.g. left margin) of the window. (Note for Windows 95/Windows NT version's users: if you use a two−button mouse hold the left button and the SPACE key instead of the middle mouse button (see picture−prompt for two−button mouse). Some controls use only a margin on the screen (e.g. Bottom5 means the bottom 5% of the graphics viewing area).

Note: if your SGI hardware stereo does not work properly you may need to install IRIX6.4 patches 2448, 2771 and 2843.

OPERATION	DESCRIPTION	KEYS
ROTATE	simple	LeftMB (MB stands for Mouse Button)
	continuous	**Shift**−Bottom5− LeftMB
SHIFT key enforces global rotation	Z−axis clockwise	LeftMB at top margin (*or* **ALT** +Z)

	Z−axis counterclockwise	LeftMB at top margin *or* **CTRL** +Z
	individual torsion angle in ICM−object	**CTRL** (or **CTRL+SHIFT)** LeftMB on reference atom
TRANSLATE	XY−plane (dragging)	MiddleMB
SHIFT key enforces global translation	drag atom in non−ICM object	**CTRL** LeftMB at the dragged atom
GRAPHICS.resLabelDrag controls residue label dragging	Z−axis	MiddleMB at right margin
ZOOM	zoom in	MiddleMB at left margin or **SHIFT** MiddleMB up
	zoom out	MiddleMB at left margin or **SHIFT** MiddleMB down
CLIPPING PLANES	front plane	**CTRL** MiddleMB
	back plane	**ALT** MiddleMB or Right5−MiddleMB
	slice/slab (move both planes)	**CTRL**+ALT MiddleMB
	unclip	**CTRL**+U
LABELING	label atom or grob	RightMB−click
	label residue	double RightMB−click
	paste atom's/grob's name to command line	**CTRL−SHIFT** RightMB (or under Gui: RightMB on atom and release on 1st item)
	paste residue name to the command line	**CTRL** double−RightMB (GUI: RightMB on residue, popup menu and release on 1st item. Use the residue selection level, R)
	set 3D cursor to the residue (move with arrows)	**CTRL−SHIFT** double RightMB
	disconnect/unselect everything	**ESC** or double RightMB−click, cursor in any empty area of the screen
CONNECT for independent movement of molecule(s) **SELECT GROB(S)** for changing size or color	connect to molecule or grob	**CTRL**+ALT RightMB−click on atom or vertex
	connect to more molecule(s)/grob(s)	**CTRL**+ALT+SHIFT RightMB−click
	select/edit grob	double RightMB−click
	add new grob to a selection	**SHIFT** double LeftMB−click on grob
	side−by−side stereo on/off	**CTRL**+S
	hardware stereo on/off	**ALT**+S
	full screen on/off	**CTRL**+F
	perspective view on/off	**CTRL**+P

MODES

MISCELLANEOUS	fog (depth cueing) on/off	**CTRL**+D
	change `resLabelStyle` preference	**CTRL**+L
	change `resLabelStyle` preference	**CTRL**+A
	change background color	**CTRL**+E / CTRL+Q
	change "skin" color of the selected grob(s)	**CTRL**+E / CTRL+Q
	change "wire" color of the selected grobs	**ALT**+E / ALT+Q
	change display modes of the selected grobs	**CTRL**+X
	delete string label pointed by the cursor	**BACKSPACE**
	gui (graphical user interface)	**CTRL**+G
	drag the box	MiddleMB−click at boxCorner

2.4. Editing pairwise sequence−structure alignments

ICM has a powerful editor for pairwise and multiple alignments. ICM alignment editor robust and safe. It protects you from unintended changes in the alignment. To edit an alignment one only needs four the types of operations:

- (optional) create space on both sides around a vertical section of the alignment
- select a block with one or several sequences to be moved (press Ctrl to add blocks)
- use the keyboard *arrows* to move the selected block with respect to the other sequences
- squeeze out the excessive gaps (an item in the alignment popup menu)

OPERATION	KEYS
set a vertical selection for ALL sequences in the alignment	**Double−Click**
add white space by hitting the Space bar	**SpaceBar**
remove white space	**Backspace**
select a sub−block for shifting	**Drag Left−Mouse−Button**
shift the selected block next to a gapped area	**Right and Left Arrows**

2.5. Constants

The values of most of the ICM−shell objects may also be represented explicitly in the ICM−shell as so called "constants" (i.e. in the `myFactors={1.2, −4., 5.88}` line, `myFactors` is an ICM−shell variable of the rarray type, while `{1.2, −4., 5.88}` is an "rarray" constant. The following constants are defined in the ICM−shell:

- **integers:** `−9999 12`
- **reals:** `12.0 −0.00003 2.`
- **logicals:** `yes no`
- **strings:** `"I see M", "Backslash (\\) and quote (\")" "line1\nline2"`

  Escape sequences which can be used inside strings:

```
\a − bell
\b − backspace
\f − formfeed
\n − newline
\r − carriage return
\t − horizontal tab
\v − vertical tab
\\ − backslash
\" − double quote
```

- **integer arrays:** `{2, −1, 6, 0} {−8, −1, 2}` The comma is compulsory before a negative number, it can be skipped otherwise. See also: `read iarray`.
- **real array:** `{ −1.6 , 2.150 3., −160.}` See also: `read rarray`
- **string arrays:** `{"do","re","mi","fa","sol"} {"\n(newline), \t (tab)","\a (bell)"}` See also: `read sarray`
- **`selections`** (find a detailed description below):

```
a_hiv?.  a_1,2.  a_*.           # objects
a_h*.a   a_m1    a_*.!w2,w15,z* # molecules
a_1.*/2:15,18:26 a_/18,his*     # residues
a_//ca,c,n a_1.c a_/2:4/!h*     # atoms
v_//phi,psi      V_2//?vt*      # variables
```

2.6. Subsets and index expressions

one can refer to an element or a subset of ten kinds of ICM−shell variables:

Variable type	Expression	Result type	Example
string	*string[i]*	*string*	`lastChar=str[Length(str)]`
	string[i1:i2]	*string*	`resName=pdbStr[18:21]`
iarray	*iarray[i]*	***integer***	`CurrSize=sizes[i]`

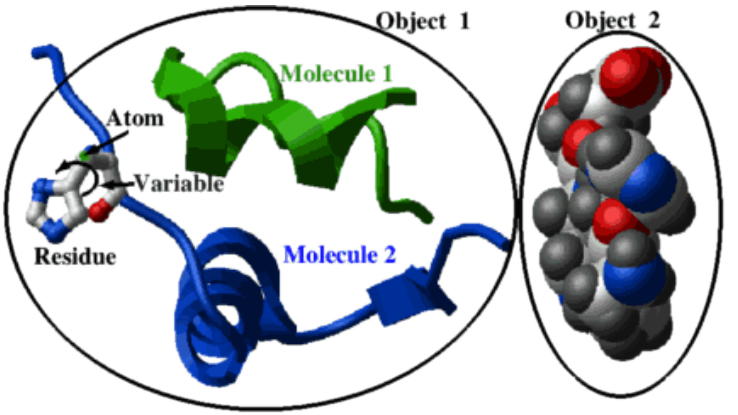
	iarray[i1:i2]	*iarray*	`frag=list[4:nitems]`
	iarray[I_]	*iarray*	`sublist=list[{1,3,5}]`
rarray	*rarray[i]*	***real***	`the=same[i]`
	rarray[i1:i2]	*rarray*	`all=as[for:iarr]`
	rarray[I_]	*rarray*	`Part=R1[{1,2,3}]`
sarray	*sarray[i]*	***string***	`best=menu[ibest]`
	sarray[i1:i2]	*sarray*	`fish=list[4:8]`
	sarray[I_]	*sarray*	`some=all[{1,2,3}]`
matrix	*matrix[i1,i2]*	***real***	`Element=M[4,5]`
	matrix[i1]	***rarray***	`atomCaVec=CoordMatr[15]`
	matrix[i1,i2:i3]	***rarray***	`thirdRow=M[3,1:5]`
	matrix[i1,?]	***rarray***	`thirdRow=M[3,?]`
	matrix[i1:i2,i3]	***rarray***	`firstColumn=mm[1:3,1]`
	matrix[?,i3]	***rarray***	`firstColumn=mm[?,1]`
	matrix[i1:i2,i3:i4]	***matrix***	`upperSqr=rot[1:2,1:2]`
sequence	*sequence[i]*	***string***	`amino4=bpti[4]`
	sequence[i1:i2]	*sequence*	`domain=seq[139:302]`
alignment	*alignment[i]*	*alignment*	`column4=globins[4]`
	alignment[i1,i2]	*string*	`AminoAcIn2ndSeq=globins[4,2]`

	alignment[i1:i2]	*alignment*	`motif=EFhand[15:27]`
profile	*profile[i]*	*profile*	`His=prof[18:18]`
	profile[i1:i2]	*profile*	`motif=prf[14:35]`
selection	*selection[i]*	*selection*	`ca18=ca[18]`
	selection[i1:i2]	*selection*	`frag=ca[14:35]`
table	*table[i]*	*table*	`show t[3]`
	table[i1:i2]	*table*	`delete t[3:5]`

Important note. When both lower and upper limits are explicitly specified, even if they are equal (e.g. *list* [3:3]), the type of the subset object remains the same. If only one element is specified, the rank may be reduced. The upper limit may be larger than the actual limit (e.g. t[3:9999]). You may also use `0` instead of the last element number (e.g. t[3:0]).

2.7. Molecule intro

Molecules are the main inhabitants of the ICM shell. The shell can contain many objects, each of which can be a soup (this expression belongs to my friend Gert Vriend) of separate molecules. Molecules, in turn contain residues and atoms. ICM can handle both **raw** objects, as they come from a PDB file or a mol−file, and a fully prepared for molecular modeling "ICM"−objects.



The non−ICM objects can be visualized, but they need to be converted into ICM−objects to perform the most interesting modeling operations. To specify the subsets of objects, molecules, residues, atoms and internal variables, you need to learn the language of molecular selections.

A quick preview of the selection language, using the picture above as an example:

```
display a_2. cpk           # object selection (the second object)
display a_1.1 ribbon green # molecule 1 from object 1
display a_1.2/his xstick   # residue his12 shown as balls and sticks
color   a_/1.2/12/n* xstick blue  # atoms: color nitrogens in blue
```

For an in−depth description of selections, read the next section.

2.8. Selections

Let us imagine that we decided to compare two structures deposited in the PDB. We will read both entries in the ICM shell, and define the following levels or organization. Each entry will form an **object,** each object will contain one or several **molecules,** protein molecules will naturally contain amino acid **residues** and residues will consist of **atoms.** Now, in the superimpose command, we will need to specify, or **select,** the molecules, residues or atoms which should be `superimposed.` The ICM shell language has a flexible way of selecting subsets of atoms, amino−acid residues, molecules, objects, as well as torsion angles and other internal geometrical parameters of molecules. Most of the ICM commands and functions dealing with molecules, for example, display, delete, minimize, etc., will operate on an arbitrary selection. What does a selection look like? For example, selection `a_2./2:14/c*` selects carbon atoms of residues from 2 to 14 of the second object. The general syntax of a selection is the following:

prefix **_** *[object(s)* **.** *] molecule(s) / residue(s) / atom(s) or variable(s)*

The object section including the *dot* (e.g. `1crn.`) may be omitted. In this case the selection will be performed in the `current` object.

There can be as many as five sections separated by **`_.`** / and **/,**

Examples:

```
a_2ins.a,b/lys,arg/ca,cb,n*   # atom selection, '*' – any string
a_2ins.a,b/2:10/n,ca,c        # atom selection
v_crn./lys,arg/phi,PSI        # variable selection
```

(Note use of `PSI` torsion in the last example.)

Storing selections in named variables.

Selections can be assigned to a variable (e.g. `x = a_//c*`) and can be combined in an expression by *logical and* (**&**) or *logical or* (|), e.g. (`a_//n* a_//ca`).

Selection Types

Three prefix types: a_ v_ and V_ . The Prefix defines one of the three selection types:

- atoms, residues, molecules and objects (`a_..`)
- free variables (`v_..`)
- all variables (`V_..`)

The a_ selection is the most popular and selects **atoms, residues, molecules** or **objects.** Therefore, there are four atom selection subtypes which are abbreviated as follows:

abbr.	selection name	example
os_	object selection	`a_ ; a_1. ; a_1crn. ; a_*.`
ms_	molecule selection	`a_1.2 ; a_a,b ; a_*.*`
rs_	residue selection	`a_/3:9 ; a_/* ; a_/"GKS"`
as_	atom selection	`a_1.2//ca,c,n ; a_//c*`

Two additional types of selections let you select amongst the free internal coordinates or all internal coordinates (both free and fixed). These selections are widely used in commands and functions related to energy minimization and sampling:

abbr.	selection name	example
vs_	selection from free internal variable	`v_ ; v_1. ; v_1.2//x* ; v_2//?vt*`
Vs_	selection from all internal coordinates	`V_ ; V_1. ; V_1crn.//!phi,psi,omg`

A selection can also be assigned to a named variable:

Example:

```
aa = a_//ca,c,n  # the backbone
show aa
```

The object and molecule sections are separated by a period, all other sections are separated by slashes. Inside each section, arguments in a list are separated by comma (,) while ranges are separated by colon (*from:to*).

Selection levels

There are four principal levels of selection: object selection, molecular selection, residue selection and atom or variable selection. The level is defined by the "lowest" section explicitly specified in a selection (e.g. `a_1.1/2:4` is a residue level selection, while `a_//ca` is an atom selection). These selections are referred to as ***os_ ms_ rs_ as_*** or ***vs_*** , respectively. If selection level is not important or the level is the lowest one (atoms or variables), selections are referred to as ***as_*** or ***vs_*.**

The selection level of the interactive graphics selections is controlled by the `GRAPHICS.selectionLevel` preference. To change it from the command line, assign this variable to an appropriate level, e.g. `GRAPHICS.selectionLevel="atom"` .

Selection levels can be changed from the **GUI** interface, by changing the selection level

Examples

Examples of different selection levels (note that object and molecule names are arbitrary):

```
a_1,3.  a_mod*.   a_*.  a_"*benz?n*".   # object selections
a_3.mol1  a_zinc  a_$molNum  a_*.*      # molecule selections
a_/3:29,as?,ala  a_/*  a_*./"VHC?[!W]A" # residue selections
a//h?,c*  a_//T v_//phi,psi             # atom or variable selections
```

For example, `a_1,3.` is an object selection, and `a_/ala` is a residue selection.

Each section may contain a **negation** symbol **!** in the beginning. It selects *all, but the specified*. You can only use the negation symbol in the first position of a section and the negation will always apply to the *whole* section. For example, `a_/!ala,gly` is right, while `a_/ala,!gly` is wrong.

If object section together with the separating period is skipped, selection addresses the current object rather than all objects.

Select by number, range, name or pattern

Matching. Objects, molecules, residues, atoms and variables may be referred to by their names. Objects and molecules can be additionally referred to by their sequential numbers (e.g. `a_1.2).` To select by a numerical name, use backslash before the name, e.g. `a_\123` . Metacharacters, such as *** ? []**, can also be used for pattern matching (e.g. `v_//?vt*).`

Full syntax. A complete description of selection syntax for each level is as follows:

2.8.1. Object selection

(**a_** *obj.* or just **a_** for the current object):

a_ *name* **.**	(a_1crn. , note the dot at the end)
a_ *namePattern.*	(a_1c?n.)
a_ *relNumber.*	(a_2. means the second object)
a_ *num1:num2.*	(`a_2:5.` range from object 2 to object 5)
a_	the *current* object, it is a special case.
a_ " *commentPattern* ".	select by pattern matching in the object *comment* field.
a_ICM.	objects of ICM type (a_!ICM. − non−ICM objects)
a_CATRACE.	objects of `"Ca−trace"` type

Other object types (e.g. `"NMR","Fiber",` etc.) can be selected or checked with the `Type` (os_ 2) function.

Example:

```
read object s_icmhome+"all"
show a_   # the current object
show a_1,2:3.
show a_s1?.
show  a_"*Th[iy]o*".//!h*
```

2.8.2. Molecule selection

a_*obj.mol*	in specified object(s),
a_*mol*	in the current object or
a_*.*mol*	in any object

by name:

a_*s_name* e.g. `a_m2` or `a_1.m2` in the current (`a_`), or the first (`a_1`) object, respectively. (Note that there is **no** dot at the end). If the name starts with a digit or one of the reserved one−letter types (see below), add backslash before the digit, e.g. `a_\123 , a_\A` .

by pattern

a_*s_namePattern* (`a_w*` − all water molecules in the current object)

by number(s)

a_*number* (`a_2` , `a_3.2,4,7`) − relative number of molecule(s)

by range(s)

a_*num1:num2* (`a_2:5` , `a_2:5,10:12`) − number range

by chemical formula (F):

a_**F***formula1*,**F***formula2*..

the chemical formula must be the same as the one returned by the ICM `String`(ms_) function **without hydrogens**, e.g.

```
  read pdb "1abe"
  show a_FC505  # selects 2 arabinose molecules
  String( a_2//!h* )
 C5O5
```

by special symbol for types of molecules:

a_*specialSymbol[,specialSymbol2..]*

- A peptides and proteins
- B molecules included in biological unit
- C select by Chain, e.g. a_1.Cabc
- H hetatm, usually ligands and water molecules
- N nucleic acids
- Q molecules which have a seQuence linked to them
- S sugars
- M Multiple sequence alignment linked to molecule exists
- L lipids
- W water including deuterated water (dod)
- U unknown (miscellanea)

Note that if a molecule name coincides with any of the above characters (i.e. `"ACHLMNQRSTUW"`), ICM gives preference to the type selection. To select by molecule name, use backslash (e.g. `a_1.\A` for chain named `"A"`)

Examples:

```
nice "1dnk"  # one peptide, two dna chains and other mols
a_A          # the peptide
a_N          # the two DNA chains
a_A,N        # the peptide and the DNA chains
rename a_1 "A"
a_\A         # chain NAMED "A"
read pdb "2ins"
delete a_W
```

Some special cases:

```
a_*   # all molecules in the current object
a_a   # molecule 'a' in the current object
a_.a  # molecules 'a' in all objects
a_*.a # the same as a_.a
```

selecting water molecules from pdb−files by their 'residue−field' number.

Water molecules in PDB files are numbered and the numbers are stored in the residue field. For consistency, we convert these numbers into residue numbers. At the same time the *names* of water molecules are built sequentially like this: `w1,w2,w3` . This way one can use both sequential numbering via molecule names and PDB−file numbering via residue numbers.

```
read pdb "1sri"
show a_w12:w15    # by molecule name, sequential numbering
show a_w*/719:721 # by original pdb number
```

converting any selection to molecules with the `Mol` function

Selection of any level, e.g. atoms, residues, and objects can be converted to molecules with the `Mol` (*selection*) function. Example:

```
Mol(Sphere(a_zinc a_1,2 8.)) # Sphere returns atoms
```

2.8.3. Residue selection

With respect to objects and molecules there are the following possibilities:

a_*obj.mol/res*	complete specification, (e.g. `a_*.*/14:19` or `a_2.3/ala).`
a_*mol/res*	the current object and the specified molecules, (e.g. `a_w*/*`)
a_/*res*	all molecules of the current object, (e.g. `a_/23:25)`

Residue field specifications (for all molecules in the current object).

by name:

a_/*resName* (e.g. `a_/his` , or `a_/\001` − here we had to start with a backslash becase the residue name looked like a number)

by pattern:

a_/*resNamePattern* (e.g. `a_/as?` − asn or asp). A useful tip for DNA or RNA selections. Quite often bases are modified. To select A,T,G,C,U and their modifications, use `a_/??a` or `a_/??t` or `a_/??g` or `a_/??c` or `a_/??u,` respectively.

by residue number(s):

a_/*numChar* (`a_/3` or `a_/15A`) − PDB residue number may contain additional characters.

by residue range(s):

a_/*numChar1:numChar2* (`a_/4:15,20:25`) − reference residue number range

by amino acid sequence pattern:

a_/"*seqPattern*" (`a_/"G?GTE"`) − selects the fragment with matching aminoacid sequence.

Example selecting all residues preceding prolines (the first expression selects dipeptides with the second proline, the second one excludes prolines):

```
show a_/"?P" a_/!pro*
```

by special symbols and expressions

by residue type

a_/**A** − residues of `"Amino"` type (N− and C−termini have different type) **displayed residues**

a_/**D** − displayed residues in the `ribbon` representation only

a_/**DD** − displayed residues in which either ribbon or some atoms are displayed

residues identical to their homology target residues

a_/**I** − if atoms of one molecular object are tethered to atoms of another object, selection `a_/I` shows those tethered residues (i.e. they contain tethered atoms) which have identical names to the residues to which they have been tethered.

by absolute number

a_/**N** *absNumber* (`a_/N15`) − absolute number (all residues

of all objects are numbered sequentially starting from one.) **by secondary structure**

a_/**S** *sec_struct_chars* − residues with certain secondary structure (e.g. `a_/SH` − only helices; `a_/SEH` − sheets and helices; `a_/S_` − only coil)

terminal residues (like N−terminal, C−terminal, and DNA 5' and 3' termini) a_/**T**

by alignment consensus

a_/**C** *resConservationCode* − selects residues according to the consensus of the *alignment* linked to a molecule. The symbols can be combined, e.g. `a_/CYnh` for conserved tyrosines, negatively−charged residues and hydrophobics. Possible codes:

- A , C ... − particular conserved amino acid types (one−letter code)
- X − all absolutely conserved residues
- h − conserved hydrophobic residues (#)
- s − conserved small residues (^)
- p − conserved polar residues (~)
- o − conserved positive residues (+)
- n − conserved negative residues (−)
- a − conserved aromatic residues (%)
- x − not conserved but in the ungapped block (.)
- g − gap in one of the sequences of the alignment (' ')

(e.g. `a_/CXh` − selects all identities in the alignment and hydrophobic residues, `a_/CACg` − all conserved alanines, cysteins and gapped regions)

by functional features

a_/**F**[*SiteChars*] or a_/**F**"*siteID*"

residue selection by the one−letter site type or the site ID, respectively. Letter F refers to the word *feature* as in the FT (feature table) field of Swissprot entries. The types along with their one−letter codes are listed in the glossary site entry. The default string, the `a_/F` selection, is defined by the `SITE.defSelect` string (you may redefine it), which defines important local features such as binding sites as opposed to domain−type sites such as signal peptides, zinc fingers and other protein domains. The PDB entries do not comply with the standard SWISSPROT site definitions, such as ACT_SITE BINDING etc., and are assigned by the user type **F** (selection `a_/FF`).

Example:

```
nice "1as6"
show site
color ribbon a_/F magenta
show a_/FF
show a_/F"cu3"     # select only site named cu3
show a_/F"MUTAGEN" # sites so defined in Swissprot
set site a_1.1 "FT SITE 15 15 My favourite residue"
```

converting selections to residue level: The `Residue` (*selection*) will convert any selection of higher level or lower level to the residue level. Example

```
a_/SH a_/pro  # a proline in a helix
Res(Sphere(a_/pro 2.))  # expand to the neighboring residues
```

2.8.4. Atom selection

(**a_**//*atoms*):

by name

a_//*name* (`a_.//ca` , `ca` is a usual name for alpha carbon)

by name pattern

a_//*namePattern* (`a_.//c*` for all carbons)

by special symbols and expressions

alternative atom positions in X−ray structures

a_//**A** *alterCharacter* − select alternative positions of the specified type (e.g. `read pdb "1cbn" ; show a_//Ab`). See also the `set comment "A"` *as_* command.

by atom code

a_//**C***atomCodeNum[:atomCodeNum2]* − select by atom code as described in the icm.cod file, e.g. `a_//C2,C4` selects aromatic and methylene hydrogens, `a_//C2:15` selects codes from 2 to 15

a_//**M***atomMmffCodeNum[:atomCodeMmffNum2]* − by mmff code

displayed atoms

* a_/**D**[*displayTypes*] − Displayed atoms (e.g. `a_//D` for all displayed atoms, or `a_//DWC` for wire or cpk). The following graphical types can be selected:

- **A** − labelled atoms
- **B** − `ball`
- **C** − `cpk`
- **D** − displayed atoms or atoms in displayed residues
- **S** − `skin`
- **W** − `wire`
- **X** − `xstick` (i.e. ball or stick)
- *no arguments* − any graphical representation

Special named selections: as_graph graphically selected atoms:

`as_graph` selection contains graphically selected objects, molecules, residues, or atoms The level of selection depends on the `GRAPHICS.selectionLevel` preference. The level can be changed from the GUI interface or from command line.

strained atoms (atoms with high energy gradient)

a_//**G** − strained atoms (Gradient vector longer than `selectMinGrad`) You can also use the `display gradient` command.

Example:

```
buildpep "his trp trp"
display
randomize v_//phi,psi
selectMinGrad = 100.
show energy
display a_//G ball
display gradient
```

hydrophobic atoms a_//**H**

aromatic atoms a_//**R** It selects heavy atoms connected by aromatic bonds and hydrogens attached to them. Example:

```
buildpep "HWYP"
display skin
color skin a_//R magenta
```

tethered atoms

a_//**T** − Tethered atoms (see also `a_//Z` − tether destination atoms)

tether−target atoms

a_//**Z** − Tether destination/target atoms (see also `a_//T` − tethered atoms)

chiral atoms a_//**X**[0123RLB] − chiral atoms. Each atom has two bits characterizing its chiral properties. If the two bits are presented as an integer, the chiral number has the following values:

- zero − a non−chiral center
- 1 − a left topoisomer (L)
- 2 − a right topoisomer (R)
- 3 − a racemic mixture of both isomers (B)

The chiral symbols can be appended. For example `a_//X123` means `a_//X1 | a_//X2 | a_//X3` . A short form of this selection, `a_//X` means all non−chiral atoms and is identical to `a_//X123` (or a_//!X0) Examples: `a_m/3:4/X1` , `a_//XLR` (only left or only right chiral centers, but no racemic centers), `a_//XB` (only racemic centers)

by absolute number

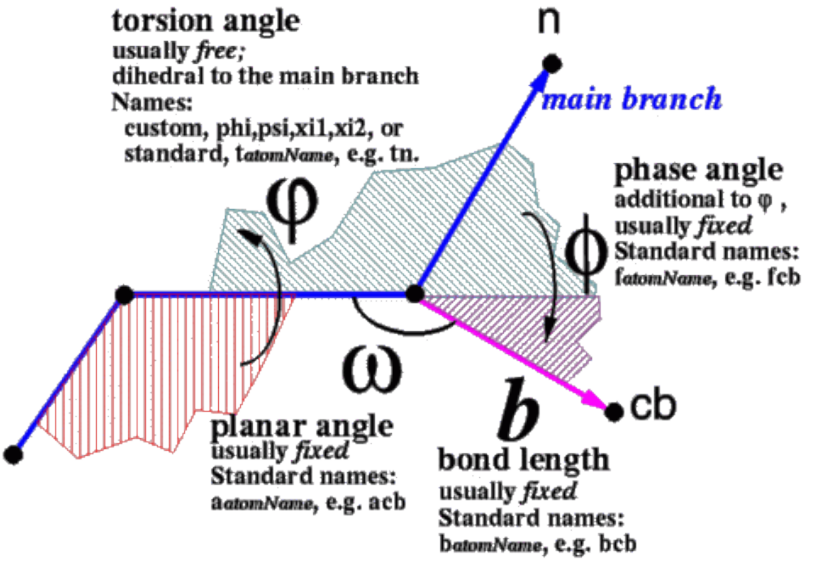
a_//*absNumber* − absolute number (all atoms of all objects are numbered sequentially starting from one)

converting to atom level: The `Atom` (*selection*) will convert any selection of higher level to the atom level.

2.8.5. Free and all variables (v_ and V_)

The ***v_selection*** selects **free variables** in molecular objects of ICM−type.

The main types of **internal coordinates** , or geometrical variables, are shown below:



The position of each atom branch is determined by the positions of the preceding atoms and three parameters: dihedral angle, planar angle and bond length. The dihedral angle for the main branch atom is the torsion angle itself, while for the secondary branch atoms the dihedral angle consists of the torsion angle plus the phase angle. The default fixation is given in the ICM−residue library and can be changed by

`fix` and `unfix` commands. Individual free variables can be rotated interactively with `Ctrl−LeftMB−Atom−Click` and drag. A *vselection* can also be assigned to a named variable:

Example:

```
aa = v_//phi,psi  # the backbone torsions
unfix only aa
unfix only v_/10:15/phi,psi
```

V_ : selecting among all internal coordinates

Finally, the **V_** *selection* selects **both free and fixed variables** in molecular objects of ICM−type. You always need this type of selection in the `unfix` command. It makes no sense to unfix variables which are free already.

Here is a list of variable selection specifications:

by name:

v_//*name* (`v_//phi`)

by name pattern:

v_//*namePattern* (`v_//x*`) use asterisk ***** for any string, and question mark **?** for any character. Example: `v_//?vt*` selects the 6 " `virtual`" variables defining rigid body rotation and translation.

torsion variables

v_//**T***torsionCodeNum[:torsionCodeNum2]* − select by torsion angle code as described in the icm.tot file, e.g. v_//T11 selects the amide group torsion angle v_//T10:15 selects torsion codes from 10 to 15

angles (planar angle variables)

v_//**A***angleCodeNum[:angleCodeNum2]* − select by planar angle code as described in the icm.bbt file.

bond length variables

v_//**B***bondCodeNum[:bondCodeNum2]* − select by bond length code as described in the icm.bst file.

Psi torsions not shifted to the next residue

v_//**PSI** − *psi* torsion angle which belongs to the residue you would expect. The reason for this definition is that from ICM point of the *psi* backbone torsion with rotation axis between Ca and C of residue *i* belongs to N−atom of the **next** residue *i+1* because N is the first atom this torsion angle moves. E.g., `v_/3/phi,psi` selection will contain the *psi* from residue 2 and then *phi* from residue 3. The definition **PSI** allows you to use the conventional attribution of angles, e.g. v_/3/phi,PSI is a pair of angles with axes around Ca atom or residue 3. **Important**. However, note that if you use selection expressions like

`v_//phi,PSI a_/2,3` it will not work (in contrast to `a_/2,3/phi,PSI`) and you will have to use the `Next` function.

Example:

```
 vPhi = v_/3/phi
 vPsi = v_/3/PSI
# BUT !!!
 vPhi = v_//phi* a_/3
 vPsi = v_//PSI  Next( a_/3 )
```

methyl group torsions

v_//**M** − torsion angles rotating Methyl−type terminal hydrogens (excluding polar hydrogen)

polar hydrogen torsions

v_//**P** − torsion angles rotating Polar hydrogens (e.g. hydroxyl group)

essential (non−hydrogen) torsions:

v_//**H** − side chain torsion angles rotating "Heavy" atoms

standard set of free torsions (excludes rings)

v_//**S** − all "Standard" free torsion angles as defined in the `icm.tot` file.

Note that `v_//M, v_//P,` and `v_//H` do not overlap, they are mutually exclusive. `v_//S` contains `v_//M, v_//P,` and `v_//H` as well as other standard torsion angles.

phase angles

v_//**F** − select **all** phase angles (usually they are fixed, so use `V_//F`)

V_//**FC** − select phase angles related to the **chiral** centers (see `set chiral` and `montecarlo chiral`)

all torsion angles

v_//**T** − select **all** free torsion angles, `V_//T` for all torsion angles including the fixed ones.

2.8.6. Functions returning selections

- `Acc` − select solvent−accessible atom/residues.
- `Atom` − convert to the atom selection
- `Deletion` − residues deleted according to the alignment
- `Insertion` − residues inserted according the alignment
- `Mol` − convert to the molecule selection
- `Next` − extract the next atom
- `Obj` − convert to the object selection
- `Res` − convert to the residue selection
- `Sphere` − expand a selection by *r_radius* or 5Å.
- `Select` − selection of atoms according to their coordinates, bfactors, or other properties

Substituting ICM−shell variables into a selection. You can insert the value of an `integer` or `string` ICM−shell variable anywhere inside your selection by using a **$** (dollar sign) prefix. (Note, this is a general ICM−shell substitution mechanism).

Examples:

```
selstr="!w*/14:19"             # a string constant
display a_$selstr
```

Logical operations. You can also assign selection to a variable, (i.e.: `backbone=a_//ca,c,n`) combine several selections using logical operators (example: `show a_/3:6 backbone`) .

2.8.7. Finding contiguous residue ranges with the String function

To identify contiguous ranges of residues in residue selection, use the `String` (*rs_*) function which will convert your selection into a string expression suitable for entering into a ICM−shell. For example, if we want to find all prolines surrounded by two other helical residues helical proline plus next and prev. residues we might do the following:

```
read pdb "1dkf"
rrange = String( a_/"?P?" ) # the result would look like "a_a.b/5:7,30:32"
rg = Split(rrange,"/,|")    # split into sarray with {"a_a.b","5:7","30:32"}
                            # bar (|) helps with multiple chains
okrg={""}
k=0  # counter for good residue triplets with HHH and ?P?
for i=2,Nof(rg)
  if Nof(Split(rg[i],":")) != 2 continue    # ignore molecular names
  if Sstructure( a_/$rg[i] ) == "HHH" then  # compare with ss−pattern
   k = k+1
    okrg[k] = rg[i]
  endif
endfor
# now ok−ranges are stored in okrg string array e.g. {"5:7"}
# to use them Sum(okrg,",")
```

2.9. Arithmetics

Most of the ICM−objects can be used in arithmetical, logical of comparison expressions. In this section we describe operations defined in the ICM−shell.

Members of the arithmetic, logical and comparison expressions

Abbreviations: `integer` (**i**), `real` (**r**), `string` (**s**), `logical` (**l**), `iarray` (**I**), `rarray` (**R**), `sarray` (**S**), `matrix` (**M**), `sequence` (**seq**), `profile` (**prf**). `alignment` (**ali**), `map` (**m**), graphics object (grob) (**g**), atom selections (**as**), selections of internal coordinates, for example torsion angles, (**vs**) , and `table` (**T**). Table arrays are abbreviated as **T.I, T.R** and **T.S,** depending on the type

2.9.1. Assignment

allows you to assign a value to a variable.

Syntax: ***ICM−shell−variable−name = Value or expression***

If the name is new, a new ICM−shell variable is created.

Examples:

```
a=1            # create new integer variable  a
b=a*a          # create variable b as product a*a
c=a*Sin(45.)   # create new real variable c
```

Assignment and operations **in place** are also possible and it allows to modify an existing variable rather than create a new one. Example:

```
i += 1  # adds one to i, better than i = i + 1
s += " and more .. "
I //= 15  # append to an iarray
R //= 1.5 # append to an rarray
S //= "one more element" # append to an sarray
```

2.9.2. Arithmetic operations

The following operations are defined in the ICM−shell:

- **addition** (+) :
  - **i+i** returns **i** (e.g. `2+3` returns `5`),
  - **i+r, r+i, r+r** return **r** (e.g. `2+3.` returns `5`),
  - **I+I** returns **I** (e.g. `{1,2}+{2,3}` returns `{3,5}`),
  - **I+R, R+I, R+R** return **R** (element by element),
  - **s+s, s+i, s+r** return **s** (i.e. "what" + "If" returns "whatIf","file"+2 return "file2"),
  - **S+S, S+I, S+R** return **S** (the above three operations for each element),
  - **M+M** returns **M** of the same dimensions (element by element addition),
  - **prf+prf** returns **prf,**
  - **grob + R3** return **grob** with coordinates translated by **R3,**
  - **map+map, map+i, map+r, i+map, r+map** returns **map** of the same dimensions.
- **subtraction** (−) :
  - **i−i** returns **i,**
  - **i−r, r−i, r−r** return **r,**

- **I−I** returns **I,**
- **I−R, R−I, R−R** returns **R** (element by element),
- **M−M** returns **M** of the same dimensions (element by element subtraction),
- **map−map, map−i, map−r, i−map, r−map** returns **map** of the same dimensions.

• **multiplication** (*) :

- **i*i** returns **i,**
- **i*r, r*i, r*r** returns **r,**
- **I*I** returns **I** (element by element, e.g. `{1,2}*{3,4}` returns `{3,8}`),
- **I*R, R*I, R*R** return **R** (element by element). The **scalar product** is returned by `Sum(R_1,R_2),` and the **vector product** is returned by `Vector(R_1,R_2)` (two 3D vectors)
- **M*M** returns a matrix product of the two matrices (M[nk]*M[km]==>M[nm]),
- **M*R, R*M** returns **R,**
- **prf*prf** returns **prf,**
- **map*r, map*i, i*map, r*map, map*map** return **map** (operations on each element),
- **grob*r, grob*i, r*grob, i*grob** return **grob** with transformed coordinates.

• **division** (/) :

- **i/i** returns **i** (integer division, e.g. 3/4 returns 0),
- **i/r, r/i, r/r** return **r** (real division, e.g. 3/4. returns 0.75),
- **I**/I returns **I** (integer division of elements),
- **I/R, R/I, R/R** return **R** (real division of elements),
- **map/r, map/i** return **map** (operations on each element),
- **grob/r, grob/i** return **grob** with transformed coordinates.

• **concatenation, appending into array** (//) :

- **i//i** returns **I[2]** (e.g. `2//3` returns `{2,3}`),
- **r//r** returns **R[2]** (e.g. `2.2//3.3` returns `{2.2,3.3}`),

- **s//s** returns **S[2]** (e.g. `"a"//"b"` returns `{"a","b"}`),
- **I//i** returns **I[n+1]** extended by the integer (e.g. `{1,2}//3` returns `{1,2,3}`),
- **I//I** returns **I[n+m]** (e.g. `{1,2}//{3,4}` returns `{1,2,3,4}`),
- **R//r** returns **R[n+1]** extended by the real (e.g. `{1.,2.}//3.` returns `{1.,2.,3.}),`
- **R//R** returns **R[n+m]** (e.g. `{1.,2.}//{3.,4.}` returns `{1.,2.,3.,4.}`),
- **S//s** returns **S[n+1]** extended by the string (e.g. `{"a","b"}//"c"` returns `{"a","b","c"}),`
- **S//S** returns **Sn+m** (e.g. `{"a","b"}//{"c","d"}` returns `{"a","b","c","d"}`),
- **M**[n,m]//**M**[n,k] returns **M[n,m+k]** (matrix concatenation row by row),
- **seq//seq** returns concatenated **seq** (similar to s+s);
- **prf//prf** returns concatenated **prf;**
- **grob//grob** returns concatenated **grob** (similar to s+s);

- *ali1//ali2* returns **projected alignment.** Projected concatenation of two alignments sharing the same sequence. The shared sequence serves as a ruler for merging the two alignments. The alignments can be of arbitrary size and number of sequences. In the simplest case of three sequences `a, b, c` and alignments `ab` and `bc,` the operation `ab//bc` will create an alignment of three sequences `a b c` . The function `Align(ab//bc,{1,3})` will extract the, so called, projected alignment of **a** and **c** through **b.** Example:

```
  ali1    //    ali2  returns   Projected ali.
a VYRWA-W     b FK-WG--KW     a  VYR-WA---W
b -FKWGKW     c AKGWAPGKW     b  -FK-WG--KW
                              c  -AKGWAPGKW
```

Additionally, character arrays (strings) can be projected from sequence to alignment and back with the `String` (..) function and numerical residue properties can be projected from sequence via alignment with the `Rarray` (..) function.

2.9.3. Logical operations

Logical operations with `table` arrays are described separately (see table in Glossary).

- **and** (**&**):
  - **l & l** returns **logical,** e.g. `yes no` returns `no`
  - **as & as** returns selection **as** with objects molecules residues present in both initial selections, (e.g. `a_2//ca a_//T` returns the tethered Ca atoms of the 2nd molecule),
  - **as & s**, multiplication by a **string mask**, e.g. a_//ca "x−" returns the *odd* Ca atoms.

- **as & seq** returns **residue subselection** of **as** with the **matching sequence**, e.g. a_*. 1crn_m returns residues matching the crambin sequence.
- **as & R** returns **atom subselection** with coordinates within a six dimensional box array **R** (see also function `Box`) , e.g.

```
read pdb "1crn"
display ribbon
color ribbon green Res( a_//* {0.,0.,0.,9.,9.,9.} )
```

  More types of selections are returned by the `Select`, `Sphere`, and `Acc` functions.
- **vs & vs** returns selection **vs** of internal coordinates present in both initial selections, (do not forget that v_ are free variables, and V_ are all variables);
- **vs & as** returns subset of initial variables **vs** which is related to selection **as,** e.g. side−chain torsion angles in the sphere around loop 14:18 can be selected as follows:

```
V_//xi* Sphere( a_/14:18 )
```

multiplication comments on logical multiplication of two selections below.

- **or** (|) :

  - **l|l** returns **l** (e.g. `yes|no` returns `yes`),
  - **as|as** returns **as** with members of both selections (e.g. `a_/4:6 | a_//ca`)
  - **vs|vs** returns **vs** with variables from both selections (e.g. `v_//phi,psi | v_/3`)
  - **vs|as** returns **vs** is equivalent to `vs | (V_//* as)`

- **not** (**!)** :

  - **!l** returns **logical** negation to the argument (e.g. `!yes` returns `no`),
  - **!as** returns **aselection** of the same level with members not included in the selection argument (e.g. `!a_//ca`)
  - **!vs** returns **vselection** with variables not included in the selection argument (e.g. ! v_//phi,psi)

Negation can also be applied to each section between slashes of *as_* or *vs_*. E.g. `a_//!h*` (all non−hydrogens).

2.9.4. In place operations.

ICM−shell variables can be modified in place by using the following operators:

operator	function	data types	example
+=	add in place	i,r,s	i += 1
−= subtract in place	i,r	r −= 2.2	
*= multiply in place	i,r	r *= 2.	
/= divide in place	i,r	r /= 2.	
//= append an element to an array	I,R,S	`t.Name //= "Jack"`	

If a variable does not exist yet, this operation will create the variable and assign a type according to the right−hand operand.

2.9.5. Comparison operators

Most of them are true comparison operators and return `logical` `yes` or `no.` In comparisons of table arrays or string arrays with strings, the comparison returns a subtable or subarray, respectively. Comparison operations with the `table` arrays are described separately (see table in Glossary).

- **equal** (**==**)**:**
  - **i==i, i==r, r==i, r==r, s==s, I==I, R==R, S==S, M==M, as==as, vs==vs**, exact equality of two objects;
  - **p==i, p==s** return **l.** Test the value of an ICM−shell `preference` . Example:

    ```
    if(wireStyle==1) print "int. or string is ok" # or
    if(wireStyle=="chemistry") print "double bonds"
    ```

  - **S**==**s**returns **S,** a sub−sarray of elements exactly matching **s** (e.g. `{"aa","b","aa","c"}=="aa"` returns `{"aa","aa"},` see also **S ~ s**),
- **not equal** (**!=)** :
  - **i != i, i != r, r != i, r != r, s != s, I != I, R != R, S != S, M != M, as != as, vs != vs** inequality of two objects;
  - **p!=i, p!=s** return **l.** Test an ICM−shell `preference` . Example:

    ```
    if(wireStyle != 2) print "No chemistry, sorry"
    ```

  - **S**!=**s** returns **S,** a sub−sarray of elements not matching **s** (e.g. `{"aa","b","aa","c"}!="aa"` returns `{"b","c"},` see also **S !~ s**).
- **greater than** (>) :
  - **i > i, i > r, r > i, r > r**
  - **s > s** lexicographic comparison for sorting ("apple" <"orange")
- **less than** (<) :
  - **i < i, i < r, r < i, r < r, s < s**
- **greater or equal** (>=) :
  - **i >= i, i >= r, r >= i, r >= r, s >= s**
- **less or equal** (<=) :
  - **i <= i, i <= r, r <= i, r <= r, s <= s**
- **fuzzy−equality, inclusion or pattern matching** (~):

- **s~s**returns **logical** `yes` if string matches a pattern.
- **S~s**returns **S** of sarray elements matching the pattern **s.** This comparison is similar to the UNIX **grep** command; it returns a subarray of lines matching the pattern rather than `yes` or `no.` Do not forget to add flanking asterisks (*) if the pattern occurs in the middle of a string. Example:

```
show {"abc","bcd","ee"} ~ "*[be]?"
# Another example
read database s_icmhome + "foldbank.db"
        # sarray SE contains sequences
CxCseqs = SE ~ "*C?C*" # all strings containing C?C pattern
```

- **fuzzy−not−equal** (**!~**) :

  - **s !~ s** returns **logical** `yes` if string does not match a pattern **s.**
  - **S !~ s** returns **S** of sarray elements **not** matching the pattern **s.** S!~s is similar to the UNIX **grep −v** command; it returns a subarray of lines not matching the pattern.

2.9.6. Advanced operations and some comments

1. Integers are automatically converted to reals in binary operations containing both integers and reals. However, in expressions like *integer1* / *integer2* (the same for iarrays) they are *not* converted into reals and the result will be different from what you might expect. For example, `3/4` returns `0,` but `3/4.` returns `0.75.`

2. In **s+i, s+r, S+I, S+R** expression numbers are automatically converted into strings. In the s+s expression the second string is simply appended to the first one.

   Examples:

```
show "one " + "two"  # result: "one two"
file = "aa"+ 4       # result: "aa4"
show {"a","bb"} + {1.2,3.2}  # result: {"a1.2","bb3.2"}
```

3. Selection arithmetics. The level of the expression *as_1 as_2 as_3* ... or *as_1* | *as_2* | ... (the same with *vs_*) is defined by the **lowest level** selection in the chain (atoms − the lowest < residues < molecules < objects). For example, in an expression **a_/10 | a_2/15/cg** the second selection is an atom−level−selection and the first one is a residue−level one. The result is the atom selection of all atoms of residue 10 plus *Cg* atom from residue 15.

4. **Selection logically multiplied by string, array, or mask**

   Multiplication of a selection to a string−mask or sequence. The resultant selection inherits level of the first argument. The mask is applied periodically to switch off some of the selected elements. For example mask "0001111" will switch off the first three elements in every seven. The 'switch off' characters may be the following: ' ' (space),'−','0'. Example masks to switch off the third element of five: `"xx xx", "11011", "++−++"` .

   Operations upon the sequence will select only the fragment with the specified sequence from the original selection. Multiplication by an array of 6 numbers {x,y,z,X,Y,Z} selects atoms within the specified box.

Example:

```
read object "crn"   # load crambin object
rs_ = a_/11:15      # define residue selection rs_
rs_ = rs_ "xx xx" # switch off the third element (res. 13)
display cpk a_//* {1. 0. 1. 5. 7. 6.} " # a box
```

5. **Transitional (or projected) alignment**

   Projected concatenation of two alignments sharing the same sequence. If two−sequence alignments share the same sequence, they may be merged with the shared sequence as a ruler. In the simplest case of three sequences a, b, c and alignments ab and bc, the operation ab//bc will create an alignment of three sequences a b c. The function `Align(ab//bc,{1,3})` will extract the, so called, projected alignment of **a** and **c** through **b.**

Examples of expressions:

```
i = i1/i2 + (i3−r4)*2.5/Pi

l_results=(l_beer l_wine !l_snacks) | l_vodka
if (l_results n_glasses >= 4) print "Hangover.."

for i=1,215        # list streets of Manhattan north from Houston
  print "Street " + i
endfor

prices = { 25. 6. 12.6 }
tips   = { 4.  1. 2.   }
print prices + tips        # the result is { 29. 7. 14.6 }
```

2.10. Flow control

ICM contains a complete set of control statements to allow looping, jumping and conditional branching.

2.10.1. Loops

Two types of loops are allowed, namely *for−loop* and *while−loop.*

For−loop

```
for  <i_index> = <i_from> ,  <i_to> [, <i_increment> ]
 ...
 ...
endfor
```

While−loop

```
while( <logical_expression> )
 ...
 ...
endwhile
```

Examples:

```
for i = 1, 9
  print "ICM−shell proudly announces that i=" i
endfor

for i = 1, 4
  print "ICM−shell proudly announces that i=" i
  for j = 1, 3
    print "ICM−shell proudly announces that nesting is possible and j=" j
  endfor
endfor

read object "crn"
for i = 1, Nof(a_/*)  # Nof(a_/*) means 'the number of residues'
  print Label(a_/$i)
endfor

i = −2
while (i != 4)
  i = i+1
  print i
endwhile

while(yes)
  print "endless loop, please wait 8−)"
endwhile
```

Any number of nested loops may be used.

2.10.2. Conditional branching

Several types of conditional statements are allowed in the ICM−shell.

if

```
if ( <logical_expression> ) <command>
```

if−then−endif

```
if ( <logical_expression> ) then
   ...
   ...
endif
```

if−then−elseif−..else−endif

```
if( <logical_expression> ) then
    ...
else
    ...
endif
```

or

```
if ( <logical_expression> ) then
  ...
elseif ( <logical_expression> ) then
```

```
  ...
elseif ( <logical_expression> ) then
  ...
else
  ...
endif
```

Note: `end if` or `else if` (instead of `endif` or `elseif`) are not accepted by ICM−shell.

Examples:

```
 JohnnySaid = "The gloves didn't fit"
 if ( JohnnySaid == "The gloves didn't fit" ) print "You must acquit"
#
 grade = "bad"
 if (grade == "excellent") then
   print "It's great!"
 elseif (grade == "good") then
   print "It's good!"
 elseif (grade == "bad") then
   print "It's not so bad!" # do not be harsh on your kids
 endif
```

2.10.3. Jumps

Three types of jump controls are possible, namely commands **break, continue** and **goto**. **break** interrupts the loop, **continue** skips commands until the nearest **endfor** or **endwhile** and continues looping, and **goto** jumps to any point below.

break

```
<for−loop> or <while−loop>
    ...
    if ( <logical expression> ) break
    ...
<end of loop>
```

continue

```
<for−loop> or <while−loop>
    ...
    if ( <logical expression> ) continue
    ...
<end of loop>
```

goto

```
...
if ( <logical expression> ) goto <label>
...
...
<label>:
...
```

Examples:

```
    for i = 1, 6
      print "currently i=", i, "and it will be increased at the next step"
      if (i == 3) then
        print "... but at this point we should stop it, sorry..."
        break
      endif
   endfor
   print "end of the loop demonstrating *break*, bye"

    for i = 1, 6
      if (i == 3) then
        print "... let us skip over step 3 and continue looping"
        continue
      endif
      print "currently i=", i, "and it will be increased at the next step"
   endfor
   print "end of the loop demonstrating *continue*, bye"

   for i = 1, 5
     if (i == 3) then
       print "... but at this point we decided to skip 3-rd step, sorry..."
       goto A
     endif
     print "currently i=", i, "and it will be increased at the next step"
A:   print " "
   endfor
   print "end of the loop demonstrating 'goto', bye"
```

Note: *go to* (instead of *goto)* is not accepted by the ICM−shell. Any combination of alphanumeric characters beginning with a letter (upper or lower case) may serve as a **label.** Also keep in mind that *goto* can jump only **forward;** the **backward** *goto* is not allowed.

2.11. ICM molecular objects

An ICM molecular object represents one or several molecules which can coexist in physical space, so that the energy of the molecular system can be calculated. For example, if you have two homologous molecules superimposed, multiple conformations of the same structure such as NMR structure determinations or alternative positions of a side chain, they must belong to different objects. The number of objects that may be loaded in ICM is limited only by the available computer memory. Objects may be of several types (see also: the `Type` (~os_ `2`) function):

- `"ICM"` − the only complete type which is good for everything including energy calculations
- `"X−Ray"` − incomplete (stripped) object created by `read pdb`. The structure is determined by X−ray crystallography. Good for graphics and geometrical analysis
- `"NMR"` − incomplete (stripped) object, structure determined from NMR data, similar to the "X−ray" type above.
- `"Model"` − incomplete (stripped) object, theoretical model also similar to the "X−ray" type above.
- `"Ca−trace"` − incomplete (stripped) object, only alpha−carbon atoms.

- `"Simplified"` − simplified representation.

ICM−molecular objects are created from residues and molecules described in the ICM residue library. Its content (sequences and names of molecules) is specified in an ICM sequence file (see also `IcmSequence` function). An ICM−object can also be created from a non−ICM object (e.g. of X−Ray type) with the `convert` command.

2.12. Energy and Penalty Terms

The energy function calculated for any conformation of an ICM molecular object consists of individual terms described in this section. For most of them ICM calculates analytical derivatives which use gradient minimization. The terms can be switched on and off with the `set terms [only] "xx,yy,.."` command, e.g.

```
set terms "el"         # activate electrostatic term
set terms only "vw,14" # reactivate only "vw" and "14" terms
```

van der Waals ("vw")

nonbonded interatomic pairwise interactions (1−5 and further, i.e. two atoms separated by more than 3 covalent bonds). If not for tests, this terms should always be used with the "14" energy term which considers 1−4 interactions. The ECEPP/3 force field is used. Parameters are specified in the `icm.vwt` file and are taken from Momany et al., 1975. Both the usual 6−12 term and a soft van der Waals terms are available. See also: `vwMethod`, `vwSoftMaxEnergy` .

1−4 van der Waals ("14")

A part of the total van der Waals energy for atoms separated by exactly three covalent bonds. Repulsion for 1−4 pairs is cut in half according to the ECEPP energy function. This term is complementary to the `"vw"` term and is usually used with the `"vw"` energy term.

Hydrogen bonding energy ("hb")

A different form of the `"vw"` term (10−12 instead of 6−12 for `"vw"`) for hydrogen bonding donors and acceptors as specified in `icm.cod` and `icm.hbt` files. Parameters are taken from Momany et al., 1975. The electrostatic contribution to a given hydrogen bond is not included in "hb" and is calculated as part of the electrostatic energy.

The cutoff distance for hydrogen bonding interactions is controlled by the `hbCutoff` parameter.

Torsion energy ("to")

dihedral angle deformation energy K*(1+−cos(n*Phi)). The parameters K, sign and n are given in `icm.tot` file. Parameters are taken from Momany et al., 1975,

Electrostatic energy ("el") This term is calculated in four different ways depending on the value of `electroMethod` preference. If `electroMethod="boundary element"` the solvation component is in `r_out` and the envelope surface area in `r_2out` .

A special case: if the van der Waals energy is calculated with the `vwMethod ="soft"` , the electrostatic energy will be automatically buffered to avoid singularities. You will see that the electrostatic term `"el"` changes upon switching from `vwMethod=1` to `vwMethod=2` . The buffering artifically increases the distance between two charged atoms to avoid having negative energy values better than the van der Waals repulsion and, therefore, will prevents collapse of oppositely charged atoms.

1. A simple electrostatic energy (`electroMethod="Coulomb").` The Coulomb law is used to evaluate the energy. The `dielectric constant` is constant.

2. the distance dependent electrostatics (`electroMethod="distance dependent" ;` *currentDielConst* = `dielConst` * *DISTANCEij*) Advantage: this term has analytical derivatives and can be used in local energy minization.

3. A better electrostatic free energy (`electroMethod="MIMEL"),` uses the `Modified IMage ELectrostatics` approximation (Abagyan and Totrov, 1994) to evaluate both the internal Coulombic energy and electrostatic polarization free energy. Disadvantage: this term has no analytical derivatives and has no effect on local energy minimization. It can be a part of the energy function in global optimization such as `montecarlo` or `ssearch` . The solvation component is stored separately in `r_out` . REBEL provides a more accurate evaluation of the electrostatic solvation energy. For small molecules, use `mimelDepth = 0.3` (default `0.5`).

4. The most accurate electrostatic free energy: (`electroMethod="boundary element"`) which uses so called boundary element method to solve the Poisson equation to calculated a electrostatic free energy of a protein surrounded by a continuous aqueous solution. In addition to the total energy, one can extract the two components: the electrostatic solvation energy from `r_out` , and the Coulomb energy can be calculated as a difference between the total electrostatic energy and r_out.

Surface term ("sf"). Map `m_ga`

Surface energy is based on atomic solvent−accessible surfaces. Depending on the `surfaceMethod` preference this term is either a surface tension which is evaluated as a product of the total solvent accessible area by the `surfaceTension` parameter (currently 0.012 kcal/mole/A^2) or is a product of atomic accessibilities by the atomic energy density parameters similar to those proposed by Wesson and Eisenberg (1992) (check `icm.hdt` file). The "sf" term is evaluated at each Monte Carlo or systematic search step, but not during local minimization (we do not calculate analytical energy derivatives).

The atomic accessible surfaces are calculated using a faster modification of the Shrake and Rupley, (1973) algorithm. This algorithm analyzes all atom neighbors for each atom and Sometimes a part of molecular system is represented with the grid energy terms (`"gc","gh"`) rather than by explicit atoms. In this case the atomic accessibilities need to be corrected.

This correction can be introduced with a special map, called `m_ga` which stores implicit neighbor information from the parts represented with the grid potentials. The `m_ga` map is calculated with the `make map potential "sf" ..` command (see the `make map potential` command), along with other grid maps.

Entropic free energy term (conformational entropy of side−chains) ("en")

Configurational entropy of side−chains is evaluated on the basis of their maximal possible entropy which is read from the residue library. Note that this term is calculated at room temperature (300 K), so that the ICM−shell variable `temperature` does not affect the entropic contribution (see Abagyan and Totrov, 1994 for values) and solvent−accessible area of a side−chain.

Phase angle bending term ("af")

Harmonic term $U*(f1-f0)^2$. Parameters U and f0 are taken from `icm.bbt` file. Sometimes referred to as *improper torsion*.

Bond stretching energy ("bs")

Harmonic term $U*(b1-b0)^2$. Parameters U and b0 taken from `icm.bst` file.

Distance restraints ("cn") a penalty term restraining two atoms to a certain distance range. The shape of the potential is *soft square well* with lower and upper bounds. This term may be used to determine three−dimensional structure from a set of interproton distances (NOEs) resulting from NMR experiments. There are local and global distance restraints (drestraints). Local restraints become weaker and vanish as the distance grows (similar to the van der Waals forces), while global restraints become stronger as you deviate further from the required distance range.

See also files: `icm.cnt` and `icm.cn` .

Disulfide bonds and covalent bridges ("ss")

a penalty term establishing the additional (extra−tree) covalent bridges. Currently there are three types of covalent bridges: disulfide bonds, peptide bonds and thioester bonds. In each case several distance constraints are imposed to enforce the correct covalent geometry. The constraints for the disulfide bonds include Sg1−Sg2, Sg1−Cb2, Sg2−Cb1, Cb1−Cb2 atom pairs. The extra CO−NH bond involves C−N, C−H, O−N and O−H constraints. Similarly, CO−SH bond involves C−S, C−H, O−C, O−H, C−C and O−H constraints. The functional form of this penalty term is identical to local distance restraints. The disulfide SS bonds are automatically formed when you load the object. The disulfide bonds may be LOCAL, i.e. when two sulfur atoms feel each other ONLY at small distances. See also: `icm.cnt`, disulfide bond, `make disulfide bond`, `make peptide bond`, `delete disulfide bond`, `delete peptide bond`.

Tethers ("tz")

Quadratic restraint E= `tzWeight` *Distance^2 between atoms in the current object and static atoms in a different object (as opposed to distance restraints "cn" between atoms in the same object). The target value of the distance is zero. See also: `read pdb`, `set tether`, and `tether` .

Multidimensional variable restraints ("rs")

Energy associated with multidimensional ellipsoidal attraction zones (in which dimension they look like soft square wells with flat bottom) in a hyperspace of internal variables (e.g. preferred side−chain or backbone torsion angles). Vrestraints are defined in `icm.rst` and `icm.rs` files and are earmarked to be used in energy calculations (as opposed as for the BPMC) with the `rse` field (as opposed to `rs`). Use `set vrestraint energy` command to assign vrestraints. Described in Abagyan, Totrov and Kuznetsov, 1994 (pp. 494,495).

Density correlation ("dc")

Penalty function associated with correlation between the static `map` (the current map is used by default) and a virtual map generated from atomic positions on the fly. The `densityCorrMethod` preference allows you to choose between several different functional forms of this term:

$$DC = 1 - Sum(D_i - <D>)(A_i - <A>) / (N * Rmsd(D) * Rmsd(A))$$

and

$$DC = 1 - Sum(D_i - <D>)(A_i - <A>) / N$$

where D_i is the map value, and A_i is the density generated dynamically from atomic positions.

The term has analytical derivatives with respect to the internal coordinates and can be efficiently locally minimized. By adding this term one can combine energy minimization with the real space fitting into electron density.

A more detailed description can be found in the `densityCorrMethod` section.

Crystallographic correlation between Fobs and Fcalc ("xr")

van der Waals grid potential for carbon probe ("gc")

van der Waals interaction between explicit non−hydrogen atoms of an ICM object and a van der Waals potential calculated on the grid. To calculate this term one needs an ICM object and map named `m_gc` which is calculated with `make map potential "gc" ..` . The calculation also counts the number of atoms in the area with Evw>0.8 * `GRID.maxVw` and stores this number in `r_2out` .

van der Waals grid potential for hydrogen probe ("gh")

hydrophobic potential ("gs")

electrostatic grid potential ("ge")

Calculates the electrostatic potential contribution from the atoms specified in the `make map potential as_` command. The contributions are calculated by the Coulomb formula with distance dependent−dielectric constant ($4*D_{ij}$)

hydrogen bonding grid potential ("gb")

Potential of mean force (`"mf"` and `pmf`)

Note that term name is `"mf",` while icm keyword for some commands is `pmf`

The mean−force `"mf"` potential was designed as a generic energy term which is calculated for pairs of atoms according to their pmf−types and interatomic distances. The definitions of the pmf−types and energy−distance dependencies for each contributing pair of atom types can be loaded from a `.pmf` file.

The list of pmf−interacting pairs is calculated dynamically and only the pairs at smaller that `vwCutoff` threshold distance are considered. **Note:** It is important that `vwCutoff` = 9.5 is used in binding score

evaluation.

There is a preference called `mfMethod` which controls if the atoms in the same molecule can interract. By default only intermolecular pairs of atoms are considered (`mfMethod` = 1). Switching `mfMethod` to `2` (or `"all"`) allows to include all atomic pairs regardless of which molecule they belong to in the "mf" term calculation.

Since this term is quite general one can prepare different pmf−parameter files for solving different problems. The default file `icm.pmf` has been derived from receptor−ligand complexes and allows pmf−scoring of docked ligands. Another file: `ident.pmf` was designed to specify attraction of the same atom types and allows to solve a problem of chemical superposition.

The relative weight of the pmf−term is controlled by the `mfWeight` parameter.

An example in which we evaluate a binding score:

```
read object "rec"
read object "anwers1"
move a_2. a_1.
vwCutoff = 9.5
mfMethod = 1
show energy "mf" a_1 a_2
e = Energy("mf")
```

An example in which flexible superposition of two molecules is performed:

```
 buildpep "his ; gly trp"  # two molecules
 read pmf "ident.pmf"
 fix v_//omg
 display
 superimpose a_1 a_2
 vwCutoff = 2. # mf uses vwCutoff to calculate lists
 montecarlo "mf" v_2//?vt*  | v_//!?vt*  # internal variables + positional for the second mole
```

See also: `mfMethod` , pmf−file, `mfWeight` .

2.13. Integer shell parameters.

Here is the alphabetically sorted dump of integer parameters defined in the ICM−shell. These parameters are used by various commands and functions and can be changed interactively, e.g.

```
 mncallsMC= 10000
 montecarlo
```

ICM−shell integer variables are the following.

2.13.1. autoSavePeriod

In the course of a `montecarlo` or `ssearch` procedures which may run for days, the current `stack` of conformations which accumulates the best energy representatives of different conformational areas is saved periodically to allow access to intermediate results of the simulations. The above parameter defines the number of stack changes after which it is saved to a disk file. Set autoSavePeriod to 1 if you want to be

conservative.

If you set `autoSavePeriod` to `0` , the stack will **not** be saved at all.

Default (10).

2.13.2. defSymGroup

defines a crystal space group number. To find the group name and symmetry operations use the `Symgroup` function. Default (0) means that the group is not defined.

Examples:

```
defSymGroup = 19  # direct assignment. You know group 19, don't you?

defSymGroup = Symgroup("P212121") # Oh, you do not! ..

defSymGroup = Symgroup("P61 2 2") # This one you do not remember for sure
```

2.13.3. i_out

an integer where some commands or functions store their integer output:

- `Rmsd` saves the number of aligned equivalent points;
- `Srmsd` saves the number of aligned equivalent points;
- `convert` saves the number of heavy atoms missing from the pdb−template (e.g. atoms of the flexible lys side−chain are not given in the pdb−file).
- `superimpose` saves number of aligned equivalent points;
- `set tether` saves the number of tethers imposed;
- `set drestraint` saves the number of distance restraints imposed;
- `set vrestraint` saves the number of variable restraints imposed;
- `make disulfide bond` saves the number of imposed disulfide bonds;
- `minimize` saves the number of function evaluations;
- `montecarlo` saves the total number of function evaluations during minimization;
- `show area skin` saves the total number of triangles in the Connolly construction.

Default (0).

2.13.4. iProc

the current of process number filled by the `fork` command. This number is zero for the parent process.

Default (0).

2.13.5. maxColorPotential

local electrostatic potential in kcal/e.u.charge units at which the surface element is colored by extreme red or extreme blue. All higher values will have the same color. This absolute scaling is convenient to develop a feeling of electrostatic properties of molecular surfaces.

If the `maxColorPotential` is set to `0.` the the `color grob potential` command will perform automated scaling to the absolute maximal value of the potential.

See also: `color grob potential`, `dsRebel` , `Potential` , `make grob potential` .

Example:

```
build string "se glu arg"  # dipeptide
maxColorPotential = 3.
dsRebel a_ yes
maxColorPotential = 6.
dsRebel a_ yes
```

2.13.6. maxMemory

maximal memory size requested by the program in megabytes. It is used to read blocks of databases in the search commands. Make sure that this parameter is reasonable. If your maxMemory is larger than what your computer actually has, expect serious delays. However, usually computers can handle it by swapping memory onto disk, which can be slow.

Recommendation: divide your available RAM by a factor from 2 to 4. Current memory resources are reported by the chkdsk command on a PC or by the top command on a UNIX workstation. Do not forget that ICM itself will *additionally* allocate some `BufferSpace` specified in the `icm.cfg` file.

Default (10.0) Mb

2.13.7. minTetherWindow

maximal number of preceding torsions strictly speaking rigid bodies which are locally minimized during the chain growth procedure (the `minimize tether` command) to create an ICM−object with ideal geometry on the basis of a set of arbitrary atom coordinates (ofter referred to as the `regularization` procedure).

Default (30).

2.13.8. mnSolutions

this parameter limits the number of hits retained by the program after a search. It is used in several icm−search functions:

- `find molecule` − chemical substurcture search
- `find pattern` − find sequence pattern in sequences of mol. objects.
- `find database` − advanced sequence similarity search
- `align` *ms_1 ms_2* − alternatives solutions for 3D superposition
- find profile − find protein Prosite profiles in a sequence
- `find prosite` − find protein Prosite patterns in a sequence

Default (100).

2.13.9. mncalls

maximal number of function calls in local minimization performed in `minimize`, and as a part of one step of a multistep procedure in `montecarlo`, `ssearch`, `convert` . The number of function evaluations required to find the local minimum varies widely depending on the terms used (i.e. the `"tz"` term makes minimization very slow, if structure is far from its target). If the minimum is found according to the `tolGrad` criterion, the procedure will be terminated anyway.

Default (100).

See also: `minimizeMethod` , `tolGrad` , `drop` .

2.13.10. mncallsMC

maximal number of function calls in the `montecarlo` command. Since the procedure performs random steps accompanied by local minimization (controlled by the `mncalls` parameter), the number of function evaluations for the whole procedure can be roughly evaluated as a product of `mncalls` and the number of MC iterations. `mncallsMC` should be sufficiently large to ensure convergence of the global optimization procedure and may range from 10,000 for a single side−chain, 100,000 for a 3−4 residue peptide to several million calls for 15−20 residue peptide or a large protein loop.

Default (`1000`). The default value is small to minimize damage of the unintentional calls of the montecarlo command.

See also: `montecarlo` , `mncalls` .

2.13.11. mnconf

maximal number of `conf`ormations in the conformational `stack` . The stack stops growing after this number is achieved and starts replacing representative conformations with higher energy values by new conformations with superior energies, if the latter are found.

Default (50)

See also: `montecarlo` , `ssearch` .

2.13.12. mnhighEnergy

maximal number of consecutive accepted trial conformations which do not change the conformational `stack` because their energies are higher than energies of the stack conformations. Therefore, the `montecarlo` procedure is walking in the high energy area and is probably wasting its time. When this threshold is reached the procedure acts according to the `highEnergyAction` parameter.

Default (50)

See also: `mnvisits` , `mnreject` , `stack` .

2.13.13. mnreject

maximal number of consecutive rejections (due to the Metropolis criterion) of trial conformations generated by the `montecarlo` procedure. When this threshold is reached the procedure acts according to the `rejectAction` parameter (which usually increases the simulation temperature).

Default (10)

See also: `mnvisits` , `mnhighEnergy` .

2.13.14. mnvisits

maximal number of visits to the same slot of the conformational `stack` in the course of a `montecarlo` procedure. When this threshold is reached the MC procedure acts according to the `visitsAction` parameter. A visit is an event when a newly generated conformation finds a slot with a similar conformation in it, but the stack conformation is not replaced by the new one because it has a better energy.

The optimal *mnvisits* parameter grows with the size of the problem (it may be several hundred for a 15−20 residue peptide).

Default (50)

See also: `mnreject` , `mnhighEnergy` .

2.13.15. nLocalDeformVar

Number of backbone torsion angle variables (excluding omegas) which are changed simultaneously to provide local deformation. This parameter can be less than the actual number of backbone torsion angles in the loop. In other words it is OK if the loop contains more than *nLocalDeformVar* variables, however, if it contains less than *nLocalDeformVar* variables, it will not be deformed.

Default (10), minimal number (8).

See also: `montecarlo local`.

2.13.16. nSsearchStep

number of steps per variable for `ssearch` . Normally the whole [−180., 180.] range is divided into `nSsearchStep` parts. In the `local` mode (i.e. the search is performed around a particular conformation) the total search range around each variable is defined by the `ssearchStep` parameter (30. deg. by default)

Default (3) .

2.13.17. nProc

Number of processors used by the parallel version of the program.

Default (1). Range [1: *maximum_number_of_processors_available*].

2.13.18. randomSeed

is a seed used by the random−number generator in the `montecarlo` , `randomize` , `Random` function. Helpful if you need to *reproduce exactly* a calculation which uses random number(s). If the variable has its zero default value, the random function is seeded from the current time. Otherwise, if you explicitly redefine it before, let us say, a `montecarlo` run, it will use the specified number.

Note that the `randomSeed` parameter can be set only once **in the very beginning of the session**. If you redefine its value in the middle of the session, it will not be used. To push the new value of the seed, use the `set randomize i_newRandomSeed` command.

Default (0).

Examples:

```
 randomSeed=2493059372  # this number you took from the previous run
 montecarlo             # simulation will reproduce the previous one
#
...
#
 set randomize 2493059372
 montecarlo
```

2.13.19. segMinLength

secondary structure `segments` shorter than this threshold will be ignored when a simplified quantitative representation of the polypeptide fold is constructed using the `assign sstructure segment` command.

Default (3).

2.13.20. sequenceBlock

length of the contiguous sequence block in sequence output.

Default (10).

See also: `sequenceLine` .

2.13.21. sequenceLine

maximum sequence length printed on each line. Usually sequence is additionally subdivided into smaller blocks.

The same parameter also controls the size of alignment block as saved by the `write alignment` command.

Example:

```
 read alignment s_icmhome+"sh3"
```

```
sequenceLine=1000
write sh3 "aaa"
```

Default (60). Values >= 1 .

See also: `sequenceBlock`

2.13.22. surfaceAccuracy

accuracy level used in surface calculations (not graphics). By reducing the level, you can speed up the accessibility calculation in the `show area surface` command. The corresponding number of dots per sphere is the following:

- Level 1 (89 dots)
- Level 2 (144 dots)
- Level 3 (233 dots)
- Level 4 (377 dots)
- Level 5 (610 dots)

Default (3)

See also: `show area surface`, `"sf" energy term`.

2.13.23. windowSize

number of elements used for sliding window averaging by the `Smooth` function.

Default (7).

2.14. Real shell variables

ICM−shell real variables are the following.

2.14.1. addBfactor

additional B−factor which may be added to the current atomic B−values to create a smoother electron density map from a set of atoms. See also: `make map`

Default (0.0)

2.14.2. alignMinCoverage

a threshold for the ratio of the aligned residues to the shorter sequence length. All alignments shorter than *alignMinCoverage*minLength* will not be reported by `find database` command.

The default value is 0.5. However the parameter can be tuned with the respect to the database and the nature of the query sequence.

- Search against the protein domain sequence database: use 0.5 or higher

- Search a multidomain sequence against long multidomain sequences: use 0.1 or lower

See also: 'alignMinMethod , `find database` .

Default (0.5)

2.14.3. alignOldStatWeight

a parameter influencing the statistical evaluation of sequence comparison significance in the `find database` command.

Statistical significance can be evaluated in two ways: first, *a priori*, i.e. before the database search and based only on the individual score of an alignment of interest and its *theoretical* distribution, or, second, *a posteriori*, i.e. on the fly and on the basis of all *empirically* observed scores of *other* alignments in the course of the database search.

The parameter ranges from 0. to 1. and sets how two different statistical criteria of alignment significance, a precomputed (the old one) and a run−time, should be mixed. Zero corresponds to only the run−time measure (the *new* way) in which the significance is evaluated on the run−time statistics of the observed alignment scores, while one corresponds to the statistics evaluated before the search using the formula from Abagyan and Batalov, 1997 . If the database is small then the run−time score statistics may be incomplete and `alignOldStatWeight` closer to 1. is a better choice. On the other hand, the run−time statistics has several principal advantages:

Precomputed statistics (1.) based on individual alignment score and length	**Run−time statistics (0.) based on distribution of scores**
works always	relies on database diversity
is trained only in 64 condition sets and ZEGA alignment	automatically adjusts to any set of conditions, e.g. `gapFunction`, or `alignMinCoverage`
does not reflect compositional bias	automatically reflects all seq. properties
does not reflect extra terms to the score	accounts for solvent accessibility correction (see `accFunction`)

The run−time statistics will fit the scores to an optimized empirical function. This function avoids the problems of the normal distribution, and certain pitfalls of a popular EVD function. The resulting P−value is a reliable estimate of the false positive rate if the database is sufficiently diverse, i.e. the fraction of sequences similar to the query is small. For example, searching a tyrosine kinase through a database of tyrosine kinases will yield incorrectly low pP−values (pP = −Log(P)).

Reliable expect−values: P * Nof(sequences) <= 0.1 .

Example:

- Swissprot has N=89,000 sequences. LogN = 4.95
- Reliable pP = LogN + 3, twilight pP is from LogN + 1. to LogN + 3.

2.14.4. axisLength

length (in Angstroms) of the X,Y,Z axes of the coordinate frame. The axes can be displayed by the `display origin` or `display virtual` command. The axes are marked **X Y Z** . Example:

```
buildpep "ala ala his his"
display
axisLength=10.
display origin
```

Default (1.5)

2.14.5. clashThreshold

a clash is defined as an interatomic distance less than a sum of van der Waals radii of two atoms of interest multiplied by the `clashThreshold` parameter. For hydrogen bonded atoms, the distance threshold is additionally reduced by `20%` .

See also: `display clash` , `show clash`, `GRAPHICS.clashWidth`

Default (0.82)

2.14.6. cnWeight

weighting factor for the interatomic `distance restraints` penalty term. See also: `tzMethod` , `drestraint` and `Bfactor` .

Default (1.0)

2.14.7. dcWeight

weighting factor for the density correlation term `"dc"`.

Default (1.0)

2.14.8. CONSENSUS_strength

regulates the strength of consensus modifying the CONSENSUS.fraction values. The CONSENSUS table controls the rules of consensus derivation from an `alignment` . This table may look like this:

```
#>T CONSENSUS
#>-symbol------fraction----residues---
   A           80          A
   C           90          C
   D           85          D
   d           60          ND
...
```

. . .

The CONSENSUS_strength (denoted ***S***) parameter can increase or decrease the `fraction` values ***f*** according to the following formula: ***f1 = f + (100−f)*(S−0.5)*** Therefore if ***S*** = 1. all fraction values become equal to 100% . This affects the `Consensus` function and the GUI representation of alignment consensus in ICM versions above 3.0.

To color structures according to the consensus, use the `color as_ alignment` command, or, interactively, left−click on a color icon and select *ColorBy* followed by *alignment.*

Default (0.5)

2.14.9. densityCutoff

The neglected fraction of the total atomic electron density in the course of calculation of the grid electron density from atomic positions. Atomic density distribution is approximated by two gaussian functions which need to be truncated for computational efficiency. See also: `make map` command and related operations with the electron density, penalty term `"dc"`

Default (0.1)

2.14.10. dielConst

dielectric constant of the solute used in Coulomb, distance−dependent, MIMEL, and boundary element `electrostatic` calculations. If `electroMethod="distance dependent"` the actual dielectric constant is a product of `dielConst` and a distance from a change.

See also: `dielConstExtern`, `term "el"`

Default (4.0)

2.14.11. dielConstExtern

dielectric constant of the solvent exterior used in MIMEL and boundary element `electrostatic` calculations.

Default (78.5)

2.14.12. drop

expected initial function drop in local `minimization`. The parameter is used to evaluate initial step size. If your function is already very close to its minimum, it is a good idea to reduce the parameter, otherwise the procedure will start with an inappropriately large step.

Default (10.0)

2.14.13. fogStart

relative Z−depth with respect to the front clipping plane at which fogging starts. With this parameter you can keep some area in front without any fog and than start gradually increasing the effect until the back clipping plane.

To activate **fog** use **Ctrl−D** . Clipping planes can be moved with `Ctrl−MiddleMB` (front plane) and MiddleMB − left 5% margin (back plane). Actually the mapping of these operations to particular keystrokes is flexible and is defined in the `icm.clr` file. For Linux it is useful to redefine the back−clipping plane movements to

```
mode   9  Right5−Mid                # Move rear clipping plane
```

Right5 means that you use the 5% right margin of your window.

Usually the fog color is the same as the background color. You can change the fog color with the

`color volume` *Color*

command.

Default (0.3)

2.14.14. gapExtension

Relative gap extension penalty used in an `alignment` procedure. The absolute gap penalty is calculated as a product of `gapExtension` and the average diagonal element of the residue comparison table

Default (0.15)

See also `gapFunction` , `Align` .

2.14.15. gapOpen

Relative gap opening penalty used in an `alignment` procedure. The absolute gap penalty is calculated as a product of `gapOpen` and the average diagonal element of the residue comparison table You may vary gapOpen between 1.8 and 2.8 to analyze dependence of your alignment on this parameter. Lower pairwise similarity may require somewhat lower gapOpen parameter. A value of 2.4 (gapExtension=0.15) was shown to be optimal for structural similarity recognition with the Gonnet et. al.) matrix, while a value of 2.0 was optimal for the Blosum50) matrix (Abagyan and Batalov, 1997).

Default (2.4).

See also `gapFunction` , `Align` .

2.14.16. hbCutoff

(Angstroms) cutoff radius for `hydrogen bonding` interactions.

Default (3.0)

2.14.17. lineWidth

the real width of lines used to display the `wire` representation of chemical bonds. See also `IMAGE.lineWidth` parameter which controls line thickness in molecular images generated by the `write postscript` command, and the `PLOT.lineWidth` which controls the width for the `plot` command.

Default (1.0)

Example:

```
build string "se nad"  # NAD molecule
lineWidth = 3.
wireStyle="chemistry"
display
```

2.14.18. mapSigmaLevel

(in Rmsd values over the mean value). Margin value used for making `graphical objects` contouring the 3D density `map` .

Default (1.5)

2.14.19. mcBell

average relative size of normally distributed `montecarlo` step from the center of an ellipsoid surrounding the multidimensional `variable restraint` zone.

Example:

```
mcBell = 1.0       # places one standard deviation at the rs border
mcBell = 2.0       # distribution is two times broader etc.
```

Default (1.0)

2.14.20. mcJump

maximum value (in degrees) of random angular distortion per variable. This local random perturbation occurs if `visitsAction`, `highEnergy` or `rejectAction` ICM−shell variables are set to the `"random"` value. Randomization is a possible action in three problematic situations in `montecarlo` procedure.

Default (30.0)

2.14.21. mcShake

amplitude [Angstrom] of Brownian type the `montecarlo` random move applied to a molecule when one of the 6 variables defining its relative position is picked. Usually these variables may be selected by `v_myMolecule//?vt*selection.` The center of mass of the molecule randomly moves in an xyz sphere of **mcShake** radius. The molecule is also randomly rotated around a random axis with an amplitude equal to *mcShake* divided by the *MolecularRadius* . This parameter is also used as a default amplitude for the `randomize` command where the six position/orientation variables are selected.

Default (2.0)

2.14.22. mcStep

`montecarlo` step size (degrees). Maximum random change of one variable. This parameter is also used as the default amplitude for the `randomize` command

Default (180.0)

2.14.23. mfWeight

the overall weighting factor for the `"mf"` penalty term. This term may contain any user−defined energy or penalty function depending on pairs of atom types and interatomic distances. The parameters for the term are stored in `icm.pmf` file.

The weighting factor will determine the "mf" term contribution with respect to the energy terms.

See also: `"mf"` term, `cnWeight`, `dcWeight`, `rsWeight`, `ssWeight`, `tzWeight`, `ssWeight` .

Default (1.0)

2.14.24. mimelDepth

The fraction of an estimated molecular radius which is taken as a radius of the probe sphere used by the `MIMEL` algorithm. The accessible surface of this probe sphere is used to calculate the distance between a charge and the effective dielectric boundary. Described in detail on p. 991−992 of (Abagyan and Totrov, 1994). For small molecules `mimelDepth = 0.3` is recommended.

Default (0.5).

2.14.25. mimelMolDensity

a coefficient used to calculate the effective molecular radius from a number of atoms. Recommendation: do not touch it, unless you are an advanced user. See also the description of the `MIMEL` method.

Default (1.0).

2.14.26. r_out

a real variable where some commands and functions (e.g. `show area`, `show volume`, `superimpose`, `minimize tether`, `Corr` , `Axis` , `Align`) store their output. Also, in the electrostatic calculations with the `MIMEL` or `REBEL` method, the solvation energy part of the electrostatic energy is returned in

r_out.

Default (0.0). See also: r_2out.

2.14.27. r_2out

a real variable where some commands and functions (e.g. Axis) store their output.

Default (0.0). See also: r_out .

2.14.28. resLabelShift

is the translation towards the viewer (normal to the graphics screen) used to display a label in front of cpk's or skin's rather than bury the label under them. The recommended value is 4. See also: resLabelStyle

Default (0.0) to be used with more popular wire representation.

2.14.29. rsWeight

weighting factor for the multidimensional variable restraints penalty term.

Default (1.0).

2.14.30. selectMinGrad

default minimal gradient vector length for gradient atom selection (a_//G). This parameter is also used by the montecarlo fast command, which requires a value of 1.5 for optimal performance.

Example:

```
read pdb "1fox"
convertObject a_ yes no yes no
show energy
 selectMinGrad=80.
show a_//G
display
display a_//G cpk
```

Default (1.5).

2.14.31. selectSphereRadius

default sphere radius (in Angstroms) for atom selections in Sphere( ) function, as well as the gaussian 3D averaging radius in the color ribbon command with ribbonColorStyle="reliability".

This parameter is also used in the compare surface command.

Default (5.0).

2.14.32. shininess

parameter defining the shininess of solid surfaces such as `cpk`, `ribbon`, `ball`, `stick`, `xstick`, and `skin` when they are `display`ed. Only values in the range [0.,128.] are accepted.

Example in which we generate a high quality CPK image:

```
buildpep "ASDW"
GRAPHICS.quality = 15.
shininess = 100.
display cpk
```

Default (20.0). Range: from 0. to 128.

2.14.33. ssThreshold

threshold distance between two Sg atoms of cystein residues. This distance controls the automatic formation of disulfide bonds in some commands (e.g. `read pdb`).

Default (2.35).

2.14.34. ssWeight

weighting factor for the disulfide bridge (`"ss"`) penalty term.

Default (1.0).

2.14.35. ssearchStep

angular increment (in degrees) for variables in the systematic search (`ssearch` command) in so called "local" mode when the search is performed around the current conformation.

Default (30.0).

2.14.36. surfaceTension

surface energy density in kcal/mole/A^2. The surface energy which is a product of this parameter by the total solvent accessible area will be stored in the `"sf"` term, if `surfaceMethod` preference is set to `"constant tension"` .

Note, that if a part of the system is represented with grid potentials, one needs a special `m_ga` grid map for correct calculations of the surface accessibilities.

Default (0.012)

2.14.37. tempLocal

`montecarlo` simulation temperature for local deformation random moves. This temperature can be set higher than the normal `temperature` since a local deformation includes a larger number of variables and

may require a higher temperature for efficient sampling. To set the same simulation temperature, specify:

```
tempLocal=temperature
```

in your script.

Default (5000.).

2.14.38. temperature

`montecarlo` simulation temperature. A new trial conformation with a higher energy than the current one is accepted with the probability of exp(−(Etrial − Enew)/RT)). RT is 0.6 kcal/mole for T = 300 Kelvin.

The effect of temperature on the `montecarlo` procedure is the following:

- to find the global minimum successfully one needs a combination of persistense if a chosen place with a good sense of when to stop searching in this place and move along to the next one.
- if the temperature is too high, the acceptance ratio improves (gets higher) and wider sampling becomes easier since more high energy conformations are accepted. The downside of this is the low "persistence" (or "lack of patience") of the search procedure. Instead of spending more time in each conformational `vicinity` to find the real global minimum, the procedure just tries a couple of sub−optimal conformations and jumps away.
- if the temperature is too low the procedure may not cover the global conformational space of interest.

Default (300.).

2.14.39. tolGrad

gradient tolerance criterion for local `minimization`. Minimization is stopped if the gradient root−mean−square deviation from zero is less than the parameter value.

Default (0.05).

2.14.40. tzWeight

the overall weighting factor for the `tether` penalty term. You may need to increase it while minimizing a highly energetically strained molecule resulting from the initial steps of the `conversion` or `regularization` procedure. Additional atom specific weights can be introduced through atomic bfactors with `tzMethod="weighted"`

Default (1.0).

2.14.41. vicinity

maximum angular root−mean−square deviation per variable (degrees) or cartesian root−mean−square deviation per atom (Angstroms) when two structures are still considered belonging to the same conformational family in `conf`ormational `stack` manipulations. The type of comparison is defined by the `compare` command.

Examples:

```
compare a_//ca,c,n  # compare by Cartesian RMSD
vicinity = 3.0      # conf. are similar if RMSD< 3 A

compare v_//phi,psi # compare by angular RMSD
vicinity = 40.0     # conf. are similar if aRMSD < 40 deg
```

Default (15.0) . Do not forget to set it to a lower value if Cartesian RMSD is `compare`d.

2.14.42. vwCutoff

(Angstroms) cutoff radius for `van der Waals` interactions and Coulomb `electrostatics` .

Default (7.5).

2.14.43. vwExpand

radius of a probe sphere used to `display` a dotted `surface` of a molecule. All van der Waals radii are expanded by this value. *vwExpand=0* corresponds to the `CPK` surface, *vwExpand=1.4* corresponds to the water−accessible surface. Be aware of the difference between the `waterRadius` and `vwExpand` parameters: waterRadius is used in

- `show energy "sf"`
- `show [area|volume] skin`
- `display skin`

while `vwExpand` is used in

- `show [area|volume] surface`
- `display surface`

Default (1.4).

2.14.44. vwSoftMaxEnergy

Parameter defining maximal energy value of van der Waals repulsion at r −> 0. for the finite approximation van der Waals function (`vwMethod` = `"soft"`). This parameter must be greater than 0. kcal/mole.

Note that in the "soft" mode, the electrostatic energy will be automatically buffered to avoid singularities. You will see that the electrostatic term `"el"` changes upon switching from `vwMethod=1` to `vwMethod=2` .

Default (7.0).

2.14.45. waterRadius

radius of water sphere which is used to calculate an analytical molecular surface (referred to as `skin`) as well as the solvent−accessible `surface` (centers of water spheres). Because of the complexity of skin calculations, it is not recommended that one play's with this parameter (of course, you rushed to do exactly

that). Be aware of the difference between the `waterRadius` and `vwExpand` parameters: `waterRadius` is used in

- `show energy "sf"`
- `show [area|volume] skin`
- `display skin`

while `vwExpand` is used in

- `display surface`
- `show [area|volume] surface`

Default (1.4).

2.14.46. wireBondSeparation

the distance between two parallel lines representing a chemical double bond if `wireStyle` = `"chemistry"`.

Default (0.15 Angstroms).

2.14.47. xrWeight

the overall weighting factor for the structure factor correlation penalty term. See also: `xrMethod` .

Default (1.0).

2.15. Logical variables

ICM−shell logical variables are the following.

2.15.1. l_antiAlias

if `yes,` invokes antialising for lines displayed in the graphics window. This feature is not supported on all the platforms.

Default (`no`).

2.15.2. l_autoLink

if `yes,` tries to link molecules and alignments/sequences automatically. In case of degeneracy, i.e. identical sequences exist with different names, a molecule can be linked to two different alignments containing its sequence etc., the autolink procedure chooses the first occurrence. Use the `link` command to impose links explicitly, and the `show link` command to see them. Links can be used by the following commands and functions:

- `superimpose`
- `Rmsd` and `Srmsd`

- `set tether ali_ ...`

Default (`yes`).

2.15.3. l_bpmc

if `yes,` use Biased Probability Monte Carlo moves in the `Monte Carlo` procedure. See Abagyan and Totrov, 1994 for reference. **Important:** the probability zones are described in the `icm.rst` file and should be assigned to a peptide before the `montecarlo` command with the

`set vrestraint` a_/*

command.

Default (`yes`).

2.15.4. l_breakRibbon

if yes, break too the `ribbon` if the distance between the reference atoms is larger than 9 Angstroms. Default (`yes`).

2.15.5. l_bufferedOutput

if `no,` suppresses paging in the output of ICM commands. Useful in batch jobs.

Default (`yes`).

2.15.6. l_bug

if `yes,` print some debug information

Default (`no`).

2.15.7. l_caseSensitivity

active in most commands and functions using string comparisons.

Default (`no`).

2.15.8. l_commands

if no, do not show commands in batch mode

Default (`yes`).

2.15.9. l_confirm

if `no,` overwrite the contents of an existing file; ask permission to overwrite it otherwise.

Default (`no`).

2.15.10. l_easyRotate

allows faster handling of images in the graphics window. If `yes,` then the currently displayed solid representations (e.g., `ribbon`, `skin`, `cpk`, etc.) are temporarily hidden if an operation like rotation or translation is undertaken. Only the `wire` representation remains allowing quick manipulation with the object in use. The previous type of display is restored when rotation or translation is completed. The parameter can be toggled by a keystroke if you assign the `l_easyRotate = !l_easyRotate` with the `set key` command.

Default (`no`).

2.15.11. l_info

if `yes,` print info messages

Default (`yes`).

2.15.12. l_minRedraw

if `no,` suppresses redrawing of a displayed structure at each `minimization` step. The new minimized structure will be redrawn only at the end of minimization. Useful when the graphics is slow or the structure is heavy.

2.15.13. l_neutralAcids

Several commands such as `read mol`, `read mol2`, `build smiles` and `set bond auto` include automated assignment of aromatic systems as well as some resonance structures in O−C=O, O−S=O, PO3, O−N=O, and NO3. The automated conversion invoked with the `l_readMolArom` variable set to `yes` reassigns the bonds in the group to be equivalent. For the acidic groups it leads to the *charged* form with two partial charges of −1/2 or −1/3. If you want to suppress this transformation for the CO2,SO2 and PO3 groups only set the `l_neutralAcids` flag to `yes` . In this case the acidic groups will be kept unchanged.

Example:

```
l_neutralAcids = yes
read mol s_icmhome+"ex_mol.mol"
wireStyle=2
display only a_  # the acidic group is uncharged
build hydrogen
```

Default (`no`).

See also: read">readmol">read mol, read mol2, build smiles and set bond auto.

2.15.14. l_out

a logical variable similar to i_out and r_out .

Default (yes).

2.15.15. l_print

if yes, show print command with arguments as well as the result of its action.

Default (no).

2.15.16. l_racemicMC

Activate switching between stereoisomers at chiral centers during montecarlo. This flag can also be dynamically activated with the chiral option of the montecarlo command. To reset the chirality status of an atom use the set chiral command

Example:

```
build string "se nter his cter"
set chiral a_/his/ca 3  # set chirality flag to 3 (means a racemic mixture)
unfix V_//FC    # unfix phases for stereoisomeric rearrangements
compare a_//*
vicinity = 1.

l_racemicMC = yes
montecarlo v_//!?vt*   # will switch between stereoisomers

display
display atom label type=6   # to see the isomers
# now you can browse the stack solutions
```

2.15.17. l_readMolArom

if yes, automatically assigns aromatic rings and resonant structures (CO2,SO2,PO3,NO2,NO3) from patterns of single and double bonds upon reading objects, mol and mol2 files or build from smiles. The automated assignment module is also called by the set bond auto command.

If this flag is set to no , the build hydrogen command will have problems with resonant structures, such as carboxyl groups, − a hydrogen will be attached to the oxygen connected with a single bond to the carbon.

Example of a recommended best convertion procedure for chemical library files:

```
 l_readMolArom = yes # it is the default, but just in case
# you also want to use l_neutralAcids = yes
 read mol s_icmhome + "ex_mol"
 for i=1,Nof(object)
   build hydrogens   # may have problems if l_readMolArom = no
```

```
   set type mmff     # also improves the aromatic system assignment
   set charge mmff
   convert           # makes an ICM object
 endfor
```

Default (yes).

See also: l_neutralAcids which allows to keep acidic groups unchanged and uncharged.

2.15.18. l_showAccessibility

show the residue accessibility string assigned to a sequence generated from a three dimensional structure in the commands show sequence , show alignment, write alignment . The relative residue accessible area is expressed by an integer number in a scale from 0 to 9 (0−fully buried, 9−fully exposed). Example:

```
read pdb "1crn"
show surface area   # calculate atomic and residue accessibilities
make sequence a_1   # generate a sequence
l_showAccessibility=yes
show 1crn_m
```

Default (yes).

2.15.19. l_showMC

display one−line info about each Monte Carlo trial conformation.

Default (yes).

2.15.20. l_showMinSteps

display every step of the local minimization procedure.

Default (no).

2.15.21. l_showSpecialChar

if yes, displays unprintable characters with the show string and list string commands in text format (like \a \t \n). This flag does not apply to the print command.

Default (no).

2.15.22. l_showSites

show the site string assigned to a sequence in the commands show sequence, show alignment, write alignment. The one−letter site codes are given below.

Default (yes).

2.15.23. l_showSstructure

show the secondary structure string assigned to a `sequence` in the commands `show sequence`, `show alignment`, `write alignment`.

Default (`no`).

2.15.24. l_showWater

if `yes,` all water molecules are shown in the output of commands such as `show molecule` or `show a_*` . Set it to `no` to skip the usually long lists of water molecules in PDB structures.

Default (`yes`).

2.15.25. l_showTerms

Obsolete. Now you can achieve the same via `s_icmPrompt` variable.

Examples:

```
s_icmPrompt = "icm/%o/%e> "  # equivalent to l_showTerms=yes
```

2.15.26. l_warn

if `yes,` print warning messages. If you want to see warning messages (i.e. `l_warn = yes`), but suppress some of the messages, use the `s_skipMessages` variable (e.g. `s_skipMessages = "[147][148]"`) .

Default (`yes`).

2.15.27. l_wrapLine

wrap long lines if `yes.` If `no` truncate long lines and add a dollar sign ($) to indicate that truncation has occurred.

Default (`yes`).

2.15.28. l_writeStartObjMC

write the starting object in the `montecarlo` command to a file. This object will have the same fixation (set of free and fixed variables) as in your montecarlo simulation. In case the variable is set to `no,` the same object can be generated if you repeat the fix and unfix command as in your simulation script.

Default (`yes`).

2.15.29. l_xrUseHydrogen

defines whether hydrogen atoms are used in calculations of crystallographic structure factors from atom coordinates (the term).

Default (`yes`).

2.16. String variables

2.16.1. s_blastdbDir

return directory with Blast−formatted sequence files for ICM sequence searches. By default the directory is set to the `$BLASTDB` system shell variable. The variable can also be explicitly defined in the `user_profile.icm` or `_startup` file. In order to start using the `$BLASTDB` shell variable, delete explicit assignment of the `s_blastdbDir` from your `_startup` file or add

```
s_blastdbDir=Getenv("BLASTDB")
```

to your `~/.icm/user_startup.icm` file.

The `find database` family of sequence/pattern search commands use the `s_blastdbDir` directory.

2.16.2. s_editor

a string to invoke an external editor.

Attention!!! Always use the call to the program which starts the program in the foreground. For example: use "jot −f" rather than just "jot", since the default is running in the background.

Examples:

```
s_editor = "vi"      # good old vi, does not require a separate window
s_editor = "jot −f"  # popular SGI editor
s_editor = "xedit"   # simple and exists for X on every platform
s_editor = "notepad" # exists for PCs
```

2.16.3. s_entryDelimiter

a string which delimits entries in the `database` output of a `table` or a set of arrays, generated by the `show database` or `write database` commands. The **%i** specification at the end will be replaced by the current number of the entry and carriage return.

Default: ("#_____ %i")

Example:

```
s_entryDelimiter="//\n"  # EMBL−database delimiter
```

2.16.4. s_errorFormat

defines the exact appearance of the ICM error messages. Specification %s corresponds to the minimal ICM error message. If %s is missing all error messages are reduced to the specified text. If **s_errorFormat** is equal to the empty string (""), all error messages will be suppressed. If icm is started in the "web" mode (i.e. with the **−w** *path* flag), the variable is automatically set to `"<hr><h3>Error: %s</h3><hr>"` .

Examples:

```
s_errorFormat=""             # do NOT print error messages
s_errorFormat=" Error> %s"   # standard error messages
s_errorFormat=" Erreur> %s"  # French version
                             # html−padding
s_errorFormat="<hr><h3>%s</h3><hr>"
s_errorFormat=" Fehler> der Betrieb ist verboten"
                             # replace all the messages by this text
```

2.16.5. s_fieldDelimiter

contains characters which are considered as field delimiters by the `Field` and `Split` functions, as well as by `read column` and `write table` commands. In "Split" and "read table" one can also specify the field delimiter explicitly.

Important. If a character is duplicated in *s_fieldDelimiter* (e.g. `s_fieldDelimiter="::"`), then multiple occurrences of this character will be ignored. Otherwise, EMPTY fields will be created between each pair of identical delimiter characters.

In `write table` s_fieldDelimiter is honored only if is a one−letter symbol, like "," or "\t".

See also the opposite operation, merging members of string array into one string: `Sum`(*S_*, *s_separator*)

Examples:

```
s_fieldDelimiter="\t"   # "aaa\t\t bbb" splits into "aaa","," bbb"
s_fieldDelimiter="\t\t" # "aaa\t\t bbb" splits into "aaa"," bbb"
```

Default (`" \t\t"` i.e. two blanks, two tabs, meaning skip multiple blanks or tabs). Another reasonable possibility is `" \t\t\n\n"` which means skip blanks,tabs and carriage returns.

2.16.6. s_helpEngine

path to the HTML help file browser program. If you have no HTML browser, the default setting is `s_helpEngine="icm",` so you can use the simple internal ascii help−file viewer `more` filter ('q' − to stop, '/' to find a string, 'Enter' − next screen). If the desired help information is not found, just type help and then use '/' plus the search pattern to perform the context search in the whole help file.

Examples:

```
s_helpEngine="/usr/bin/netscape"
s_helpEngine="mozilla"  # make sure you can start it in the UNIX shell
s_helpEngine="icm"      # why would one need more?
```

2.16.7. s_icmhome

defines the home directory of the ICM program. This directory contains all standard ICM databases, all scripts, examples, documentation, initial configuration files (later users can override them with the files stored in the `s_userDir` directory.

The Linux icm−rpm package creates `s_icmhome` in `/usr/icm` directory.

2.16.8. s_inxDir

defines directory from which icm − index files for large sequence or chemical databases are stored. This variable is used by the `write index` command. By default `s_inxDir` is set to `s_icmhome` + `"/data/inx/"` .

See also: `read index` , `write index table`, `write index` .

2.16.9. s_icmPrompt

defines the ICM−prompt string. This string contains text and a bunch of wild cards for:

- **%o** − name of the current molecular **object**
- **%e** − list of the active **energy** terms (see the `set terms` command)
- **%t** − **time** spent in ICM (may be convenient for scripts)
- **%T** − astronomical **Time**
- **%%** − **%** character
- **%#** − icm−command order number

Be smart, see the `energy` or penalty `terms` you are using by adding **%e** to the prompt string.

Examples:

```
s_icmPrompt="%## "                    # for askets
s_icmPrompt=""                        # for super−askets
s_icmPrompt="%T> "                    # for anxious paranoiac freaks
s_icmPrompt="MY_ICM/%o/%e/%T/%#> "    # for the verbose
s_icmPrompt="Hi−hi|%e−^%o+%T>   "     # for the messy
s_icmPrompt="Icm command number %#> " # for the retarded
s_icmPrompt="Hey dude, type something" # for dudes
s_icmPrompt="%o/%e> "                 # for humble and wise researches
```

Default: `"icm/%o> "`

2.16.10. s_imageViewer

defines the command to view the image files (`tiff, png, targa` and `rgb` formats) if the `display` option is specified. An alternative to the default is the `"xv"` program. See also the `write image` command.

Default for SGIs (`"imgview").`

2.16.11. s_labelHeader

defines a prefix string for all labels. For example, when displaying CPK atoms you may move the label to the right of the atom center by

```
s_labelHeader="     "
```

Default (`""` − an empty string).

2.16.12. s_lib

ICM library name root. If you redefine it to say "new", ICM will start to look for the following library files: new.cod, new.bbt, new.bbs, ... etc. in the $ICMHOME directory.

Default (`"icm"`).

2.16.13. s_logDir

when you quit an icm−session, a `_seslog.icm` file is automatically stored. If the `s_logDir` variable is empty, it is stored to the `s_userDir` + `"/log/"` directory. However one can redirect it to the current working directory (`"."`) or any other directory.

The same logic applies to the `_crashlog.icm` file which is created when ICM crashes.

Examples:

```
s_logDir = "." # _seslog.icm stored in the current working directory
s_logDir = ""  # to the current working directory
```

2.16.14. s_out

a string where some commands store their string/text output. See also: `printf` `read database` `read string`, `read table`, and `read unix`,

Default (`"is where the string/text is stored"`).

2.16.15. s_pdbDir

directory containing the PDB database of 3D structures. These files can also be easily downloaded directly from the PDB site if the variables are set as in the example below. PDB distributions can exist in several styles (all files in the same directory, or divided etc.). The style is defined by the `pdbDirStyle` preference.

The pdb directory also contains the `derived_data` subdirectory with useful files (pdb sequences, index files etc.)

Example:

```
s_pdbDir ="ftp://ftp.rcsb.org/pub/pdb/data/structures/divided/pdb/"
```

```
 pdbDirStyle = "ab/pdb1abc.ent.Z"

 s_pdbDir = "/data/pdb/"
 read sarray s_pdbDir+"/derived_data/index/source.idx"
 source = Tolower(Trim(Field(source,1)))
 for i=1,Nof(source)
   read pdb source[i]
#  do some analysis
   delete a_*.
 endfor
```

Default (`"/data/pdb/").` It is usually redefined in the _startup file.

2.16.16. s_projectDir

a **relative** path to the directory in which icm−projects (all the icm−objects in a session) are stored. This path is appended to the `s_userDir` directory.

2.16.17. s_printCommand

a command to print text or postscript files. This command is invoked if the `print` option is specified in the `write image postscript` or `write postscript` commands. Customize this string. Default (`"lp −c"`).

Example:

```
 s_printCommand = "lp −c −d ColorPrn22"
 write image postscript print  # save image and print
```

2.16.18. s_prositeDat

is a file containing the full file name of the `prosite` database of protein patterns. This file is not large and is distributed with ICM. If you have your own copy of prosite, redefine the variable and delete prosite.dat in the $ICMHOME directory to avoid redundancy.

Default (`"prosite.dat"`). It is usually redefined to `s_icmhome+"prosite.dat"` in the `_startup` file.

2.16.19. s_psViewer

a PostScript viewer used while you are in ICM session. A command to invoke is to be:

```
 unix $s_psViewer </tt><i>your PostScript file name</i>
```

Default (`"/usr/opt/bin/gs −q"`).

2.16.20. s_reslib

name of the icm residue library. The file will be loaded from the $ICMHOME directory.

Default (`"icm").`

2.16.21. s_skipMessages : ignore specific error messages

In ICM all error and warning messages are numbered (e.g. `" Warning> [123] .. "`). You may specify a set of message numbers which you want to suppress. While the messages are suppressed the error code can still be returned with the `Error`(number) function.

Example:

```
a = 1
if = 2       # deliberately generate error
 Error> [2073] illegal IF: wrong condition in  if=2

s_skipMessages = "[2073]"
if = 2        # now no message is generated
if Error(number)==2073  quit

a = yes      # generates another error
 Error> [696] wrong assignment or name conflict
s_skipMessages = "[2073][696]"
a = yes      # hides the error message

234*2352352532
Warning> [147] number 2352352532 is too big for an integer (>2147483647)
0
s_skipMessages = "[2073][696][147]"   # suppress the warning
234*2352352532
0
```

See also: `errorAction` , `s_errorFormat` .

Default (`"[3000][3012]"` just to show an example).

2.16.22. s_tempDir

scratch directory for temporary files (some montecarlo files will be saved there).

Default (`"/usr/tmp/").`

2.16.23. s_translateString

a set of characters used in the ascii representation of numerical values of arrays, matrices and maps. See also the `String` function and the `show map` command.

Default (`".:*0#"`).

2.16.24. s_userDir

The path to the user directory containing ICM−related and ICM−generated data files.

The suggested _startup file sets this variable to a subdirectory `.icm` of the user $HOME directory (`$USERPROFILE` for Windows), but you may set it anywhere you want.

Default ("$HOME/.icm/").

2.16.25. s_usrlib (obsolete)

an obsolete variable. The new mechanism to add new icm residue libraries uses the LIBRARY.res sarray. You can generate the entries using the write library command.

Default ("usr").

2.16.26. s_webEntrezLink

defines the NCBI Entrez link.

See also: webEntrezOption, Default ("http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6.

2.16.27. s_webViewer

an HTML browser invoked by ICM by the following commands: web dbEntryCode, web T_, write html.

Examples:

```
s_webViewer="/usr/bin/netscape"
s_webViewer="Mozilla"
```

Default ("netscape").

2.16.28. s_xpdbDir

path to the ICM XPDB database of compact binary ICM objects which are annotated with the site information. The advantage of the XPDB database is the speed of reading and smaller size than PDB. XPDB entries are read about **80** times faster!

Here we compare the execution times for the pdb and xpdb files:

```
eos:/home/ruben/icm> time ./icm -s -e 'read object "/data/xpdb/1ffk.ob"'
0.450u 0.090s 0:00.54 100.0%
eos:/home/ruben/icm> time ./icm -s -e 'read pdb "/data/pdb/ff/pdb1ffk.ent.Z"'
38.800u 0.430s 0:42.11 93.1%
```

2.17. Preferences

Preferences are multiple choices. You can show and list them. You can change a preference by assigning it to:

- the item number
- the item name
- "**nextItem**" string

- 0 (the same as **"nextItem")**

Examples:

```
 resLabelStyle = 3              # 3-rd choice
 resLabelStyle = "Ala 5"        # assign by string
 resLabelStyle = "nextItem"     # go to the next item in the list
```

2.17.1. atomLabelStyle

style of atom labels invoked by clicking on an atom or the `display atom label as_` command. You may display name, electric charge (q) and/or `mmff` atom type. Options are the following:

1. `"cb1"` <== default
2. `"cb1 q"` (atomic charge)
3. `"cb1:FC"` (formal charge and chirality)
4. `"cb1 all"` (different atomic properties)
5. `"cb1 mmff q"`
6. `"C"` (chemical atom name for non−H and non−C atoms, formal charge and chirality)
7. `"[C]"` (chem. name, formal charge and chirality on a rectangle)

The last two choices use periodic table convention to label atoms, and the label is positioned into the center of atom. In the latter case ("[C]") a rectangle of the background color is used to highlight the label. Be careful since in the latter case the selection mark (green cross) is hidden.

Examples:

```
 build string "se his"
 atomLabelStyle = "[C]"
 wireStyle = "chemistry"
 lineWidth = 3.
 display atom label wire black # press Ctrl-A
 color background white
 write postscript "tm"         # save the results
#
 atomLabelStyle = "C"
 display xstick
 set type mmff                 # press Ctrl-A again
```

2.17.2. alignMethod

alignment method used in the `Align` and `Score` functions and `find database` command (as described in Batalov and Abagyan, 1999).

1. "ZEGA"
2. "H−align" <− the best choice
3. "frame−H−align" # allows to align DNA sequence against protein sequence or protein sequence database

See also:

- `gapFunction`,
- `accFunction`,
- `alignMinCoverage` (0.5) − minimal ratio of the aligned residues with respect to the shorter sequence length.

2.17.3. atomSingleStyle

display style of isolated atoms in the `wire` mode.

1. "tetrahedron"
2. "cross"
3. "dot"

The size of the first two representation is controlled by the `GRAPHICS.ballRadius` parameter and the line width (especially important for the "dot" style) is controlled by the `lineWidth` parameter.

2.17.4. dcMethod

defines the algorithm for the `density correlation` calculation which is the correlation between the static `density distribution` and a virtual map generated from atomic positions on the fly.

1. `"exact"` <− default
2. `"unnormalized"`

Explanation:

1. The `"exact"` density correlation penalty function uses the Pearson's correlation coefficient. The correlation coefficient is then shifted by +1 so that the function ranges from `0.` to `2.` rather than from `1.` to `−1.`

   $$DC = 1 - Sum(D_i - <D>)(A_i - <A>)/(N * Rmsd(D)*Rmsd(A))$$

   The term has analytical derivatives with respect to the internal coordinates and can be efficiently locally minimized. This term requires additional memory allocation equal to the current map size and is two times slower than the unnormalized term.

2. The "unnormalized" density correlation. Formula:

   $$DC = 1 - Sum(D_i - <D>)(A_i - <A>)/ N$$

   where D_i is a map value in point i , and A_i represents the density generated dynamically from atomic positions.

   The differences from the `"exact"` term are the following:

   - scaling is arbitrary in contrast to `"exact"` term. Therefore you have to estimate a reasonable `dcWeight` value if `"dc"` is optimized along with the other energy or penalty terms.

- The "unnormalized" term does not require additional memory and is two times faster than the "exact" term. The term has analytical derivatives with respect to the internal coordinates and can be efficiently locally minimized.

2.17.5. electroMethod

defines method used for the electrostatic energy evaluation. Four options are available:

1. "Coulomb"
2. "distance dependent" <− default
3. "MIMEL"
4. "boundary element"

The meaning:

1. The Coulomb electrostatics is defined as $U = q_1 * q_2 / D * r_{12}$ with D = dielConst .
2. In the distance−dependent dielectric model D in the above formula is set to dielConst*r, where r is an interatomic distance.
3. The "MIMEL" electrostatics allows to evaluate the free energy of a molecule in water environment by the Modified IMage ELectrostatics approximation at every iteration of the Monte Carlo, or search procedure. This energy will only be calculated for a static structure or at the end of local minimization (so called "double energy scheme", see Abagyan and Totrov, 1994 section (e) on p.992, or Abagyan, Totrov and Kuznetsov, 1994 p. 10, for reference).). The MIMEL energy consists of the Coulomb energy, which is calculated for all the atom pairs at the current dielConst value, and the electrostatic solvation energy which is a sum of "selfEnergy" and "crossEnergy" and is returned in the r_out real variable upon completion of the calculation in the show energy command. A more accurate evaluation of the electrostatic solvation energy can be obtained with the boundary element method.
4. The boundary element method provides an accurate solution of the Poisson equation. The dielectric boundary is defined by the accurate analytical molecular surface (skin) and all the local charges stay exactly where they are. The boundary element method does not rely on any 3D grid and is free from dependence on the grid size. The ICM implementation of the boundary element method is fast and accurate. During the local minimization the derivatives with respect to the internal coordinates are not calculated (similar to the MIMEL method). The distance dependent dielectric model is used during minimization instead. At the end of the local minimization the electrostatic energy is replaced by the more rigorous boundary element energy.

2.17.6. errorAction

action taken after an error has occurred.

1. = "none" # error flag is set (see the Error() function)
2. = "break" <− default # exit from loops and macros
3. = "exit" # exit from a script into shell
4. = "quit" # quit ICM: useful for CGIs

Specific error messages can be suppressed with the s_skipMessages (e.g. s_skipMessages = "[696][2073]")

See also: `s_errorFormat`, `interruptAction`

2.17.7. ffMethod

force field used in the `show energy`, `minimize`, and `montecarlo` commands.

1. = `"ecepp"` <− default
2. = `"mmff"`
3. = "icmff" a new experimental force field obtained by reparametrization of the mmff force field into the internal coordinate space and derivation of the parameters specific for a particular covalent geometry.

Note that `minimize cartesian` temporarily enforces ffMethod = "mmff", since the ecepp force field is not applicable to the carterian minimization.

To use the force fields you need to do the following:

- "ecepp"
  - ♦ `read library` (if it is not included in your _startup.icm file)
  - ♦ modify terms with the `set terms` command.
  - ♦ use `show energy` , `minimize,` or `montecarlo.`
- "mmff" in cartesian space (free covalent geometry). The command requires at least the `"vw,af,bb,bs"` terms and needs correct atom types and charges.
  - ♦ `read library mmff`
  - ♦ assign atom types: `set type mmff a_` . This operation requires correct
- chemical structure (when you build the molecule, make sure it is complete),
- bond types (check graphically with wireMethod=2, and change with the `set bond type` command), and
- formal charges (check graphically with the `atomLabelStyle=3,` and assign with the `set charge formal ..` command).
  - ♦ assign charges: `set charge mmff a_`
  - ♦ modify terms with the `set terms` command. The full set is: `set terms "vw,el,to,af,bb,bs"`
  - ♦ use `show energy` , `minimize,` or `montecarlo.`
- "mmff" in the internal coordinate space according to the current fixation. The use of the mmff force field is not recommended.

- "icmff". This new force field is designed to be used with the fixed covalent geometry and is faster than both mmff−cartesian and "ecepp". The icmff force field is still experimental and should be used with caution. The vacuum part of icmff requires only three terms: "vw,to,el". The solvation terms "sf,en" can be added.

  Icmff calculates parameters on the fly for a particular geometry. To use this force field use the following procedures:

- assign mmff types and charges, and load the mmff libraries (see above)
- to generate the starting conformation, minimize your molecule with `ffMethod = 2` and `minimize cartesian "14,to,bb,bs,af"` .
- set ffMethod to 3 and `set terms ""vw,to,el,sf,en" only` .

- use show energy or montecarlo

2.17.8. gcMethod

method defining how the `m_gc` map is used in the `"gc"` grid energy calculation. The `"gc"` method allows to calculate interactions of a molecule with grid energy field representing another molecule (the first method), or treat the `m_gc` map as the electron density map.

1. `"vw"` <− default choice: current object interacts with the van der Waals field. Positive values repel, negative attract; Contribution from one non−hydrogen atom is `Eatom = 1.*Egc`
2. `"density"` : treats the `m_gc` map as positive electron density and pulls the object into it. The contributions of atoms are proportional to atomic number (the number of electrons), hydrogens are ignored: `Eatom = −AtomicNumber*Egc`
3. `"field"` : uses user−defined atomic `field` value, which can be set by the `set field` command and extracted with the `Field` (as_) command, as the relative weight of each atom. Anticipates that van der Waals type of the map (attractive negative values, repulsive positive) as in the first method. `Eatom = Field(atom)*Egc`

2.17.9. highEnergyAction

action taken upon achievement of the maximal allowed number of `montecarlo` steps resulting in no modification of a stack `mnhighEnergy` , (it means that conformations are dissimilar to those in the stack and have higher energy). Four actions can be taken:

1. " `heat`"
2. " `stackjump`" <− default
3. " `random`"
4. " `exit`"

2.17.10. interruptAction

action taken upon ICM−interrupt (^\ Control backslash).

1. = `"break loop"`
2. = `"break all loops"` <− default
3. = `"exit macro"`
4. = `"exit to the main macro"`
5. = `"exit all macros"`

2.17.11. mfMethod

atom pair selection algorithm used when `"mf"` energy term is calculated by the `show energy`, `montecarlo`, or `minimize` commands.

Allowed values:

- `"intermolecular"` (or `1`) <− default
- `"all"` (or `2`)

(e.g. `mfMethod = 2`)

In contrast to the `"vw"` term, only intermolecular atom pairs are considered by default, since usually intramolecular interactions are calculated with the standard energy terms.

In the `"all"` mode the atom pairs are taken from the van der Waals interaction lists calculated dynamically in the `show energy`, `montecarlo`, or `minimize` commands. All atom pairs except atoms separated by 1 or 2 bonds (so called 1−2 and 1−3 interactions) and within the `vwCutoff` distance are taken into account.

See also: `term "mf"`, pmf−file, `mfWeight` .

2.17.12. minimizeMethod

algorithm used for local `energy` minimization which takes place in the `minimize` command, and is a part of one step of a multistep procedure such as `montecarlo`, `ssearch`, and `convert` .

Allowed values:

1. `"conjugate"`
2. `"newton"`
3. `"auto"` <− default

`"conjugate"` means conjugate gradient minimization. Uses analytical first derivatives and takes 6* *n_free_variables* memory.

`"newton"` − quasi−Newton method. It uses analytical first derivatives and takes *n_free_variables*n_free_variables* memory. We recommend this method for energy minimization of small molecules.

`"auto"` <− default; use the more efficient quasi−Newton if the number of free variables (Nof(v_//*) is less than 100 (additional memory requirement of about 2 MB) and switch to the conjugate gradient method if the number of free variables is more than 100.

2.17.13. pdbDirStyle

The style of your Protein Data Bank directory/directories. ICM will understand all of the listed styles, including distributions with compressed *.gz , *.bz2 and *.Z files. In all cases, if the `s_pdbDir` variable is set correctly, it is sufficient to refer to the file by its four−character code, e.g.

`read pdb "1abc"`

1. "1abc.pdb"
2. "pdb1abc.ent" "ab/pdb1abc.ent"
3. "ab/pdb1abc.ent.Z"
4. "ab/pdb1abc.ent.gz"
5. "PDB website"

Do not forget to set the right pdb−style in your `_startup` file.

2.17.14. rejectAction

what to do, if the MC procedure rejects `mnreject` trial conformations in a row. Four actions can be taken:

1. " `heat`" <− default choice
2. " `stackjump`"
3. " `random`"
4. " `exit`"

2.17.15. resLabelStyle

style of residue labels invoked by double clicking on the residue or `display residue label` *rs_* command. Possibilities:

1. `"A5"` <− default choice
2. `"Ala 5"`
3. `"ALA 5"`
4. `"Ala"`
5. `"ALA"`
6. `"Alanine 5"`
7. `"5"`
8. `"A"`
9. `" A"`
10. `"Mol"` − displays MOLECULAR name.

See also : `resLabelShift`, `atomLabelStyle` .

2.17.16. ribbonColorStyle

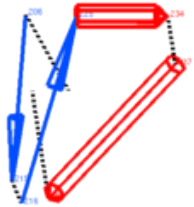
− sets the ribbon coloring scheme.

1 = "none"	default. colors by secondary structure type or explicit color
2 = "NtoC"	colors each chain gradually blue−to−red from N− to C− (or from 5' to 3' for DNA)
3 = "alignment"	if there is an alignment linked to a protein, color gapped backbone regions gray
4 = "reliability"	3D gaussian averaging with `selectSphereRadius` of alignment strength in space

If `ribbonColorStyle` equals to 4, the conserved areas will be colored blue, while the most divergent will be red, and the intermediate conservation areas will be colored white. Example:

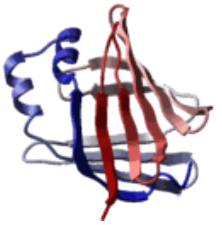
```
nice "1eoc.a/"
make sequence a_1.1
read pdb sequence "3pcc.a/"
aa = Align(3pcc_a 1eoc_a)
ribbonColorStyle=3   # color gaps gray
color ribbon
ribbonColorStyle=4   # see alignment strength
color ribbon
```

2.17.17. ribbonStyle



specifies type of representation when `display ribbon` command is used. Options are the following:

1. `"ribbon"` <− default choice
2. `"cylinders"`
3. `"pencils"`
4. `"numbers"`



The first choice is a solid `ribbon` representation.

The second representation draws alpha−helices as cylinders. If a helix is too curved, ICM tries to split it into more straight helices. The radius of a helix depends on the helical curvature and is calculated to include all C atoms. Therefore, wide cylinders contain more curved helices. One can break a helix in any place with the 'assignsstructure{assign sstructure} command. (e.g. `assign sstructure a_/182 "_"` to break a helix by residue 182).

The third and the fourth, "pencils" and "number" refers to a style where secondary structure elements are represented by vectors (see Abagyan and Maiorov, 1988).

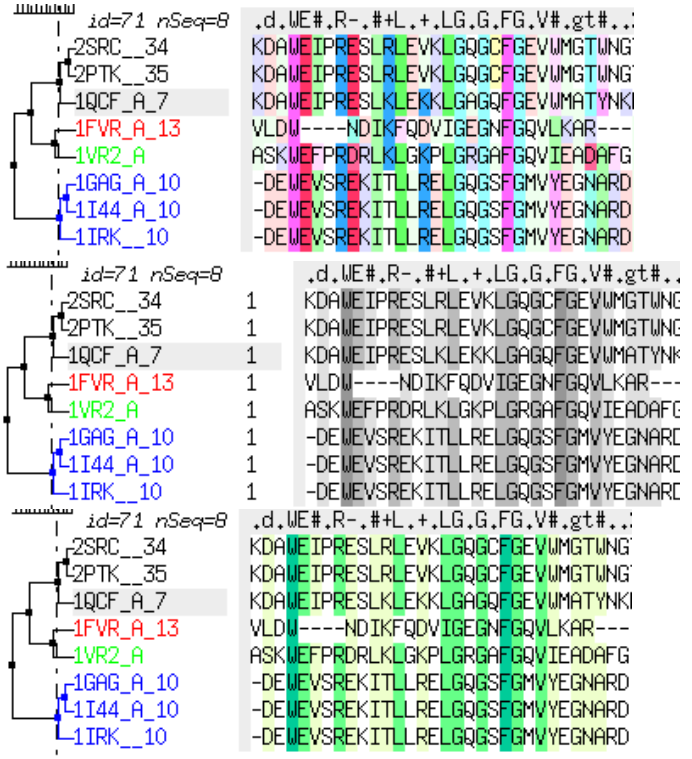
Note The segment parameters must be **pre−calculated** with the `assign sstructure segment` command. The segment description is used in `fast searches` for related topologies in the databank. The last option ("both") will display both representations of the backbone topology.

2.17.18. sequenceColorScheme

defines the color scheme selection which is used to color alignment in ICM. The following preferences are defined:

1. `"no color"`
2. `"residue type"`
3. `"icm−combo"`
4. `"consensus strength"`
5. `"greyscale"`

The actual color table containing the correspondence between colors, residues and consensus symbols is stored in the CONSENSUSCOLOR table. The strength of the consensus is regulated by the `CONSENSUS_strength` parameter. The last three preferences are illustrated below.



2.17.19. shineStyle

defines how solid surfaces of `cpk` , `skin` and `grobs` reflect light. Possibilities:

1. `"white"` <- default
2. `"color"`

The first option gives a more shiny and greasy look.

2.17.20. surfaceMethod

defines how the `surface energy` is calculated. Options available:

1. `"constant tension"`
2. `"atomic solvation"` <- default choice
3. `"apolar"`

Explanations:

1. "constant tension" means that the energy terms are just the product of the total solvent−accessible surface by the surfaceTension parameter. This term is intended to represent the surface energy if electrostatics takes the solvent polarization energy into account (see electroMethod)
2. "atomic solvation" option is designed to evaluate the solvation energy purely on the basis of the atomic accessible surfaces instead of using the proper electrostatic evaluation of the polarization free energy. This fast but approximate scheme was proposed by Wesson and Eisenberg, (1992) . Atomic surface parameters derived from the experimental vacuum−water transfer energies are given in the icm.hdt file.
3. "apolar" option is designed to evaluate the stabilization energy, which is the difference between denatured and folded states. The "atomic solvation" energy should be used with the van der Waals term while the "apolar" energy takes it into account and should be used without any other energy terms. The "apolar" atomic surface parameters were derived from the experimental octanol−water transfer energies and are given in the icm.hdt file.

Note, that if a part of the system is represented with grid potentials, one needs a special m_ga grid map for correct calculations of the surface accessibilities.

2.17.21. tzMethod

method of imposing and calculating tethers. The three alternatives are the following

1. "simple" : equal weight tethers to 3D points

2. "weighted" : individual weights are calculated from atomic B−factors by dividing $8*PI^2$ by the B−factor value. All the weights additionally are multiplied by the tzWeight shell variable.

3. "z_only" : tethers are imposed only in the Z−direction towards the target Z−coordinate. These type of tethers pulls a molecule into a z−plane. This may be useful if you are trying to generate a flat projection of a three−dimensional molecule.

4. "function" : tethers can take a form of distance restraints with individual weights, upper and lower bounds. The three parameters are controlled by the following properties of the **target** atoms (not the source atoms as in the "weighted" case): individual weights are directly taked from bfactor values, the upper bounds from the area fields, and the lower bounds from the charge field. To set those values, use the set bfactor, set area and set charge commands respectively.

   applying linear force to atoms: to exert a constant force to an atom, set the formal charge of the target atom to a special value of 5. The b−factors will continue to serve as individual force constants and the direction of force will correspond to the vector from the origin to the target pdb−atom with this special value of formal charge.

Example for the "z_only" method in which we generate a more or less flat image of a chemical.

```
build smiles "c1c(ccc(c1)N(=O)=O)N2CCC(CC2)=CC(=O)NNC(=O)Nc3cc(ccc3)C(F)(F)F"
tzMethod = "z_only"
set tether a_   # sets tethers to x,y,z=0. coordinates for each atom
minimize "vw,tz" 200
dsChem a_//!h*
```

```
#linear force. Use interface to set the linear force flag (formal charge) and bfactors
copy a_ "tzcopy"
tzMethod = "function" # will use bfactor and formal charge features of a_tzcopy. atoms
set tether a_/1/ca a_tzcopy./1/ca  # drag the target atom where you want
set charge formal a_tzcopy./1/ca 5. # number 5. signals ICM to interpret it as linear force
set bfactor a_tzcopy./1/ca 5000.    # the force constant
set tether a_/1/cb a_tzcopy./1/cb   # combine with normal tethers.
display tether a_
minimize v_//?vt* "tz"
```

2.17.22. varLabelStyle

style of labels for free torsions, angles and bonds (i.e. internal variables) `display variable label vs` command. Possibilities:

1. `"greek"` <− default choice
2. `"name"`
3. `"value"`

2.17.23. visitsAction

what to do, if one `stack conf`ormation is overvisited, i.e. `mnvisits` has been reached. The following actions are allowed:

1. `"random"`
2. `"heat"` <− default choice
3. `"stackjump"`
4. `"exit"`

Explanation of actions:

- `"heat"` − double the simulation temperature
- `"stackjump"` − jump to the conformation of the least visited slot in the stack.
- `"random"` − randomize all free variables according to the `mcJump` parameter
- `"exit"` − exit the MC procedure

2.17.24. vwMethod

specifies the function type of the van der Waals term ("vw"). The following three functions can be chosen:

1. `"exact"` <− default choice:

   $F_{vw} = A/r^{12} - B/r^{6}$. This is the usual van der Waals formula tending to infinity at r close to 0.

2. `"soft":`

   $F_{soft} = F_{vw}$, for $F_{vw} <= 0.$ and $F_{soft} = F_{vw} * (t/(t+F_{vw}))$ for $F_{vw} > 0.$ (repulsion).

   This form preserves the function for the most populated part of the curve but smoothly reaches the limit `t` (defined by the `vwSoftMaxEnergy` real system variable)

3. "old soft":

   another smooth approximation with the finite value at r=0, depending on the well depth.

2.17.25. webEntrezOption

defines how to interpret the NCBI Entrez links.

1. "none"
2. "g:GenPept" <− default
3. "r:Report"
4. "f:FASTA"
5. "a:ASN.1"
6. "d:Entrez document summary"
7. "m:MEDLINE links"
8. "p:protein neighbors"
9. "n:nucleotide links"
10. "t:structure links"
11. "c:genome links"

See also: `s_webEntrezLink`, `web`, `show html`, `write html`.

2.17.26. wireStyle

style of the `display wire` mode. The choices are the following:

1. "wire" <− default choice
2. "chemistry"
3. "tree"

Style "chemistry" shows different types of chemical bonds. Style "tree" shows a directed graph of the ICM−molecular tree. Yellow triangle indicates the entry atom of an ICM object. The tree can be rerooted with the `write library a_newEntryAtom` command. The topology of the complete tree including the virtual atoms can be shown with the `display virtual` command.

Note: The "tree" graph does **not** exist for objects of non−ICM type, e.g. those created by the `read pdb` command, and this preference will have no effect. The tree representation elucidates the ICM topology graph imposed on molecules and is crucial in the `modify` command, since it removes a branch up−tree from the specified entry atom, and replaces it by another branch. Use `Ctrl−W` to toggle between these styles (see `set key` command). The line width is controlled by the `lineWidth` parameter.

2.17.27. xrMethod

The penalty function of correspondence between observed and calculated structure factors.

1. "corr Fc:Fo" <− default
2. "corr Fc2:Fo2"

2.18. Tables (structures)

The following predefined icm−shell tables are collections of different icm−shell−objects related to a certain topic. Note that these tables (as opposed to user−defined ICM `table`s) usually only have the header section. You can `show` and `list` them. You can also change any table element by the usual icm assignment:

Examples:

```
 IMAGE.color = yes       # this member is a logical
 IMAGE.stereoBase = 2.5  # redefine real distance between stereo panels
```

2.18.1. CONSENSUS

The consensus *symbol* is established if the percentage of specified *residues* in a give column exceeds the *fraction* given in the 2nd column. In rows were we provide two symbols (e.g. "−n"), the first (e.g. '−') is used in alignment representations, while the letter form of this symbol (e.g. 'n') is used in residue selections, (e.g. `a_/Cn`) The first matched consensus condition takes precedence. In an example below, if `Q` is found in more than 85% or sequences, its consensus symbol is `Q,` if the percentage is between 60 and 85, the symbol becomes `q,` and if no consensus is establish, the symbol becomes the dot character ('.').

```
#>T CONSENSUS
#>-symbol------fraction----residues---
   A           85          A
   C           85          C
   Q           85          Q
...
   d           60          ND
   -n          70          ED
   +o          60          RK
   gj          60          G
   q           70          Q
   p           60          P
   t           60          TSN
   "#h"        85          WLVIMAFCYHP
   %f          65          WLVIMAFCYHP
   " g"        85          −
```

See also: `CONSENSUSCOLOR` , `CONSENSUS_strength` , `color rs_ alignment`.

2.18.2. CONSENSUSCOLOR

contains coloring schemes of residues according the a multiple sequence alignment (see the `align` command). This table is saved together with the GUI preferences. Residue color is defined by two factors: its type, as listed in the first column of the table, AND the consensus character under which this residue is aligned. The consensus symbols are defined by the `CONSENSUS` table and are listed in the third column of the CONSENSUSCOLOR table. In this scheme the same residue can be colored differently depending on the alignment in a current position.

```
#>T CONSENSUSCOLOR
#>-residue-----color-------symbols----
   *           *           *         # separator between sections
```

```
ED          "#ff0000"   "−EDp"    # E and D residues will be colored red under '−','E' or '
KR          "#0000ff"   "+KRp"
```

2.18.3. FILTER

contains filters which can be applied to the input stream in the `read` command. Components have names corresponding to standard file name extensions; their `string` value is a unix filter. Token **`%s`** is a placeholder for the file name. The provided defaults can be redefined in your `_startup` file. You can also add your own extensions and filters by doing the following:

```
z = "pcat %s"     # define the action for the unix packed files
group table append FILTER header z  # append new filter to the structure
```

The mechanism ICM employs allows to keep the transformed files intact and avoid creating temporary files when possible (e.g. uuencode unix command always creates an output file). Existing extensions and defaults are given below. You may need to redefine the defaults by adding the exact path to the utility or using alternatives.

FILTER.Z

allows you to read the compressed files (*.Z) directly leaving the compressed file intact. The default value: `"zcat %s"` . If you do not have zcat utility, try

FILTER.Z = "uncompress −c %s"

FILTER.gz

The default value is `"gunzip −c %s"` .

FILTER.uue

The default value is

```
"sed 's:begin .*:begin 600 /tmp/UUPtm:' %s | uudecode &cat /tmp/UUPtm &rm −f /tmp/UUPtm"
```

This works for UNIX file system, write your own on the PC, if needed.

2.18.4. FTP

`table` which controls reading from `ftp`.

FTP.createFile

(default `no`). This flag is not active yet. The file is always created in the `s_tempDir` directory.

FTP.keepFile

(default `no`). If `yes,` the temporary file is kept in the `s_tempDir` directory. Otherwise the file is deleted.

FTP.proxy

`string` path to the proxy server for connections through firewall. Default: "" (empty string).

2.18.5. GRAPHICS

display parameters for different graphics representations.

GRAPHICS.ballRadius

radius (in Angstroms) of a small ball `display`ed as a part of `ball` or `xstick` graphical representations of a molecule.

Default (0.15)

GRAPHICS.clashWidth

relative width of a displayed `clash` . This parameter can be changed from the **File/Preferences/DisplayGeneral** menu.

See also: `lineWidth` , `GRAPHICS.grobLineWidth` , `GRAPHICS.hbondWidth` , `GRAPHICS.mapLineWidth` , `GRAPHICS.wireWidth` .

Default (1.)

GRAPHICS.displayLineLabels

enables/disables the display of edge lengths (inter−point distances) of a `grob` generated with the `Grob`(`"distance"` ..) function. This parameter can be changed from the **File/Preferences/DisplayGeneral** menu.

See also: `Grob` ("distance" ..)

Default (yes)

GRAPHICS.displayMapBox

controls if the bounding box of a map is displayed (see `display map`).

Default (yes)

GRAPHICS.dnaBallRadius

DNA bases in ribbon representation are shown as balls controlled by the above `real` parameter. You can undisplay them with the: `undisplay ribbon base` command.

Default: 1.5

GRAPHICS.dnaRibbonRatio

`real` ratio of depth to width for the DNA `ribbon` .

Default: 0.3

GRAPHICS.dnaRibbonWidth

`real` width (in Angstroms) of the DNA `ribbon` .

Default: 2.

GRAPHICS.dnaRibbonWorm

`logical` which, if yes, makes the DNA backbone `ribbon` round, rather than rectangular.

Default: no

GRAPHICS.dnaStickRadius

`real` radius of the sticks representing bases in DNA `ribbon` .

Default: 0.72

GRAPHICS.grobLineWidth

relative width of displayed lines of 3D meshes (grobs). Also affects the interatomic distance display. This parameter can be changed from the **File/Preferences/DisplayGeneral** menu.

See also: `lineWidth` , `GRAPHICS.clashWidth` , `GRAPHICS.hbondWidth` , `GRAPHICS.mapLineWidth` .

Default (1.)

GRAPHICS.hbondStyle

determines the style in which hydrogen bonds are displayed. Here hbond−Donor, Hydrogen, and hbond−Acceptor atoms will be referred to as D, H and A, respectively,

```
GRAPHICS.hbondStyle = "dash"
       1 = "dash"      # the default choice. Just a line
       2 = "length"    # show the D−A distance in addition
       3 = "length and angle"  # show both the distance and the 180. − <D−H.. A> angle
```

The best possible value for a non−linearity angle is 0. . The display dialog has a small button to roll through this preference. See also: `GRAPHICS.hbondWidth` .

GRAPHICS.hbondWidth

relative width of a displayed `hbond` . This parameter can be changed from the **File/Preferences/DisplayGeneral** menu.

See also: `lineWidth` , `hbond` `display hbond`, `GRAPHICS.grobLineWidth` , `GRAPHICS.clashWidth` , `GRAPHICS.mapLineWidth` .

Default (1.)

GRAPHICS.hydrogenDisplay

determines the default hydrogen display mode for the `display` command.

```
GRAPHICS.hydrogenDisplay = "polar"
       1 = "all"   # all hydrogens are shown
       2 = "polar" <-- current choice  # polar displayed, the non-polar hidden
       3 = "none"  # no hydrogens are displayed
```

GRAPHICS.light

a `rarray` of 13 elements between 0. and 1. which controls the main properties of lighting model in GL. The sections of this array can be changed with four sliders of the Display tab in a top tool bar. The following elements are defined:

Elements	Property	Range	Default	Comment
GRAPHICS.light[1]	shininess	0.,1.	1.	property of the solid material
GRAPHICS.light[2:4]	ambient light	0.,1.	{0.15 0.15 0.15}	intensity of RGB for ambient light
GRAPHICS.light[5:7]	diffuse light	0.,1.	{0.6 0.6 0.6}	intensity of RGB for diffuse light
GRAPHICS.light[8:10]	specular light	0.,1.	{0.35 0.35 0.35}	intensity of RGB for specular light
GRAPHICS.light[11:13]	emission	0.,1.	{0. 0. 0.}	intensity of RGB for emitted light

The first element defines the shininess of solid surfaces such as `cpk`, `ribbon`, `ball`, `stick`, `xstick`, and `skin` when they are `display`ed. The other elements contain triplets of R,G,B (red green blue) values from 0. to 1. for the four types of visual effects. If R,G and B channels do not have equal intensity (e.g. `GRAPHICS.light[5:7] = {0.2 0.2 0.6}`) the corresponding light effect will have color (blue in the example above).

To re−render the solid graphics with new parameters, use the

```
display new reflection
```

command.

Example:

```
build string "se his trp glu"
display cpk
color background blue
GRAPHICS.light[5:7] = {0.2 0.2 0.6}
display new reflection
```

GRAPHICS.mapLineWidth

relative width of lines and dots of a displayed `map` . This parameter can be changed from the **File/Preferences/DisplayGeneral** menu.

See also: `lineWidth` , `GRAPHICS.grobLineWidth` , `map` , `GRAPHICS.hbondWidth` .

Default (1.)

GRAPHICS.quality

`integer` parameter controlling quality (density of graphical elements) of such representations as cpk, ball, stick, `ribbon` . Do not make it larger than about 20 or smaller than 1. This parameter supersedes the previous `ballQuality` parameter.

We recomment to make this parameter at least `15` if you want to make a high quality image. You can also increase the number of image resolution by making the image window 2,3,4 times larger (in the example below it is 2 times larger) than the displayed window.

```
GRAPHICS.quality = 15
display ribbon

# press Ctrl-D  for the fog effect, move clipping planes, change fogStart

write image png window=2*View(window)
```

Default: 5.

GRAPHICS.rainbowBarStyle

determines if and where the color bar will appear after a molecule is colored by an array. Coloring by an array is one of the options of the `display` and `color` commands.

1. = "left" <− default choice
2. = "right"
3. = "no text"
4. = "no bar"

The bar can be dragged (use middlebutton), removed (point into the bar and press BACKSPACE), just like a string label. To assign your own numbers to the bar, you may choose option `"no text"` and use several `display s_label` commands. The bar, if displayed, is exported to TIF, RGB `images` and `postscript`.

GRAPHICS.resLabelDrag

if `yes,` enables dragging of the displayed residue labels with the middle mouse button. The labels can be reset to their initial positions with the `set residue label distance` rs_

command. The intial position is defined by the relative displacements of {0. 0. 0.} from the special "residue label−carrying" atom of the residue, see the `set label as_` command. See also `resLabelStyle`

Default (no).

GRAPHICS.ribbonRatio

real ratio of depth to width for the protein ribbon .

Default: 0.3

GRAPHICS.ribbonWidth

real width of the protein ribbon .

Default: 1.

GRAPHICS.ribbonWorm

logical parameter, if yes, makes the ribbon round, rather than rectangular.

Default: no

GRAPHICS.selectionLevel

preference for the selection level of as_graph selection. The atoms, residues, molecules or objects selected interactively in the graphics window are automatically stored in the as_graph variable. The preference may have the following values.

```
GRAPHICS.selectionLevel = "atom"
      1 = "object"
      2 = "molecule"
      3 = "residue"
      4 = "atom" # default
      5 = "variable"
```

The GRAPHICS.selectionLevel can be switched either interactively, e.g.

```
GRAPHICS.selectionLevel = 3
```

or from GUI by selecting the level combo box with the following choices: O (object), M (molecule), R (residue), X (atom), or an icon of a torsion (variable).

GRAPHICS.selectionStyle

preference for the style in which the graphical selection is shown. The preference may have the following values.

```
GRAPHICS.selectionStyle = "color"
      1 = "none"
      2 = "cross"
      3 = "color" # the default choice
      4 = "both"
```

In the 1−st mode ("none") only a single selection mark is shown. It is convenient when you do not want multiple selection marks to overwhelm the image. The 3−rd mode is incovenient if you want to try different colored displays for the selected fragments.

GRAPHICS.stereoMode

1. "up−and−down"
2. "line interleaved" "in−a−window"

a simple hardware stereo mode for workstations with a horizontal frame splitter. In the "up−and−down" mode a longer frame with two stereo images on top of each other is generated and the two halves are then superimposed with the splitter. This mode does not require anything from a graphics card, but does require a frame splitter. A frame splitter box was connected between a monitor and a graphics card output. This mode has an unpleasant side effect, the rest of the screen (beyond the OpenGl window) becomes stretched and the lower part of the screen is superimposed on the top half.

The "line interleaved" mode can be used with a new type of frame splitter at the line level. In this case the odd lines from one stereo−image are interleaved with the even lines of another. The side−effect of this mode is that the intensity is reduced in half since at each moment one sees only one half of the lines. The splitter device for this mode can be purchased from Virex (www.virex.com). This mode produces a dark stereo image but is easily available (requires stereo goggles, e.g. from Virex).

The "in−a−window" mode is used in SGI workstations and in a Linux workstation with an advanced graphics card supporting a quad graphics buffer. In this mode the hardware stereo regime applies only to an OpenGl window. This is the best mode but it requires an expensive graphics card (plus the stereo goggles).

Note: LCD screens can not display a stereo image since the image is not continuously updated at high frequency. This technical problem may be solved in the future (so we hear).

GRAPHICS.stickRadius

radius (in Angstroms) of a cylinder displayed as a part of stick or xstick graphical representation of a molecule.

Individual (residue−wide) control of stick radii.

In order to modify the default values of the radii from the command line set the 3rd field of the residue of interest to the new value. For example:

```
set field as_Residue_Selection number=3 r_newStickRadius
```

In this case the ball radius will be changed according to the radio of the **default** parameters (e.g. GRAPHICS.ballRaduis/GRAPHICS.stickRadius)

Default (0.4).

GRAPHICS.wormRadius

radius of coiled segments (i.e. those where the secondary structure is marked as "_") of a polypeptide chain in ribbon representation.

Default (0.3).

2.18.6. GRID

parameters for the grid energy calculations (see also `"gh,gc,ge,gs,sf" energy terms`).

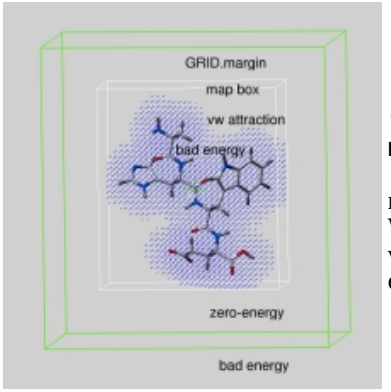
GRID.gcghExteriorPenalty

A preference to allow automatically impose a repulsive penalty outside the area covered by the van der Waals maps (`m_gc` and `m_gh`).

1. = `"repulsive"` <− the default
2. = `"zero"`

In the default mode a volume penalty is imposed automatically outside the map box expanded by the `GRID.margin` . The penalty potential is set to the `GRID.maxVw` value.

GRID.margin



`real` parameter determining the extra penalty−free space around the `map` bounding box if `GRID.gcghExteriorPenalty = "repulsive"` (see above). For any atom which gets outside the map−bounding box expanded by `GRID.margin,` its grid van der Waals energy (`"gc"` or `"gh"`) is penalized by the `GRID.maxVw` value. This is the same penalty value which atoms get if they severely clash with other atoms.

Therefore, if you set up grid energy calculations it is essential either to create a big enough box or set a sufficient margin to allow ligand rearrangements near the receptor surface. If `GRID.margin` is very large, your ligand will be "on the loose" and may spend too much time flying in open air. It is recommended that the margin is not larger than the diameter of your ligand.

Default: `0.00` A

GRID.maxEl

`real` truncation parameter. Default: `20.0` kcal/mole.

GRID.minEl

Default: −20.0 kcal/mole.

GRID.maxVw

The truncation level of the van der Waals repulsion energy precalculated in the `"gc"` grid energy term. This number also is used as a penalty for the atoms outside the map box expanded by `GRID.margin` .

Default: 3.0 kcal/mole.

2.18.7. GROB

Parameters related to `graphics objects`. See also the `Grob` family of functions.

GROB.atomSphereRadius

default radius (in Angstroms) which is used to select a patch on the surface of a grob. Used in the `color` *grob as_selection color* command.

Default: `4.0.`

GROB.relArrowSize

a `real` relative arrow size ([0.,1.]). Default: `0.2.`

GROB.arrowRadius

a `real` arrow radius in Angstoms used by the `Grob`("ARROW", R_) function. Default: `0.5.`

GROB.relArrowHead

a `real` ratio of the arrow head radius to the arrow radius. This parameter is used by the `Grob`("ARROW", R_) function. Default: `3.0.`

2.18.8. GUI

table contains some settings for the GUI. Most of the settings are stored automatically in the `s_userDir` + `"/config/icm.cfg"` file

GUI.workspaceTabStyle

allows to change the style of ICM−object tabs created in the workspace panel of ICM GUI.

1. = "icon title" # default
2. = "icon"
3. = "title"

2.18.9. IMAGE

table contains settings used by the following commands creating image files:

- `write image`,

- `write postscript`,
- `display movie image`.

IMAGE.quality

this `integer` parameter allows to improve quality of vectorized postscript images saved by the `write postscript` command. Actually this parameter only changes one number in the header of a postscript file. You can also manually edit the file to correct this number. This number defines the number of divisions of larger triangles into smaller ones accompanied by interpolation of colors which occurs during printer interpretation of the postscript stream to provide smooth continuous transitions. The optimal value of this parameter depends on the maximal triangle size. It may grow as large as 100 for a single triangle on a page. Typically for a molecular image with molecular surface `IMAGE.quality=3` is sufficient.

Important. Do not set the parameter to values higher than 5 for the molecular image, your printer will die!

Default: `3`

IMAGE.printerDPI

this `integer` parameter the printer resolution in Dot Per Inch (DPI). Important for the `write image postscript` command.

Default: `300`

IMAGE.lineWidth

this `real` parameter specifies the default line width for the postscript lines.

Default: `1.0`

IMAGE.scale

`real` variable. If non zero, controls the image scale with respect to the screen image size. The screen image resolution (or Dots−Per−Inch) is usually 72. Let's assume printer DPI to be 300 (see the `IMAGE.printerDPI` parameter). In this case `IMAGE.scale=1.` will make the printed image the same pixel size (which is about 4 times smaller) than the screen image. For pixel images saved by `write image postscript` command integer `IMAGE.scale` values (2., 3., 4.) are preferable. That is what auto mode (IMAGE.scale=0.0) is trying to do. This consideration is NOT important for the vectorized postscript images created by the `write postscript` command.

Default: `0.0` (i.e. auto mode: maximum size fitting the page in given `IMAGE.orientation`)

IMAGE.stereoBase

`real` variable to define the stereo base (separation between two stereo panels) in the `write image postscript` and `write postscript` command.

Default: `2.35` inches, (~ 60mm)

IMAGE.stereoAngle

`real` variable to define stereo angle (relative rotation of two stereo images) in the `write image postscript` and `write postscript` command.

Default: `6.0` degrees.

IMAGE.gammaCorrection

`real` variable to to lighten or darken the image by changing the *gamma* parameter. A gamma value that is greater than `1.0` will lighten the printed picture, while a gamma value that is less that `1.0` will darken it. You may adjust your gamma correction parameter for your printer with respect to your display and add this setting to the `_startup`

Default: `2.0`

IMAGE.color

`logical` to save color or black_and_white ('bw') images. You can override this parameter by using the explicit `bw` option in the `write image` command.

Default: `yes`

IMAGE.compress

`logical` to toggle simple lossless compression, standard for .tif files. This compression is required to be implemented in all TIFF−reading programs.

Default: `yes`

IMAGE.generateAlpha

`logical` to toggle generation of the alpha (opacity) channel for the SGI `rgb`, `tif` and `png` image files to make the pixels of the background color transparent.

Be careful. The alpha channel is set to 1. for every pixel in your image which has the same color as the background. Therefore there is a danger that the same color will be accidently used inside your image. If you nevertheless want to generate the alpha−channel, use a rare color your background (not black, but rather green, e.g. `rgb = {0.,0.976,0.}`.

Default: `yes`

IMAGE.stereoText

`logical` to make text labels for only one panel or both panels of the stereo diagram.

Default: `yes`

IMAGE.previewer

a `string` parameter to specify the external filter which creates a rough binary (pixmap) postscript preview and adds it to the header of the ICM−generated high resolution bitmap or vectorized postscript files saved by the `write image postscript`, and `write postscript` , respectively . This preview information is compliant with EPSI (encapsulated Postscript interchange file format) and is useful to see a draft image instead of a empty rectangle upon inclusion of the postscript file into other drawing and imaging software like IRIS showcase.

Default: `"gs −sDEVICE=pgmraw −q −dNOPAUSE −sOutputFile=− −r%d −− %s"`

IMAGE.previewResolution

`integer` resolution of the rough bitmap preview added to the vectorized postscript file in *lines per inch*. Recommendations:

- 10 − very rough (1/10th of an inch)
- 20 − a reasonable preview but no fine details
- 30 − a fine preview, do not increase it any higher since the file will become too large.

IMAGE.orientation

`preference` to specify image orientation.

1. = "portrait" <− default
2. = "landscape"
3. = "auto"

Default: "portrait"

IMAGE.paperSize

`preference` to specify paper size.

1. = "Letter (8.5x11")" <− default
2. = "Legal (8.5x14")"
3. = "11x17""
4. = "A4 (210x297mm)"
5. = "A3 (297x420mm)"

Default: "Letter (8.5x11")"

IMAGE.rgb2bw

`rarray` of 6 elements defining translation of rgb colors into black and white ('bw') grades. The array is {RED_scale, GREEN_scale, BLUE_scale, RED_bias, GREEN_bias, BLUE_bias} and the default values are {0.3125, 0.5, 0.1875, 0., 0., 0.}.

2.18.10. LIBRARY

table containing string paths of the icm parameter files, which are loaded by the `read library [mmff]` command. The library files will be taken from the `s_icmhome` directory if no explicit directory is provided. Extensions are automatically added. Defaults:

```
LIBRARY.bbt="icm"  # bond bending types
LIBRARY.bci="icm"  # mmff bond charge increments
LIBRARY.bst="icm"  # bond stretching types
LIBRARY.clr="icm"  # colors, gui controls
LIBRARY.cmp="icm"  # amino-acid comparison matrix
LIBRARY.cnt="icm"  # distant restraint types
LIBRARY.cod="icm"  # atom codes
LIBRARY.hbt="icm"  # hydrogen bonding types
LIBRARY.hdt="icm"  # hydration types
LIBRARY.lps="icm.lps"  # loop database, rebuilt with write model [append]
LIBRARY.men="icm.gui"  # GUI commands
LIBRARY.mmbbt= "mmff"  # mmff bond bending
LIBRARY.mmbst= "mmff"  # mmff bond stretching
LIBRARY.mmtot= "mmff"  # mmff torsions
LIBRARY.mmvwt= "mmff"  # mmff van der Waals
LIBRARY.rst="icm"  # variable restraint types
LIBRARY.tor="icm"  # precomputed icmff torsion params
LIBRARY.tot="icm"  # torsion types
LIBRARY.vwt="icm"  # van der Waals types
LIBRARY.res={"icm","usr"}
```

Example:

```
LIBRARY.res=LIBRARY.res // "./benz.res" # just append
LIBRARY.cod="./newCodes.cod"
read library
```

2.18.11. OBJECT

Controls atom requisites which are written to a file in the `write object` command. Extensions are automatically added. Defaults:

```
OBJECT.bfactor  =yes
OBJECT.charge   =yes
OBJECT.occupancy=yes
OBJECT.site     =yes
OBJECT.display  =no
OBJECT.library  =no
OBJECT.auto     =no
```

Example:

```
OBJECT.auto = no
OBJECT.display = yes
read object "crn"
display ribbon a_/1:40
set plane 2
display cpk a_/12
write object "tm"  # graphics and planes are written
```

```
delete a_*.
read object "tm"
```

2.18.12. PLOT

Contains settings used by the `plot` command. All real sizes are expressed in the Postscript "points" equal to 1/72" (about 1/3 mm).

PLOT.numberOffset

`integer` offset for the X−coordinate with the `number` option. This option is used in a number of macros generating multisection plots for amino−acid sequences.

Default (0).

PLOT.fontSize

`real` font size. Any reasonable number from 3. (1 mm, use a magnifying glass then) to 96.

Default (10.0).

PLOT.lineWidth

`real` line width for graphs (not the frame and tics)

Default (1.0).

PLOT.markSize

`real` mark size in points. Allowed mark types: line, cross, square, triangle, diamond, circle, star, dstar, bar, dot, SQUARE, TRIANGLE, DIAMOND, CIRCLE, STAR, DSTAR, BAR. Uppercase words indicate filled marks.

Default (1.0).

PLOT.Yratio

`real` aspect ratio of the ICM plot frame. Using `link` option of the `plot` command is equivalent to setting this variable to 1.0. If `PLOT.Yratio` is set to 0. , the ratio will be set automatically to fill out the available box optimally.

Default (0.8).

PLOT.logo

`logical` switch for the ICM−logo on the plot.

Default (`yes`).

PLOT.color

`logical` to generate a color plot. Usually it does not make sense to switch it off because your b/w printer will interpret the color postscript just fine anyway.

PLOT.orientation

`preference` for the plot orientation. Currently inactive. Default (`yes`).

PLOT.seriesLabels

`preference` to indicate position of a series/color legend inside the plot frame. You can provide individual names for each series in the optional `string array` argument of the `plot` command. (e.g. plot M_XY1Y2 {"Title","X","Y","Ser 1","Ser 2"}) Available choices:

- 1 = "none"
- 2 = "right" <− default choice
- 3 = "left"
- 4 = "top"
- 5 = "bottom"

PLOT.font

`preference` for the title/legend font. The font size can only be redefined by editing the *.eps file (search for the number before the `scalefont` string). Available choices:

- 1 = "Times−Bold"
- 2 = "Times−Roman" <− default choice
- 3 = "Helvetica"
- 4 = "Courier"
- 5 = "Symbol"

PLOT.labelFont

`preference` for the data point label font. You can also redefine the font size with the `PLOT.fontSize` variable. Available choices:

- 1 = "Times−Bold"
- 2 = "Times−Roman" <− default choice
- 3 = "Helvetica"
- 4 = "Courier"
- 5 = "Symbol"

PLOT.rainbowStyle

`preference` defining the color spectrum used by the `plot area` command. This command lets you plot a function of 2 arguments and show the function value by color. By default the plot command uses the minimal and maximal values of the provided matrix. You can enforce the range with the `color` option. Available choices:

- 1 = "black/white"
- 2 = "blue/white/red" <− default choice
- 3 = "blue/rainbow/red"

Example:

```
 read matrix  # def.mat is the default one
 PLOT.rainbowStyle=1
 plot area def display   # grey−scale, automatical min and max
 PLOT.rainbowStyle=3
 plot area def color={−10.,0.} display  # enforce new range
 PLOT.rainbowStyle=2
 plot area def transparent={−2.,8.} display
# low values − blue, middle [−2.,8.] − invisible, large red
```

PLOT.box

`rarray` of the origin and relative sizes of the ICM plot frame: { X_origin, Y_origin, X_size, Y_size }. Box `{0. 0. 1. 1.}` fits the page optimally.

Default ({0. 0. 1. 1.}).

2.18.13. SITE

This table contains parameters and preferences used to display the `site`s, or important residues.

SITE.defSelect

string of significant site types (shown as one letter abbreviations) Sequence identity in the alignment positions which have one of those sites is additionally rewarded in the alignment score calculation.

Default: `"ABFGLMstepm"`

SITE.labelOffset

(default 5. A) the `real` offset of the site label with respect to the residue label atom.

SITE.labelStyle

the style `preference` of the displayed site information:

1. "none"
2. "symbol" # one letter symbol, see `site` .
3. "TYPE" # < −− default choice
4. "RES.TYPE"
5. "comment"
6. "full"

SITE.labelWrap

0.5 (inactive)

SITE.showSeqSkip

the `string` of the `site` types skipped in the `show sequence` (or alignment) commands.

2.18.14. WEBLINK

This table contains definitions of types of web links used in the `web`, `show html`, and `write html` commands. The table is read from `"WEBLINK.tab"` file from the `$ICMHOME` directory. Change this file for your own definitions. The weblink specification is used to extend the argument string substituted for %s (e.g. "IL2_HUMAN" element of the table array linked according to the type

`SP %s "http://www.aaa?%s"` will be transformed into the `<a href="http://www.aaa?IL2_HUMAN">IL2_HUMAN</a>` link. If %Ns specification is used, only N characters of the argument string will be retain in the link. For example,

`PDB %s "http://www.pdb?%4s"` and `1xyz_a15_25` (specifying chain and residue range) will be translated into

`<a href="http://www.pdb?1xyz">1xyz</a>_a15_25` which in your browser will look like this:

"AUTO" is another type which can be used in the link S_ "TYPE" ... expression. In this case the DB type is automatically recognized according the database reference string pattern (see also `WEBAUTOLINK`). An example table:

```
#>T WEBLINK
#>-DB------DR--LINK-------
 PDB      %s  http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6&uid=pdb|%4s|&Dop
 NCBI     g%s http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6&uid=%s&Dopt=g
 EMBL     %s  http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6&uid=emb|%s|&Dopt
 SP       %s  http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6&uid=sp||%s&Dopt=
 SPA      %s  http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=s&form=6&uid=sp|%s|&Dopt=
 PROSITE %s  http://saturn.med.nyu.edu/srs/srsc?[PROSITE-acc:%s]
 MED      %s  http://www3.ncbi.nlm.nih.gov/htbin-post/Entrez/query?db=m&form=6&uid=%s
```

Example:

```
 read table "seqcomp.tab"  #contains references to different databases
 web SR link SR.NA1 "PDB" SR.NA2 "AUTO"
```

2.18.15. WEBAUTOLINK

This table contains definitions of web link string patterns for automatic recognition in the `web`, `show html`, and `write html` commands. The table is read from the "WEBLINK.tab" file in the `$ICMHOME` directory. Change the file for your own definitions. Recognition is not perfect because the patterns overlap.

Example:

```
read table "seqcomp.tab"  #contains references to different databases
web SR link SR.NA1 "AUTO" SR.NA2 "AUTO"
```

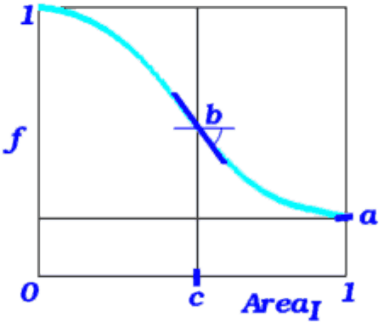
2.19. Other shell variables

2.19.1. defCell

the `real array` of the default cell parameters. This definition is used in the `Resolution` and `MaxHKL` functions if cell parameters are not provided as arguments.

Default: {1. 1. 1. 90. 90. 90.}

2.19.2. accFunction



the `real array` of the solvent accessibility penalty parameters (as described in Batalov and Abagyan, 1999).

It contains the values of *a*, *b*, *c* and *E* damping parameters for aminoacid substitution scores. Generally, if a residue is completely buried (*Area=0)*, its substitution scores will be used without changes. If it is completely exposed, its substitution scores will be multiplied by the minimal possible value of *a*. Between these cases the substitution scores are modulated by a smooth ("arctangent") function with a saddle point at *Area=c*, where the slope will be −*b*. The fourth parameter is reserved for development.

This definition is effectively implemented in the `Align`(*seq_1 seq_2* `area`) }, `Score` functions and `find database` command.

Default: {0.33 2.35 0.211, −15.0}.

See also: `alignMethod` .

2.19.3. gapFunction

the `real array` of the gap penalty parameters, which represent a piecewise−linear concave function (as described in Batalov and Abagyan, 1999).

ATTENTION: at the present time this `gapFunction` is only active when `alignMethod` =2.

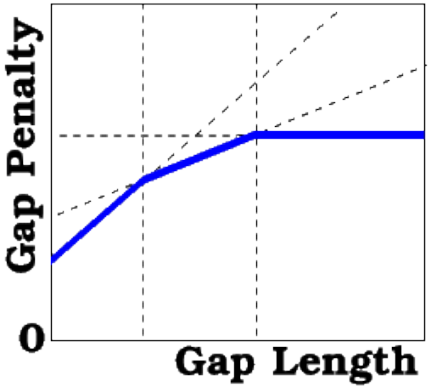
The first two values replace `gapOpen` and `gapExtension` traditional values. If present, the third element of the array represents the length of the gap, starting at which further `gapExtensions` become equal to the fourth element of the array. Likewise, if more elements are present, they represent pairs of the threshold lengths of the gap and the new **gapExtensions** values. For example,

```
gapFunction = {2.4 0.15 10. 0.05 20. 0.}
```

means that

- gap penalty=2.25+0.15*L for L={ 0..10} (and for L=1 it is 2.4= `gapOpen`),

- gap penalty=3.25+0.05*L for L={11..20} and
- gap penalty=4.25 for L>20



The calculations are fastest for the traditional two−element `gapFunction.` The three− or four−element `gapFunction` invokes the optimized routines and is 50−70% slower. The general kind `gapFunction` costs approximately 70−90% additional time for every pair of `gapFunction` values. If the last `gapExtension` is zero, it may be omitted. This definition is effectively implemented in the `Align` , `Score` functions and `find database` search command.

Default: {2.4 0.15}.

Recommended (put it in your `_startup` file): gapFunction = {2.4 0.15 10.}

This set will produce fast and structure−like alignments.

See also `alignMethod`, and `accFunction` (the accessibility attenuation parameters).

2.19.4. I_out

an `integer array` in which the output of some commands is stored.

2.19.5. M_out

`matrix` in which the output of some commands is stored.

2.19.6. R_out

`real array` in which the output of some commands is stored.

2.19.7. S_out

`string array` in which the output of some commands is stored.

2.19.8. swissFields

`string array` of SWISS−PROT fields to be read by default in `read sequence swiss`

2.19.9. readMolNames

`string array` in which the SDF−file comment fields containing database compound identifier and description are preset. There is a standard place where database compound identifier should be stored in SDF (MOL)−files. This is the first line of the entry. However most of the database providers got used to leaving this line empty. Instead they put identifier and description in the end of the file in the following fashion:

```
...
M  END
> <CAT_NO>
R150002

> <NAME>
(5−OXO−HEXAHYDRO−PYRANO[3,2−B]PYRROL−1−YL)−ACETIC ACID METHYL ESTER

$$$$
```

In this particular case before using such database set

```
readMolNames = {"<CAT_NO>" "<NAME>"} # useful for Sigma−Aldrich files
```

Another example:

```
readMolNames = {"<CODE>" "<IUPAC_NAME>"} # useful for ACD database
```

2.19.10. Named Atom/Residue/Molecule/Object Selections

Examples:

```
cc = a_//ca                 # created named selection variable cc
show cc a_/3:15           # use it in the expression
```

In this case the named selection **cc** is a true ICM−shell variable, not just an alias for the Ca selection. Please do not confuse it with another useful mechanism which allows you to use a **string** in a selection. This mechanism is used in scripts and macros.

Example:

```
cc = "a_//ca"      # in this case cc is a string, not a selection
show $cc a_/3:15 # $cc is replaced by a_//ca before parsing
```

2.19.11. as_out

an atom/residue/molecule/object `selection` variable where some commands or functions store their output:

- `Rmsd`
- `Srmsd`
- `superimpose`
- `set tether`

- `show drestraint`
- `show tethers`

If atoms a_1./3/ca,c,n relate to atoms a_2./45/ca,c,n, then the first set will end up in `as_out` and the second in `as2_out.`

2.19.12. as2_out

the second set of atoms (`selection`) returned by the following commands and functions:

- `Rmsd`
- `Srmsd`
- `superimpose`
- `set tether`
- `show drestraint`
- `show tethers`

See also `as_out` above.

2.19.13. Named Selections of Internal Variables (Dihedrals, Angles and Bonds)

2.19.14. vs_out

The variable selection where some commands or functions store their output:

- `read variable` saves a selection of loaded variables;

2.20. Commands

2.20.1. add/insert table rows.

`add` *T_ i_row* [*row_selection*]

add/insert rows to table *T_* after position *i_row* (0 if you need to insert the first line). If the 3rd argument is not provided, adds an empty row. The *row_selection* can contain rows from the *same* table or from a *different* table with matching column structure. In the latter case, the columns can be named differently, but the number of columns and their types must match (see example below). The defaults for an empty line are empty string or zero value for strings or numbers, respectively.

Examples:

```
group table t {1 2 3} "a" {"b","d","e"} "b"
show t
 #>T t
 #>-a----------b----------
    1          b
    2          d
    3          e
```

```
add t 0 # insert empty line before 1st
show t
 #>T t
 #>-a----------b----------
    0          ""
    1          b
    2          d
    3          e

group table t {1 2 3} "a" {"b","d","e"} "b" # redo the table
add t 2 t[1]  # insert a duplicate of 1st row after the 2nd
 #>T t
 #>-a----------b----------
    1          b
    2          d
    1          b
    3          e

group table t {1 2 3}  "a"  {"b","d","e"} "b"  # redo the table
group table tt {1 2 3} "aa" {"b","d","e"} "bb" # another table
# column names are different, but the structure is the same
add t 2 tt[1:2]  # or add t 2 tt.aa<3
show t
 #>T t
 #>-a----------b----------
    1          b
    2          d
    1          b
    2          d
    3          e
```

2.20.2. alias

`alias` *abbreviation word1 word2 ...*

create alias

`alias delete` *abbreviation*

delete alias

It is important that the abbreviation is not used in the ICM−shell. The same names can not be given later to ICM−shell objects.

Alias may contain arguments $0, $1, $2, etc. ICM−shell will pick space−separated words following the alias name and substitute $1, $2, etc. arguments by the specified argument. $0 stands for all the arguments after the alias name.

Examples:

```
 alias seq sequence                    # seq will invoke sequence
 alias delete seq                      # delete alias name seq
 alias dsb display a_//ca,c,n          # abbreviate several words to
                                       # reduce typing efforts
```

```
                                        # aliases with arguments
alias NORM ($1-Mean($1))/Rmsd($1)
show NORM {6,7,8,4,6,5,6,7,5,6}         # make sure there is no space
```

2.20.3. align

align number: renumber residues sequentially

`align number` *rs_residuesToBeRenumbered* [*i_firstNumber*]

`align number` *ms_chainsToBeRenumbered* [*i_firstNumber*]

renumber selected residues, or residues in selected molecules or objects sequentially in all of them from starting one or the specified first number. May be useful to deal with messy numbering in some pdb−files. Example:

```
read pdb "1crn"
align number a_1            # renumber all res. 1 to N
align number a_1/10:20 101  # just the selected residues from 101
align number a_1       101  # renumber all res. 101 to 100+N
```

`align number` *ms_chainsToBeRenumbered seq_master* [*i_offset*]
renumber the residues of the selected molecule according to *seq_master* master sequence which is aligned to the sequence of the selected chain. The alignment (pairwise or multiple) need to be linked to the molecule/chain and both the chain sequence and the master sequence need to be covered by the alignment. The molecular sequence can be generated with the `make sequence` [*ms_chainsToBeRenumbered*] command. The can be either aligned anew the the master sequence with the `Align` function or appended to a multiple sequence alignment using alignment projection.

This command may be useful in cases in which a structural model does not represent the entire sequence because of omitted loops, N− and C− termini, while you still want to keep the numbering according to the full master sequence. You might want to use the command also on models by homology generated with the `build model` command.

Example:

```
seqmaster = Sequence("ACDEFGHIKLMNPQRST")
buildpep             "--DEFGH-----PQRST"  # dashes are skipped
make sequence a_1 name="seqmodel"         # sequence is auto-linked
a = Align(seqmodel,seqmaster)             # linked alignment
align number a_1 seqmaster
# Info> residues of a_def.m renumbered by sequence 'seqmaster' from alignment 'a'
display residue label
```

align: ICM multiple alignment algorithm

`align ali_SequenceGroupName` [`tree=` *s_epsFileName*]

make a multiple alignment of specified sequences a sequence group resulting from the `group sequence` *s_groupName* command. For pairwise alignment use the `Align`(*seq1* seq2) function. The algorithm includes the following steps (inspired by corridor discussions with Des Higgins, Toby Gibson and Julie Thompson):

1. align **all** sequence pairs with the ICM ZEGA algorithm, and calculate pairwise `distance`s between each pair of aligned sequence with the Dayhoff formula, e.g. the distance between two identical sequences will be 0. , while the distance between two 30% different sequences will be around 0.5. The distance goes to an arbitrary number of 10. for completely unrelated sequences. The distance matrix $\boldsymbol{D_{ij}}$ can later be extracted from the alignment with the `Distance`(*ali_*) function.
2. build an evolutionary tree from $\boldsymbol{D_{ij}}$ with the "neighbor−joining algorithm" of Saitou, N., Nei, M. (1987) to determine the order of the alignment and calculate relative weights of sequences and profiles from the branch lengths. The tree will be saved in the file defined by the `tree` option (aligTree.eps file by default). The so−called `Newick tree` description `string` will be saved in `s_out` .
3. traverse the tree from top to bottom, aligning the closest sequences, sequence and profile or two profiles. After each Needleman and Wunsch alignment, build the profile.
4. generate the final neighbor−joining evolutionary tree and write the PostScript file with the tree to disk.

Examples:

```
read sequences s_icmhome+"zincFinger"
list sequences               # see them, then ...
group sequence alZnFing      # group them, then ...
align alZnFing               # align them, then ...
unix gs aligTree.eps         # ... evolutionary tree ready
                             # (gs is a PostScript previewer)
```

EST,DNA alignment and assembly

`align new` *ali_sequenceGroup* [*seq_seed*]

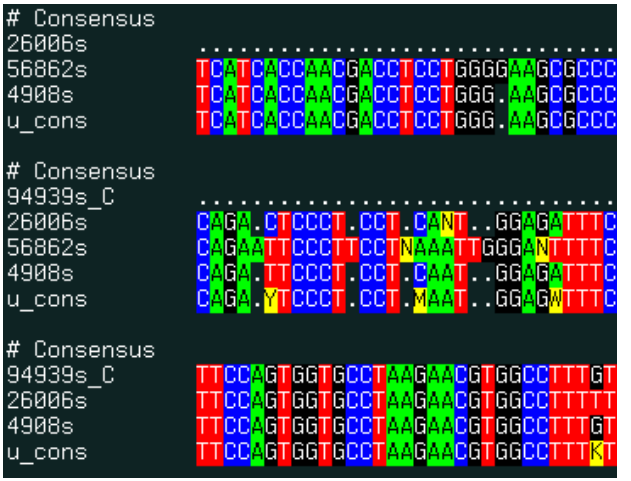
multiple alignment of ESTs and genomic DNA and consensus derivation. This command uses the external the sim4 program to generate pairwise alignments between expressed DNA sequence and a genomic sequence. The sim4 program can be downloaded from the `http://globin.cse.psu.edu/globin/html/docs/sim4.html` site.

The procedure has the following steps:

- sequences are sorted by length
- the longest sequence is chosen as the seed sequence unless it is explicitly provided
- the longest sequence from the remaining set is aligned to the seed sequence using the external `sim4` program.
- the output of this program is parsed and translated into the icm alignment
- the **consensus** sequence is created and becomes the master sequence
- the procedure is repeated until all the sequences are processed

- the multiple sequence alignment is further cleaned to compress spurious gaps when possible. This cleaning makes the consensus much more compact.

The result of this command is best displayed with the `show color` *`ali_`* command.



An example:

```
read sequence "http://www.ncbi.nlm.nih.gov/UniGene/" + \
    "download.cgi?ID=5198/tt> #
read sequence "../Hs5198"
group sequence unique u # squeeze out obvious redundancies and form group 'u'
align new u             # form multiple alignment and build consensus
show color u
```

See also:

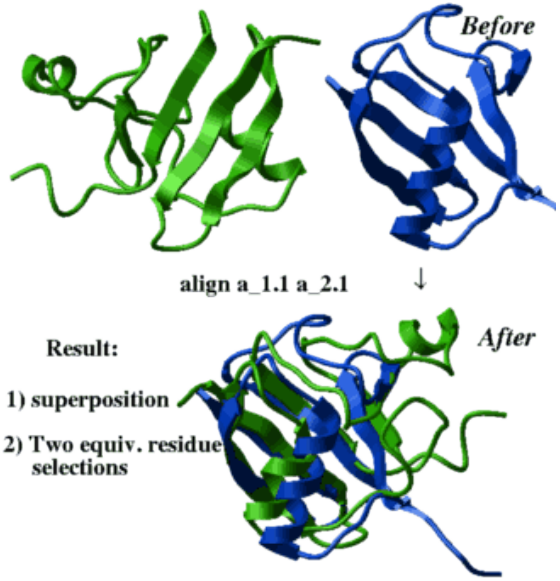
- `filtering, group sequence unique=".."`
- `Trans` ()
- show [color] *ali_*

align two molecules by their backbone topology

`align` [`distance`] *ms_1 ms_2* [`i_windowSize=`15] [`r_seqWeight=`0.5]

This command finds the residue *alignment* (or residue−to−residue correspondence) for two arbitrary molecules having superimposable parts of the backbone conformations. The structural alignment identification and optimal superposition is primarily based on the C−alpha−atom coordinates, but the sequence information can be added with a certain weight (the default value of *r_seqWeight* is 0.5 which was found optimal on a benchmark). The structural alignment algorithm is based on the ZEGA (zero−end−gap−alignment) dynamic programming

procedure in which substitution scores for each i,j−pair of residues contain two terms:



- structural similarity in a *i_windowSize* window between two fragments surrounding residues i and j, respectively. This similarity is calculated as local `Rmsd` of the residue label atoms (these atoms are C−alpha atoms by default but can be reset to other atoms with the `set label` command, e.g. `set label a_*.//cb`). If the option `distance` is specified the deviation of the interatomic distances between equivalent *pairs* of atoms (so called *distance rmsd*) is calculated instead of a more traditional root−mean square deviation between atom coordinates of equivalent atoms. The latter method is less accurate but an order of magnitude faster.

- sequence similarity (if *r_seqWeight* > 0.). Average local sequence alignment score in the *i_windowSize* window is calculated for i,j−centered pair of fragments. In this sense this sequence similarity is different from the one used in pure sequence alignment (see the `Align` function), in which just the i,j residue pair is evaluated. The default value of *r_seqWeight* of 0.5 is rather mild (about a half of the structural signal).

The output:

- `ali_out` contains structural alignment (if sequences linked to the molecules do not exist, they will be created on the fly). The alignment can be further edited with the interactive alignment `alignment editor`.

- `as_out` contains the residue selection of the aligned residues in the first molecule

- `as2_out` contains the residue selection of the aligned residues in the second molecule

- `M_out` , the matrix of local structural/sequence similarity in a window is retained and can be visualized by:

```
make grob color 10.*M_out name="g_mat # x,y,z scales
display g_mat
# or
plot area M_out display grid link
```

See also:

- `Align`(*seq_1 seq_2* `distance|superimpose`). This function creates the first unrefined structural alignment as described above.
- `find alignment` which refines initial structural alignment.

The overall result of the `align` command is equivalent to:

```
a = Align(... superimpose )  # superposition/RMSD based local str. alignment
a = Align(... distance    )  # distance RMSD based local str. alignment

find a superimpose 4.0 0.5
```

Example:

```
read object s_xpdbDir + "/1brl.b/"
read object s_xpdbDir+"/1nfp"
rm a_*.!A
display a_*.//ca,c,n
color molecule a_*.
align a_2.1 a_1.1
center
show String(as_out) String(as2_out)
color red as_out
color blue as2_out
show ali_out
```

align heavy command for multiple alternative structural alignments.

`align heavy` *rs_1 rs_2* [*r_rmsd*] [*i_windowSize* [*i_minFragment*]] [*r_elongationWeight*]

This method, as opposed to the default `align ms_1 ms_2` generates many possible solutions and does not depend on sequential order of the secondary structure elements. However, it leads to a combinatorial explosion and is intrinsically less stable computationally, and generally requires more time. The command finds the optimal 3D superposition between two arbitrary molecules/fragments (two residue selections *rs_1* and *rs_2*).

The procedure generates structural fragments of certain initial length and superimposes all of them to calculate the structural similarity distance. Then the "islands" of similarity are merged into larger pieces. This process is controlled by the following arguments: *i_windowSize* is the residue length of structural fragments for the initial fragment superposition. Fragment pairs with the rms deviation less than *r_rmsd* are then combined, giving composite solutions of total residue length larger than *i_minFragment.* Acception or rejection of the composite solutions is governed by the following score (the smaller, the better)

score = rmsd − (1.37 + Sqrt(1.16 * length − 15.1)), length >= 14

If ***length>14*** , we use linear extrapolation of the score dependence:

score = rmsd − (1.37 + 1.068*(length−13))

The score is required to be less than *r_rmsd.* Practically, for longer fragments one can find much larger RMS deviations according to the length correction of the score.

Defaults:

- *r_rmsd* = 1. A
- *i_windowSize* = 15 residues
- *i_minFragment = i_windowSize*
- *r_elongationWeight=0.1*

There may be several different reasonable solutions. All the solutions are sorted, shown and stored in the memory. The two output selections `as_out` and `as2_out` contain the best scoring solution. Any solution can be `load`ed and displayed. Additionally, a residue alignment is created for each solution. The decision about which residues are aligned is based on the overall score described above for the of combined fragments.

See also: How to optimally superimpose without the residue alignment

Example:

```
read pdb "4fxc"
read pdb "1ubq"
display a_*.//ca,c,n
color molecule a_*.
align heavy a_1.1 a_2.1 12 1.5 .1
center
load solution 2            # load the second best solution
color red  as_out
color blue as2_out
for i=1,10
  load solution i
  color molecule a_*.
  color red  as_out
  color blue as2_out
  pause                     # rotate and hit 'return'

endfor
```

Note. Increase *i_minFragment* parameter (12 in the above example) to something like 20 if the program hangs for too long. Interrupt execution with the ICM−interrupt (**Ctrl** \) if you want only the top solutions.

2.20.4. append two tables by share column

`append` t1.A t2.B

Append rows of table *t2* to table *t1* by rows corresponding to unique column *t2.B* . The *t1.A* column values do not need to be unique.

```
group table people {"J","C","M"} "p" {"MS","MS","MS"} "orgid"
group table orgs  {"MS"} "id" {"Molsoft"} "name"
append people.orgid orgs.id
```

```
people
 #>T people
 #>-p----------orgid-------name-------
    J           MS          Molsoft
    C           MS          Molsoft
    M           MS          Molsoft
```

2.20.5. assign

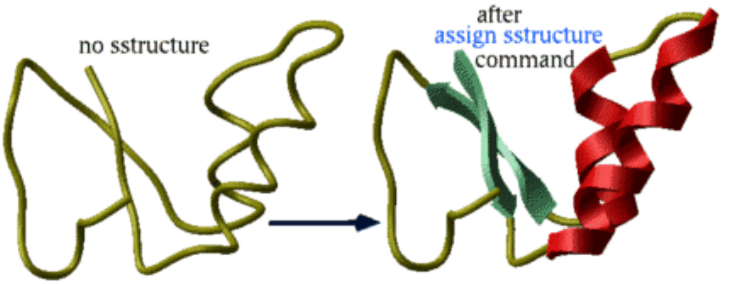
assign sstructure: derive secondary structure from a pattern of hydrogen bonds

`assign sstructure` *rs_* [{ *s_SecondaryStructTypeCharacter* | *s_SSstring* }]

Manual assignment of a desired secondary structure annotation to a residue fragment

assign specified secondary structure to the selected residues `rs_` , e.g.

```
read pdb "1est"
assign sstructure a_/* "_"  # make everything look like a coil
cool a_
assign sstructure a_/1:10 "HHHH_EEEEE"
cool a_
```



This command does not change the geometry of the model, it only formally assigns secondary structure symbols to residues.

Note: to **change the conformation** of the selected residue fragment, according to a desired secondary string, use the ICM −object and the `set` command applied to both sequences and molecular objects.

Automated derivation and assignment of secondary structure from atomic coordinates

`assign sstructure` *rs_*

If the secondary structure string is not specified, apply ICM modification of the DSSP algorithm of automatic secondary structure assignment `(Kabsch and Sander, 1983)` based on the observed pattern of hydrogen bonds in a three dimensional structure.

The DSSP algorithm in its original form overassigns the helical regions. For example, in the structure of T4 lysozyme (PDB code **103l**) DSSP assigns to one helix the whole region a_/93:112 which actually consists of two helices a_/93:105 and a_/108:112 forming a sharp angle of 64 degrees. ICM employs a modified algorithm which patches the above problem of the original DSSP algorithm. Assigned secondary structure types are the following: "H" − alpha helix, "G" − 3/10 helix, "I" − pi helix, "E" − beta strand, "B" − beta−bridge, "_" or "C" − coil.

Examples:

```
nice "1est"       # notice that many loops look like beta-strands
assign sstructure # now the problem is fixed
cool a_
```

See the `set rs_ s_SecStructPattern` command to actually set new phi, psi angles to a peptide backbone according to the string of secondary structure.

assign sstructure segment

`assign sstructure segment` [*ms_molecules*]

create simplified description of protein topology (referred to as `segment` representation). Segments shorter than `segMinLength` are ignored. The `current object` is the default.

See also `show segment`, `ribbonStyle`, `display ribbon`.

2.20.6. break

is one of the `ICM flow control` statements. It permits a loop (e.g. `for` or `while`) to be `broken` before calculations have completed.

Examples:

```
  for i = 1, 8
    print "Now i = ", i, "and it goes up"
    if (i == 4) then
      print "... but at i=4 it breaks, Ouch!"
      break
    endif
  endfor
```

See also `goto.`

2.20.7. build

The build family of functions allows to create molecular objects

- from sequence file (`build s_seqfile`)
- from sequence string (`build string`)
- from a linear chemical notation (`build smiles`)
- from a sequence and a template *by homology* (`build model`)

It also adds implied hydrogens (`build hydrogen`) to a molecule and to find a loop in a database (`build loop`)

build from sequence file

`build` [*s_IcmSeqFileName*] [`library=` { *s_libFile* | *S_libFiles*}] [`delete`]

reads *s_IcmSeqFileName.se* `ICM-sequence file` and builds an ICM molecular object. This sequence file is different from a simple sequence file and contains three (sometimes four) character residue names

defined in the `icm.res` residue library file (try `show residue types` to see the list). Use macro `buildpep` if you want to build an object from a string with one letter coded sequences or a named sequence (see the `build string` command below). The `buildpep` macro also allows to easily create several molecules by using a semicolon `;` separator. To get a D−amino acid instead of L−ones simply use D as a prefix: `Dala Darg.` Specify N− or C−terminal modifiers directly in the file if needed. The build command will create them in some default conformation (extended backbone with different molecules oriented around the origin as a bunch of flowers). Several molecules can be specified in the ICM sequence file.

Residue names can contain numbers (i.e. 4me). However, the residue numbers with a modification character, such as 44a, 44b should contain a slash before the modification character (i.e. 44/a , 44/b). An example in which we create a sequence of residues ala and 4me with numbers 2a and 2b, respectively: "se 2a ala 2b 4me".

Option `library=` lets you temporarily switch the library file. It can also be done by redefining the `LIBRARY.res` array of the `LIBRARY` table.

Option `delete` temporarily sets the `l_confirm` flag to `no` and the old object with the same name gets overwritten.

Examples:

```
 build          # def.se file
 build "alpha"  # alpha.se file
 build "wierd" library="mod.res"  # get residues from mod.res
#
 LIBRARY.res = {"icm","./myres"}
 build "a"
```

Use a convenient macro `buildpep` to build one or several−chain peptides with one− or three− letter code. E.g.

```
 buildpep "ASFGDH;FFF"  # two molecules
 buildpep "ala his trp" # one chain of three residues
```

build model by homology

`build model` *seq_1 seq_2 ... ms_Templates ...* [*ali_1 ...*] [`margin=` { i_maxLoopLength, i_maxNterm, i_maxCterm, *i_expandGaps* }

build a comparative model (homology model) of the input sequences based on the similarity to the given molecular objects. The margin arguments:

name	default	description
i_maxLoopLength	999	longer loops are dropped
i_maxNterm	1	the maximal length of the N−terminal model sequence which extends beyond the template
i_maxCterm	1	the maximal length of the C−terminal model sequence which extends beyond the template
i_expandGaps	1	additional widening of the gaps in the alignment. End gaps are not expanded

Possible modes:

- simple one−to−one mode: build model seq_1 [ms_1] [ali_1]
- N sequences − N corresponding molecules: build model seq_1 seq_2 .. seq_N ms_1,2,..N

Example:

```
 l_autoLink = yes
 read pdb "x"
 read alignment "sx"
 build model ly6 a_
 ribbonColorStyle = "alignment" # grey−gaps, magenta−insertions
 display ribbon
#
 read pdb "2ins"  # multichain
 read sequence unix cat
> a
GIVEQCCASV CSLYQLENYC N
> b
VNQHLCGSHL VEALYLVCGE RGFFYTPKA
> c
GIVEQCCASV CSLYQLENYC N
> d
VNQHLCGSHL VEALYLVCGE RGFFYTPKA
^D
 build model  a b c d a_1.
# Now optimize the side chains
 selectMinGrad = 1.5
 set vrestraint a_/*
 montecarlo fast v_/!I/x*
# !I means residues which are not Identical to their template residues
# use  refineModel  to energetically optimize the model
```

The algorithm performs the following steps:

Alignment adjustment: modifies the alignment according to *i_expandGaps*, and prepare a sequence with the ends and the long loops truncated according to the alignment and the { *i_maxLoopLength* , *i_maxNterm* , *i_maxCterm* } parameters.

Building a straight polypeptide from the model sequence: builds a full−atom polypeptide chain for this new sequence. The residues in your model are numbered according to the template and all the inserted loops residues are indexed with 'a','b', etc. E.g. the numbering may look like this: `200,201,203,204,204a,204b,204c,205` ... This numbering allows one to follow more easily the correspondence between the template and the model. If you do not like this numbering scheme, just use the

```
align number a_/*
```

command and the model residues will be renumbered from 1 to the number of residues.

Backbone topology transfer: inherits the backbone conformation from the aligned (but not necessarily identical) parts of the known template

Identical side−chain building: inherits conformations of sidechains identical to their template in the alignment

Non−identical side−chain placement: assigns the most likely rotamer to the side chains not identical in alignment. If you want to do more than that apply:

```
set vrestraint a_/*  # assigns the rotamer probabilities
montecarlo fast v_/Cx/x* # x* selects for all chi (xi) angles
```

You can also manually re−optimize any side chains either interactively (right−mouse click on a residue atom, then select Shake Amino−Acid Side−Chain) or from a script, e.g. for residue 14:

```
set vrestraint a_/*  # assigns the rotamer probabilities
montecarlo v_/14/x*
ssearch v_/14/x*     # systematic conformational search for the 14−th sidechain
```

Loop searches:

searches the `icm.lps` which may contain entire PDB−database for suitable loops with matching loop ends and as close loop sequence as possible, inserts them into the model and modifies the side−chains according to the model sequence.

The loop file can be easily customized, updated and rebuilt with the `write model [append]` command in a loop over protein structures. To use your custom loop file, redefine the `LIBRARY.lps` variable.

Loop refinement and storing alternatives:

adjusts the best loops found and keeps a stack of loop alternatives which can later be tested (see the Homology gui−menu)

The output

The build model command returns the following variables:

`LoopTable` master table containing list of all the loops, their conformation in alphanumeric code, a measure of the deviation of the database loop ends and the model attachment sites, the loop length and the numerical conformation type (not really important). E.g.

```
#>T LoopTable
#>−1_Loop−−−−−−2_Conf−−−−−−3_Rmsd−−−−−−4_Nof−−−−−−−5_Type−−−−−
   a_ly6.a/7:10 31R21       0.1         11          1
   a_ly6.a/60:63 1RRR32      0.1         8           1
   a_ly6.a/43:46 211331RRRR  0.240658    4           1
```

Individual loop tables

Tables called `LOOP1` , `LOOP2` , etc. for each inserted loop. The tables contain the coded conformational string, relative energy, the position of the offset in the structure database file (`offset`) to be able to extract this loop again, and the `rmsd` of the loop ends. Example:

```
icm/ly6> LOOP1
#>T LOOP1
#>−Conf−−−−−−−−energy−−−−−−offset−−−−−−rmsd−−−−−−−
   31R21       0.          3623594     0.092104
```

```
31RR2       1.519275    3427772     0.083372
R1121       1.612712    3750108     0.097777
R1R32       1.639177    1529882     0.087113
R1RR2       1.880638    3806768     0.079335
31R32       3.714823    4561270     0.053853
R3RR2       4.531406    4003324     0.042881
```

Writing and restoring the tethers

You can write both template and the model and the tethers between them to files (see section write tethers .

Trouble shooting

`build model` may crash. A possible reason of the crash is that the pdb file is not correctly parsed due to formatting errors. Many pdb files still have formatting errors, especially those which are generated by other programs or prepared manually. In this case the `read pdb` command is trying to interpret the field shifts and, as with any guess work, frequently gets it wrong. For example, try `2ins` and you will see that the atom or residue names are shifted. To fix the problem, try to use the `exact` option of the `read pdb` command.

build loop to a model by homology

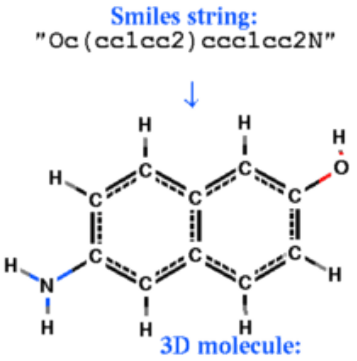
`build loop` *rs_fragments*

rebuild specified loop based in a PDB−database search (see `build model`).

An example:

```
read object s_icmhome+"crn"
build loop a_/20:26  # rebuild this loop
```

`build` [`smiles` | `sln`] *s_smiles_or_sln* [`name=` *s_ObjName*]



create an ICM−object from the `smiles−string` or `sln−string`, respectively.

Set `l_readMolArom` to `no` if you do not want to assign aromatic rings from a pattern of single and double bonds (and formal charge and bond symmetrization for CO2, SO2, NO2or3, PO3) upon building. To suppress suppress the symmetrization and consequential charging of CO2, set the `l_neutralAcids` flag to `yes` .

Examples:

```
  build smiles "CCO"   # ethanol

  build smiles "Oc(cc1cc2)ccc1cc2N"

  build smiles "Oc(cc1cc2)cc(ccc3)c1c3c2"

                # dicoronene
  build smiles "c1c2ccc3ccc4c5c6c(ccc7c6c(c2c35)c2c1c1c3c5c6c"+\
               "(c1)ccc1c6c6c(cc1)ccc1ccc(c5c61)cc3c2c7)cc4"

                # NAD
  build smiles "[O-]P(=O)(OCC1OC(C(O)C1O)N1C=2N=CN=C(N)C=2N=C1)"+\
               "OP(=O)([O-])OCC1OC(C(O)C1O)N=1C=CC=C(C=1)C(=O)N"

                # Hexabenzo(bc,ef,hi,kl,no,qr)coronene
  build smiles "c1c2c3c4c(ccc3)c3c5c(c6c7c(ccc6)c6c8c(ccc6)c6c9"+\
               "c(ccc6)c(cc1)c2c1c9c8c7c5c41)ccc3"

                # rubrene
  build smiles "c1c2c(c3ccccc3)c3c(c(c4ccccc4)c4c(cccc4)c3c3ccccc3)"+\
               "c(c2ccc1)c1ccccc1"
```

Usually the build smiles command is not sufficient. The molecule needs to be optimized in the mmff force field and several conformations need to be sampled. The quick way of doing it is shown below.

```
 build smiles "CC=1C(=O)C=CC(C=1)=O"
 strip a_
 build hydrogen
 set type mmff
 set charge mmff
 convert
 read library mmff
 tolGrad = 0.001
 ffMethod = "mmff"
 minimize cartesian
```

A more rigorous way of doing the conversion is done with this macro:

```
macro scan2Dto3Dconvert
  oldGrad = tolGrad
  tolGrad = 0.0001
  ffMethod = "mmff"
  vwMethod = "soft"
  unfix V_//a* !V_//avt*
  v =  Value( v_//a* !V_//avt* )
  m = Matrix( Nof( v) 2 )
  m[?,1] = v
  m[?,2] = Rarray( Nof( v) 170. )
  v = Min (Transpose( m ) )
  set v_//a* !V_//avt* v
  delete m v
  fix V_//a* !V_//avt*
  delete stack
  store conf 1
  for i=2,5
    load conf 1
    randomize a_// 0.03
    randomize v_//
```

```
    store conf i
  endfor
  minimize stack "vw,14,to,hb"
  errorAction = "none" # avoid crashing on cartesian min.
  minimize cartesian stack 3000 "vw,14,to,hb,bb,bs,af"
  if(!Error()) then
    load conf 0
  else
    load conf 1 # try to restore a good conformation
  endif
  vwMethod = "exact"
  minimize cartesian 3000 "vw,14,to,hb,el,bb,bs,af"
  if(Error()) print "ERROR> 2Dto3D failed"
  errorAction = "break"
  delete stack
  tolGrad = oldGrad
  randomize a_//* 0.01
endmacro
```

See also the `Smiles` function and the `find molecule s_Smiles1 S_Smiles2` command to find a substructure

build object from string

`build string` *s_IcmSequence* [`name=` *s_ObjName*] [`delete`]

create an ICM−object from a *s_IcmSequence* string (see the `build` command above). To get a D−amino acid instead of L−ones simply use D as a prefix: Dala Darg. Specify N− or C−terminal modifiers directly in the file if needed. The build command will create them in some default conformation.

Option `delete` temporarily sets the `l_confirm` flag to `no` and the old object with the same name gets overwritten.

Examples:

```
   build string "se nh3+ ala his coo−" name="pep"  # one peptide named a_pep.
   build string "ml a \nse nh3+ his coo− \nml b \nse trp" # molecules a and b
   build string IcmSequence("GHFDSFSDRT","nter","cooh") # translate and add termini
#
# Using alias  BS   build string "se $0"
   BS ala his trp
#
# Using alias  BSS  build string IcmSequence( $0 )
   BSS "SFGDFAGSFG"   # quoted one−letter code string
   read sequence "GTPA_HUMAN.seq"
   BSS GTPA_HUMAN     # sequence name
```

build hydrogens according to topology and formal charges.

`build hydrogen` [*as_heavyAtoms*] [*i_forcedNofHydrogens*]

add hydrogens to the specified heavy atoms according to their type and `formal charge`. All heavy atoms of the current object are used by default. If your have hydrogens already and their configuration is wrong, you can delete them with the `delete hydrogen` command. The number of hydrogens may be

enforced if the optional *i_forcedNofHydrogens* argument is specified. See also the `set bond type` command.

Examples:

```
read mol2 s_icmhome+ "ex_mol2"  # several small molecules
display a_4.
build hydrogen a_4.  # added and displayed
```

2.20.8. call icm script

`call` *s_ScriptFileName* [`only`]

invokes and executes an ICM−script file. End the script with the `quit` command, unless you want to continue to work interactively, or use it in other script.

Option `only` allows you to suppress opening the script file if the `call` command is inside a block which is not executed. By default the script file is opened and loaded into the ICM history stack anyway, but the commands from the file are not executed.

The absolute path of the script can be return by the `Path` (`last`) function.

Calling scripts inside conditional expressions.

Examples:

```
call _startup             # execute commands from _startup file


if Version() !~ "* R *" goto skip:    # Rebel is not licensed
  call _rebel only  # only means do not read _rebel if skipped.
skip:
```

2.20.9. center

`center` [{ *as_* | *grob* }] [`only`] [`static`] [`margin=` *r_margin*]

centers and zooms the screen on selected atoms *as_* or graphics objects. Default objects: all existing atoms and graphics objects. The *r_margin* argument is given in Angstrom units and can be used to set a relative size of the selection and the frame. Normally all dimensions of the molecule/grob are taken into account, so that the molecule can be rotated without changing scale.

Options:

- `only` : **do not rescale**, translate only, i.e. move the selected atoms to the center of the graphics window
- `static` : scale only according to the visible X−Y dimensions and the margin. Do not take the Z−dimension into account in the size calculation as if you do not intend to rotate objects. That implies an assumption that the orientation of molecules/grobs/maps will not be changed.

Examples:

```
nice "1est"
center
center Sphere ( a_/15:18 )
center a_/1:2 only  # keep the scale

read grob s_icmhome+"beethoven" # a genius
display g_beethoven smooth
center g_beethoven static   # 10 A margin
```

2.20.10. clear

clear terminal screen (no big deal).

2.20.11. color family of commands

The color command allows you to color different shell objects, their parts, or different graphical representations with by colors specified in various ways.

color: main command

The main color command:

`color` [{ *as_* | *g_grobName* }] [`wire` | `hbond` | `cpk` | `ball` | `stick` | `xstick` | `surface` | `skin` | `site` | `ribbon` [*base*]] [*color_specification*]

The color can be specified as

color_name | *s_ColorName* | color[*i_index*] | *i_Color* | *r_Color* | *I_Color* | *R_Color* | `*rgbr=`R_3rgb [*window = R_MinMax*]

color selected atoms (*as_*) or graphics object(s) according to specified color. The window={minValue,maxValue} option allows to provide a range for color mapping. Example:

```
color ribbon a_/ Bfactor(a_/ simple) window=-0.5//2.
```

This command will clamp Bfactor(a_/ simple) values which are normally around zero, but may range from large negative values to large values, to the [−0.5,2.] range.

The defaults:

- objects: the current object (`a_`) only (to color all objects, use `a_*.`)
- graphic representation: all except ribbon. To color `ribbon` specify use `color ribbon`
- color: the default coloring (atoms − by atom type, which can be changed in the `icm.clr` file; `ribbon` − by secondary structure)

Examples of how the defaults work:

```
nice "1crn"
display       # also displays wire
```

```
color         # all except ribbon colored by atom type
color ribbon  # only ribbon of a_ by secondary structure type
color ribbon red         # only ribbon as specified
color a_1,2. ribbon red  # only ribbon as specified
```

color_name. Color may be just a word (such as black, white, grey, blue, red, yellow, green, orange, magenta, ...) or string (as "green"), or integer (convenient for automatic coloring within ICM loops), or integer array, or real array (to color according to a certain property, as electric charge or Bfactor). Default: color by atom type; in ribbon representation by secondary structure type.

In DNA and RNA ribbons, bases can be colored separately (e.g. `color ribbon base a_1/* white`), the default coloring being A−red, C−cyan, G−blue, T or U−gold. Colors themselves and all the defaults may be changed in the `icm.clr` file. Different color specifications with examples:

color `red` unquoted color name

color `"red"` quoted color name or a string variable

color `color[4]` use color number 4 from the list of "**named**" colors (first section of the `icm.clr` file). You can show the colors with their numbers by the `show color` command and their total number is accessible via the `Nof( color)` function. This mode is useful if you need to color selected elements with contrasting colors rather than with a smooth spectrum.

Example:

```
display a__crn.             # load and display molecule
show colors
color a_/1:5/* color[89]
for i=1,Nof(a_/*)
 color a_/$i color[i]       # gay coloring
endfor
```

color 3 (integer) color number from the "**rainbow**" section of the `icm.clr` file. Currently there are 128 colors (i=0,127) in this section and they form a smooth transition from blue to red via white (not really a rainbow). You may change the "rainbow" colors in the icm.clr file. Number 128 becomes blue again. Execute these lines to see how it goes:

```
display "Colors"
for i=1,255
  color background i
  print i
endfor
```

color `4.5` (real) similar to the previous type. The color is interpolated. 4.5 will be the average between the "rainbow color" 4 and "rainbow color" 5.

`color` *selection* `{1,3,5}` or `color` *selection* `{1.,3.,5.}` color each element of the selection by `I_Color` or `R_Color`. The scale is determined by the minimal and the maximal elements of the array, independently of the array length. First the numbers in the array are scaled so that its minimum corresponds to the first color in the "rainbow" section and its maximum to the last color. Then the scaled numbers are applied sequentially to the elements of the selection. If the number of elements in the array is shorter than the number of elements in the selection, the array is applied periodically. In the opposite situation the

excessive numbers are not used for coloring but (attention!) they will be used for scaling. Therefore, if you want to influence scaling you may append extremes to the color−property array. See also: `GRAPHICS.rainbowBarStyle` which determines if and where the color bar will appear.

Example:

```
display a__crn.             # load and display molecule
cc=Charge(a_//*)//{−1.,1.}  # add explicit min. and max. charges
color a_//* cc
```

color `rgb={0.2 0.5 0.1}` find the closest color with the following rgb components.

color `rgb="ff0000"` string representation of rgb color (like in html), each of the three colors (red,green,blue) is defined by **two** characters in hexadecimal form.

color background

`color background` [*Color* | *s_Color* | *i_Color*] colors the background to the specified color.

Examples:

```
buildpep "ASDWER"     # hexapeptide
color a_/1:4 green    # the first four residues in green
color                 # return to default colors by atom type

                      # load, display crambin from the PDB file 1crn
display a__1crn. only
                      # color atoms according to their B−factor
color a_1crn.//* Bfactor(a_1crn.//*)
                      # crambin's ribbon
                      # from blue N−term to red C−term gradually
display a_/* ribbon only
color a_/* Rarray(Count(1 Nof(a_/* ))) ribbon

                      # another crambin's ribbon
                      # from blue N−term to red C−term gradually
color background blue
                      # thick worm representation
assign sstructure a_/* "_"
GRAPHICS.wormRadius= 0.9
display a_/* ribbon only
color a_/* Count(1 Nof(a_/* )) ribbon
```

color by alignment

`color` *selection* [`wire` |`cpk` |`skin` |`ribbon` |`xstick` |`ball` |`stick` |`surface` ..] `alignment`

color specified graphics representations of the selected residues by the colors of an alignment as you see it in the alignment window of the Graphics User Interface. The color of a residue is controled by the following factors:

- residue type
- consensus character at the residue position in the alignment

- colors as provided by the `CONSENSUSCOLOR` table.

Note that the CONSENSUSCOLOR table can be divided into sub−sections, and the active subsection can be selected from GUI.

Example:

```
read sequence s_icmhome+"sh3"
nice "1fyn"
make sequence a_1  # extract 1st sequence
group sequence sh3
align sh3

color a_1 ribbon alignment
display skin white a_1 a_1
color a_1 alignment   # colors all representations including skin
```

color cursor

`color cursor` [*colorName*]

colors the residue cursor which can be displayed with the `display cursor` *rs_* [*colorName*] command.

Example:

```
nice "1crn"
display cursor a_/21  # use arrows to move the res. cursor
color cursor blue
```

See also: `display cursor`, `Res( cursor )`

color grob : special ways to color grobs

`color grob unique` : *color grob M_rgbMatrix `color` *grob* `map` *map_name I_transferFunction R_2mapValueBounds* [*color*] : *color grob *potential [*fast] ms_sourceAtoms [*reverse] `color` *grob as_closeAtoms color*

automatic assignment of different colors to different grobs

`color grob unique`

In addition to the main `color` command which colors grobs there is a special command to automatically assign the displayed `grob`s to different colors. See example for the `split` command.

color grob by matrix of RGB values for each vertex.

`color` *g_grob M_rgbMatrix*

a special command to color `grob`s by colors defined for every vertex by three RGB numbers. This type of matrix is returned by the `Color(` *g_grob)* command. This command allows for gradual disappearance of a

grob into background.

Example:

```
   g = Grob("SPHERE",3.,5)  # a wire sphere
   display g smooth
   color g  Random(Nof(g),3, 0., 1.) # color randomly
   M_colors = Color(g)               # extract current colors
# make the sphere disappear (modern poetry)
   for i=1,20    # shineStyle = "color" makes it disappear completely
     color g (1.-i/20.)*M_colors
   endfor
   for i=20,1,-1 # bring the sphere back
     color g (1.-i/20.)*M_colors
   endfor
```

color grob by proximity to atoms

`color` *grob as_closeAtoms color*

color vertices of the *grob* which are less than `GROB.atomSphereRadius` to any of the selected atoms. The default value for the radius is 4A.

color grob by map: coloring surfaces by 3D scalar field

`color` *grob* `map` *map_Name I_transferFunction R_2mapValueBounds* [*color*]

color vertices of the *grob* by the values of the *map_Name* . The map values at each grid point are first clamped into the *R_2mapValueBounds* range, then this range is divided according to the number of elements in the transfer function and each point is colored according to the value of the transfer function.

The new color will be *mixed* with the current color of grob points. Therefore if you want to color each of 3 RGB channels with a different normalized property value, first color the grob black, and then color with the `red` , `green` , or `blue` color depending on which channel you intend to use. Note that zero in the tranfer function correspond to *no color* . Corresponding grob nodes will not be colored.

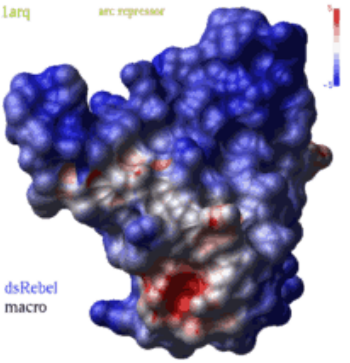
Transfer function is the same to the one in `color map` but has certain differences. This function (e.g. `{0 0 0 1 2 3}`) contains any number of positive integers. 0 means "do not color", and each positive value is a scaling factor for the *color* provided as an argument, or a parameter to select a color from a predefined rainbow. In the above example, the *R_2mapValueBounds* range will be divided into 6 ranges and each value range will be colored accoringly.

Example in which we color the vertices of a grob by inverted values of truncated hydrophobic potential:

```
# create g_pocket
  make map "gs" Sphere( g_pocket )
  compress g_pocket 1.
  color g_pocket black
  color g_pocket map -m_gs { 0,0,0,3,4,5 } { 0. 0.5  } green
  h = Transpose( Color( g_pocket ) )[2]  # extract hydrophobicity
```

color grob potential : coloring grob by electrostatic potential

`color` *grob* `potential` [`fast`] [`reverse` | `simple`] *ms_sourceAtoms*



(REBEL feature) calculates electrostatic potential `waterRadius` away from the surface of the *g_skin* graphics object and color surface elements according to this potential from red to blue. **Important** the location of the center of the water probe is determined by the grob normal (you can change it with the `set g_ reverse` command). If you compute the potential at a blob outside the molecule but with the normals point outwards, use the `reverse` option. To compute potential without any positional correction including normals use the `simple` option.

The potential is calculated either by the REBEL boundary element solution of the Poisson equation, or, if option `fast` is specified, by a simple Coulomb formula with the `dielConstExtern` dielectric constant (78.5 by default).

The local value of potential is clamped to the range [`-maxColorPotential, +maxColorPotential`]. It means that a potential larger than `maxColorPotential` is represented by the same blue color, while values smaller than `maxColorPotential` are represented by the same red color. The real range is reported by the command and you can adjust `maxColorPotential` to cover the whole range. To suppress the absolute maxColorPotential threshold and use auto−scaling instead set `maxColorPotential` to 0. The color bar with values will appear according to the `GRAPHICS.rainbowBarStyle` preference. There are two macros to generate potential−colored skins: `rebel` and `rebelAllAtom`

The second one (given below) considers all the atoms (including hydrogens) with their charges.

The mean value of the potential at the surface is returned in `r_out` , and the root mean square deviation of the potential is return in `r_2out` shell variables, respectively. The averaging is free from bias due to uneven density of grob points. It uses equal size cubes distributed evenly over the surface. The number of representative cubes used for the calculation is return in `i_out` .

Examples:

```
macro rebelAllAtom ms_
  display ms_
  make grob skin ms_ ms_
  make boundary ms_
  color grob potential ms_  # HERE
  display grob smooth
endmacro

read object "crn"
rebelAllAtom a_1
```

See also: `electroMethod`, `make boundary`, `delete boundary`, `show energy "el"`, `Potential( )`.

color label

`color label` [*as_*] [*Color* | *s_Color* | `color` [*integer*] | *i_Color* | *r_Color* | *I_Color* | *R_Color*]

Color labels associated with the selected residues or atoms.

Examples:

```
read object "crn"
display a_//n,ca,c white
display label residue
color label a_/* Count(1 Nof(a_/*))
color label a_/5:10 magenta
```

See also: `display label`, `resLabelStyle.`

color map

`color map` [*s_mapName*] [*I_colorTransferFunction*] [*R2_fromTo*] [`auto`]

color the current or the specified map according to the color transfer function supplied as *I_colorTransferFunction.*

The default: By default the maps are colored in such a way that points with zero map values become transparent while values above and below zero are colored by shades of blue or red, respectively.

The *R2_fromTo* array of two elements allows to set the lower and the upper boundaries for the red and blue colors, respectively. All values above and below will be trimmed to the range. For electrostatic maps the array is set to `{-5.,5.}` by default.

In the `auto` mode all grid points are divided to Nof(*I_colorTransferFunction*) color classes according to the normalized function value (sigma units around the mean value) and each class is colored as specified in the *I_colorTransferFunction* (0 means transparent).

If the number of *I_colorTransferFunction* elements is odd (2* *n+1*) the class boundaries are the following:

- −infinity
- Mean− *n* *sigma,
- Mean−(*n* −1)*sigma,
- Mean−(*n* −2)*sigma,
- ...
- Mean− *1*sigma,*
- Mean
- Mean+ *1*sigma,*
- ...
- Mean+(*n* −1)*sigma,
- Mean+(*n*)*sigma.
- +infinity

For even number of elements (2* *n*), boundaries are shifted by half a sigma, so that the middle class is between Mean−0.5*sigma and Mean+0.5*sigma. Color codes are in arbitrary units since the array is normalized so that the highest value corresponds to the red color. Deep blue is 1. Zero is always the transparent color (no coloring). The spectrum is defined in the `icm.clr` file. Examples of coloring:

- `{0 0 0 0 0,0 0 0 3 10}` default map coloring, color only high densities (blue from 3 to 4 Sigma, red >4 Sigma). Comma only shows you where the mean is.
- `{0 1 0}` color only Mean+− 0.5*sigma nodes, ignore high and low densities.
- `{1 0 2}` color low and high densities by different colors, ignore densities around the mean.
- `{1 2 3 0 5 6 7}` similar the previous one, but with more grades

Example:

```
color map {1 2 0 4 5}
```

color molecule

`color molecule` [*ms_molecules*]

a special command to color the displayed and selected molecules differently. It is a bit tricky (solely for your convenience): if there are both proteins and small "hetero"−molecules (e.g. waters), the colors will not be wasted on little guys. If all the molecules are non−protein (i.e. no residues defined as amino−acids, or a_/A is empty) , than they will be colored differently.

color ribbon

`color ribbon`

color the displayed `ribbon` . See also `base`, `GRAPHICS.dnaBallRadius`, `GRAPHICS.dnaStickRadius`, and other DNA settings in `GRAPHICS.`

color volume

`color volume` [*Color* | *s_Color* | *i_Color*]

determines the color of the `fog` in the depthcueing mode (activated with `Ctrl−D`). For example, if you want that distant parts of you structure are darker (black fog), but the background is sky−blue, you will do the following:

Examples:

```
color background blue
color volume black
```

2.20.12. compare: setting conformation comparison parameters for the montecarlo command

`compare` { *as_* | *vs_* } *options*

The goal of the two following `compare` commands is to provide a desired **setting before the `montecarlo` command** . This command defines a filter which is used to decide how many and what conformations from the stochastic optimization trajectory are kept as low energy representatives of a certain area in conformational space. This metric is also used for the subsequent **stack** manipulations, e.g. `compress stack`.

The `compare` command defines the distance measure between molecular conformations which is used to form a set of different low energy conformers in the course of the stochastic global optimization procedure. The defined distance is compared with the `vicinity` parameter and determines whether two conformations should be considered different or similar (i.e. belonging to the same slot in the conformational stack). The compare command determines the spectrum of conformations that will be retained in the stack, accumulated during a `montecarlo` procedure. The default comparison set is a set of all free torsion variables (see `compare` *vs_*). Other methods compare atom RMSD with and without superposition, and compare only the atoms in the vicinity of a static object (`compare surface`).

compare by deviations of cartesian coordinates

`compare` [`static`] *as_*

The command needs to be run when Cartesian root−mean−square deviation for positions of selected atoms (*as_*) as a distance measure between stack conformations. Set the `vicinity` parameter to about 2.0 Angstrom if you want to consider conformations deviating by more than 2 A as different conformational families.

By default the selected atoms in different conformations will be optimally *superimposed before* the coordinate RMSD is calculated. The `static` option suppresses superposition and measures absolute deviation of the coordinates between conformations. The `static` option is relevant for ligand atoms in docking simulations to a static receptor.

The result of this procedure is that an internal flag is set to perform cartesian RMSD calculations during `montecarlo` run, and a set of selected atoms is marked for comparison.

compare by coordinate deviations of the surface patches only

`compare` [`surface`] *as_*

Similarly to `compare static` *as_* it will look at absolute deviations of coordinates, but the comparison will be applied dynamically only to a **patch subselection** of the atoms in the current object in the `selectSphereRadius` (default 5. A) proximity to the non−current−object atoms of the *as_* selection. The selection typically would look like this: `a_`*activeIcmObject*`.//ca | a_`*staticPdbReceptorObject*`.//ca`

Example:

```
compare a_runObj.//ca | a_recName.//ca surface
```

compare by deviations of internal coordinates/torsions.

`compare` *vs_*

use angular root−mean−square deviation for selected internal variables (usually torsion angles) as distance (set `vicinity` to at least 30.0 degrees accordingly)

Examples:

```
compare v_//phi,psi            # compare ONLY the backbone angles
vicinity=30.0                  # consider two conformations
                               # with phi−psi RMSD < 30. as similar

compare a_2//ca static         # compare Cartesian deviations
                               # of the second molecule's alpha−carbon atoms
                               # without prior optimal superposition
vicinity=3.0                   # consider two conformations with second
                               # molecule deviation < 3 A as similar
```

compare surface: dynamically selecting comparison atoms

`compare surface` *as_currentObjSelection* | as_staticReferenceObject.

dynamically calculates a subset of *as_currentObjSelection* **near** *as_staticReferenceObject* for comparison by static RMSD inside `montecarlo` command.

This is useful for protein−protein docking simulations when you want to measure the `sRmsd` distance between the current conformation and the stack conformations ONLY for the interface residues of the moving molecule. The interface residues are dynamically determined as those which are close to the static receptor specified in the second part of the selection. This static receptor should reside in a separate object.

The *vicinity* size is determined by the `selectSphereRadius` parameter

An example in which we sRmsd−compare only those carbons of barstar which are next to the barnase surface.

```
 read pdb "1bgs"     # a complex
 read pdb "1a19.a/"  # the protein ligand only
 convert
...     # make maps and other actions to prepare protein−protein docking
 compare a_//c* | a_1.1 surface  # will use only
 selectSphereRadius = 7.
...
 montecarlo
```

2.20.13. compress

compress grobs or stacks

`compress` *g_grobName1 g_grobName2* .. [`r_minimalEdgeLength=`.5] : *compress *grob [*selection] [r_minimalEdgeLength=.5]

simplify a grob by eliminating/merging small triangles into bigger ones. This procedure allows to generate very "low−resolution" molecular surfaces. The default value of the *r_minimalEdgeLength* is 0.5 Angstroms. Typically compression with the 1. A minimal edge parameter reduces the number of triangles by an order of magnitude. The compression algorithm does not change the connectivity of the surface.

Therefore you can still `split` the compressed grob and find the fully enclosed cavities. It is important to use the `make grob skin` command with the `smooth` option since it closes the cusps.

The compress command returns the new number of verteces in `i_out` and the new number of triangles in `r_out` variables, respectively (for the last compressed grob only).

Example:

```
read pdb "1crn"
make grob skin smooth # creates 28832 triangles
display g_1crn
compress g_1crn 1. # from 28832 to only 3082 triangles
display g_1crn
compress g_1crn 4. # another 3−fold reduction
display g_1crn
```

`compress stack` [`fast`] [*i_fromConfNumber i_toConfNumber*]

Remove similar and/or high energy conformations from the conformational stack. During a `montecarlo` run, some conformations of the generated conformational stack may be substituted by newly calculated ones with lower energies. New conformations may violate the initially correct distribution of the conformations in the slots of the stack as defined by the `vicinity` parameter and by comparison mode specified by the `compare` command. The **compress** command compares all the pairs of the stack conformations, identifies pairs of conformations in which two conformations are separated by a distance less than the `vicinity` threshold, and removes the higher energy stack conformation from each close pair. Optional arguments *i_fromConfNumber* and *i_toConfNumber* define a subset of the conformations in the stack which are to be analyzed and compressed (if any). The whole stack (from the first to the last conformations) is processed by default.

Note that if two close conformations are compressed into the better energy one, the number of visits of the resulting conformation will be a **sum** of the two numbers of visits.

The `fast` option applies an iterative compression algorithm which can be several orders of magnitude faster but the result may slightly differ form the default compress. The fast algorithm algorithm performs the following steps:

1. sort conformations by energy
2. start from the lowest energy conformation
3. find all conformations with higher energy than the current conformation within `vicinity` .
4. delete similar conformations with higher energies and compress stack
5. move to the next conformation in the new sorted stack, make it current and go back to step 3

See also How to merge and compress several conformational stacks

Example (define a distance and compress) we generate two stacks, merge them and re−compress two sets with a different comparison criterion:

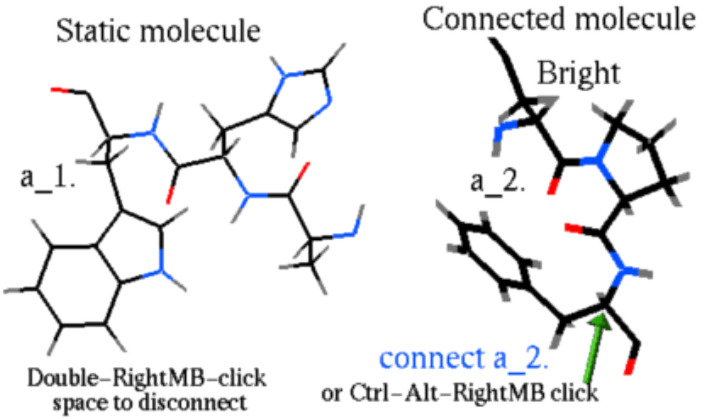
```
buildpep "VTLFVALY"
mncallsMC = 5000
montecarlo   # generates stack, compar
write stack "f1"
```

```
delete stack # clean up and
montecarlo   # generates another stack
read stack append "f1"  #
compare v_/2:5/phi,psi  # compare settings are different
vicinity = 40.          #
compress stack fast
vicinity = 20.          # new vicinity
compress stack
```

2.20.14. connect

`connect` [`append`] [`none`] [{ *ms_molecule* | *grob* }]

connects selected molecules to the mouse for independent rotation (by the LeftMouseButton) and translation (MiddleMouseButton) with respect to the original coordinate frame.



Option `append` will add selected molecule to the previously connected molecules

Note, that rotations/translations in the connect mode actually **change the atomic coordinates** of the selected molecules and keep the coordinate system unchanged in your graphics window.

To restore the usual global mode (i.e. all objects/molecules are disconnected and the mouse does not change their absolute positions, but rather the point of view), hit the Esc key when the cursor is in the graphics window. To restore the global mode **temporarily** press the `Shift` button. Connect can also be activated by a `--Ctrl-Alt-RightMB-Click` on any atom of the chosen molecule (see `graphics controls`).

Use: `connect none` to switch back to the global connection

2.20.15. continue

`continue`

skip commands until the nearest `endfor` or `endwhile`. Note, that in contrast to FORTRAN (god bless it), it is NOT a dummy operator.

Example:

```
for i=1,10
  if i==3 continue  # do not print 3
  print i
endfor
```

See also: `flow control statements`.

2.20.16. convert

`convert` [`exact`] [`charge`] [`tether`] [os_non−ICM−object] [*s_newObjectName*]

converts an incomplete non−ICM−object (e.g. object of type 'X−Ray' resulting from the `read pdb` command) into a true ICM−object for which you may calculate energy, build a molecular surface and perform all operations.

There are two principally different modes of conversion. In the default mode the program looks at the **residue name** and tries to find a full−atom description of this residue in the `icm.res` file. This search is suppressed with the `exact` option.

Hydrogen atoms will be added if the converted residues are known to the program and described in the `icm.res` library. If the object selection is omitted, the current object will be converted. If default *s_newObjectName* is generated by adding number `"1"` to the source object name.

The default `convert` command is best used to convert `PDB` entries which have explicit residue descriptions and usually do not have hydrogen coordinates. In this mode each residue name is searched in the icm.res file and the coordinates of the present heavy atoms are used to calculate the internal geometrical variables (bond lengths, bond angles, phase and torsion angles) for the full atom model.

The `exact` option: converting protein with unusual amino−acids

Some pdb−entries may contain non−amino acid residues, or *modified* amino−acid residues which do not need to be replaced by standard full atom library entries with *the same name* . In this case use the `exact` option. This option suppresses interpretation by short residue name and converts the **existing** atoms and bonds in single−residue molecules (amino acids in peptides and proteins will still be extended by hydrogens upon conversion, to suppress that conversion write the molecule as mol and read it back, then `convert exact`). Option exact may be necessary because chemical compounds with a four−letter short name identical to one of the amino−acid residues, could be mistakenly converted into an amino−acid with a corresponding name.

The `charge` option

Normally, upon convertion, the atomic charges are taken from the `icm.res` library entries. Option `charge` tells the program to inherit atomic charges from the *os_non−ICM−object.* For small molecules, use `set charge`, `set bond type` and, possibly, `build hydrogens` before conversion of a new compound. `i_out` will contain the number of heavy atoms missing from the pdb−template.

Additional cleanup

Actually more precedures need to be performed to prepare a functional object from crystallographic coordinates, e.g. identifying optimal positions of added polar hydrogens, assigning the most isomeric form of `histidine` , and finding a correct orientation of side−chain groups for glutamine and asparagine.

We recommend the `convertObject` macro instead of the plain `convert` command to achieve those goals.

Refining the model

To refine a model use the `refineModel` macro.

`convertObject` macro

The `convertObject` macro is a convenient next layer on the convert command. The macro may convert only a few molecules out of your pdb file, optimize hydrogens and do some other useful improvements of the model.

Comparing convert, minimize tether and regularization.

It is important to understand the difference between the **convert** command, the `minimize tether` command and the `regularization procedure` implemented in the macro `regul` .

All three create ICM−objects from PDB coordinates, but details of generated conformations and the amount of energy strain will differ.

We recommend to use `convertObject` macro for most serious applications involving energy optimization.

convert

- uses all−atom residue templates (including hydrogens) from the icm.res library
- creates temporary ICM−library descriptions for unknown residues
- makes geometry **identical** to the PDB coordinates: bond length and bond angles may be distorted.
- the converted structure will be energy strained because of common imperfections of the PDB entries and the hydrogen atoms added by the procedure
- C−alpha−only structures will not be properly converted because a special prediction algorithm is required to extrapolate the coordinates of all atoms from `C−alpha` atom positions.
- these objects are good enough for graphics, skin, secondary structure assignment, rigid body docking. They are not good for loop modeling and side−chain modeling.
- needs to be followed by polar hydrogen placement and histidine state prediction (implemented in the `convertObject` macro)

`minimize tether` threading a regular polypeptide through an incomplete/gapped set of coordinates.

- you need to create a sequence file first and use the `build` command;
- you will need to create the missing residues manually, say, with the `write library` command;
- build will use all−atom residue templates including hydrogens, and will preserves the fixation;
- the linear chain with *fixed idealized covalent geometry* or, actually, any fixation you define, will be threaded onto the PDB coordinates in the best possible way;

- Ca−atom PDB structures will be handled properly if all backbone torsion angles are unfixed;
- the resulting ICM−object will be strained and will need further relaxation.

full regularization and refinement

- uses `minimize tether` to create the starting conformation;
- employs a multistep energy minimization (annealing) of the structure to relief energy strain;
- these are the best objects that can create in ICM for further simulations.

(see macro `regul` for details).

Examples:

```
read pdb "1a28.a/"           # reading just the first molecule
convertObject yes yes no no  # the best way to prepare for docking
                             # convert + optimizes polar H, His and Pro

read pdb "1crn"         # X−ray object, no hydrogens, no energy parameters
convert                 # a_1crn_icm ICM−object will be created
convert a_1. "new"      # a_new. ICM−object will be created
convert a_1. exact      # keep modified residues as is

read mol2 s_icmhome+"ex_mol2"
set object a_catjuc.
build hydrogen
set type mmff
set charge mmff
convert
```

Converting a chemical compound from a mol/sdf or mol2 files.

To convert a chemical from GUI menus, follow these steps:

- make sure that bond types and formal charges are correct
- select the `MolMechanics.ICM−Convert.Chemical` menu item, check the parameters and press OK. Normally to convert from 2D to 3D you need to optimize the ligand. ICM will perform a multiple start global optimization using the MMFF94 force field (internally it runs the `convert2Dto3D` macro). If you want to preserve the geometry, select the `keepGeometry` option.

Command line conversion To perform the same conversion in a *batch* run the `convert2Dto3D` macro, or, to make a conversion without full optimization from a command line or script, issue the following commands:

```
# assuming that bond types and formal charges are correct
build hydrogen
set type mmff
set charge mmff
randomize a_//!vt* 0.01 # sometimes it helps to avoid singularities
convert
set v_//T3 180.  # making flat peptide bonds
fix v_//T3       # optional
```

Converting a chemical compound and rerooting the tree at the same time

`convert` *as_rootAtom*

if an atom selection is provided instead of the object selection, the tree will be rerooted to the selected atom. The converted molecule will have the *as_rootAtom* located at the root of molecular tree so that it is convenient to `modify` another molecule with the converted molecule.

If you need to reroot an ICM object, do the following:

- strip it to a non−ICM object: e.g. `strip virtual`
- re−root and convert, e.g. convert a_//hb1 .

2.20.17. copy

copies stuff which CANNOT be copied by direct assignment such as: `a=b`

`copy` [`strip`] [`tether`] *os_* [*s_newObjectName*] [`delete`]

create a copy of *os_* with the specified name. Default source object is the current object. The default name is `"copy"` (object `a_copy.`)

Option `delete` (must be specified at the end of the line) forces the command to overwrite the object with the same name if there is a name conflict.

Option `strip` applies the `strip` operation to the copied object. The stripped object has a PDB type and is much smaller in memory.

Option `tether` applies tethers from the source object to the atoms of the copy−object. For further refinement see the `refineModel` macro.

Examples:

```
read pdb "1crn"
copy a_          # creates a_copy.
copy a_1. "aaa"   # create a copy  a_aaa.

read object "rough"         # unrefined object
copy a_ strip delete tether # create a_copy. and tether to it
```

2.20.18. crypt

`crypt key=` *s_password* { *s_fileName* | `string=` *s_string* }

encrypts the file *s_fileName* or string *s_string* in place (the size of the encrypted file/string is exactly the same), adds extension .e to the file name. If string is encrypted, its name is not changed. Apply the operation again to restore the file or string. You may encrypt both text and binary files. Note that this command has nothing to do with the unix crypt utility. ICM uses different algorithm.

Example:

```
crypt key="HeyMan" "_secretScript"    # encrypt and create *.e file
crypt key="HeyMan" "_secretScript.e"  # decrypt it

ss="Secret rumour: Div(Rot(F))=0 !"
crypt key="fomka" string = ss  # encrypt
show ss
crypt key="fomka" string = ss  # decrypt
show ss
```

2.20.19. delete ICM shell objects

delete shell objects or their parts.

delete ICM−shell object

`delete` [`alias`][`alignment`][`factor`][`grob`][`iarray`][`integer`][`logical`][`macro`][`map`][`matrix`][`profile`][`rarray`][`sarray`][`sequence`][`string`] { *name1* | *s_namePattern1* } *name2* ...

ICM−shell objects have unique names; to delete some of them just type

`delete` [`mute`] { icm−shell−objectName1 | *s_namePattern1* } icm−shell−objectName2 ...

You may use name patterns with **wildcards** (see `pattern matching`) and add explicit specification of the ICM−shell object type, if you want the search to match only the objects of particular type. If the ICM−shell object type is not specified, all the shell−variables will be considered.

Option `mute` will temporarily switch off the `l_confirm` flag.

Examples:

```
delete aaa           # delete ICM−shell object aaa
delete a b c         # delete ICM−shell objects a, b and c
delete "*"           # delete ALL ICM−shell objects added by user
delete "mc?a*" mute  # delete ICM−shell objects matching the pattern
delete rarrays       # delete ALL real array
delete objects       # delete ALL molecular objects, same as delete a_*.
delete rarray "a*"   # delete real arrays starting with 'a'
```

delete alias

`delete alias`

see `alias delete` *`alias_name`* . Example:

```
alias ls list
alias delete ls
```

delete selection variable

`delete` *as_selectionName*

or

`delete` *vs_selectionName*

delete named variable with atom or v_ selections. The number of named selections is limited to about 10 in each category, therefore you may need to delete them from time to time.

Important: keep in mind that deleting the named selection is not the same as deleting actual objects, molecules or atoms selected by them. To delete atoms selected by a named variable in an non−ICM object, add keyword `atom` (see `delete atom nameSelection`)

Examples:

```
buildpep "ASFGD"      # build a molecule
vsel = v_//phi,psi    # this is a vselection
delete vsel

asel = a_//c*,n*      # this an aselection (atom selection)
delete asel           # delete variable asel, do not touch the atoms
delete atom asel      # delete atoms in a non−ICM object
```

delete atom

`delete` *as_atoms* : *delete *atoms as_namedSelection

delete selected atoms in a non−ICM object. The selection here must be a constant atom selection, rather than a named selection (e.g. you can say `delete a_/1:10/*` but NOT `aaa = a_/1:10/*` , `delete aaa`).

To delete a named variable, use `delete atom` *name* Example:

```
read pdb "1crn"
delete a_/1:10/*

aaa = a_/18:20
delete atom aaa
```

delete directory

`delete directory` *s_Directory*

delete directory. Example:

```
delete directory "/home/doe/temp/"
```

See also: `make directory`, `set directory`, `Path`(directory)

delete history lines

`delete session`

deletes all previous history lines. Example:

```
call _macro
delete session
```

delete hydrogen

`delete hydrogen` *as_*

delete selected hydrogen atoms in a non−ICM object. See also `build hydrogen`. To delete hydrogens in an ICM object, `strip` it first.

delete object

`delete` { `object` | *os_* }

delete molecular object. Make sure that you specify an object selection (`a_1crn.` is correct, `a_1crn.*` or `a_1crn.//*` is INCORRECT.) To delete an object from a selection variable (`as_out,as2_out` or `as_graph,` or any use defined aselection variable), use `delete atom` *as_namedSelection* (e.g. `delete atom as_graph`) or specify the selection level explicitly.

Examples:

```
delete object          # delete ALL molecular objects
delete a_*.            # delete ALL molecular objects
delete a_2,4.          # delete objects number 2 and 4
delete a_2a*.          # delete objects with names starting from 2a

read pdb "1crn"        # load crambin
convert                # create the second object named 1crn_icm
                       # from the pdb object
delete a_1.            # delete the 1st pdb−object
delete Object( as_graph )  # graphical selection
```

delete molecule

`delete` [`molecule`] *ms_*

delete separate molecules from molecular objects. The integer reference number(s) of molecule(s) which can be shown by the `show molecule` command and used in molecule selections are redefined after deleting or moving molecules from or in the ICM−tree, respectively.

To delete a molecule from a selection variable (as_out,as2_out or as_graph, or any use defined aselection variable), use `delete atoms` *as_namedSelection* (e.g. `delete atom as_graph`) for non−ICM objects, or use the `Mol` function to specify the selection level explicitly (e.g. `Mol( as_graph )`).

Examples:

```
read pdb "2ins"        # load insulin with water molecules
delete a_2ins.w*       # delete water molecules
delete atoms as_graph  # deletes selected non-ICM atoms/molecules
delete Mol( as_graph )  # deletes selected non-ICM atoms/molecules
```

delete bond

`delete bond` *as_singleAtom1 as_singleAtom2*

delete a covalent bond between two selected atoms. This command is used to correct erroneous connectivity guessed by the `read pdb` command. It is particularly important when you are going to create a new ICM-residue using the `write library` command and the entry to it in the `icm.res` or your own residue file (it has the same format). In interactive graphics mode you may type `delete bond` and then click two atoms with the CTRL button pressed.

Examples:

```
read pdb "newmol"              # automatic bond determination is not perfect
delete bond a_/3/cg1 a_/5/ce2  # disconnect two carbon atoms
```

See also: `make bond` and `make bond` *atom_chain* .

delete boundary

`delete boundary`

an auxiliary command to free additional memory allocated by the `make boundary` command.

delete conf

`delete conf` *i_stackConfNumber* [*i_stackConfNumberTo*]

delete a specified conformation from the stack or a series of conformations starting from *i_stackConfNumber* to *i_stackConfNumberTo*

delete drestraint

`delete drestraint` [*as_1* [*as_2*]]

delete distance restraints formed between specified atom selections *as_1* and *as_2*. If no selection is specified all distance restraints are deleted

Examples:

```
delete drestraint a_mol1 a_mol2       # intermolecular restraints
```

delete label

`delete label` *i_StringLabelNumber*

delete graphics string label (text in the graphics window). These strings have no unique identification names, they are just numbered. Numbers are compressed as you delete some labels from the middle of the list.

Examples:

```
delete label 1  # delete the first displayed label
```

See also:

`show label`	to find out the label number and
`display label`	to create and display a string label.

delete sequence

`delete sequence` [*seq_1 seq_2* ..]

`delete sequence selection`

delete the sequences selected through GUI.

`delete sequence` *i_NofLastSequences*

`delete sequence` [*i_minLength i_maxLength*]

- no arguments: delete all ICM−sequences
- one integer argument: delete last *i_NofLastSequences* sequences
- two integer argument: delete sequences shorter than *i_minLength* or longer *i_maxLength*

Deleting some sequences from an alignment `delete` *alignmentName* `only selection` : *delete alignmentName *only seq1 seq2 ... To delete sequences *selected* via the graphics user interface from an alignment without deleting them from the shell. Example

```
delete sh3 only Fyn
delete sh3 only selection
```

delete site

`delete site` [{ *s_siteString* | *i_siteNumber*| *I_siteNumbers* }] *ms_*

delete the `sites` of the selected molecules. The sites can be specified by their name, or number. All sites are deleted by default.

Example:

```
nice "1est"          # has 13 sites.
delete site a_1.1 12
delete site a_1.1 {3,4,5}
delete site a_1.1 "FT CONFLICT 178 178"  # blanks are unimportant
delete sites         # delete all of them
```

delete sstructure

`delete sstructure` *seq_1 seq_2 ..* : *delete *sstructure *select

delete the assigned secondary structure to prepare the sequence for the secondary structure prediction (see the `Sstructure` function).

The `selection` option allows to delete secondary structure only for the sequences selected through GUI.

delete disulfide bond

`delete disulfide bond` [*all*] [{ *rs_Cys1 rs_Cys2* | *as_atomSg1 as_atomSg2* }]

delete specified or all disulfide bridges in ICM objects.

Examples:

```
        # SS-bond specified by residue, or
delete disulfide bond a_/15 a_/29
        # by atoms
delete disulfide bond a_/15/sg a_/29/sg
        # remove all SS-bonds in the current object
delete disulfide bond all
```

See also: `make disulfide bond` and **(important!)** `disulfide bond`.

delete peptide bond

`delete peptide bond` [*as_N as_C*]

delete specified extra peptide bonds in ICM objects (e.g. imposed to form a cyclic peptide).

Example:

```
delete peptide bond a_/15/c a_/29/n
```

See also: `make peptide bond` and `peptide bond`.

delete stack

`delete stack`

delete `stack of conformations`.

See also `read stack`, `write stack`, and `delete conf`.

delete table

`delete` { *T_table* | *table_expression* }

delete the specified complete table or just the entries selected by the expression.

Examples:

```
group table t {1 2 3} "a" {4. 5. 7.} "b"
delete t.a == 2       # the second entry
show t
delete t              # the whole thing
```

delete term

`delete term` *s_terms*

switch off the specified terms of the energy/penalty function.

Examples:

```
delete terms "tz,sf"    # do not consider tethers and solvation contributions
```

delete tether

`delete tether` [*as_*]

delete tethers of the specified atoms (*as_*), if no selection is specified all tethers are deleted.

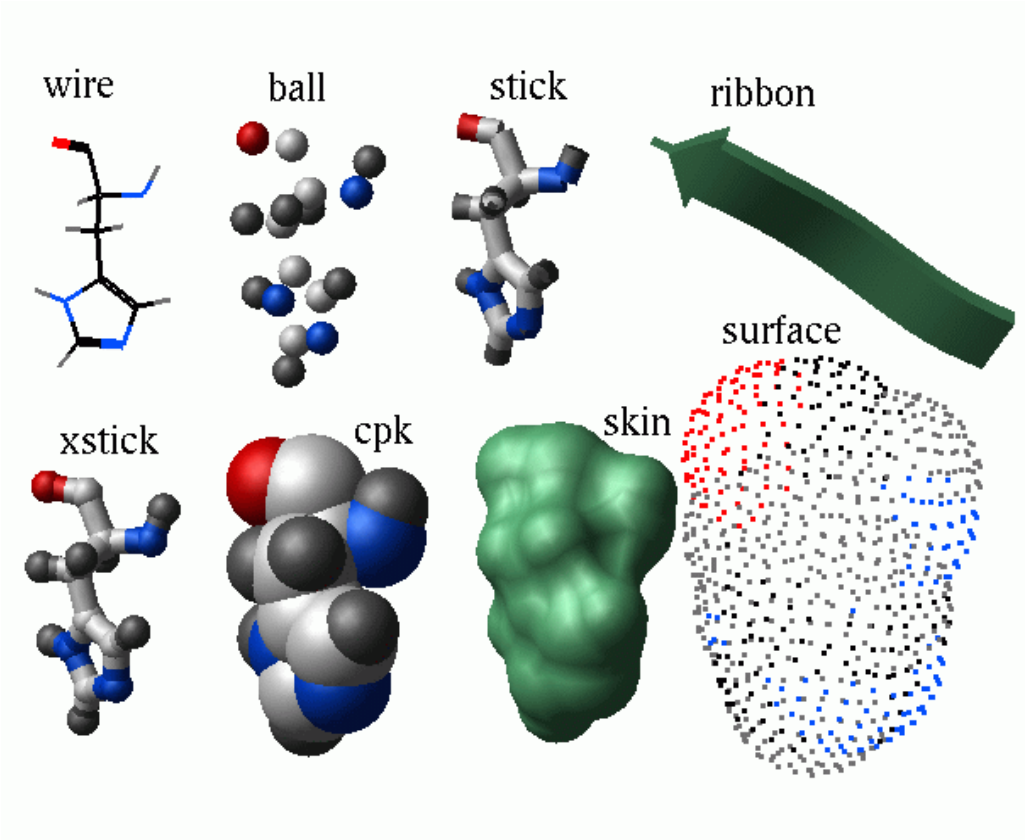
2.20.20. display

display molecules or graphical objects

display model

`display` [`wire` |`cpk` |`ball` |`stick` |`xstick` |`surface` |`skin` |`ribbon` [`base`]] [*as_* [*as_2*]] [*color*] [`virtual`] [`plane`] [`center` [*center_options*]] : *display [*transparent] [*stick|*skin|*ribbon [*base]] [as_ [as_2]]

display specified graphics primitives for selected atoms or residues.



Once something is displayed and your cursor is in the graphics window you may rotate, translate, zoom and move both clipping planes with the mouse and keystrokes.

To refer to the base part of DNA/RNA represented as `ribbon` , use the additional specifier called **base,** which can be separately displayed and colored. E.g.

```
makeDnaRna "ACTG" "mydna" yes yes "dna"
display ribbon base
color ribbon base a_1 blue
```

Display surface atoms may be defined by TWO arbitrary selections (it would mean: display surface of atoms *as_1* as they are surrounded by atoms *as_2*) Note that the `GRAPHICS.hydrogenDisplay` preference may affect the displayed atoms. To be able to display all atoms set `GRAPHICS.hydrogenDisplay` to `"all"`.

Defaults: wire representation, all atoms (corrected by the GRAPHICS.hydrogenDisplay), coloring according to atom type.

color options

The color can be specified by a number of ways (see the `color` command for a more detailed description) : *Color* (e.g. `red`), s_Color (e.g. "red"), numerical color:

i_Color | *r_Color* | *I_Color* | *R_Color* [`window=` *R_2minmax*]

The window array of min and max values allows to clamp the value you want to map to a color to the specified range.

Other options:

center : will perform the `center` command on the displayed object(s).

transparent : will display the ribbons, skins or sticks as transparent objects,

```
read pdb "1crn"
display transparent ribbon
display skin transparent
```

plane : will display the object the way it was saved, e.g.

Example:

```
 nice "1crn"
# Display something and save the object with the graphical information
 color ribbon green
 display a_/3:5 cpk
 write object auto "tm"
 q
% icm
 read object "tm" # now contains graphics information
 display plane
```

intensity= ***r_fraction*** **:** renders the image with fractional intensity by merging the source display image with the background.

virtual : additionally displays the coordinate axes, `virtual` atoms and virtual bonds starting from the origin. It is a good way to visualize the whole ICM molecular tree as it grows from the origin. This option is applicable only to the ICM molecular objects.

More examples:

```
 buildpep "AFSGDH;QWRTEY"       # two peptides
 display                        # display current object and color atoms
                                # according to atom type
 display a_1 red                # display the first molecule and color it red
 display skin a_/5 a_* yellow   # display skin of the 5th residue
                                # as surrounded by all the atoms
 display ribbon                 # display ribbon for all the residues

 read pdb "2drp"                # a pdb file
 assign sstructure a_1/123:134,153:165 "H"       # No sstructure in 2drp
```

```
 assign sstructure a_1/109:114,117:121,141:144,147:151 "E"
 display a_1 ribbon red                          # two Zn-fingers
 display a_1/113,116,143,146/!n,c,o xstick blue  # Cys residues
 display a_1/129,134,159,164/!n,c,o xstick navy  # His residues
 display a_2,3 cpk magenta                       # Zn-atoms
 adna1=a_4//p,c3[*],c4[*],c5[*],o3[*],o5[*]      # two DNA chains
 adna2=a_5//p,c3[*],c4[*],c5[*],o3[*],o5[*]
 display adna1 xstick white
 display adna2 xstick aquamarine
 display adna1 adna1 surface white
 display adna2 adna2 surface aquamarine
 center
 display "Zn-finger peptides complexed with DNA" pink

# display 4 chains of insulin as 4 thick worms colored from N-to C-terminus
 read pdb "2ins"
 color background blue
 assign sstructure a_/* "_"  # thick worm representation
 GRAPHICS.wormRadius= 0.9
 display a_/* ribbon only
 color a_1/* Count(1 Nof(a_1/* )) ribbon
 color a_2/* Count(1 Nof(a_2/* )) ribbon
 color a_3/* Count(1 Nof(a_3/* )) ribbon
 color a_4/* Count(1 Nof(a_4/* )) ribbon

# examples of DNA and RNA ribbons
 nice "4tna"
 resLabelStyle = "A"
 display residue label
 color residue label a_/??u gold # ??u also selects modified Us
 color residue label a_/??a red
```

display new: refresh or unclip view

`display new` : *display *restore `display restore plane`

commands to mimic some of the interactive controls. These commands are primarily used in GUI commands (see icm.gui file) and scripts/macros.

new : rebuilds some graphical representations (e.g. your as_graph has been changed in the shell and you need to refresh the image, or you changed the orientation and want to redisplay the labels elevated above the skin surface by `resLabelShift`).

restore : a softer action than `new` .

restore plane : moves the clipping planes beyond the displayed objects (keystroke: `Ctrl-U,` or the `'Unclip'` button) .

display off-screen

`display off` [*i_Width i_Height*]

Sometimes you want to generate some images in a script **without** opening an explicit graphics window. The `display off` command opens an off-screen rendering buffer of *i_Width* by *i_Height* size in pixels, in which all the usual `display/color/undisplay/center` commands work as usual. **NOTE:** one

cannot have both off−screen and on−screen displays in one ICM session.

An example script (can also be performed interactively):

```
display off 400 300
nice "1est"
rotate view Rot( {0. 1. 1.} 50.)
write image "est1"
unix xv est1.tif
set window 700 800  # NB: 'center all' will be applied
write image "est2"
unix xv est2.tif
display a_/4/o cpk
center a_/3,4
write image "est3" rgb
unix xv est3.rgb
build string "se ala trp"
display off 400 300
display skin
write image "est3" rgb delete
unix xv est3.rgb
```

display origin

display the axis of the coordinate frame. The length of the arrows is defined by the `axisLength` parameter. Use `undisplay origin` to undisplay it. E.g.

```
read pdb "1crn"
display
display origin
undisplay origin
```

display box

`display box` [*R_6boxCorners*]

display graphics box specified by x,y,z coordinates of two opposite corners of a parallelepiped. This box can be resized and translated interactively with the Left and Middle mouse buttons:

- Resizing: Grab **a corner of the box with the Left−Mouse−Button** and drag it to resize the box
- Translating: Grab a corner or a center of the box with the **Middle−Mouse−Button** and translate

Example:

```
buildpep "ala his trp"
display box Box( a_/1 )  # change it interactively
```

See also the `Box` () function which returns six parameters describing the box.

Examples:

```
build string "se ala his"  # a peptide
display
display box                      # the default box position/size
```

```
   display box {0. 0. 0. 2. 2. 2.}  #  or
   display box Box(a_/2 1.2)  # surround the a_/2 by a box with 1.2A margin
```

display cursor

`display cursor` [*rs_*] [*color*] [*s_Symbol*]

display the residue cursor at the specified single residue *rs_*. Move the cursor with the left and the right arrows. You may redefine the color (default 'red') and the cursor symbol (default '#').

display clash

`display clash` [*as_1* [*as_2*]] [*r_clashThreshold*]

display all the interatomic distances between two atom selections which are shorter than the sum of van der Waals radii multiplied by the *r_clashThreshold* parameter. The default value is taken from the `clashThreshold` variable. Initially it is set to `0.82` but can be redefined. IMPORTANT: this will work only for the ICM−objects. For hydrogen bonded atoms the threshold is additionally multiplied by `0.8`. Use the `show energy "vw"` command (and pay attention to the current fixation) to precalculate interaction lists.

This command may show some irrelevant short contacts. `calcEnergyStrain` , `display gradient` , etc. seem to be more informative.

See also: `GRAPHICS.clashWidth` , `clashThreshold` , `show clash`, `undisplay` and atom energy gradient (force) analysis with: `show a_//G` or `display a_//G`.

Example:

```
 read object "crn"
 show energy "vw"
 display clash a_/11 a_/!11 0.75  # distances < (R1+R2)*0.75
# this is an alternative method which analyzes the gradient
 selectMinGrad = 100.   # analyzes forces greater than 100
 display ribbon grey
 display Res( a_//G )
 display gradient a_//G
 color Res( a_//G ) ribbon magenta
```

display drestraint

`display drestraint` *as_*

displays drestraints, disulfide bonds, and peptide bonds imposed on selected atoms.

See also: `read drestraint`, `set drestraint`, `make disulfide bond`, `make peptide bond`, `make drestraint`.

Example:

```
  build string "se ala his trp"
  display
```

```
set drestraint a_def.a1/3/hz2 a_def.a1/1/hb3 2
display drestraint
minimize "vw,14,to,cn"
```

display gradient

`display gradient` *as_*

display vectors of energy derivative with respect to atom positions or selected atoms `as_` .

Important: the gradient must be **pre−calculated** by using one of the following commands: `show energy` or `minimize` . The values of gradient components (lengths of vectors for each atom) can be shown by `show gradient` *as_*. When a gradient vector is displayed, two transformations are performed: it is scaled and colored to represent the range of values in the most convenient and natural way while still being able to deal with a wide range of gradient values from negligible to 10 to the thirtieth power, as may be the case for a strong van der Waals clash. When all gradient vectors are under 20 kcal/mole*A they will be colored by the "cold" colors (blue...green...yellow) and will be assigned a length less than 2 Angstroms. If you see a red and long vector you may have a problem. Check it by zooming in and using `show gradient` *as_*. You can also select only atoms with gradient greater than the threshold value `selectMinGrad` by typing `a_//G` and display only specified strained atoms. It helps to get rid of little blue arrows for unstrained atoms.

Examples:

```
buildpep "ala his trp glu leu"
randomize v_//phi,psi
show energy
selectMinGrad= 200.
display gradient a_//G
```

display grob

`display grob` [`solid`][`smooth`][`dot`][`reverse`] [`transparent`]

`display` *g_Name1 g_Name2 ... options*

`display grob selection` ... *options*

display all, specified, or graphically selected graphics object(s) . They are referred to as **grob** in the ICM−shell and as "3D meshes" in the GUI interface. The `display grobs` command will display all existing graphics objects. Options:

- `dot` will show only dot−vertices of the object.
- `reverse` to invert lighting; this option will change directions of the grob surface normals (will turn the grob inside−out)
- `smooth` enforces the Gouraud shading method to smooth the solid surface.
- `solid` allows solid surface representation of the object and requires that the original object has information about triangles forming the solid surface.
- `transparent` makes solid grob transparent

One can also `color` and `undisplay` graphics objects, as well as `connect` to them.

Examples:

```
   read matrix "def.mat"    # 2D sin(r^2)/r^2 function of a grid
   make grob solid def      # convert matrix into a graphics object g_def
   display g_def smooth     # a hat of the 22st century
   display g_def reverse    # shine light from inside the head
   display grob transparent # like Lenin in Mausoleum
# now you can double-LeftMB-click on it and Alt-X it to your satisfaction
```

display hbond

`display hbond` [*as_*] [*r_maxHbondDistance*] [`only`]

Only `hydrogen bonds` of the `current object` may be displayed. Before calling this command, you should use any of the following commands: `show hbond`, `show energy`, `minimize` to calculate the list of hydrogen bonds. The real argument *r_maxHbondDistance* defines an upper bound of the distance between a hydrogen and a potential hydrogen acceptor to place the pair to the hydrogen bond list. (Default value of *r_maxHbondDistance* parameter is 2.5 A.) The list is recalculated for each new loaded molecular object. Hydrogen bonds on display are colored according to their hydrogen-acceptor distances. The option `only` allows to display hydrogen bonds without corresponding molecular object. Longer and shorter H-X distances in the hydrogen bond are color-coded, from red to blue, respectively.

For ICM object the hydrogen bonds are calculated much faster.

See also: `undisplay hbonds`, `show hbonds`.

display label

`display` [{ `atom` | `residue` }] `label` [*selection*]

`display variable label` *v_selection*

a graphics label with atom name, residue name, variable name for all or selected atoms, residues or variables respectively. The text of this label is not user-defined, although you can control it in two different ways. First, residue label style can be set using either `Ctrl-L` in the graphics window or `resLabelStyle` preference , and variable label style either by `Ctrl-V,` or setting `varLabelStyle` preference. Second, the ICM-shell string variable `s_labelHeader` defines a prefix string for all labels. For example, if you display CPK atoms you may move the label to the right from the atom center by `s_labelHeader=" "` .

The `_aliases` file has convenient aliases (e.g. `ds` for display, `unds` for undisplay, `re` , for residue, `va` for variable) for those of us who like typing commands. In this case you may just type `ds va la` to display variable labels, etc.

Examples:

```
buildpep "FAHSGDH"
display residue label #
undisplay label
display residue label a_/his
display variable label v_//phi,psi
```

```
 display variable label v_//* as_graph
 display atom label a_/1:3/*
 undisplay label
# or with aliases:
 ds re la a_/1,3
 unds la
 .. etc.
```

display map

`display` { `map` | *map_name* } [*I_colorTransferFunction*] [*R_2RangeOfMapValues*]

displays a real function defined on a three−dimensional grid (i.e., an electron density `map`). Optional `iarray` argument defines a color transfer function according to deviation from the mean.

If you provide an explicit range of map values (*R_2RangeOfMapValues*), the map values will be clamped into this range, divided into `Nof`(*I_colorTransferFunction*) subranges, and colored according to the values of *I_colorTransferFunction* :

- 0 − transparent/invisible
- 1 − blue
- maxNumer − red

To undisplay the bounding box reset the `GRAPHICS.displayMapBox` parameter.

See also the `color map` command.

Example:

```
build string "se his arg"
make map potential "el"  Box( a_/1,2/* , 3. )
display a_
display map m_el {3 2 0}  # high values are invisible
display map m_el {0 3 2 0} {−2.,2.}
make grob m_el 2.
display g_el
```

In the `display map m_el {0 1 2 3 4 0} {−3.,3.}` example, the values will be clamped into the −2.,2. range. The range will be individed into 6 sub−ranges: `−infnty:−2., −2.:−1, −1:0, 0:1, 1:2, 2:+infnty` . The first and the last ranges will be invisible (color 0). The four ranges in the middle will be colored from blue to red. (BTW, the above example does not make much sense for the electrostatic field. `{1 2 3 0 4 5 6} {−3.,3.}` makes more sense.

See also related commands: `read`, `write`, `delete`, `list`, `show map`, `set`, `make` (1), `make` (2) and file format `icm.map` .

display movie : simulation trajectory

`display movie` [`sstructure`] [`image` [= *s_framePath*] [`rgb` | `targa` | `png` | `gif`]] [*s_MovieName*] [*i_From* [*i_To*]] [*r_Smooth1* [*r_Smooth2*]] [*as_1*] [`center` [*as_2*]]

lets you play, stop and reverse a Monte Carlo simulation trajectory as well as write a series of images for future assembly of those images into movies. To obtain the movie info use

`read movie` *s_MovieName*

Integers *i_From* and *i_To* specify the frame range. Real values *r_Smooth1* and *r_Smooth2* determine minimum and maximum smoothing parameters (i.e. number of additional frames, inserted if conformation change is too dramatic). Specifying atom selection *as_1* defines a certain fragment on to the initial conformation, of which subsequent conformations are superimposed. Option `center` with selection *as_2* determines a fragment for graphics window centering (all, if `center` without *as_2*). When playing a movie, you can use ICM interrupt (`Ctrl-\`) to stop, and then toggle stepwise frame playing, reverse, or quit playing. The default is to play a whole movie without smoothing, superimposition or centering.

Option `image` allows to automatically save a series of image files in the specified directory s_framePath or in the default `s_tempDir` directory. Allowed image formats are: `rgb, targa, png, gif` . The file extensions will correspond to the image file format. The image file names consist of the default path and name, appended with the frame number. Example:

```
display movie image="/tmp/f"
/tmp/f_1.png
/tmp/f_2.png
...
s_tempDir = "/home/jack/X"
display movie image rgb
/home/jack/X_1.rgb
/home/jack/X_2.rgb
...
```

All the other image preferences may be predefined by the `IMAGE` table.

Option `sstructure` will dynamically reassign secondary structure while going through conformations of each frames. This option is very useful if you perform peptide/protein simulation and want to see if secondary structure elements are forming transiently.

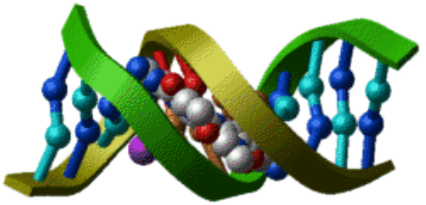
See also: `movie file`.

Examples:

```
       # seq. alpha.se
build "alpha"
display ribbon wire a_//!h*
read movie s_icmhome+"alpha"
       # reduces the size of TIFF files
IMAGE.compress=yes
IMAGE.color   =yes
       # a separate directory is actually better
s_tempDir = "/usr/tmp/"
       # create a series of /usr/tmp/X*.tif files
display movie "alpha" center image="X"
IMAGE.color   =no
       # now a series of black/white /usr/tmp/alpha*.rgb files
display movie center image rgb i
```

display ribbon

`display ribbon` [`base`] *rs_ color*



display `ribbon` . Option `base` is used for displaying cartoon representations of the bases on the DNA/RNA ribbons.

See also `base`, `GRAPHICS.dnaBallRadius`, `GRAPHICS.dnaStickRadius`, and other dna settings in `GRAPHICS.`

display site

`display site` *rs_ color*

display `site` information. Switch between different types of the site information with the `SITE.labelStyle` preference.

display skin or dotted surface

`display` { `skin` | `surface` } *as_1 as_2*

display analytical molecular surface, also referred to as `skin`, or solvent accessible `surfacearea` . Each `display skin` command will delete the previously displayed skin in the current `plane`. To display several different skins, use the `set plane` command to change the current graphics plane before you issue the display skin command. You can also convert the skin into a `grob` with the `make grob skin` command. You can co−display many grobs on the same plane, as well as make the grob transparent. This grob can be further split into individual shells with the `split` command. See also: How to display and characterize protein cavities.

Example:

```
build string "se ala his glu"  # test tripeptide
display                        # the wire model
display skin a_/1 a_/1         # skin around the 1st residue or just press <F1>
set plane 2                    # key with your cursor in the graphics window
display skin a_/3 a_/3         # skin around the 3st residue
                               # now you can toggle planes with F2 and F1
display surface                # solvent−accessible surface
```

display string

`display` *s_StringText* [`auxiliary`] [*color* `font=` *i_FontSize*] [*r_XscreenPosition r_YscreenPosition*]

display a text string in the graphics window. Relative X and Y screen coordinates (ranging from −1. to 1.) of the string beginning may be specified to display the string in a given location. Defaults are x = −0.9, y = 0.9, i.e. upper left corner of the screen.

The string can be dragged later to any location by the middle mouse button. Two fonts are at your disposal: the default font (usually times) and the auxiliary font (usually symbol). Both fonts can be redefined by the `set font` command. You can also switch to the auxiliary font and back inside the string by backslash−A (**\A).** (.e.g "Red: \Aa\A−helix"). You can also list and delete your string labels by the `list label` and `delete label` commands.

Examples:

```
display "Crambin"                              # a simple string

display "Act.site of \Ab\A−lactamase" yellow # Greek beta letter

display Name(a_1.) red 28, 0. 0.9              # first object name
                                               # in the middle
                                               # (font size=28)
```

display tethers

`display tethers` [*as_*] [*r_minDeviation*]

displays tethers assigned to the selected atoms *as_* with deviation larger than *r_minDeviation.* Tethers can be imposed between atoms of an ICM−object and atoms belonging to another object, which is static and may be a non−ICM−object. (0. by default).

display window

`display window` [*i_xLeft i_yDown i_xSize i_ySize*]

displays an empty window of the specified size and position. This command is convenient for demo scripts. See also: `set window`

2.20.21. elseif

`elseif`

is one of the ICM flow control statements, used to realize conditional statements. See also: if, then, and endif .

2.20.22. endfor

endfor

is one of the ICM flow control statements, used to perform a loop in ICM−shell calculations. See also for.

2.20.23. endif

endif

is one of the ICM flow control statements, used to realize conditional statements. See also if, elseif, and then .

2.20.24. endmacro

A command ending a macro .

Examples:

```
   macro threeEssentialsOfLife          # declare new macro
                                        # define essentials
      l_info=no
      modes={"\n\tOoops!!\n","\n\tOuch!!\n","\n\tWow!!\n"}
                                        # randomly pick a line
      print modes[Random(1,3)]
   endmacro
   threeEssentialsOfLife                # invoke macro
```

2.20.25. edit

edit *icmShellVariable*

interactively edit the ICM−shell variable using your favorite editor defined by the s_editor variable.

Examples:

```
   edit mncalls   # actually it is easier to type: mncalls=333
   edit FILTER    # edit a system table, do not change names of components
#
   read table "pdb1"  # read table with search results
   edit SR            # edit table SR
```

2.20.26. endwhile

endwhile

is one of the `ICM flow control` statements, used to perform a `loop` in ICM−shell calculations. See also `while`.

2.20.27. exit

`exit` [*s_message*]

exit from a `script` file to interactive mode. Do not confuse this command with the `exit` option in, say, `highEnergyAction` preference.

Similar to `return` [`error` *s_message*] from a `macro` .

To quit the program, use the `quit` command.

2.20.28. find

a family of commands for sequence and pattern searches, chemical matching, 3D pharmacophore matching, and alignment optimization.

find alignment : automated structural alignment

`find` *ali_initial* [`superimpose`] [`r_threshold=` 3. [`r_retainRatio=` 0.5]]

find the best structural alignment of two proteins by refining the inaccurate initial alignment *ali_initial* with the goal of finding the largest possible subset of residues which have similar local backbone fold in 3D space.

Option `superimpose` automatically superimposes molecules according to the found structural alignment upon completion of the iterations. This command needs a starting alignment of 2 sequences `link`ed to the molecules with at least one atom per residue. If `Ca` atoms are not found the atoms carrying the residue label (see the `set label` command) are used.

Low gap penalties of 1.8 and 0.1 are recommended for the initial sequence alignment.

Algorithm : At each step aligned pairs of atoms which are further than *r_threshold* from each other are disconnected so that at least *r_retainRatio* pairs are be retained. Then the molecules are superimposed again and new residue pairs are tested and accepted if it leads to a lower overall rmsd. Warning: the result strongly depends on the relevance of the starting alignment to the best 3D alignment. Sometimes 3D irrelevant sequence alignment pairs do not tend to disconnect to allow transformation into a global 3D alignment: e.g. if only one pair of elongated helixes is aligned in the starting alignment and it is only a small part of an optimal alignment which would be completely different, it might not be eventually found.

See also other types of structural searches and superpositions:

- `find segment,fold search` finds structural similarity on the basis of secondary structure elements (no sequence).
- `qsearch` and `find pdb`: search a database of a single structure for a fragment with a given sequence pattern and partial structural similarity (e.g. loop ends match).

- `superimpose:` performs structural superposition, the command can do it on the basis of sequence alignment on the fly.

Example:

```
read pdb "1nfp"
read pdb "1brl.b/"
rm !Mol(a_*./A )
make sequences a_*.
aa=Align(1brl_1_b 1nfp_m1)
ds a_1.//ca,c,n grey
ds a_2.//ca,c,n green
superimpose a_1.1 a_2.1 aa
center
find aa superimpose
show aa

gapExtension=0.05
ab=Align(1brl_1_b 1nfp_m1)
find ab 4. 0.7 superimpose
show ab                          # better
```

find database: sequence and pattern searches

`find database` [*r_probabilityThreshold*] *options* : *find *database *exact [distance= i_nOfMutations]] options `find database pattern=`{ *s_pattern* | *S_patterns* } *options* : *find *database *write [s_database]

fast sequence or `pattern` search through a sequence database.

The default `find database` sequence search program performs a full gapped optimal sequence alignment, which is a global alignment with zero−end−gap penalties (ZEGA). These alignments are more rigorous (not heuristic) than popular BLAST of FASTA searches. The latest statistics of structural significance of sequence alignments derived for a number of residue substitution matrices will be applied (Abagyan and Batalov, 1997) to assess the probability that a matching fragment shares the same 3D fold. The *r_probabilityThreshold* (default `0.00001` or 5.) option defines the lowest acceptable probability of hit. You can also provide a `−logP` number (e.g. `5.5`) instead of a small probability (`10^−5`). Threshold of 10/DatabaseSize is usually a safe threshold (no guarantees though). Practically 10^{-5} is a safe threshold for a SWISSPROT search (65,000 sequences). At 10^{-4} you may find interesting hits, but a more serious analysis may be required to confirm its significance.

The second version of the command with the `exact` keyword performs a very fast search for identical or almost identical sequences. The `distance=` *i_maxNofMutations* parameter specifies the allowed number of mutations.

The third version of the command searches for string patterns in a sequence database. The `sequence patterns` can contain while cards (e.g. "A?[LIV]?\{3,5\}[!P]"). This search is very fast.

The fourth command `find database write` is used to export ALL sequences from the blast−formatted files into to an external FASTA file defined by `output=` string (default *s_databasePath.seq*). This option is the inverse of the `write index sequence` command which creates several BLAST files from a FASTA file.

The common options are as follows: [*s_databasePath* (`"pdbseq"`)] [*seq_1* ..] [*ali_1* ..] [`output=` *s_outputFileNameRoot*] [`name=` *s_tableName*] [`unique`] [`delete`] [`protein` | `nucleotide` | `type`]

- DATABASE: *s_databasePath* (default: "pdbseq" files in the $BLASTDB directory) defines the path of the three files with the compressed sequence files. For compatibility these three files (.bsq, .atb, .ahd) are the same as generated by the `setdb` (BLAST) command. The available files can be vied with the `list database` command, by default the "swiss" file is taken from the $BLASTDB directory. If the environment variable $BLASTDB is set, the three files will be taken from this directory. To read database files from any directory, specify its explicit path (e.g. "./myLocalDb" or "/home/user/myHomeDb1") **Note:** when the PDB sequences are updated, the blast files go into `s_userDir` + "/blastdb" , On Linux the database is at "~/.icm/blastdb/pdbseq" . To make this directory the default blast directory, reset the `s_blastdbDir` to "`/your_home/.icm/blastdb/`". In GUI, choose **File;Preferences;Directories** and modify the `s_blastdbDir` variable.

- QUERY: *seq_1* .. (list of sequences), or *ali_1* .. (list of alignments), or keyword `selection` determines which sequences will be searched against the database. The default (no argument) means that all the sequences currently present in the ICM−shell (see `list sequence`) will be searched. The `selection` can be made from the ICM GUI.

- OUTPUT FILES: option `output=` *s_projName* to redefine the name of the project. The default name of the output files is the name root of the database file. The following files are saved

```
projName_seq  # query sequence(s)
projName.seq  # a sorted list of database sequences truncated to the matching fragment
projName.tab  # the result table
```

- TABLE: option name= *s_resultTableName* defines the names of output table which is created after the search. The table contains the boundaries of the hits, sequence identities etc.

- option `margin=` *i_seqMargin* in the pattern search defines the length of flanking sequences added to the matching fragment and saved in the *s_projectName.seq* file for further retrieval. Specify a very large number to store complete sequences.

- option `delete` will overwrite the output files without asking, as if `l_confirm=no` .

- option `unique` makes the program ignore hits with sequences 100% identical to the query set (if one sequence is a fragment of another, they are is still considered 100% identical).

- option `protein` or `nucleotide` limits the search to database sequences only of this type. It is important for PDB sequence database since it contains both protein and nucleic acid sequences.

- option `type` automatically selects `protein` or `nucleotide` based on the *query* sequence type, but only if you search with a *single* sequence.

Other important variables:

- `alignMinCoverage` (default 0.5) a threshold for the ratio of the aligned residues to the shorter sequence length.

- `alignOldStatWeight` (default 1.) a parameter influencing the statistical evaluation of sequence comparison. To use run−time statistics use alignOldStatWeight=0.
- Up to `mnSolutions` hits will be retained in the final table of hits.
- The parallel version of the program will use `nProc` CPUs (but not more than is available in your computer). The expected time is inversely proportional to the number of CPUs.
- `maxMemory` is a real ICM−shell−variable defining the size of the database buffer memory in Mb used by the command. If this size is smaller than the database, the sequences will be loaded in chunks.

The output table looks like this and contains the following fields:

```
#>T SR
#> NA1 NA2             MI     MX   LMIN    LN     H      ID      SC      pP   DE
1hiv_a POL_HV1H2      57    155     99  0.665  0.099  100.0  103.69   30.00 "POL PROT.."
1hiv_a POL_HV1BR      69    167     99  0.664  0.098   99.0  103.62   30.00 "POL PROT..
<i>... lines skipped ...</i>
1hiv_a POL_MLVAV       9    102     99  0.648  0.078   27.3   23.41    5.31 "PROTEASE.."
1hiv_a VPRT_MPMV     172    272     99  0.799  0.290   29.3   21.95    4.82 "PROTEASE.."
1hiv_a VPRT_SRV1     172    269     99  0.799  0.290   27.3   21.65    4.72 "PROTEASE.."
1hiv_a GPDA_RABIT     33    145     99  0.785  0.264   28.3   20.98    4.50 "GLYCEROL3P"
```

- **NA1** − the query sequence (a single command can search several query sequences)
- **NA2** − the name of the database sequence
- **MI** : MX − the matching fragment boundaries in the database sequence
- **QMI** : QMX − the matching fragment boundaries in the query sequence
- **LMIN** − the shortest sequence length in a pair (query, database sequence)
- **LN** − log−correction factor (not used in pP but you may want to use it to resort the table).
- **H** − the fraction of the database sequence covered by the alignment with the query. If you search against a database of domains this number should be close to 1 (e.g. the hit is less significant if your query is only a part of a domain). It can be taken into account by multiplying pP by this number.
- **ID** − percent sequence identity (number of identical residue pairs in the alignment divided by LMIN)
- **SC** − normalized alignment score which is used to calculated the Probability. The score depends on the residue substitution matrix and gap penalties. (see the `Score` function).
- **pP** = $-\log_{10}$(`Probability`)
- **DE** − the database sequence definition

Examples:

```
read sequence "GTPA_HUMAN.seq"
find database "/blast/swiss" output="gtpa1"
find database pattern="C?[DN]?\{4\}[FY]?C?C" "/blast/brku" margin = 5

unknown1=Sequence("TTCCPSIVARSNFNVCRLPGTPEAICATYTGCIIIPGATCPGDYAN")
find database exact unknown1 "/blast/brku" margin=1
```

find molecule: chemical substructure search

`find molecule` *s_Smile1* { *s_Smile2* | *S_Smiles2* } [`atom`] [`bond`] [`simple`] : *find *molecule *reverse ms_1 s_smile

Identify a complete match of the source molecule represented by a `smiles` string in another smiles string or an array of smiles strings representing a database of chemicals. Make sure that you unselect hydrogens in your smiles string.

Options:

`atom`	allow superpositions of all atom types
`bond`	allow superpositions of all bond types
`reverse`	searches

The following setup is optional:

- prepare the target strings with the `Smiles( a_//![hdt]* )` function (exclude hydrogen, deuterium and tritium)
- search the source string made without hydrogens

Only up to `mnSolutions` hits will be retained in the final table of hits. Change this shell variable if necessary. The function will return the results in the following variables:

- `i_out` − contains the number of hits
- `I_out` − contains the integer array of the hit numbers

An example:

```
squery = "CC=1C(=O)C=CC(C=1)=O"
read sarray s_icmhome+"chemDbSmiles"
find molecule squery chemDbSmiles # check I_out and i_out
```

The smiles string can also be generated with the Smiles function after conversion, e.g.:

```
read mol s_icmhome+ "ex_mol"
convert a_1.
squery = Smiles( a_1.//!h*,d*,t* )
```

`find molecule` [`tether`] *as_subFragmentQuery as_IcmTargetContainingQueryFragment*

You can also use the alternative set of arguments and use molecular selections instead of the smiles strings. The atoms of *as_IcmTargetContainingQueryFragment* aligned to each sequential atom of the query molecule will be stored in the `S_out` array. The atom selection of the target will also be returned in the `as_out` selection.

The `tether` option: After the equivalent sets of atoms in two molecules are identified, tethers can imposed pulling atoms of *as_IcmMolContainingQueryFragment* to the equivalent atoms of passive atoms *as_subFragmentQuery* . The matching atoms of the second selection *as_IcmMolContainingQueryFragment* which are pulled by tethers to the *as_subFragmentQuery* template positions can be superimposed with the `minimize "tz"` *v_positionalVariables* command.

An example:

```
build string name="a" "se nter his cooh"   # query template
build string name="b" "se nter his trp cooh" # target
find molecule a_a./his/cg,nd1,ce1,ne2,cd2 a_b. tether
display as_out xstick # the tethered atoms of the target
display a_*.
minimize "tz" a_b.//?vt*
show Rmsd( a_b.//* )  # will show the RMSD of the equivalent atoms
```

See also: `Smiles` function and the `build smiles` command.

find pdb: fragment search

`find pdb` *rs_fragment os_objectWhereToSearch s_3D_align_mask* [*s_sequencePattern* [*s_SecStructPattern*]] [*r_RMSD_tolerance*]

A PDB database searching engine. Find a fragment (e.g. a loop) with certain geometry, sequence and/or secondary structure. Arguments:

- *rs_fragment:* the search fragment template
- *os_objectWhereToSearch:* the other object. In the `qsearch` macro this argument contains the current object from the `qsearch` database (see also `s_qsearchDir` directory containing converted pdb−objects).
- *s_3D_align_mask:* marks the residues to be used in the 3D superposition and comparison in terms of *r_RMSD_tolerance* (see below). The number of '**x**'**s** (or 'ON' bits) in the mask must be equal to the query fragment length (it may be discontinuous), while the total mask length should be equal to the found fragment length. For example, if you search for an 11−residue loop with the same geometry of 3−residue ends, but any geometry of the middle part your mask must be `"xxx-----xxx".` If you want to match geometry of the middle part you would invert the mask: `"---xxxxx---",` etc.
- *s_sequencePattern:* Use `"*"` for any sequence. Otherwise you may use regular expressions, for example: `"?A[!P]???$".`
- *s_SecStructPattern:* Use `"*"` for any secondary structure pattern. Otherwise, specify a regular expression, for example "?HHH___EE[!_]".
- *r_RMSD_tolerance:* RMSD threshold to accept a fragment as a solution. To avoid time−consuming `optimal 3D superposition` during the search, **distance Rmsd** (i.e. root−mean−square deviation between two Ca−atom distance matrices of the compared fragments) is used as a measure of spatial similarity on the preliminary stage of each comparison. However, in the resulting list of hits, collected in *SearchSummary* `string array` the optimal 3D superposition coordinate `Rmsd` is presented. Therefore, RMSDs in the output list may exceed the specified threshold.

Hits will be stored in `s_out` . The following just illustrate the syntax, it does not make much sense, since you need to loop through a database of objects to find something interesting.

Example:

```
read object "crn"
read object "complex"         # object in which to search
find pdb a_1./16:18,20:22 a_2. "xxx----xxx" "C?[LIVM]????G??" "*" 2.5
```

See also: `qsearch` macro.

find prosite or profile

`find prosite` [`append`] *seq_* [*r_minScore*] [*i_mnHits*]

find matching `prosite` patterns, store results in the SITES `table` . Option `append` indicates that the results should be appended to the existing SITES table. The default *r_minScore* is 0.7 . The default *i_mnHits* is defined by the `mnSolutions` parameter.

Examples:

```
read sequence "zincFing.seq"
find prosite 1znf_m
show SITES
```

find pattern

`find pattern` [`number`] [`mute`] *s_sequencePattern* [*i_mnHits*] [{ *os_objectWhereToSearch* | *seq_Name* | *s_seqNamePattern* } ...]

find specified sequence pattern (i.e. "[AG]????GK[ST]" for ATP/GTP−binding site motif A) in sequences or objects. Hits will be stored in `s_out` . `r_out` contains the number of found hits divided by the expected number of hits, as suggested by random distribution of amino−acids with frequencies from the Swissprot database. This "found/expected ratio" is also reported if `l_info=yes.` If this number is 1. it does not mean anything, 10. means that you can publish the finding and two paragraphs of speculations, 10000. means that somebody else has already found this hit. Pattern language:

- ^ sequence beginning
- $ sequence ending
- ? one character
- * any number of any characters
- [ACD] alternatives
- [!ACD] all but the specified residues
- *char* \{ *i_min*, *i_max* \} : repetition. E.g. ?\{5,8\} from 5 to 8 of any character.

Other arguments and options:

- `number` − just report the number of hits instead of reporting each match
- `mute` − suppress terminal output (used in scripts)
- *i_mnHits* − (default `mnSolutions`)
- *os_objectWhereToSearch* − the target molecular object.
- *seq_Name* − the target sequence. By default, the search is performed among **all** currently loaded sequences.

- *seqNamePattern* − the target sequence name pattern to search through many sequences loaded to the shell.

Returned values

- `s_out` − text output of all matches
- `i_out` − the number of hits
- `r_out` − the ratio to the random expectation (it r_out>1. it means that the number of hits is larger than the random expectation).

See also the `searchPatternPdb` macro.

Examples:

```
read sequence s_pdbDir + "/derived_data/pdb_seqres.txt"  # all pdb−sequences
find pattern "[AG]????GK[ST]"   # search for ATP/GTP−binding sites
searchPatternPdb "^[LIVAFM]?\{115,128\}[!P]A$"
    # ^ : seq.start; ?\{115,128\} from 115 to 128 of any res.; $ : seq.end
```

See also: `read prosite`, `s_prositeDat` .

find segment: database search for a similar protein fold

`find segment` *ms_source* [*os_objectWhereToSearch_2*] [*r_maxRMSD*] [*i_minNofAlignedResidues* [*i_accuracyParam*]]

find similar 3D structural motif with the given minimal length. The topology of the specified molecule *ms_source* is searched for either in the second object or, by default, in the whole segment databank (`foldbank.seg`) which currently contains 2177 protein folds. Only structures with unique polypeptide sequences are included in the fold databank. You may create, save or append to the `foldbank.seg` a simplified topology description of your own file or a set of files (see `write segment`, `read segment`). The optional *r_maxRMSD* argument specifies a root−mean−square deviation threshold of the coordinates of the ends of secondary structure vectors (default 3.0 A). Default *i_minNofAlignedResidues* is 30 residues. Argument *i_accuracyParam* (do not use it without special needs) defines the number of distances for each reference point which are taken into account in the distance RMSD calculation. Default value equals 3 (distances).

Examples:

```
read object s_icmhome+"crn" # crambin
assign sstructure segment   # broken line through seq.str.−elements
Info>   9 segment elements for  a_crn.m : EHHE
read segment s_icmhome + "/foldbank"
find segment a_1           # default threshold RMSD less than 3A
                           # default minimal overlap is 30 residues
find segment a_1 15 2.     # threshold RMSD 2A ; more solutions,
                           #  minimal overlap 15 residues
nice "2plh.m/"             # looks just like crambin!
```

2.20.29. fix

`fix` *vs_*

fix (exclude from the free variable list) specified variables (such as bond lengths, angles and phases or torsions) in an ICM−object. This operation can be applied to the `current object` only (use `set object os_object` first). See also: `unfix` .

Examples:

```
set v_//omg 180.               # set all omega torsions to the ideal value
fix v_//omg                    # fix all omega torsions

fix v_/8:16,32:40/phi,PSI,omg*  # fix the backbone in two fragments
```

Note using `PSI` torsion reference for correct residue attribution.

2.20.30. for

`for`

is one of the `ICM flow control` statements, used to start a `loop` in the ICM−shell. See also `while`, `endfor` .

2.20.31. fork

a powerful tool for parallelization of ICM−shell scripts.

`fork` [*i_nExtraProcesses*]

spawns one or the specified number of extra copies of ICM. This command will only work in a non interactive mode, i.e. you should run icm like this:

```
icm _multiProc  # from the unix shell or
unix icm _multiProc  # from the interactive ICM-shell
```

The `iProc` shell variable will contain the current process number. The parent process has *iProc* = 0.

An example script _multiProc with a hypothetical macro bigDatabaseJob which takes two arguments: the number of database chunks, the current chunk number, and the output file name:

```
read libraries
macro bigDatabaseJob i_nChunks i_Chunk s_outFile  # definition
 ...
endmacro

read sequence "hot"
fork 4
           # spawn 4 extra processes, total 5
bigDatabaseJob 5  iProc  "out"+iProc
           # work on section iProc,
           # save results to files out1 out2 ..
```

```
wait       # also quits all extra processes
unix cat out1 out2 out3 out4 out5 >! out.tab
read table "out.tab"
....
quit
```

2.20.32. fprintf

`fprintf` [`append`] *s_file s_formatString arg1 arg1 arg2 arg3 ...*

formatted print to a file. The specifications for *s_formatString* are described in the `printf` command section. In contrast to the `print` and `printf` commands, the result of the fprintf command is not shown. E.g.

```
fprintf        "a.txt" "%s\n"      "Day Temparature"
fprintf append "a.txt" "%s %.2f\n" "Monday", 22.4
fprintf append "a.txt" "%s %.2f\n" "Tuesday", 27.334
```

2.20.33. global command

`global` *any_ICM_command*

guarantees that the new ICM shell variables created or read to the shell are at the main shell level, rather than nested inside macros.

By adding `global` to any `read` command in a `macro` you make the `keep` *variableName_or_type* command at the end of the macro unnecessary.
Example:

```
macro read_alignment s_file
  global read alignment s_file
endmacro
```

2.20.34. goto

`goto`

is one of the `ICM flow control` statements, used to `jump` over a block of ICM−shell statements. See also `break` , `continue` .

2.20.35. group

group sequence

`group sequence` [{ *seq1 seq2 ...* | *s_seqNamePattern* | *alignment*] *GroupName* [`unique` { *i_MinNofMutations* | *r_MinDistance* } [`delete`]]

group sequences into a sequence group to perform a multiple alignment with the align command.

Option `unique` allows you to select only the different sequences. If no argument follows the word `unique,` only identical sequences will be dismissed, otherwise they will be compared and retained if the

number of differences is greater than *i_MinNofMutations* (integer argument) or the distance between two sequences is greater than *r_MinDistance* (real argument). The comparison criterion is complex and has the following set of preferences which may be useful in extracting a representative subset of sequences from a PDB−database:

- **longer** sequence is better that shorter
- if the names contain the X−ray **resolution** 2 digit suffixes (like a19 and 9lyz24, for resolutions 1.9 and 2.4 respectively), higher resolution is better (1.9 is better than 2.4).

  Note Resolution suffixes are added by the `read pdb sequence resolution` command
- higher number in a pdb−file name is preferable, i.e. 9lyz is better than 3lyz. (I would not die for this principle, though).
- identical chains have alphabetical preferences (e.g. 9lyz_a is better than 9lyz_b).

Suboption `delete` tells the program to delete from ICM−shell all the sequences which were found redundant by the `unique` option.

Examples:

```
read sequences s_icmhome+"seqs.seq" # load sequences
group sequence aaa                  # group ALL the sequences into aaa
group sequence seq3 seq1 seq2 aaa   # explicit version of the previous line
align aaa                           # multiple alignment

read sequences s_icmhome+"azurins.msf" # some of sequences are very close
                                    # but not identical
group sequence myAzur unique 0.15   # 0.15 is a Dayhoff−corrected minimum
                                    # intersequence distance threshold
group sequence myAzur unique 26     # all sequence pairs differ in
                                    # more than 26 positions
group sequence myAzur unique delete # duplicates will be removed
```

group sequence unique=: clustering, redundancy removal and assembly

`group sequence unique=` "nt,junk,simple,overlap[> *nRes*]"] [`i_wordLen=`6 [`i_dictDepth=`10 [`i_nofMutations=`0]]] [`delete`] [`nosort`] [{ *seq1 seq2 ...* | *s_seqNamePattern* | *alignment*] *GroupName*

If you read a very large **redundant** set of sequences and sequence fragments some of which may (i) overlap or (ii) be included in another sequence, you may want to remove all the redundant fragments, and merge the overlapping sequences into a smaller number of longer sequences. In a simple case, if the number of sequences is not too large (less than a few hundred), this removal of redundancies and fragments in your sequence set, can be performed with the `group sequence unique ..` command described in the previous section.

To work on much larger sequences sets and allows to merge overlapping sequences a more advanced algorithm is needed. This ultra−fast removal of redundant protein or DNA sequences, may also assemble the sequences into larger consensus sequences and is invoked by `group sequence unique=` *"options"* command.

The command returns the result as a sequence group *GroupName*. Will work on tens of thousands of sequences at once. The important features of the command:

- it can cluster/unique millions of sequences very quickly (your computer just needs enough memory).
- larger sequences incorporate the matching smaller ones.
- merged or absorbed sequence names are added to the description of their master unless `nosort` is specified
- merging (option "overlap") protein sequences requires sticky C−terminus letter 'X'
- the algorithm is based on a dictionary approach and allows to have mismatches
- matching rules:
    - for proteins: any letter matches 'X', B=(D or N) and Z=(E or Q)
    - for nucleic acids: any letter matches 'N'
    - if possible, 'X','N','B','Z' are replaced by a more specific letter from the matched sequence

Options (they can be combined in a comma−separated string, e.g. `"nt,simple,junk"`):

- `delete` − the non−unique sequences are deleted not only from the group but also from the shell
- `nosort` − do not merge descriptions of the merged sequences
- `unique= "simple"` − the fastest mode. It will eliminate `only` the exact duplicates.
- `unique= "nt"` means that DNA or RNA sequences are compared (the program assumes protein sequences by default and a corresponding *i_wordLen* of six). This implies the alphabet of A,C,G,T (or U) and the word length should therefore be increased. The default nucleic acid sequence word length of 13 allows to fit the entire dictionary into the memory of 256 Mbyte. If your computer has less memory, reduce the *i_wordLen* to a smaller value.

- `unique="junk"` this option tells the program to remove sequences that do not contain any meaningful sequence. This means that they are mostly composed of 'X's or 'N's and the intermittent sequence is shorter than *i_wordLen.* This option is almost always useful.

- `unique="stripX"` this option tells the program to strip X (or N for nucleotide) character stretches from the beginning and from the end of the sequence. Those will be compressed into just one character. Useful if your sequences were *dusted* or repeat−masked.

- `unique="noX"` this option tells the program to skip the sequence quality enhancements (replacement of 'X','N','B','Z' by a more specific letter from the other very similar sequence).

- `unique="complement"` with this option the complementary nucleic acid sequences will also be considered and removed if redundant. This option **can not be combined with the "overlap" option**.

- `unique="overlap[>numberOfRes]"` Merge overlapping fragments in in addition of deleting the subfragments from the set. The number of overlaping nucleotides or amino acids can be redefined, e.g. `unique ="overlap>25"`
    - Two **aminoacid sequences** are merged only if there is the overlap is greater than the threshold (12 aminoacids by default) and the overlapping C−terminal residue is 'X'.

      An example of the allowed merge for protein sequences:

      ```
      s1     VTIKIGGQLKEALLDXGADDTVLEEMSLPGX-------
      ```

```
s2     ----------EALLDTGADDTVLZEMSLPGRWKPKMIG
result VTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIG
```

If for some reason your ESTs do not terminate with 'X's, they can be added by the following procedure:

```
for i=1,Nof(sequence )
  sequence[i] = sequence[i] //Sequence("X")
endfor
```

- Two **nucleic acid sequences** are merged if the overlap is 30 by default. There are NO special requirements for an 'X' nucleotide flanking the sequences.

- *i_wordLen* (6 by default, 14 if the `unique="nt"` option is specified). The length of a word in the dictionary. The memory occupied by the dictionary depends exponentially on his length.
- *i_dictDepth* (10 by default) limits the number of sequence fragments referenced referenced from a single 'word'. This option prevents the dictionary from growing to much in memory (what the product of *i_wordLen* * i_dictDepth) .
- *i_nofMutations* (zero by default) the maximal number of mutations/mismatches between sequences which are considered to be redundant.

See also:

- `Trans`(*seq_* frame) − to translate a DNA sequence
- `align new` # to align a cluster and generate the consensus
- `Find`(*sequence* , *s_keyword*) # to find a retired sequence with the *s_keyword* in its title among the newly formed sequences
- `show [color]` *ali_*

group table

`group table` [`copy` | `append`] [*t_tableName*] [*array* [*s_name*] *array* [*s_name*] ..] `header` [*shellObj s_name shellObj s_name* ..]

create a new `table` from individual arrays or append new columns or table header elements to an existing table. This example shows how an ICM table including both header elements and columns may look like:

```
group table t {1 2} "a" {"one","two"} "b" header "trash" "comment" 2001 "year"
 Info> table  t  (2 headers, 2 arrays) has been created
  Headers: t.comment t.year
  Arrays : t.a t.b

show t
 #>s t.comment                    # TWO HEADER ELEMENTS
 trash
 #>i t.year
  2001
 #>T t
 #>-a----------b----------        # TABLE ITSELF
    1           one
    2           two
show t.comment t.year
```

```
trash
  2001
```

Options:

- `copy:` make a copy of the original ICM−shell object and move it to the table.
- `append:` add specified ICM−shell objects to the table (default: overwrite).

In the header section each ICM−shell object should be followed by a string specifying the variable name. The empty string will be interpreted as an indication to keep the name of the variable. Unnamed constants such as {1 2 3} or "adsfasdf" will be automatically assigned unique names. See also: `split`, `Table` .

More examples:

```
a=1   # integer a
b=2.  # real b
group table copy t header a "ii" b "rr"
      # create table t with t.ii and t.rr header objects
show t
group table t header a "" b ""
      # t with t.a and t.b header objects
show t
group table t {1 2 3} {2. 3. 4.}
      # t with automatically named table
      # arrays t.1 and t.2
show t
group table t {1 2 3} "a" {2. 3. 4.} "b"
      # t with table arrays t.a and t.b
show t
split t # split the table into individual arrays
```

See also: `group by column`

group table by column with non−unique values

`group` t.keyColumnToGroupBy [t.columnToApplyFuncTo [_function,name]] ...

Group a table by unique values of the key column *t.keyColumnToGroupBy* . Then apply the specified functions to other specified columns.

The following functions can be applied to the numerical arrays:
`uniq|mean|min|max|first|last|rmsd|sum`

The string arrays can be grouped with the following subset of the above functions:

`uniq|min|max|first|last`

The `uniq` function is the default, and it means that the unique column values with the same *key* field will be accumulated by the group command.

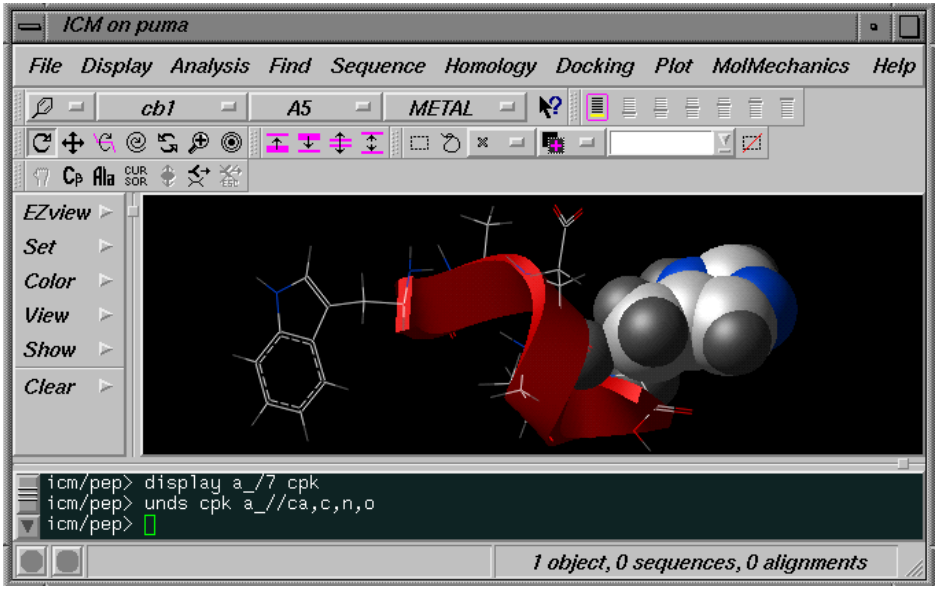
Example:

```
group table t {1 2 1 1 2} {1. 2. 3. 4. 5.}
```

```
t
 #>T t
 #>-A----------B----------
    1           1.
    2           2.
    1           3.
    1           4.
    2           5.

group t.A
t
 #>T t
 #>-A----------B----------
    1           1.,3.,4.
    2           2.,5.

group table t {1 2 1 1 2} {1. 2. 3. 4. 5.}
group t.A t.B "sum,C"  # sum t.B values and call the column C
#>T t
#>-A----------C----------
   1           8.
   2           7.
```

2.20.36. gui

`gui [ simple ]`



start menu−driven graphical user interface from command line. The GUI runs the icm.gui file containing all the commands invoked by menus or pop−ups.

Option `simple` allows you to keep your terminal window separate from the graphics window.

```
% icmgl
 gui simple
```

You can also invoke gui from the command line, e.g.:

```
icm -g # or
icm -g mymenus.gui
icm -G mymenus.gui  # keep the original terminal window
```

Terminal window and fonts

`icm -g` (or `gui` command) invokes a GUI frame *with its own built-in terminal window* . To influence the font size in this terminal window, modify `XTermFont` record of the `icm.cfg` configuration file, e.g.

```
XTermFont *-fixed-medium-*-*-*-24-*
```

If you prefer to keep the original terminal window use the `icm -G` option or invoke the `gui simple` command from ICM shell (I keep `alias guis gui simple` in my personal configuration file). In this case you can change the font of the terminal window with standard means of the window manager.

3D Graphics window

GUI has a GL-graphics window which can be undisplayed with the

```
 undisplay window
```

command or from GUI by choosing `Clear/No_graphics` menu item.

Programming GUI

To program GUI you need to modify a single file, called `icm.gui` . This file resides in the `$ICMHOME` directory. The icm.gui file contains sections for each menu item. It the menu item requires a dialog, a widget is automatically generated.

The `icm.gui` section consists of the following fields:

Field	Example	Description
MENU	Display.Advanced.Pockets	this menu item will be added in the top menu bar
SIDE	Display.Advanced.Pockets	alternative to MENU, will be added in the **side** menu bar
OPTN	Apply	optional. Allows to specify special kinds of dialogs.
SYNT	display g_pocket	the ICM-command executed upon pressing 'OK' or 'Apply'.

An example:

```
MENU Display.Color.White
SYNT color white
```

To see how to specify arguments in a dialog, see the `icm.gui` file.

2.20.37. help

get help from `icm.htm` file. Set `s_helpEngine` variable to "icm" (internal help in the text window), "netscape" or any other web−browser.

help

`help` [`input=` *s_fileName*] [*word1 word2 ...*]

get full help in either text or html form, redirect it to the specified file, if the `input` option is specified. If you need help on a complex expression like `read sequence` , merge the words into one, e.g. `help readsequence` . Do **not** use plural forms of the nouns. Examples:

```
help Random
help readsequence
```

The built−in help engine does not know about keywords. It is recommended to use the on−line version of the ICM manual which has a well−developed Index (download the newest version of the manual, `man.tar.gz` from the Molsoft ftp site).

help commands

`help commands` [*s_Pattern*]

generates concise list of syntax lines for all or specified commands.

help functions

`help functions` [*s_Pattern*]

generates concise list of syntax lines for all or specified functions.

Examples:

```
help                    # type  /stereo, and then letter n or Bar

help help               # how to get help

help commands           # list syntax of all commands

help commands  "rea*"   # list syntax of all read commands

help functions          # list syntax of all functions

help functions Matrix   # list syntax of the Matrix family of functions

help                    # start the browser to use its own search means
help montecarlo         # just the command name
help real constant

help readpdb

help Split
```

```
s_helpEngine = "netscape" # view help via netscape
help input="myHelp.htm" real constant
```

2.20.38. history

`history` [`unique`] [*i_NumberOfLines*]

display previous commands. Option `unique` squeezes out the repetitive commands. For example:

```
history 20              # show last 20 lines
history unique
```

To delete all previous history lines, use the `delete session` command. In this case the `write session` command will save only the new history lines.

2.20.39. if

`if`

is one of the `ICM flow control` statements, used to perform `conditional statements`. See also: `then`, `elseif`, and `endif` .

2.20.40. keep

`keep` ICM−shell−variable−name1 ..

retain specified ICM_shell variables or their classes (e.g. real, rarray etc.). This command is used in macros to avoid automatic deletion of all the local ICM−shell variables.

Also note that four classes of standard ICM−shell variables, `real`s, `integer`s, `logical`s, and `preference`s, are automatically restored to their initial values by default. You can use the keep command to retain their new values.

Examples:

```
macro rdseq s_pdbName  # extract sequence from a pdb−file
  read pdb sequence s_pdbName
  rz = Resolution(s_pdbName,pdb)
  mncalls = 10         # the existing standard shell variable
  keep rz, sequence    # retain all the sequences and rz
  keep mncalls         # retain its new value
endmacro
```

2.20.41. link internal variables of molecular object

`link` *vs_variablesToBeLinked*

impose a chain of equality constraints (*v[1] = v[2] = v[3] = ... = v[n]*) on the specified variables (or, in other words, keep the specified variables equal to each other). If one of the variables is changed all the others will be changed. Energy derivatives are modified accordingly. This command is great for modeling

periodic structures (e.g. (Pro−Glu)n).

Examples:

```
buildpep "ala ala ala ala ala ala ala ala ala ala"  # 10 alanines
link v_//phi                   # all the phi angles should be equal
link v_//psi                   # all the psi angles should be equal
montecarlo v_/2/phi,PSI v_*    # sample just one residue
```

Be careful with selections of `psi` variables in peptides since they are assigned in ICM to the first atom of the *next* residue. `PSI` specification goes around that attribution.

2.20.42. link residues to sequences and alignments

`link` *ms_molecules* { *ali_* | *seq1 seq2 ...*}

link or associate protein molecules with separate sequences or sequences grouped in an *alignment.* If alignment *ali_* is given, molecules are also linked to this alignment (note that the same sequence can be involved in several different alignments). Amino−acid sequences of *ms_molecules* will be compared with specified ICM−shell sequences and identical pairs will be linked. Make sure that you specify **one** molecule selection, use logical or (|) between the two selections if necessary. Linking molecules with alignments allows an automatic residue−residue assignment by the following commands and functions: `superimpose`, `set tether`, `Rmsd` and `Srmsd` . Alignments can be prepared in advance either automatically by the `align` command or `Align` function, and/or modified by manual editing of the alignment file.

Use the `ribbonColorStyle="reliability"` option and `color ribbon` to display the local strength of the alignment. The strength parameter will be 3D averaged with the `selectSphereRadius` radius.

The following illustrates the first step of homology modeling.

Example:

```
build "newseq"                # that is what you want to build by homology
read pdb "template.pdb"       # that is the known pdb−template
read alignment "seq3Dali.ali" # prepared/modified sequence alignment
                              # of the two structures
set object a_1.               # this is the first molecule that we
                              # are going to model
link a_*. seq3Dali            # establish links between sequences
                              # and objects
set tether a_1,2.1 seq3Dali   # impose tethers according to the alignment
minimize tether               # fold it according to the template
```

See also: `l_autoLink`

2.20.43. list

`list`[`alignment`][`command`][`factor`][`function`][`grob`][`iarray`][`integer`][`logical`][`macro`][`map`][`matrix`][`object`][`profile`][`rarray`][`sarray`][

`sequence`] [`string`] [*name1 name2 ...*]

list ICM−shell objects matching the name pattern (all if name−pattern is omitted). The plural form can be used for more natural expressions. 'list commands' actually means list all legal words known by ICM (ICM command words).

Examples:

```
 list                          # list the "most wanted" object-types
 list functions
 list sequences                # if you have aliases, you can
                               # type 'ls se' instead
 list "*my*"                   # all ICM-shell variables containing "my"
```

2.20.44. list the content of the icm binary file

`list binary` [*s_binaryFileName*]

list the table of contents of the icm−binary multi−object file. The default name is −"icm.icb" and the default extension is `".icb"` . To read the whole archive, use the `read binary` command. For a subset of objects, add the `name=` *S_listOfNames* option.

Note that the archive can also store graphical view parameters, tethers between the objects, and a string buffer with the last session.

Example:

```
list binary s_icmhome + "example_docking"
 Binary file version: 1
    1 mn_saveAll                    integer                4
    2 a                             integer                4
    3 S_LoopString                  sarray                28
    4 S_LoopVar                     sarray                28
    5 S_currentDockProj             sarray               396
    6 g_image_mesh_12               grob                100992
    7 g_image_mesh_13               grob                 88596
    8 m_gb                          map                 114280
    9 m_gs                          map                 114280
   10 biotin                        object                5490
   11 DOCK1_rec                     object              265167
   12 displayView                   graphical view         293
   13 s_last_session                string                5322

read binary name={"biotin","DOCK1_rec"} "example_docking"
```

2.20.45. list available sequence databases

`list database`

gives a list of BLAST databases which can be used by the `find database` command for fast sequence database searches. Normally, your system administrator should update the `BLAST` sequence files. ICM just needs a path to this directory which is defined by the $BLASTDB system variable. The output of the command is saved in the `S_out` array. This array can further be processed with the `Field` function.

Example:

```
list database
dblist = Field(S_out, 2) # sarray contains search databases
show dblist
a=Sequence("PDPPLELAVEVKQPEDRKPYLWIKWSP")
find database a dblist[2]
```

Trouble−shooting: If you get an error message, check the following:

- check if you have a directory with the blast−formatted files.
- make sure that your `s_dbDir` variable is defined in your `_startup` file and it contains the path to this directory (do not forget the last slash, e.g. `/data/blast/dbf/`). You can always assign it manually from the command line.

2.20.46. load

load things from the program memory (to load from disk files use `read` command). The opposite action to load is `store`.

load conformation from stack

`load conf` *i_confNumber* [`sstructure`]

assign the *i_confNumber−th* conformation from the conformational stack and to the current object (e.g. when you browse conformations accumulated after a `montecarlo` run). If *i_confNumber* is zero, the best energy conformation will be loaded. Montecarlo stack conformations are sorted according to energy values, however you may create your stack manually with an arbitrary order.

Option `sstructure` will automatically recalculate the secondary structure according to the hydrogen bonding pattens.

Note that the full energy of this conformation which had been stored in the `stack` can be accessed by the `Energy("func")` function.

Example:

```
read stack "f1"             # read conformational stack
load conf 0                 # set molecule into the best energy conformation
display a_//ca,c,n          # display the backbone
for i=1,Nof(conf)           # go through all the conformations
  load conf i               # load them one by one
  print Energy("func")      # extract its energy
  pause                     # wait for RETURN
endfor
```

load movie frame conformation

`load frame` *i_movieFrameNumber* [*s_movieFileName*] [`sstructure`]

load specified frame from the movie. Note that the full energy of this conformation which had been stored by the simulation procedure can be accessed by the `Energy("func")` function. Option `sstructure` will automatically recalculate the secondary structure according to the hydrogen bonding pattens.

Examples:

```
build "alpha"     # build extended chain of the Baldwin peptide
read movie "alpha"
display movie "alpha" center # a-ha! conf in frame 541 is interesting
load frame 541 "f1"          # extract conformation from frame 541
print Energy("func")         # print its energy without recalculating
```

load a structural alignment solution

`load solution` [*i_solutionNumber*]

loads the specified solution previously stored by the `align` *`rs_residue1 rs_residue2`* .. command. The two output selections as_out and as2_out contain equivalent residues of the specified solution. The second object will be superimposed according to the Ca atoms of the found equivalent residues.

Example:

```
read pdb "4fxc"
read pdb "1ubq"
display a_*.//ca,c,n
color molecule a_*.
align a_1.1 a_2.1 12 1.5 .1
center
load solution 2          # load the second best solution
color red  as_out
color blue as2_out
for i=1,10
  load solution i
  color molecule a_*.
  color red  as_out
  color blue as2_out
  pause                  # rotate and hit 'return'

endfor
```

2.20.47. ICM-shell macros

macro define a new macro command.

Syntax:

`macro` *macroName* [`mute`] *prefix1_macroArg1* [**(** *default1* **)**] *prefix2_macroArg2* [(default2)] ...

```
  # commands
  # commands
endmacro
```

To invoke macro just type its name and provide arguments if necessary. Argument names should have explicit prefixes (i_ , r_ , s_ , l_ , p_ , I_ , R_ , S_ , M_ , seq_ , prf_ , ali_ , m_ , g_ , sf_ , as_ , rs_ , ms_ , os_ , vs_ , see `above`) to specify their type. If your argument list is incomplete, you will be prompted for the missing argument. Type `q` or enter **empty string** to `quit` the macro without execution. The following features make ICM macros extremely convenient to use:

- no need to explicitly define types of arguments (implicit definition by name)
- one may specify an arbitrary subset of arguments and in arbitrary order if the arguments have different types
- automatic prompting of the missing arguments
- an easy and flexible way to provide defaults in parenthesis after the argument
- automatic restoration of all the changed standard ICM−shell variables upon execution.
- new variables defined in the macro are local and will be automatically deleted upon execution, unless they are protected with the `keep` command.

Defaults can be provided in parentheses as simple constants (i.e. i_window (8)), or as the whole expressions (i.e. i_1 (mncalls) r_a (Sin(*2.)) i_2) . Default expressions can also be omitted.

Options

- `auto` automatically use defaults for the arguments missing in the command string. Example: **nice "2ins"**. Since the second logical argument l_wormStyle is missing its default value `no` will be used automatically.
- `mute` will suppress automatic prompting. Do not use parenthesized defaults with this option.

The predefined standard ICM−shell `integer`, `real`, and `logical` variables, as well as `preferences` (i.e. i_out, l_warn, wireStyle, PLOT.logo etc.) are be automatically restored upon completion, if changed in the macro, to retain the new value use the `keep` command. Note that the string variables should be restored explicitly. Many `macros` are supplied with the program.

Examples:

```
# display molecule as a worm colored from N− to C− term.
 macro dsWorm ms_ (a_*) r_wormRadius (0.9)
  GRAPHICS.ribbonWorm = yes
  GRAPHICS.wormRadius= r_wormRadius
  display ms_ ribbon only
  for i=1,Nof(ms_)           # color each molecule separately
    color Res(ms_[i]) Count(Nof(Res(ms_[i]))) ribbon
  endfor
 endmacro
```

To invoke the macro, type

```
 read object "crn"
 dsWorm a_1 0.7
```

or just

```
 dsWorm  # and press Enter
```

A set of `ICM macros` is given in the `_macro` file.

2.20.48. make

is a family of commands which create new objects of parts of them.

make bond: forming a covalent bond

`make bond` *as_singleAtom1 as_singleAtom2* [`type=` *i_type*]

adds a covalent bond between two selected atoms in a non−ICM molecular object (e.g. X−ray or NMR pdb−entries) or resets the bond type. The command is used to correct erroneous connectivity guessed by the `read pdb` command. This correction makes the molecule displayed in the graphics window look better and is necessary before conversion into an ICM molecular library entry (see `icm.res` or user library files) using the `write library` command. It can also be useful to display a connected Ca−trace. In interactive graphics mode you may type `make bond` and then click two atoms with the Control button pressed.

The `type=` option allows to set the bond type (*i_type* `={1|2|3|4}` , for a single (default), double, triple and aromatic bond, respectively.

make bonds in an atomic chain

`make bond` *as_chainOfAtoms*

connects specified atoms in a linear chain. Useful for PDB entries containing only Ca atoms.

Examples:

```
read pdb "4cro"        # contains only Ps and Ca's
display                # Milky sausage
make bond a_4cro.//p   # connect P atoms of the DNA backbone
make bond a_4cro.//ca  # connect Ca atoms of the protein backbone
```

See also: `delete bond`.

make boundary: Poisson electrostatics

a command to prepare for the boundary element electrostatic calculation

`make boundary` [*as_*]

this is an auxiliary command which is required if you need to calculate the electrostatic free energy with the boundary element method several times. Optional atom selection `as_` from which the electrostatic field is calculated can be specified. This may be the case if the charge distribution changes but the shape does not. However, the boundary does depend on the dielectric constant parameters such as `dielConst` and `dielConstExtern` . If you intend to change them the boundary need to be remade every time. This command does not generate any output by itself, it just creates the internal table which can later be used by the `show energy` command or the `Potential( )` function.

The dielectric boundary is a smooth analytical surface which is built with the contour−buildup algorithm (`toa96{` Totrov,Abagyan, 1996). The surface looks like the `skin` surface, but uses different radii which

were optimized against experimental LogP data. Both skin and the dielectric boundary uses the same water radius (the `waterRadius` parameter). The "electrostatic" radii used by ICM to calculate the boundary are stored in the `icm.vwt` file.

See also: REBEL, `electroMethod`, `delete boundary`, `show energy"`, `term "el"`, `Potential( )`.

Examples:

```
electroMethod="boundary element"
read object "rinsr"
delete a_w*       # get rid of water molecules
make boundary a_1 # calculate parameters of the dielectric boundary
show energy "el"  # electrostatic energy by BEM
e1=Energy("el")   # extract the energy
set charge a_/33/cd*,hd*,ne*,he*,cz,nh*,hh* 0.  # uncharge arg33
show energy "el"  # electrostatic energy of the uncharged Arg33
e2=Energy("el")   # extract the energy
print e1-e2
delete boundary  # memory cleanup
```

make directory

`make directory` *s_Directory*

make specified directory. Example:

```
make directory "/home/doe/temp/"
```

See also: `set directory`, `delete directory`, `Path`(directory)

make disulfide bond

`make disulfide bond` [`only`] *as_atomSg1 as_atomSg2*

form breakable disulfide bonds between two sets of specified sulfur Sg atoms, regardless of the distance between them. Forming the bond means that two Hg hydrogens of Cys residues are dismissed, a covalent bond between two Sg is declared (but not enforced) and four local distance restraints (see `icm.cnt`) are imposed. These restraints are indeed local, since two Sg atoms only start feeling each other when they are really close, otherwise the energy contribution is close to zero . Option `only` causes deletion of previously formed disulfide bonds, otherwise the new one is added to the existing list of disulfide bonds.

Examples:

```
build string "se cys ala cys" # sequence containing two cysteins
display                       # display an extended ICM model of the sequence
                              # set only one SS-bond, disregard all previous
make disulfide bond a_/1 a_/3 only
montecarlo                    # MC search for plausible conformations
```

See also: `delete disulfide bond` and **(important!)** `disulfide bond`.

make drestraint: extract distances structure

`make drestraint` *as_select1 as_select2 r_LowerBound r_UpperBound r_LowerCorrection r_UpperCorrection* [*s_fileNameRoot*]

create two files containing the list of all the atom pairs specified by two selections (i.e. a_* a_* − all the pairs; a_1//* a_2//* atom pairs between molecules 1 and 2 for which the interatomic distance lies between *r_LowerBound* and *r_UpperBound.*

Note: it is critical that both selections are in the **same** object. Only `tethers` can pull to atoms of a different object.

For each pair of atoms a `distance restraint type` is created with lower bound less than the actual interatomic distance by *r_LowerCorrection* and upper bound greater than the actual interatomic distance by *r_UpperCorrection.* This command can be used for example to impose loose distance constraints between two subunits.

The number of the formed drestraints is returned in the `i_out` variable.

See also: `set drestraint` as_1 as_2 i_Type

if you want to impose a specific drestraint.

Examples:

```
 read object "complex"  # load a two molecule complex for refinement
                        # extract all Ca-Ca pairs between 2 and 5 A
                        # for each pair at distance D create distance
                        # restraint type with lower bound D-2.5 and
                        # upper bound D+2.5
 make drestraint a_1//ca a_2//ca 2. 5. 2.5 2.5
```

make factor: FFT calculation of diffraction amplitudes and phases

`make factor` *map_Source* { *I_3Maximal_hkl* | *r_resolution* } [*s_factorTableName* [*s_ReName* [*s_ImName*]]]

calculate structure amplitudes and phases from the given electron density map by the Fast Fourier transformation. The table ' *s_factorTableName'* with h,k,l and structure factors will be created (further referred to as **T** for brevity). It will contain the following members:

- three `integer arrays` of Miller indices: **T.h T.k T.l**
- two `rarray` of real and imaginary parts of the calculated structure factors. Default names: **T.ac** and **T.bc,** respectively. Alternative names can be explicitly provided in the command line.

If structure factor table *s_factorTableName* already exists, structure factor real and imaginary components are created or updated in place. Any other arrays containing experimental, derivative or control information may be added to the table and participate in selections and sorting.

Example:

```
read map "crn"               # load "crn.map"
set symmetry m_crn 1
make factor { 5 5 5 } "F"    # h_max=k_max=l_max=5
                             # F.h, F.k, F.l, F.ac, F.bc are created
show F
group table append F Sqrt(F.ac*F.ac + F.bc*F.bc) "Fc" Atan2(F.bc,F.ac) "Ph"
sort F.Fc
show F
```

make grob map command to contour electron density

`make grob` [`solid`] *m_map* [`name=` *s_grobName*] [`box`] [I_indexBox[1:6]] [{ *r_sigmaThreshold* | `exact` *r_absThreshold* }]

Create graphics object by contouring electron density map at a given threshold.

threshold: By default the contouring level is calculated as the mean map value (returned by `Mean` (*m_map*)) plus `mapSigmaLevel` times root−mean−square deviation value. If a real value argument is provided, the `mapSigmaLevel` shell variable is redefined. Option `exact` allows to specify *absolute* value at the contouring is performed. Example:

```
buildpep "his glu"
make map potential Box( a_ 3.)
make grob m_atoms 3. # 3 sigmas above the mean
#  make grob m_atoms .2 exact # countour at 0.2 level
#  .2 or .1 exact is useful to detect almost closed pockets
display g_atoms
#
make grob m_atoms exact 0.15 # at value of 0.15
display g_atoms
```

Defaults:

- create simple chicken wire map (sections in three sets of planes, NOT solid)
- take the `current map`;
- generate the name of the grob which is the same as the map name except for the `g_` prefix;
- contour the whole map
- use threshold value from the ICM−shell real variable `mapSigmaLevel` .

Option `solid` tells the program to create a solid triangulated surface which can later be displayed by `display grob solid` command. The threshold is expressed in the units of standard deviations from the mean map value, i.e. 1.0 stands for one sigma over the mean. *I_indexBox* [1:6] is optional 6−dimensional `iarray` containing { i_startSection i_startRow i_startColumn i_NofSections i_NofRows i_NofColumns }. It overrides the default, contouring the whole map.

Option `box` adds surrounding box to the grob.

make grob image command to create a vectorized graphics object.

`make grob image` [`name=` *s_grobName*]

create a vectorized `graphics object (grob)` from the displayed wire or solid objects. The information about colors will be inherited. Very useful if you want to export wire, `ribbon` or CPK into another graphics program, since graphics objects can be `written` in portable Wavefront (.obj) format. Further, graphics objects can exist independently on the molecules which may be sometimes convenient. Also, underlying lines and vertexes can be revealed. The graphics object created from the displayed solid representations assigns and retains color information as lit in a given projection. These colors can not be changed. Use special `make grob skin` command to generate a more elaborate graphics object from `skin` .

Examples:

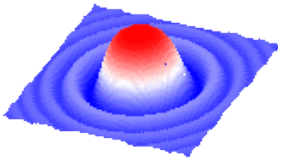
```
 ds a__crn.//!h* ribbon  # ribbon
 make grob image name="g_rib"
 display g_rib smooth only # try select g_rib and Ctrl-X,Ctrl-E/W etc.
# option smooth eliminates the jaggies.
 write g_rib              # save to a file
```

make grob matrix

`make grob` [`solid`] [`bar` [`box`]] [`color`] *M_matrixName* [*r_istep r_jstep*] [[`name=`] *s_grobName*]

Create a three−dimensional plot from *M_matrixName*, so that x=i* *r_istep*, y=j* *r_jstep* and F(x,y)= *M_matrixName[i,j]*. Options:

- `bar` : generate rectangular bars for each i,j matrix value instead of a smooth surface.
- `box` : add a box around the 3D histogram
- `color` : color grob by value according to the `PLOT.rainbowStyle` preference.
- `solid` : tells the program to triangulate the surface



Examples:

```
 read matrix s_icmhome+"def"
 make grob g_def solid
 display
# OR
```

```
read matrix "ram"                    # phi-psi energy surface
make grob ram 1. 1. 0.1              # create the surface
display g_ram magenta                # display it
make grob solid ram 1. 1. 0.08 name="g"   # create the surface
display g solid gold                 # display it
```

make grob potential

`make grob potential` [`solid`] [*as_1* [*as_2*]] [*r_gridCellSize* [*r_margin* [*r_polentialLevel*]]] [[`name=`] *s_grobName*]

create `graphics object` of isopotential contours of electrostatic potential which takes not only the point charges but also the dielectric surface charges resulting from polarization of the solvent. This potential need to be calculated in advance by the `boundary element` algorithm. Contours can be displayed in the `wire` and solid representations (see also `display grob`). The default parameters are:

- *r_gridCellSize* 0.5 A (you may want to increase it up to 2A for speed).
- *r_margin* 5.0 A (you may want to reduce it for speed).
- *r_polentialLevel* 0. kcal/mole/electron_charge_units.

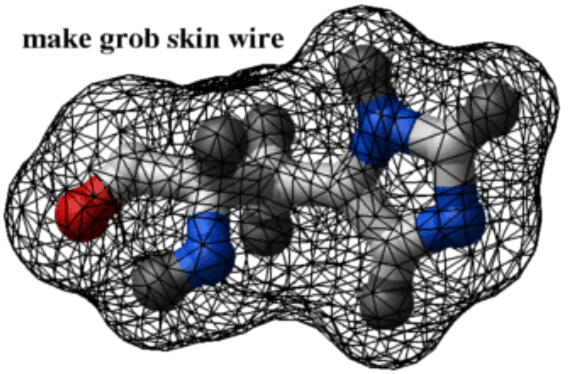
See also: `make map potential`, `electroMethod`, `make boundary`, `show energy "el"`, `term "el"`, `Potential( )`.

Examples:

```
build string "se his arg glu"
electroMethod="boundary element" # REBEL algorithm
make boundary
make grob potential solid 2. 4. 0.1 name="g_equipot1"
display g_equipot1 transparent blue
make grob potential solid 2. 4., -0.1 name="g_equipot2"
display g_equipot2 transparent red
ds xstick residue label
```

`make grob skin` [`wire` | `smooth`] [*as_1* [*as_2*]] [[`name=`] *s_grobName*]

create `grob` containing the specified molecular surface (referred to as skin). If the `wire` option is given the transparent wire grob will be created (solid grob is the default). It will have the same default color. The disconnected parts of this grob may later be `split` . The grob will be named by the default name g_*objName* unless the name is explicitly specified.



The `smooth` option allows to close the cusps. This closure is necessary to enable the `compress` grob operation.

The `compress` *g_* command allows to dramatically simplify the triangulated surface and reduce the

number of triangles. Typically `compress g_ 1.` will reduce the number of triangles by an order of magnitude.
A grob can later be colored with the `color grob potential` command.

Examples:

```
read object "crn"
          # skin around a substructure, (just as an example)
make grob skin a_/1:44 a_/1:44
split g_crn
display g_crn2  a_//*
show Area(g_crn2), Abs(Volume(g_crn2))

make grob skin a_ a_ name="gg1" # display gg1 now
make grob skin wire  name="gg2" # display gg2 now

make grob smooth
compress g_crn 1. # simplifies the surface
```

make key

`make key` { *s_smiles* | *as_* } [*S_arrayOfFragmentSmiles*]

generates a binary chemical key, i.e. a bit−string in which each bit corresponds to a chemical substructure, converts the bit−mask into the hexadecimal string and saves this hex−string in `s_out` . The bit−string with chemical substructure information can then be used to calculate the Tanimoto similary distance with another chemical key.

By default the `make key` command uses a built−in array of 96 substructures, and generates a 24−character hex−string (each hex−character codes for 4 bits), however any string array of subfragment smile−strings (*S_arrayOfFragmentSmiles*) can be provided.

The hex−string can be converted back into an array of bits packed into integers with the `Iarray`({ s_chemkey | S_chemkey } `key`) function.

The bit−distance between two arrays of bit−strings represented by two iarrays can be calculated with the `Distance`(`Iarray`(*S_1* key) `Iarray`(*S_2* key) *i_nBits* [`key`]) or `Distance`(`Iarray`(*S_1* key) `Iarray`(*S_2* key) *i_nBits* `simple`) functions, where the number of bits, *i_nBits*, is usually `96,` unless you use a user defined array of fragments. There is also a weighted form of the chemical key distance (see the `Distance` function). By default, or with the `key` option, the function returns matrix with the Tanimoto similary distance (0. all bits are the same, 1. no bits in common), while with the `simple` option the second chemical key is considered as a sub−fragment and the distance becomes `0.` (identity) if the sub−frament is present in the first bit−mask.

Examples:

```
read mol s_icmhome+"ex_mol.mol"
build hydrogen
set type mmff
convert
```

```
smil = Smiles(a_)
make key s
skey = s_out
```

make map

`make map` *R_6cellParameters I_3NofSteps* [*R_6box* | *I_6box*] ["zxy"] [*as_*] [`name=` *s_mapName*]

create an electron density distribution for atom selection `as_` (all atoms of the current object by default) on a three−dimensional grid. See also `make map potential` for a rough electron density map. The electron density is calculated from the cartesian coordinates of the selected atoms using a 2−gaussian approximation. If the `l_xrUseHydrogen` logical is set to `no` , hydrogen atoms are ignored. The following parameters are taken into account:

- the shape of the gaussian is influenced by the individual atomic b−factors (see `set bfactor`).
- `addBfactor` is added to individual atomic B−factors

R_6cellParameters is a real array containing { *a b c alpha beta gamma* } parameters. Optional *R_6box* or *I_6box* arrays define the corner of the map box (closest to the origin) and its sizes ({ *x1 y1 z1 dx dy dz* } or { *nx ny nz dnx dny dnz* }, respectively). The whole cell is taken by default.

Examples:

```
read object "crn"
make map {5. 5. 5. 90. 90. 90.} 0.5 a_//ca,c,n
```

make map factor : calculate electron density map from structure factors

`make map factor` [*T_factor*] [*m_map*]

calculate an electron density distribution on a three−dimensional grid from a structure `factor` table of the Miller indices, reflection amplitudes and phases. Requires that the map is created before with the `make map` command. If optional arguments are not given the `current map` and/or `current factor` will be used. A new empty map can be created from an empty selection by the

```
make map a_!*
```

parameters # see the `make map` command.

make map potential: grid energies

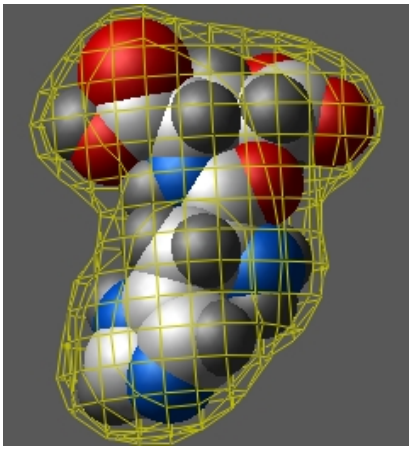
`make map potential` [*s_terms*] [*as_*] [*R_6box*] [*r_gridCellSize*]

create a property `map` for the *as_* selection. This command is used for low−resolution surface generation or to make grid potential maps for fast docking. The optional arguments are the following:

- *s_terms* : a smooth gaussian atom density map is generated by default, otherwise the grid energy maps specified by the

2−letter terms are calculated, e.g. `"gc,gh,gs,ge"`) . The names of the generated maps are standard and can not be changed.

- *as_* selection : All atoms of the current object are taken by default.
- *r_gridCellSize* : by default is 0.5 A for small objects, the default increases with the size of the object. We do not recommend to use values over 7 A for very large objects.
- *R_6box* : default it is a box around the selected atoms plus 3A margnins. The box defines coordinates of the two opposite corners of a box (see also the `Box` function).



`m_atoms` contoured at `0.3` `exact` level. The `0.5` level is closer to the van der Waals surface.

- default (no terms specified): atomic density map `m_atoms` ; if contoured, `m_atoms` generates a smooth gaussian envelope around a molecule (see Figures)

```
 buildpep "his arg"
 display cpk
 make map potential Box( a_ 3.)

# wire surface
 make grob m_atoms 0.3 exact  # contours near vw−raduis.
 display g_atoms

# solid surface
 make grob m_atoms solid 0.5 exact
 display g_atoms smooth
```

- term "el", map m_el : Coulomb electrostatic grid, contributions truncated at +−100. kcal/mol.

```
 build string "se his arg" "test"
 make map potential "el"  Box( a_/1,2/* , 3. )
 display a_
 display map m_el {1 2 3}
 make grob m_el exact  # contouring at 0. potential
 display g_el
```

- term "gh" : van der Waals grid for a hydrogen probe, grid potential is truncated from above according to the `GRID.maxVw` parameter;

- term "gc", map m_gc : van der Waals grid for a carbon probe; grid potential is truncated from above according to the `GRID.maxVw` parameter;

- term "ge", map m_ge : electrostatic grid; grid potential is truncated from above and below according to the `GRID.maxEl` and `GRID.minEl` parameters;
- term "gb", map m_gb : hydrogen bonding grid;
- term "sf", map m_ga : surface accessibility grid. This map is not an independent term, but allows to correctly calculate atomic accessible areas if a part of the system is presented by the grid potentials. If a map named `m_ga` is present it will be automatically taken into account in energy calculations of the `"sf"` term.

Fine−tuning the maps Sometimes you want the van der Waals grids, "gh" and "gc", generated from the whole receptor, while the "ge" or "gb" grids generated only from a small region of the receptor. In this case you can run the command two times with different source−atom selection.

Example:

```
make map potential "gh,gc" a_1 Box()
make map potential "gb,ge,gs" a_1/15:18,33:47 Box()
write m_ge m_gc m_ge  # write three maps at once
```

An alternative method is to use the `Bracket`(*m, R_6box*) function which sets everything beyond the box to zero. Example:

```
make map potential "gh,gc,gb,ge,gs" a_1 Box()
m_ge = Bracket(m_ge, Box( a_1/15:18,33:47 )) # redefine m_ge
```

make peptide bond

`make peptide bond` *as_C as_N_or_S*

form the peptide bond between two selected C− and N− atoms, or the thioester bond between C− and S− atoms. The bonds may be formed between the terminal amino− and carboxy− groups (a_/1/n and the last c), as well as between such amino acid side−chains groups as a_/lys/nz and a_/asp,asn/cd, a_/glu,gln/cg. See also: `delete peptide bond` How to modify an ICM−object .

Example:

```
build string "se nh3+ gly gly gly gly his coo−"
display
make peptide bond a_/nh3*/n a_/his/c       # form a cyclic peptide
display drestraint
minimize "ss"
minimize "vw,14,hb,el,to,ss"
#
# form thioester bond
#
build string "se cys ala ala ala glu"
display
make peptide bond a_/1/sg a_/5/cd
minimize "ss"  # term "ss" is responsible for the extra drestraints
```

make sequence: extract from pdb or icm structure

`make sequence` *ms_* [`name=` { *s_name* | *S_names* }] [`resolution`]

creates sequences (or, more strictly speaking, ICM−shell objects of 'sequence' type) of residues composing selected molecules *ms_*. One−letter equivalents of full residue names are specified in the `icm.res` library. Option `resolution` adds the X−ray resolution value multiplied by 10 to the name (e.g. 2ins_a25 for resolution of 2.5A) or `'No'` for NMR and theoretical structures. The `group sequence` command will automatically prefer a sequence from structure with better `resolution.` This resolution digits The resolution is not appended if option `name=` is specified.

The `make sequence` command also extracts both the secondary structure and the `site` information.

See also: `read pdb sequence`

Examples:

```
make sequence a_2ins.a,b        # two seqs 2ins_a and 2ins_b created
make sequence a_2ins.a,b resolution # resolution*10 added to the name
make sequence a_1.1 name="aa" # sequence named: aa
make sequence a_2ins.a,b name={"aa","bb"} # seqs named: aa and bb
```

make tree

`make tree` *ali_name* [*s_epsFile*]

reconstruct the evolutionary tree from the specified sequence alignment using the neighbor−joining method (Saitou and Nei, 1987). Create a PostScript image of this tree which will be saved in the *ali_name*`.eps` file. See also: the `align` command.

Examples:

```
read alignment msf s_icmhome+"azurins" # read alignment
make tree azurins              # draw evolutionary tree
```

`make tree` M_squareDistanceMatrix[1:n,1:n] [S_objectNames[1:n]] [*s_epsFile*]

reconstruct the evolutionary tree for arbitrary objects from the **matrix of pairwise distances**. The names of individual objects may be provided in a string array for a nicer PostScript picture. This command is cool.

See also: `Disgeo` function.

Examples:

```
read matrix "dist"            # read a distance matrix [n,n]
make tree dist
unix gs dist.eps
```

make unique: reorder atoms in a unique order.

Example:

```
read mol s_icmhome+"ex_mol"
make unique
#
build hydrogen
set type mmff
convert
Smiles(a_)  # unique smiles string
```

2.20.49. minimize

`minimize` [`stack`] [*i_mncalls*] [*vs_*] [*s_termString*] [*as_1* [*as_2*]]

minimize locally the sum of currently active, or specified, terms of the energy/penalty function with respect to variables specified by *vs_*, or all the free variables, if variable selection is skipped.

Optional arguments:

`stack`: If option `stack` is specified, the procedure extracts each `stack` conformation, minimizes it and replace the stack conformation with the optimized ones. The stack can be generated with the `montecarlo` procedure, manually created with the `store conf` command, or `read` from a stack file. This command allows to refine your set of alternative conformations all at once.

i_mncalls : defines the maximal number of iterations. The minimization procedure can terminate earlier if the gradient becomes lower than the `tolGrad` parameter. If *i_mncalls* is not provided, the default parameter `mncalls` defines the maximal number of function evaluations during the minimization.

vs_ : variable selection If selection of variables *vs_* selection is specified, the object will be refixed but the initial fixation will be restored after minimization.

s_termString : redefines the set of terms used in the minimization dynamically (e.g. `minimize "tz"`). You may check the active terms with the `show terms` command, or change them before the minimization with the `set terms ".."` command. By the way, the active terms can be shown as a part of your command line prompt if you add the `%e` specification to `s_icmPrompt` variable (like `s_icmPrompt="icm/%o/%e> "`).

atom pair filter: By default all the atoms and all the atom pairs within distance thresholds `vwCutoff` and `hbCutoff` are involved in the calculation. However, two explicit atom selections [*as_1* [*as_2*]] may impose a mask on atom pairs involved in the calculation of the pairwise energy or penalty terms. The default for the skipped *as_1* is all the atoms. If only the *as_1* is specified, the *as_2* is assumed to be all atoms. Using atom selections is dangerous and is not recommended since there are many combinations which do not make sense and give unpredictable results.

the algorithm: the `minimizeMethod` preference. The type of algorithm (conjugate gradient, quasi Newton, or automatic switching between the two) is defined by the `minimizeMethod` preference. The progress bar will show you the progress of the procedure. If minimizeMethod="auto", the progress bar of the minimization procedure will show the 'C' character in a row of dots and colons when the quasi−Newton

method switches to the conjugate gradient method.

Dots show progression of the minimization procedure, while colons mark recalculations of neighbor lists. The lists are updated if at least one of the atoms deviates from its previous position by more than 1.5 A. Both basic methods use the analytical derivatives of the terms with respect to free internal variables.

The procedure is terminated if the gradient falls below the `tolGrad` parameter or if the maximal number of function evaluations is reached.

the output `l_showMinSteps` flag and `i_out` : The actual number of function evaluations during minimization is saved in the `i_out` variable. The `l_showMinSteps` flag allows to see every iteration of the minimization procedure. To speed up the procedure you may switch off the `l_minRedraw` flag to suppress redrawing of the molecule for each new conformation.

Examples:

```
buildpep "HHAS;TW"  # create object from "def.se" sequence file
minimize v_//xi*    # do not touch the backbone torsions
minimize            # use all variables
minimize 500        # run longer until number of calls is 500
```

minimize cartesian: full conformational optimization

`minimize cartesian` [`stack`] [`type`] [`charge`] [*i_mncalls*] [*s_termString*]

minimize the `mmff` energy for a fully flexible molecule in the space of atomic cartesian coordinates. Before running this command please make sure that the atomic types and charges are set and the `mmff` libraries are loaded.

The *i_mncalls* and *s_termString* have the same meaning as in the previous command. Options:

- `stack` : if option `stack` is specified, the procedure extracts each `stack` conformation, minimizes it and stores back to the stack.
- `type` : if option `type` is specified the `set type mmff` command is executed and mmff atoms are assigned.
- `charge` : if option `charge` is specified the `set charge mmff` command is executed and mmff partial charges are assigned
- *i_mncalls* : redefines the maximal number of minimization iterations (`mncalls`)
- *s_termString* : allows to dynamically redefine the default energy terms.

Example:

```
build string "se nter his cooh"
display
minimize cartesian type charge
```

The `drop` and `tolGrad` minimization parameters will still apply.

minimize loop after build model

`minimize loop` *i_loopNumber*

to use this command you must run the `build model` command first. The `build model` command may not be able to find a perfectly matching loop. Two sorts of problems may appear: the imperfections of the loop attachments and the clashes of the loop to the body of the model.

The `minimize loop` command optimizes the covalent geometry at the junctions and the clashes through an interative procedure which maintains the loop closure.

The energy function used by the command is not as detailed as the full atom energy. It is advisable to perform a regularization (e.g. `regul a_`) and full atom refinement.

To save all the graphical frames during this minimization set the `autoSavePeriod` variable to the special value of `99` . In this case png image files named `f_x_y.png` , where `x` is the loop number and `y` is the frame number, will be saved in the current working directory.

minimize stack: minimize each stack conformation

minimize *stack* [*s_terms*] [*mncalls*]

execute these steps:

1. `load` each `stack` conformation
2. locally `minimize` it
3. `store` each conformation back to the stack

As a result, both the geometries and the energies are updated with the optimized ones. Example:

```
read stack "a"
minimize stack 400
```

One can achieve the same result with a shell script like this:

```
read stack "a"
for i=1,Nof(conf)
  load conf i
  minimize 400
  store conf i
endfor
```

minimize tether: threading a model with idealized geometry through a pdb−structure

`minimize tether` [*vs_*]

regularization procedure. It creates a conformation (i.e. determines free variables) that minimizes distances between atoms and their tethering points. If initial model was built from standard amino−acids with idealized covalent geometry , this procedure will create a model with standard bonds and angles which fits the best to the target set of atom coordinates. The `tethers` may be imposed by the `set tether` command. An integer variable `minTetherWindow` defines the maximal number of preceding torsions

which are locally minimized to best−fit the pdb−model. Optional variable selection *vs_* allows to perform fitting only for the selected fragment of the model. This may be convenient if you want to re−fit only a local fragment. Variable `r_out` contains the RMS deviation between the template and the model.

2.20.50. menu

a tool for making clickable strings in the graphics window.

`menu` [*i_string1 i_string2 ...*]

this command declares the listed string labels as active and returns the chosen string number in `i_out.` If no arguments are specified, only the last string will be "clickable". See also _demo_main file.

Examples:

```
while(yes)
display string "Menu"
display string "Fish"    −0.7, 0.6   yellow # 2
display string "Pork"    −0.7, 0.5   yellow # 3
display string "Pasta"   −0.7, 0.4   yellow # 4
display string "Quit"    −0.7, 0.3   yellow # 5
menu 2 3 4 5
choice=i_out
delete label
if    (choice == 2) then
  display "Good choice.\n Our fish is the best.\nClick here"
  menu
  delete label
elseif(choice == 3) then
  display "Good choice.\n Our pork is the best.\nClick here"
  menu
  delete label
elseif(choice == 4) then
  display "Good choice.\n Our pasta is the best.\nClick here"
  menu
  delete label
elseif(choice == 5) then
  quit
endif
endwhile
```

2.20.51. modify

modify chemical structure of a molecule by replacing one part with a specified group or "residue" from `icm.res` or user residue library. Prerequisites:

- modify works only for ICM objects. `convert` your object to ICM type if necessary
- modify deletes the atoms which need to be replaced, so you do not need to delete them explicitly

modify atom with a library group

`modify` *as_exitAtom s_NewRadical*

replace the branch starting from the specified atom by another library radical. Suitable for standard biochemical modifications, such as glycosylation, phosphorylation, etc. (Note that to myristoylate N−terminus you need to use "myr" as N−terminal residue, i.e. `build string "se myr ala ala coo−"`).

Examples:

```
read object "crn"
display a_/8:13
color red a_/11  # serine
                     # O-glycosylation ("acgl", "xyl", "agal", "bgal")
modify  a_crn.m/11/og "acgl" #  beta-D-N-acetylglucosaminide
modify  a_crn.m/11/og "xyl"  # add Xylose
                     # Phosphorylation
build string "se ser thr tyr asp lys his"
modify a_/ser/og  "pho"
modify a_/thr/og1 "pho"
modify a_/tyr/oh  "pho"
modify a_/asp/od2 "pho"
modify a_/lys/hz2 "pho"
modify a_/his/hd1 "pho"
```

modify: single or multiple residue mutations `modify` *rs_ s_NewResidueName*

replace selected residue(s) `rs_` by another residue *s_NewResidueName*. The backbone conformation is not changed, unless the new residue is "pro" and the phi angle is outside [−90.,−30.] range.

You can replace amino acids (the usual list of three letter codes), as well as nucleotides: `"rpa" "rpg" "rpc" "rpu"` for RNA and `"dpa" "dpg" "dpc" "dpt"` for DNA.

Examples:

```
# Peptides and proteins
#
 modify a_/15,18 "his"          # substitute residue 15 and 18 with histidines
 modify a_/ala "val"            # substitute all alanines with valines
#
# DNA or RNA
#
 read pdb "4tna"
 convert
 modify a_4tna1./66 "rpu"        # substitute nucleotide 66 by Uracyl
```

modify by grafting parts of objects `modify` *as_atom1 as_atom2*

replace a fragment of the molecular tree in an ICM−object starting from a specified single atom *as_atom1* (e.g. a_/15/cg) by a subtree starting from another single atom *as_atom2*. This subtree is simply copied and not altered in any way. It is recommended to perform molecular building operation interactively and with your molecule displayed in the graphics window. Type `modify` and `Ctrl−click` the atom starting the branch to be replaced and then the atom starting the branch to be grafted. It does not matter where you take the modification group from. It may be the same molecule, a group in another object, etc. You may want to load a residue containing the group of interest directly from the `icm.res` residue library by doing.

Examples:

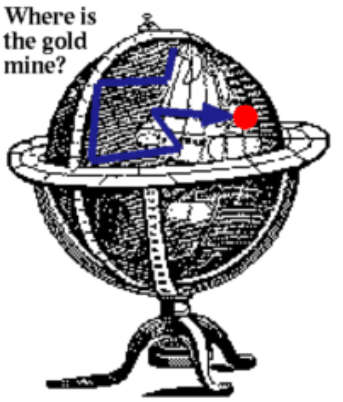
```
show residue types     # find out what residues are available
build string "se ret"  # create a new object with retinol molecule.
```

After the modification you can remove objects (such as `"ret"` in the above example) used for construction. Be careful if modifying atoms within ring systems; the results may not always be obvious unless you know how the ICM−tree is constructed (you'll be kindly warned anyway). However, the whole ring can be modified or grafted without any difficulty.

Examples:

```
buildpep "MIPEAY"  # build a molecule
display              # display it to click two atoms and watch

modify a_/1/ce a_/1/ha      # replace methyl group of Met−1 by a hydrogen
modify a_/2/hd13 a_/2/cg2   # methylate hd13 hydrogen of Ile
modify a_/3/hg1 a_/6/oh     # turn proline into hydroxyproline
```

2.20.52. montecarlo



a generic command to sample conformational space of a molecule with the ICM global optimization procedure.

`montecarlo` [*OPTIONS*] [*vs_MC* [*vs_minimize*]] [`local` *rs_loop*]

runs Monte Carlo simulation for specified variables *vs_MC*, with local minimization with respect to the *vs_minimize* variables following after each random move.

Each iteration of the procedure consists of

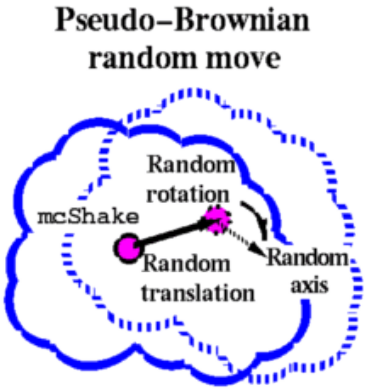
1. a random move of one of 4 types;
   - change one internal variable by a random value (e.g., montecarlo v_//x*)
   - change a group of angles described as a `vrestraint` according to its probability distribution (e.g. set vrestraint a_/* ; montecarlo v_//*)
   - change the six positional variables (e.g. montecarlo v_2//?vt*) defining position of a molecule in space

(the so called pseudo−Brownian move).

- change the loop conformation (e.g.

```
set vrestraint a_/16:24
montecarlo v_/16:24 local a_/16:24
```

2. local energy minimization;
3. calculation of the complete energy potentially including surface and advanced electrostatics terms (REBEL or MIMEL);
4. acceptance or rejection of this iteration based on the energy and the temperature.



Three possibilities for variable selections arguments:

- no variable selections: both *vs_MC* and *vs_minimize* will be set to all free variables. Some vs_MC variables, such as torsions rotating methyl groups, NH2 groups , will be automatically filtered out, since it is enough to just locally minimize them.
- one variable selection: the specified selection will be considered as the *vs_MC* , *vs_minimize* will be **the same** *vs_MC*.
- two variable selections: the first one is *vs_MC* selection, the second one is *vs_minimize*. **Important:** if two selections are explicitly specified, only *vs_MC vs_minimize* will be set free. It means that during the montecarlo procedure the object will be fixed differently than before. After the command, the status of variables will be returned as they were before the montecarlo procedure. There are two basic possibilities: unfix on the fly or unfix first and then run montecarlo:

```
 montecarlo vs_MC vs_minimize # unfix on the fly
# OR
 unfix only vs_minimize # prepare fixation (vs_MC is a subset of vs_minimize)
 montecarlo vs_MC  # now one selection suffices and
                   # the object set of free variables is not changed
```

OPTIONS: `append`

appends to the existing conformational `stack` (overwrites by default).

`chiral`

temporarily activates the `l_racemicMC` variable

`fast :`

rapid side−chain optimization. This option allows to accelerate the calculation by minimizing only the strained variables after each step. Needs the `selectMinGrad` parameter to be set to 1.5. Example:

```
build string "se ala his trp glu"
selectMinGrad=1.5
set vrestraint a_/*
montecarlo fast v_//x*
```

This mode is useful for side chain optimization in homology modeling.

`bfactor :`

you can use the `bfactor` option to sample 'hot' parts of structure with higher probabilities. The relative frequences are taken from the b−factors of the atoms belonging to the mc−variables. Example:

```
buildpep "ala his trp glu"  # default b-factor=20
set bfactor a_/2  1000.     # make 2nd his hot
montecarlo bfactor
```

To preserve the old bfactors, save them before the simulation and restore after. E.g.

```
b_old = Bfactor(a_//*)   # save
..
set bfactor a_/10:20 200.
montecarlo bfactor
..
set bfactor a_//* b_old  # restore
```

`local`

`local` [`dash`] [a_/residueRange1,residueRange2...]

(this option is specified after the main variable selections [*vs_MC* [*vs_minimize*]]) option `local` makes local deformation type movement for specified regions (e.g. two loops a_/15:22,41:55). Sub−option `dash` chooses angles for random deformation symmetrically with respect to the loop center. Note, that to avoid movements of the flanking regions around the loop, you need to set tethers for those regions. The local deformation only applies to the random move, but the subsequence local energy minimization may move the flaking areas (in particular to the C−terminus side) away from their correct positions. The simplest way to set the tethers for the flanking residues (40:45 in the example below) is the following:

```
copy a_ tether      # create a copy of your current object
                    # and tether all atoms the original positions
delete tether a_//h* | a_/40:45
set terms "tz"      # add "tz" to the list of terms
montecarlo v_/40:45 local a_/40:45
```

`movie`

records all accepted conformations sequentially in a binary `*.mov` file. Later one can `read movie`, `display movie`, and operate with individual frames, e.g.

```
for i=1,Nof(frames)
  load conf i       # to extract a frame
  display skin white center
  write image png "f"+i
endfor
```

`mute`

suppresses the text output about every random move

`output`

shorten the output by print out only the steps with the **DY** (down/yes) outcome. The steps in which any of the simulation limits is reached are also shown. This option may considerably shorten log files of very long simulations.

r_exitEnergy real argument determines if you want your procedure to exit upon achievement of equal or lower energy value . For example, if you know energy of the minimum, you may want to stop the search when this value is achieved. E.g.

```
buildpep "AHWEND"   # hexapeptide
set vrestraint a_/* # BPMC−probability zones
montecarlo 10. # stop after energy of 10. is reached
```

two atom selections: montecarlo .. as_1 as_2

(option is NOT recommended for beginners) Atom selection arguments [*as_select1* [*as_select2]]* impose a filter on atom pairs considered in the terms of internal energy like "vw,el,hb,sf". There are three possibilities:

- *no selections* − the whole object (all atoms) is considered (the default)
- *as_select* − interactions of the specified atoms with ALL atoms in the object.
- *as_select1 as_select2* − interactions between two selections. For example, `a_dom1 a_dom1` would consider only the internal energy of the domain `dom1.`

`reverse`

this option makes a more intellegent random move in singlechain or a multichain molecule. By default if an angle is randomly changed near the beginning of a molecule, the second part of this chain moves. With the `reverse` the random move can occur in such a way that a part of the chain *above* a randomly chosen angle will stay the same, while the chain *below* the angle will move. Actually, the parts will be compared by molecular mass and the heavier part will be more likely to stay where it is than the lighter part. The probability that a part stays static is propotional to the number of atoms of this part. It is important that the virtual variables (`v_//?vt*` are not fixed).

This option is very useful in docking, since the receptor is static and the moving molecule should try to preserve the majority of current interactions. Also, the `reverse` option helps if one simulates the N−terminus of a multichain protein, or a docking of a peptide to a protein. Example:

```
read pdb "1aya"  # read a complex
delete a_!1,2    # keep only SH2 domain and a peptide
convert          # make an ICM object with hydrogen
set vrestraint a_/*         # set prob. zones
montecarlo reverse v_2 v_2  # re−dock the peptide
```

If you move the **1st** molecule, do not forget to unfix the `fvt1` variables of all other molecules, e.g.:

```
..
unfix only v_1 | v_*//fvt1
montecarlo reverse
```

If you always want to keep the C−terminus static and move the N−terminus, use the `superimpose` option (see below).

`superimpose` *as_3atoms_per_molecule*

superimposes new generated conformations after every move. Usually if you change backbone torsion at the N−terminus, the whole molecule moves. This option allows to generate conformational changes at the N−terminal part of a peptide while its C−terminus occupies the same position in space. After each random move the first 3 atoms selected in molecule(s) will be superimposed on their initial position and the 6 positional variables (v_//?vt*) will be updated accordingly. The setup:

1. unselect the virtual variables from the MC selection (v_//!?vt*)
2. specify three or more atoms beyond the N−term. of interest for superposition
3. add virtual variables to the minimization selection (it is usually the default) to allow positional adjustments during minimization (the movements of C−terminus are suppressed only in the MC move, not in the following minimization).
4. if minimization is used (mncalls > 1), make a copy of the molecule and tether the C−terminus to it.

Example:

```
 mncalls = 1 # move N−term residues a_/1:5 and while keeping
             # the rest in the same position
 montecarlo v_//!?vt* superimpose a_/6/c,ca,o
             # virtual variables should be available for minimization
 montecarlo v_/1:3/!omg,?vt* superimpose a_/6/c,ca,o
# Now a more realistic example
 build string "se ala his trp ala ala ala ala"
 display
 display residue label
 mncalls = 200
 copy a_1. "original"
 set tether a_/5:7 a_original./5:7
 set terms "tz"
 set vrestraint a_/*
 mncallsMC=100000
 montecarlo v_/1:4/!omg,?vt*  superimpose a_/5:7/ca
```

The following ICM−shell variables and commands are important for the procedure.

- `mncallsMC`,
- `mncalls`,
- `temperature`,
- `mcBell` to make rs−zones narrower or wider than in `icm.res` file
- `mcJump`
- `mcShake` − the average amplitude of the pseudo−Brownian move
- `mcStep` − an amplitude of the unbiased step
- `l_bpmc` − if no, makes simple random steps (one angle by a random value)
- `l_writeStartObjMC` − if yes, write the starting object with its fixation and geometry to a file.
- `mnvisits` three limits and three actions follow

- visitsAction,
- mnhighEnergy,
- highEnergyAction,
- mnreject,
- rejectAction,
- vicinity,
- compare.

EXPLANATION OF THE OUTPUT (below are 3 example lines with numbered fields):

```
1 2       3    4     5   6    7   9    9       10        11     12    13    14
DY Visi    600  16   gln  xi3 70   −98   94   −322.04   −324.56   35   4.87 51559
__ __      600  32   ile BPMC ipt  ipt  ipt   −324.56   −290.80   18  65.72 51577
_Y Visi    600  16   gln BPMC qmm  qmt  qmm   −324.56   −323.93   41   3.78 51618
```

1. DY = Down Yes, i.e. energy has decreased after change and new conf. is accepted

   __ = up no , i.e. energy has increased and new conf. is not accepted

   _Y = up Yes, i.e. energy has increased, but new conf. is accepted

2. stack operation code indicates the outcome of comparison of the current conformation with the stack.
   - Impr : the conformation is close to one in the stack and has a better energy. Visited and improved
   - New : the conformation added as a new stack conformation
   - Sbst : not found, full stack, the worst is substituted for the current
   - Visi : visited and not improved
   - Vlm : visited and not improved, repetition limit mnvisits is achieved
   - High : not found, worse than the worst stack stucture
   - __ : NO in calling routine (has nothing to do with stack)
   - NLim : NO limit of sequential rejections is reached (has nothing to do with stack)
   - VLim : NO Vlm (number of visits>mnvisits)
   - HLim : NO High. mnHighEnergy limit is reached.
3. current temperature in Kelvin;
4. number of selected residue
5. selected residue name
6. name of randomly selected angle or BPMC to indicate the biased probability move
7. internal coordinate value or name of the multidimensional zone before random change;
8. internal coordinate value or name of the multidimensional zone after the random change but before minimization;
9. internal coordinate value or name of the multidimensional zone after the minimization;
10. energy before the random change;
11. energy after the random change and subsequent minimization;
12. number of function calls made during minimization;
13. gradient RMS deviation (normal completion is with low or zero gradient);
14. total number of function calls in the simulation.

The logic of stack operations is the following. There are three possible events for each slot of a stack:

1. new slot creation
2. energy improvement of the current slot conformational family
3. replacement of the looser conformational family by a better energy conformation

The starting conformation is placed to the first slot, if the stack is empty. At every simulation iteration, distances (either coordinate RMSD or angular RMSD, as defined by the `compare` command) are calculated between the current conformation and all slots. If any of the distances is less than the `vicinity` parameter, then the energies are compared and if the current conformation has the better energy, the stack conformation is replaced by the current one, otherwise the visit counter of the slot is incremented. If no similar structures are found, the conformation is appended to the stack, i.e. a new slot is created. If the stack is full, i.e. number of slots reached `mnconf` parameter, then the worst−energy structure will be substituted by the current, provided the latter has lower energy. Otherwise, no action is taken and *number_of_high_energy_conformation* counter is incremented (see also `mnhighEnergy`).

2.20.53. move

Move objects, molecules between objects.

move ms_molecule: change tree topology

`move` *ms_moleculeToReconnect as_terminalAtom*

changes the topology of the basic ICM−tree by reconnecting the first `virtual` bond of a specified molecule to a given atom. This allows you to move two molecules together as one rigid body. By default, all the molecules are connected to the origin [0,0,0] through virtual bonds. The molecule can be connected only to the terminal atom, usually a hydrogen. The molecule can not be connected to itself (naturally, do not even try it). This operation is defined only for ICM molecular objects.

Examples:

```
build "twomol"          # two molecules connected by virtual bonds
                        # to the origin
move a_2 a_1/1/hn2      # graft the second molecule to a hydrogen
                        # on another molecule
                        # now the second molecule will move together
                        # with the a_1/1/hn2 branch
                        # if you change v_1//?vt* variables
```

move : move multiple molecules between objects or merge two objects

`move` *ms_MoleculesToMove os_destination* : *move os_ObjectToMove os_destination

move one, several or all selected molecules (*ms_MoleculesToMove* or *os_ObjectToMove)* to the specified object *os_destination.* When all the molecules are moved from the source object, the empty object is deleted. The *ms_MoleculesToMove* molecule or object are **appended** to the end of the *os_destination* object and their `virtual torsion tvt1` becomes virtual phase `fvt1.` This command is used to create one object from several components.

Examples:

```
                        # 1st object
```

```
read object "crn"
                          # 2nd object
build string "se ala his leu"
move a_2. a_1.            # take the 2nd obj and merge
                          # it with the 1st one

read pdb "1sis"
read pdb "2eti"
set object a_1.
move a_2. a_1.     # two PDB structures became one
                   # ICM molecular object
display virtual
```

2.20.54. pause

`pause` [*i_numberOfSeconds*] [*s_message*]

suspends execution for specified number of seconds. If no argument is specified, the program will wait until RETURN is pressed.

Examples:

```
pause 5 "You have 5 secs"    # pause for 5 seconds

                             # How to analyze the conformational stack
display a_//ca,c,n           # display backbone
for i=1,Nof(stack)           # for all stack conformation
  load conf i                # load and redisplay each of them
  pause "Press Return. N"+i  # gives you time to inspect the structure
endfor                       # go on to the next conformation
```

Debugging shell scripts

The `pause` command also can set the program into a debugger mode in which you will be prompted to confirm each command by pressing RETURN. In the debugger mode the `l_commands` flag will be automatically set to `yes` and restored upon quitting. This is how to do it:

- To start the debugger mode, add to your script: `pause "START DEBUGGER"`
- To quit the debugger mode, type or add to your script: `pause "QUIT DEBUGGER"`

2.20.55. plot

create a PostScript file with a plot.

`plot` { *R_Xdata R_Ydata* | *M_XmultpleYdata* } [*S_PointLabels*] [*S_PlotAxisTitles*] [{ *R_4Tics* | *R_8Tics* }] [*s_epsFileName*] [*options*]

- **Simple input:** Two compulsory arguments *R_Xdata R_Ydata* contain the X and Y coordinates. Both arrays may also be `integer arrays`.
- **Matrix input:** allows you to specify several data sets. The *M_XmultpleYdata* matrix may contain either X,Y1,Y2,..Yn columns or just Y1,Y2,..Yn columns if option `number` is used. Matrix

M[2,n] or M[n,2] is equivalent to the simple input *R_Xdata R_Ydata* (Note that function `Histogram( )` returns such a matrix). Additional convenience: by default, different data sets will be shown in different colors and a panel with series/color correspondence will appear at the position specified by the `PLOT.seriesLabels` preference (choose "none" to suppress the panel). To avoid ambiguity do not use explicit *S_PointLabels* with the matrix input.

- **Axis and Tics:** 8−array *R_Tics[1:8]* contains information about X and Y axis: { *Xfrom, Xto, XmajorTics, XminorTics, Yfrom, Yto, YmajorTics, YminorTics* }. If only 4 numbers are provided, they are interpreted as { *Xfrom, Xto, XmajorTics, XminorTics* } while the Y axis tic marks are determined automatically. By default, if this argument is missing, the tic marks for both axes are calculated automatically. Example:

```
x={1. 3. 4. 7. 11. 18.}
y=Sqrt(x)
plot x y {0.,30.,2.,4.}              # only X−axis marks are defined
plot x y {0.,30.,2.,4.,0.,10.,1.,5.} # both axes are explicitly defined
```

- **Title and legends**: string array *S_PlotAxesTitles[1:3+NofSeries]* contains { "Title", "X title", "Y title" } in the simplest case. If multiple series are plotted using *M_XmultpleYdata* or **number** *M_multpleYdata* arguments, each series may be named with additional components of the array: { "Title", "X title", "Y title","Y1 title","Y2 title",..}.

- **Plot controls**: Optional *S_PointLabels* has the same number of elements as *R_Xdata* or *R_Ydata* and may contain either string to be displayed at the corresponding X Y point, or control information about marker type, color and size. The control string must start with underscore (_). To display both symbols and string labels, duplicate X and Y arrays (e.g. X//X, Y//Y) and supply the first S_PointLabel section with the symbol information and the second one with the string label information.

  Examples of string labels:

```
s={"1crn", "2ins", "1gpu", "3kgb","4fbr","6cia"}       # text labels: show as is
s={"_red SQUARE 0.4", "", "", "_green DIAMOND","",""}  # control labels
s={"_line" "" "" "_red line" "" "" "_blue line" "" ""} # control labels
```

  The empty string tells the program to inherit all the settings for the previous point. Individual components of the string label are (i) color, (ii) mark type and (iii) mark size. Omitted components are not changed. Allowed mark types: **line, cross, square, triangle, diamond, circle, star, dstar, bar, dot, SQUARE, TRIANGLE, DIAMOND, CIRCLE, STAR, DSTAR, BAR.** Uppercase words indicate filled marks.

Options.

- `append` − append the plot to an existing plot file.

- `display` − view the created postscript file with an external viewer defined by the `s_psViewer` variable.

- `grid,` or `grid="x",` or `grid="y"` − draw grid at the major tics for the specified axis. Default: for both axes ("xy").

- `exact` − data points can reside exactly at a margin.
- `regression` − draw linear regression line.
- `frame` − draw NO frame around the plot (paradox isn't it? yeaah we are tricky).
- `origin` − make origin at (0,0) point.
- `link` − enforce 1:1 aspect ratio, equivalent to `PLOT.Yratio` = 1.0 .
- `comment=` *S_xyXYtext* − this option allows to draw one line of text along all the four sides of the plot box. The string array may contain up to four strings {s_x,s_y,s_X,s_Y}:
    1. s_x: lower horizontal string, i.e. comment={"xxxxxxx"}
    2. s_y: left vertical string, i.e. comment={"","yyy"}
    3. s_X: upper horizontal string, i.e. comment={"","","XXXXXXX"}
    4. s_Y: right vertical string, i.e. comment={"x","y","X","YYY"}

  This option may be used to draw amino acid sequence around a contact plot box or a dot plot box.
- `number` generates the sequential numbering for X−array if this array is missing and sets a natural X tic style. In case of matrix input (see above) option `number` allows to omit the X−array.

String variable *s_epsFileName* with extension `.eps` defines the name of a PostScript file where the resulting plot is to be written to. The default of *s_epsFileName* is `"def.eps".`

Examples:

```
x = Rarray(90,0.,360.)             # an array of angles with 4 deg. steps
plot x Sin(x) display
plot x//x Sin(x)//Cos(x) display   # quick and dirty way to have two data sets.
                                     # Now let us get rid of the defect
s = Sarray(2*Nof(x))               # S_PointLabels for both arrays
s[Nof(x)+1] = "_red line"          # restart line for the first point
                                   # of the second set
plot x//x Sin(x)//Cos(x) s display # much better

plot Transpose(x)//Transpose(Sin(x))//Transpose(Cos(x)) display

read object "crn"
crn_m = Sequence(a_/A)             # a_/A ignores termini
plot comment=String(crn_m)+Sstructure(a_/A) number Turn(crn_m) display # try it
plot comment=String(crn_m)+Sstructure(a_/A) number Turn(crn_m) {"Turn prediction","Res","P"}
unix gs def.eps                    # to see it again
```

See also: `Histogram`, `plotRama` macro in the `_macro` file, and examples in the `_demo_plot` file.

2.20.56. plot area: show matrix values with color

`plot area` *M_XYdata options* [*S_TitleXY*] [{ *R_4Tics* | *R_8Tics* }] [*s_epsFileName*]

plot 2D data from the matrix and mark values by color. Other arguments are the same as in the `plot` command. Distribution of colors is controlled by the `PLOT.rainbowStyle` preference. By default the minimal and maximal values of matrix *M_XYdata* are used as extremes for coloring. **Options**:

- `color=` *R_2MinMax* option allows you to enforce specific boundaries represented by the color range. For example, if you chose the "blue/red" PLOT.rainbowStyle the matrix value smaller than or equal to the first element of the *R_MinMax* array will be colored blue, while the matrix values larger than or equal to the second element of the array will be colored red, the middle values will be color with intermediate colors. The real array of boundaries contains two elements.

```
PLOT.rainbowStyle = "blue/white/red"
color={1. 3.}  # <= 1. are blue; above 3. red
color={3. 1.}  # >= 3. are blue; <= 1. are red
```

- `link` − enforce square shape (1:1 aspect ratio) of each cell, overrides `PLOT.Yratio`.

- `comment=` *S_xyXYtext*

  this option allows to draw one line of text along all the four sides of the plot box. The string array may contain up to four strings {s_x,s_y,s_X,s_Y}:

  1. s_x: lower horizontal string, i.e. comment={"xxxxxxx"}
  2. s_y: left vertical string, i.e. comment={"","yyy"}
  3. s_X: upper horizontal string, i.e. comment={"","","XXXXXXX"}
  4. s_Y: right vertical string, i.e. comment={"x","y","X","YYY"}

  This option may be used to draw amino acid sequence around a contact plot box or a dot plot box.

- `transparent=` *R_2range* option allows you to make a certain range of matrix values invisible. If *R_2range[1]* < *R_2range[2]*, the specified range will be excluded from the plot, while the values beyond the range will be shown. If *R_2range[1]* > *R_2range[2]*, the specified range will be shown by color, while the values beyond the range will be excluded.

  Example:

```
transparent={1. 3.}  # values WITHIN  the range are not shown
transparent={3. 1.}  # values OUTSIDE the range are not shown
```

Data can also be transformed and clamped with the `Trim( )` function.

Examples:

```
read matrix "def.mat"
PLOT.rainbowStyle = "blue/white/red"
plot area def display  # min/max = {-3.,17.}
plot area def color = { 0., 20.} display
plot area def color={-0.,15.} transparent={-10.,5.} display
plot area def[1:12,1:10] link display comment={"X","Y axis"}
#
#
N=210
M=Matrix(N N)
for i=1,N
  M[i,?]=Sin((Power(i-12.1 2)+Power(Count(N)-12.1 2)))
endfor
plot area M link display
    # just a nice test, default boundaries are used
```

```
read pdb "1crn"
MDIST=Distance(Xyz(a_//ca))
s=String(Sequence(a_1./A) )
PLOT.rainbowStyle = "blue/rainbow/red"
                  # contact map for 1crn, values below 4.8 and
                  # above 10. A are not shown
plot area MDIST area color = {4.5 15.} transparent={10.,4.8} \
       display link grid comment=s//s
```

2.20.57. print

`print` *arg1 arg2 arg3 ...*

The arguments may be variables or constants of `integer`, `real`, `string`, `logical`, `iarray`, `rarray`, `sarray`, `matrix`, `sequence`, or `alignment` type.

Examples:

```
print "no. of atoms=", i_out, "GRAPHICS.wormRadius=", GRAPHICS.wormRadius
```

2.20.58. printf

a family of three functions for the formatted print:

- printf s_formatString args ... # prints to stdout and s_out
- sprintf [append] s_formatString args ... # prints to s_out only
- fprintf [append] s_file s_formatString args ... # write to a file

`printf` *s_formatString arg1 arg1 arg2 arg3 ...*

formatted print, mostly follows the C−language printf syntax. The arguments may be variables or constants of only `integer`, `real`, `string` type.

s_formatString may contain

- **plain characters** that are directly reproduced
- **ambiguous characters**: \\ − backslash, \" − double quote, %% − percent
- **escape sequences** for more tricky characters (\a − bell, \b − backspace, \f − formfeed, \n − newline, \r − carriage return, \t − horizontal tab, \v − vertical tab) and
- **conversion specifications** for each argument of the printf command. Each specification starts from **%** and may be followed by **−** sign for left adjustment, and precision specification (e.g. %−**5**.2f).
- %c − unsigned character
- %s − string
- %d %D − integer
- %[−] *i1*.*i2f* − float (real) in decimal notation
- %g %G − real in either f or e style, precision specifies the number of significant digits.
- %e %E − real in [−]d.ddde+dd style
- %o %O − unsigned octal
- %u %U − unsigned decimal
- %x %X − unsigned hexadecimal

The output is directed to the screen and is also saved in the `s_out` string which can be later written or appended to a file.

Examples:

```
 printf "Resol. = %4.1f N_ml= %-3d\n", a, n
 write append s_out "log"                    # append to the log file
```

See also: `sprintf [append] [s_]` (prints to the `s_out` string by default) `fprintf [append] s_file` (directly prints to a file).

2.20.59. print image

`print image` [`window=` *I_xyPixelSizes*]

print the current screen image to the printer defined by the `s_printCommand` ICM string variable. Use option `window=` to increase the resolution (however in this case bear in mind that the lines will get thinner and labels smaller). Be kind to your printer and color the background white (e.g. `Ctrl-E`). See also: `write image` `s_printCommand`, `View ( window).`

Example:

```
 nice "4fgf"
 color background white # or press Ctrl-E
 print image
# or
 s_printCommand  = "lp -c -ddepartmentalColorPrinter"
 print image window=View(window)*2 # increase resolution two-fold
```

2.20.60. quit

`quit`

Terminates ICM session.

2.20.61. randomize

randomize internal variables in molecules

`randomize` *vs_ r_angAmplitude*

randomly distort current values of specified variables with either specified or default amplitude in degrees for angles and in Angstroms for bonds. The range is [CurrentValue − *r_angAmplitude*, CurrentValue + *r_angAmplitude*]. Default amplitude is defined by `mcJump` ICM−shell variable (30.0).

randomize variables in range

`randomize` *vs_* r_angMin, *r_angMax*

assigns random values within specified range to selected variables.

randomize atom positions

`randomize` *as_ r_amplitude*

translates the specified atoms `as_` randomly and isotropically according to Gaussian distribution with the specified sigma.

randomize molecule positions

`randomize` *ms_ r_amplitude*

translates and rotates the specified molecules *ms_* randomly and isotropically according to Gaussian distribution with the specified sigma. We call it a Pseudo−Brownian random move. The same moves are used in the montecarlo docking protocol.

Examples:

```
randomize v_//!omg 50.   # distort all variables with
                         # 50 degrees amplitude

randomize v_/14:21/phi,PSI −70., −50. # range [−70.,−50.]

randomize a_2

randomize a_/tyr/!ca,c,n,o
```

(Note use of `PSI` torsion in the last example.)

2.20.62. read

read stuff from a disk file, pipe or string.

ICM offers several ways of reading information in:

read from file

`read` ... *s_fileName* [`mute`]

reading from a file. Just say way what and from what file. The file name is a string and must be quoted. Usually, the extension can be omitted if it is standard. Also, in several cases the program will try to find the requested file in a special directory (`s_pdbDir` for a PDB file, `s_xpdbDir` for an xpdb object, etc.), if is not found in the current one.

Option *mute will temporarily switch `l_info` to `no` .

Examples:

```
read pdb "1crn"
     # s_pdbDir will also be searched.
     # It will also read "1crn.brk.Z"
```

```
     # you may specify file extension explicitly
read iarray "a.a" mute
```

read binary and read binary list

`read binary` [*name = S_objNames*] [*s_fileName*] [`mute`] [`display`]

reads icm−portable binary project file. ICM allows to save multiple ICM−shell objects to a single compact cross−platform binary file. To list the objects in this archive, use the `list binary` command. Options:

`name=` *S_objNames*	name={"g1","m_gb"}	reads a subset of objects
`mute`	read binary mute	temporarily switches `l_info` to `no`
`display`	read binary display	displays molecules as they were saved

`read binary list` [*name = s_outputTableName*] *s_fileName* creates a table of content for the icm objects stored in a binary file. It the table name is not specified, `T_out` table is created. From the GUI interface you can double click on a table row to download a particular object from the file.

```
read binary         # reads the default icm.icb file
read binary "aaa"   # reads all objects from aaa.icb
read binary name={"biotin","DOCK1_rec"} "example_docking"
read binary "example_docking" display  # reads and displays as saved

read binary list "example_docking" name="TOC_ex_docking"
```

read from string

`read` ... `input=` *s_bufferString* [`name=` *s_newName*]

reading from an ICM string. Replacing file by a string is useful in CGI scripts, because the input information is easily accessible as an ICM string. Option `name=` *s_newName* allows to specify a name of the new ICM−shell object.

Examples:

```
s_mat="1 2\n3 5\n0 6"
read matrix input=s_mat name="m23" # matrix m23 is created
s_seq = "> a\nAFSGFASG\n> b\nQRWTERQWTE\n"
read sequence input=s_seq  # read sequences a and b
show a b
```

read through filters: assign action by file extension.

`read` ... *s_compressed_or_encoded_files*

of any type directly. The files will be uncompressed on the fly, if the file extension and the corresponding filtering command are found in the the `FILTER` table. ICM understands `.gz` (`gzip`), `.bz2` (`bzip2`) and `.Z` (`compress`) compression.

Examples:

```
read object "aa.ob.gz"
```

```
read pdb "/data/pdb/pdb1crn.ent.Z"
```

read all

`read all` *s_allFileName*

reading from a `mixed file` containing several ICM−shell objects (including tables) or data types. Legal types and separators:

- #>i `integer_name`
- #>r `real_name`
- #>s `string_name`
- #>l `logical_name`
- #>p `preference_name`
- #>I `iarray_name`
- #>R `rarray_name`
- #>S `sarray_name`
- #>M `matrix_name`
- #>seq `sequence_name`
- #>prf `profile_name`
- #>ali `alignment_name`
- #>m `map_name`
- #>g `grob_name`
- #>T `table_name` # the column layout
- #>col `table_name` # the column layout
- #>db `table_name` # the database layout
- #> `brk` # a protein−data−bank file content
- #> `var` # internal variables (torsions, angles, bonds) for the current ICM−object

Example:

```
read all "a.all"  # the file is given below
```

The `a.all` file may look like this:

```
#>r lineWidth
  1.00
#>R box4
 0. 0. 1. 1.
#>s tt.h
this is a header string of table tt. The arrays follow.
#>i tt.n
15
#>T tt
#> name bd nlines
icm 1985 160000
bee 1998 100000
inet 2000 80000
```

Such a file can be created with the

`write append` *icmShellObject file.all*

command

read index table

`read` { `sequence` | `mol` | `mol2` } *T_selectedEntries*

extract database entries selected via index `table expression`, e.g.

```
 read index "/data/inx/SWISS.inx"
 read sequence SWISS[2:15]
 read sequence SWISS.ID ~ "IL2_*" | SWISS.ID == "ML2_HUMAN"
 # or
 read index "NCI3D"
 read mol2 NCI3D.DE ~ "^benz*"
```

See the `readMolNames` sarray for details on database compound name storage conventions.

Index file contains an integer position of the first character of an entry (ST as in STart), and the entry length (LE as in LEngth). Accepted types of the database index files are single files with multiple entries:

```
#>s Swiss.DIR
/data/swissprot/seq
#>s Swiss.EXT
.dat
#>T Swiss
#>--ID---------ST-------DA------LE-
104K_THEPA      0       906     1094
..
```

read ftp

`read` .. "ftp−path/file"

reading directly from **ftp** port. The ICM can read not only from files directly accessible from your computer but also files from remote locations via ftp. ICM includes a simple FTP client to simplify access to the databases on the internet. Files names may be specified as an ftp style URL:

`ftp://[` *user* [: *password*]@] *hostname* [: *port*]/ *path/* file

If the password portion is omitted, the password will be prompted for. If both the user and password are omitted, anonymous ftp is used. In all cases passive (PASV) ftp transfers are used. If port is omitted, standard port (:21) is used.

Example:

```
 read sarray "ftp://ftp.rcsb.org/pub/pdb/data/structures/divided/pdb/"+\
             "ab/pdb1ab1.ent.Z"
 read sequence "ftp://embl−heidelberg.de/toby/ph.seq"
```

URL−header may be used in existing mechanism of access to PDB:

```
 s_pdbDir ="ftp://ftp.rcsb.org/pub/pdb/data/structures/divided/pdb/"
 pdbDirStyle = "ab/pdb1abc.ent.Z"
```

```
read pdb "1crn"
```

Remote files are stored in your local `s_tempDir` directory. Do not forget to delete them from time to time. The system table `FTP` can be configured to delete temporary files and deal with firewalls.

read http

`read` .. "http−path/file"

reading from **http** port via lynx.

Example:

```
read pdb "http://www.pdb.bnl.gov/pdb−bin/send−pdb?id=1crn"
```

*

read unix

`read` .. `unix` *unix_command*

reading from a unix pipe. (Note that you can read unix shell variables directly with the `Getenv`(*s_varName)}* function).

Examples:

```
read unix date
if(s_out[1:3]=="Sun")print "Go to church"

read column unix grep "^DY" f1.ou | awk '{print $11, $12}'
show def
```

read unix cat

`read` .. `unix` *cat*

reading from a buffer pasted with the mouse is a special case of reading from a unix pipe. Basically, just mark anything ICM−readable in any window, paste it to your ICM session and press `Ctrl−D.` Note that a file name which is usually used to name the ICM−shell object is missing now, therefore it may be named 'def' (i.e. default), rename it afterwards.

Examples:

```
  read alignment unix cat
  cd59n LQCYNCPNP−−TADCKTAVNCSSDFDACLITKAG−−−−−−−−LQVYNKCWK
  ly6n  LECYQCYGVPFETSCP−SITCPYPDGVCVTQEAAVIVDSQTRKVKNNLCLP
  ^D
  show def
  rename def cd_ly

  read sequence unix cat
> cd59
```

```
  LQCYNCPNPTADCKTAVNCSSDFDACLITKAG
  LQVYNKCWKFEHCNFNDVTTRLRENELTYYCCKKDLCNFNEQLEN
  ^D

# read unix cat or read string are two equivalent ways to
# load text to the  s_out string
  read string
  This is the text which will end up
  in you s_out string.
  ^D

# read a mixed, read all −type, input and create two ICM−shell variables:
read all unix cat
#>s ss
strrr
#>i aa
234
^D
```

read alignment

`read alignment` [`fasta` | `pir` | `msf`] [*s_aliFileNameRoot*] [`name=` *s_aliName*]

read alignment file in a natural, pir or msf `formats`. Upon reading, all the sequences are created as separate ICM−shell objects. The alignment is created as a separate object for msf−formatted files. In the case of other formats the alignment object is created if lengths of all the sequences together with dashed ("−−−") insertions are equal to each other.

read color

`read color` *s_clrFile*

If you want to have an alternative color file (say, "icmw.clr"), you can reread the colors.

Example:

```
 read color "icmw"
```

read comp_matrix

`read comp_matrix` [*s_cmpFileNameRoot*]

reads cmp−formatted file (`*.cmp`) containing one or several residue comparison matrices.

read conf: conformations from file

`read conf` [*i_stackConf*] [*s_stackFileNameRoot*]

reads and sets one specified conformation from the conformational stack file `*.cnf`. If *i_stackConf* is omitted the best energy conformation is extracted. This command will work with both compressed and uncompressed (old) stack file formats.

See also `read stack`.

read csd

`read csd` [*s_csdFileNameRoot* [*s_csdJournalFileName*]] [*i_NofObjectsLimit* [*i_startingObject*]]

reads the output of the Cambridge Structural Database (CSD) search utility, namely, FDAT−formatted file (*.dat) and the optional session journal−file (*.jnl). Information about atomic coordinates, connectivity, parameters and symmetry of crystallographic cell is taken from the FDAT file. The journal file contains information about chemical names of compounds. If not provided, the REFCODE csd−name is assigned to the compound name of the ICM−object. (See also `Name` ([*os_* ,] `real`)). Optional *i_NofObjectsLimit* and *i_startingObject* arguments allow you to extract a subset of several objects from a certain position of a multi−entry file. You can loop through all the objects by reading the chunks of up to about 1000 objects by doing the following:

```
 offset = 1
 while( yes )                 # infinite loop
   read csd "large" 100 offset  # read the next 100 objects
   if(Nof(object) == 0 ) break  # exit upon reading all obj.
#
#    do whatever you want
#
   offset = offset + 100
   delete a_*.
 endwhile
```

The object created is not of the ICM−type, use `convert` or `write library` to create an object or an ICM−library entry, respectively. Note that you can also read compressed CSD files (see `FILTER`).

Examples:

```
          # all objects from ex_csd.dat and ex_csd.jnl
 read csd "ex_csd"
          # only the first obj. ; explicit name for the journal file
 read csd "ex_csd" "ex_csd" 1
```

To see how to generate all the symmetry−related molecules in the cell, see the `transform` command.

read database

`read database` [`field=` *S_fields*] [`group` [`name=` *s_tableName*]] *s_databaseFileName*

read a text database with strings and numbers and create appropriate arrays. The field names in the database become names of the arrays upon reading. The list of array names will be stored in `s_out` . Option `group` indicates that a `table` should be formed (or ICM−shell structure) of the constituent arrays. This table will be renamed if option `name` is specified.

You may also `group` arrays of the database to form a `table` with a separate command. That will allow you to `sort` all the arrays and search all the fields by the `Find`( ) function.

Examples:

```
 read database field ={"NA","RZ"} s_icmhome+"foldbank.db" group name="tt"
 read database field ={"RZ","NA"} s_icmhome+"foldbank.db" group
```

```
 show foldbank
#
# ANOTHER EXAMPLE
 read database "LIST.db"
 show database $s_out  # you may also list the arrays explicitly
 write database $s_out "out.db"
```

See also: `read column`, `write database`, `show database`.

read drestraint

`read drestraint` [`only`][*s_cnFileNameRoot*]

read `distance restraints` (often referred to as *cn*) from an a `.cn` file. Do not forget to read drestraint types first. Option `only` tells the program to delete previous distance restraint settings.

read drestraint type

`read drestraint type` [`only`] [*s_cntFileNameRoot*]

read distance restraint types from a `*.cnt` file. Option `only` tells the program to delete all previous distance restraint types settings.

read factor

`read factor` [*s_factorFileNameRoot*]

reads the Xplor−formatted structure factor file. The input is free−field, and each reflection record may be extended over several lines.

Example:

```
INDEx 1 2 3  FOBS=9.0   SIGMA=3.3  Phase=50.0   Fom=0.8
INDEx 2 −3 1 FOBS=31.0   SIGMA=2.3  Phase=20.0   Fom=0.3
INDEx 5 6 6  FOBS=44.0   SIGMA=2.0
```

To read the ICM−formatted structure factor table, just use the `read table` command. ICM will recognize the file type.

read grob

`read grob` [*s_groFileNameRoot*]

read `graphics object` from a `file`. To avoid conflicts with existing names of ICM−shell variables, prefix `g_` is added to the *s_groFileNameRoot.* The default file name root is "def". Allowed input formats: ICM (`*.gro`) or wavefront (*.obj).

Examples:

```
 read grob "icos"  # load icosahedron from icos.gro file
 display g_icos    # usually g_ prefix is added to the file name
```

read iarray

`read iarray` *s_iarrayFileName* [`name=` *s_IName*]

read `integer array` from a file. File `format` is free.

read index

`read index` *s_indexTableFile* [`database=` *s_newDataBaseFileName*]

read the index file for quick access to a database. The optional argument allows to access the database file at a location different from those specified in the course of indexing with the `write index` command.

Examples:

```
 group table NCBI_ {"ID","DE","SQ"} "fd" \
       header "/data/nr/" "DIR" {"nr"} "FI" "" "EXT"
# we created control table t
  write index fasta NBCI_ "/data/nr/NR.inx"
                  # make index and save to a file
  read index "/data/icm/inx/NR.inx"
                  # read index
  show NR[2:5]
                  # usage of the last optional argument
                  # move the data file, keep the index file
  unix mv /data/nr/nr /newdisk/data1/nr/nr
  read index "/data/icm/inx/NR.inx" database="/newdisk/data1/nr/nr"
```

read library

`read library` [*s_libraryFileNameRoot*] : *read *library [*residue | *atom | *color | *drestraint | *vrestraint | *charge | *energy] [s_libraryFileNameRoot]

reads the ICM library files:

- `icm.res` and user residue libraries. Several residue libraries can be used. The `LIBRARY.res` string array defines the residue library files which are loaded into ICM. For example, to add your library file `jack.res` to the existing residue libraries, you can do the following:

  ```
  LIBRARY.res = LIBRARY.res // "/home/jack/jack.res"
  read library
  ```

- `icm.bbt` − bond bend angle bending and improper torsion deformation parameters
- `icm.bst` − bond stretching parameters
- `icm.cod` − atom codes and types
- `icm.tot` − torsion angle energy parameters
- `icm.hbt` − hydrogen bonding parameters
- `icm.hdt` − surface−based hydration parameters
- `icm.cmp` − residue comparison matrix(es)
- `icm.cnt` − distance restraint types (cn)
- `icm.vwt` − van der Waals energy parameters (keyword `energy`)
- `icm.rst` − multidimensional variable restraints zones

The default library path is defined by the `s_icmhome` variable and the name is defined by the `s_lib` string ICM−shell variable.

Examples:

```
read library   # reads all library files according to LIBRARY table
LIBRARY.res = {"icm","/home/jack/jack.res"}
read library residue            # to re−read only residue libraries
read library atom "new.cod"     # re−read different atom codes
read library color "new.clr"    # different colors
read library drestraint "new.cnt" # drestraint types
read library vrestraint "new.rst" # vrestraint types
read library charge "new.bci"     # charge increments
```

read library mmff

`read library mmff` [*s_libraryFileNameRoot*]

reads the following additional library files for the `mmff94` force field:

- mmff.bbt
- mmff.bst
- mmff.tor
- mmff.tot
- mmff.vwt

To calculate the `mmff` energy one needs to assign `atom types`, and `charges`. The force field is switched with the `ffMethod` preference. An example:

Example:

```
build string "se nter his cooh"
read library mmff
set type mmff
set charge mmff
display
minimize cartesian
```

read map

`read map` [`reverse` | `xplor`] [*s_mapFileNameRoot*] [`name=` *s_mapName*]

read ICM−electron−density `map file` and create an ICM−shell variable of the `map` type. ICM understands the following map formats:

- CCP4 binary maps
- Xplor text format

If you read an external binary map file in CCP4 format, ICM will automatically recognize the ~Endian (the order of bits in numbers) and perform the conversion required. Option *reverse forcibly changes the *Endian* for binary maps generated outside ICM under a different operating system. We can not support many other popular map formats, or sub−types of the CCP4 or Xplor formats generated by different

program. Use the **mapman** program (Kleywegt, G.J. and Jones, T.A. (1996). xdlMAPMAN and xdlDATAMAN − programs for reformatting, analysis and manipulation of biomacromolecular electron−density maps and reflection data sets. Acta Cryst D52, 826−828) to reformat the map to one of the two supported formats if necessary. **Reading many maps at once**

`read map` [`reverse`] [*s_mapFileNames*] [`name=` *s_mapNames*]

read multiple files specified in comma−separated string (e.g. `"./map/gc,./map/ge"`) and rename the maps by matching names from a comma−separated string. Examples:

```
read map "gc1,ge1,gh1" name="m_gc,m_ge,m_gh"

read map "./gc1,./map/ge1,./gh1" name="m_gc,m_ge,m_gh"
```

read matrix

`read matrix` [*s_matrixFileNameRoot*] [`name=` *s_MName*]

read ICM−matrix `file` and create an ICM−shell variable of the `matrix` type.

read mol

`read mol` [`exact`] [*s_FileNameRoot*] [`number=` { *i_number* | *I_from_to*}] [`name=` *s_rootName*]

read multi−molecule MDL `mol` −file (a.k.a. SD−file) and create stripped molecular objects (they need further `conversion`). The molecules are named according to the first line of the name section of the mol/sd format. If this line is empty, the root name is taken from the option `name=` *s_rootName.* If none provided the molecules are named 'm1', 'm2', 'm3',..., sequentially. If possible `readMolNames` is utilized.

In the default mode a pattern of single and double bonds is interpreted in order to identify aromatic systems. Then appropriate bond types are changed to aromatic (hit `Ctrl−W` to see the effect). This aromatic system assignment, however, is irreversible. If you `write mol` after that the new bond types will be saved.

Set `l_readMolArom` to `no` if you do not want to assign aromatic rings upon reading. (and formal charge and bond symmetrization for CO2, SO2, NO2or3, PO3). To suppress suppress the symmetrization and consequential charging of CO2, set the `l_neutralAcids` to `yes` .

S_out contains all properties: All the property fields specified in the mol file, e.g.

```
<logp>
2.344
<cas>
234
```

will be stored in the `S_out` array (one string for each object). The string can be further split into fields to extract the values, e.g.

```
 cas  = Trim(Field(S_out,"cas_rn",1,"\n")) # sarray of cas numbers
 logp = Rarray(Field(S_out,"logp",1,"\n")) # rarray of logp values
```

Do not forget that ICM converts all strings to low−case.

Options:

- `exact:` enforces the exact mol/sd format. The default reading mode is more tolerant to common format violations.
- `auto:` automatically assigns compound names, if the name line is missing. The name is composed of the file name root and the order number of a compound.

Examples:

```
read mol "ex_mol.mol"  # you may skip the extension
logP = Rarray(Trim(Field(S_out,"logp",1,"\n"))) # rarray of LogP values
build hydrogen
wireStyle="chemistry"
display a_
```

If you do not need to create molecular objects, but need to create a molecular spreadsheet instead, use the `read table mol` command.

See also: `l_readMolArom`, `l_neutralAcids`, `read table mol`

read mol2

`read mol2` [*s_FileNameRoot*]

read Tripos' Sybyl `mol2` −formatted file (extension .ml2) and create stripped molecular objects (they need further `conversion` to become ICM−objects).

Set `l_readMolArom` to `no` if you do not want to assign aromatic rings upon reading. (and formal charge and bond symmetrization for CO2, SO2, NO2or3, PO3). To suppress suppress the symmetrization and consequential charging of the acidic groups like CO2, SO3, PO3 set the `l_neutralAcids` to `yes` . These will work only if the input files contain only single and double bonds (no aromatic types).

Examples:

```
read mol2 "ex_mol2"  # this example file is provided
```

read movie

`read movie` [*s_movFileNameRoot*]

read ICM−movie `file` with the Monte Carlo simulation trajectory.

See also: `display movie`.

read movie write

`read movie` [*s_movie1*] `write` [*append*] *i_fromFrame i_toFrame s_movie2*

a movie **editing** tool. Read ICM−movie `file` with the MC simulation trajectory, grab a fragment [*i_fromFrame:i_toFrame*] and append it to some other file *s_movie2.*

read object

`read object` [*s_objFileNameRoot*] [`number=` { *i_objNumber* | *I_objNumbers*}] [`delete`] [`name=` *s_*]

read previously formed and saved ICM−molecular−object `file`. If ICM object file contains several objects, all the objects are read. If argument *i_objNumber* is specified only the specified object is read.

The names of the loaded objects from are stored in the `S_out` array, and the number of new objects in `i_out.`

Options:

- `delete` : temporarily sets `l_confirm` to `no` and, consequently, overwrites objects with the same name without a confirmation.
- `number` = i|I : reads one or several objects for a multi−object file
- `name` = s_ : redefines the object name

See also: `build` command to create an object from the sequence and `copy object` command to copy the existing object.

Example:

```
read object "1crn"
read object s_xpdbDir+"4tna" name="tmp" delete

build string "se glu" name="glu"
build string "se his" name="his"
write object a_1. "obb"
write object a_2. "obb" append
delete object a_*.
read object "obb" number=2
S_objNames = S_out
show a_$S_objNames[1].
```

read pdb

`read pdb` [`charge`] [`all`] [`sstructure`] [*s_pdbFileNameRoot* [.mol/res1:res2/at1,at2,..]]

read pdb−formatted file and create a molecular object. You can read all the information from the file or only the part you need to save program memory:

- the whole object: read pdb "/data/pdb/2ins"
- one or several chains: read pdb "/data/pdb/2ins.a,b/" (if chain is not named, refer to it as 'm')
- chain fragment: read pdb "2ins.a/3:16"
- certain atoms: read pdb "2ins./3:17/ca,c,n" (you may use name patterns with **wildcards** too)

Structures determined by NMR are usually represented by several models separated by MODEL and ENDMDL fields. By default only the first model will be read in.

Options:

- `all` : may be used to load all NMR models. Each model will be placed into a separate object. Object names will be automatically generated.
- `delete` : temporarily sets `l_confirm` to `no` and, consequently, overwrites objects with the same name without a confirmation.
- `sstructure` : redefines the secondary structure by analyzing the pattern of hydrogen bonds (see `assign sstructure`)

Deleting alternative atoms Frequently there are alternative atoms in PDB objects. Sometimes you want to get rid of all secondary alternatives and make the 1st alternative the detault. To achieve follow this example:

```
read pdb "1hyt"
set comment a_//Aa,A1 " "  # clear the alter-symbol of the main alternative
delete a_//A               # delete atoms with non-space alter-symbol
write pdb "clean"          # this object does not have alternatives
```

Error detection.

ICM detects chain missing residues according to the differences between SEQRES sequence and the residues with coordinates and returns the total number of missing residues in the `i_out` system variable. E.g.

```
read pdb "1amo.a/"
make sequence a_1.1  # sequence 1amo_1_a extracted
if(i_out>1) then
  read pdb sequence "1amo"  # sequence 1amo_a read
  a=Align(1amo_a 1amo_1_a)
  build model 1amo_a a_1.1 a   # patch the missing fragments
endif
```

See also: `convert` command to turn it into an ICM-molecular object and the `FILTER` preference to see how to read the compressed pdb-files directly.

The fields parsed by ICM.

ICM parses most of the information from the PDB database entry and allows to manipulate with this information in the ICM-shell. The following fields are parsed:

- ATOM : all atom properties including alternative chains. To show the info: `show a_//*`. Function to extract the atom properties:
  - `Bfactor:` b-factors
  - `Charge:` charges
  - `Occupancy:` charges
  - `Name:` atom names

  You can also `select` by many different properties of atoms, residues, molecules and objects directly in the selection expression or via the `Select` function.

- HETATM : all properties including alternative chains
- EXPDTA : assigned as the ICM−object type. ICM function: `Type`(*os_*).
- REMARK 2: resolution is extracted. ICM function `Resolution`(*a_*).
- REMARK 4: is shown as info upon reading.
- REMARK 800: description of `SITE`s is extracted. Can be viewed by `show site`. You can select these `site`s by a_/F" *siteID"*
- COMPND : assigned to the object comment field. Editable and reassignable with the `set comment`. The comment is returned by the ICM function `Namex` . You may directly select with the a_"searchString". expression.
- SSBOND:
- DBREF: database reference information shown upon reading
- SITE : `site`s can be shown with the `show site`, can be selected with the `a_/F` expression.
- HELIX : returned with the ICM `Sstructure` function.
- SHEET : returned with the ICM `Sstructure` function.
- SEQRES: this sequence can differ from the sequences extracted from the ATOM records. It is read with the `read pdb sequence` command and becomes an ICM−shell `sequence`
- SCALE,TVECT,MTRIX: read but not used, the CRYST1 and ORIGX information is used instead.
- CRYST1,ORIGX : the `transformation vector` is returned by the ICM function `Symgroup` and can be applied with the `transform` command.

Treatment of water molecules. Water molecules become molecules named sequentially `w1,w2,w3...` Their original numbers which are stored in the residue field become their 'residue' numbers, e.g. to select water molecule number 225 and 312, do not use the `w..` names of water molecues, but use the `a_w*/225,312` selection instead.

Option `charge` tells the program to load atomic charge from the occupancy field and reset occupancies to 1., and atomic radii from the B−factor field.

Option `sstructure` tells the program to automatically assign the secondary structure if it is not provided in the PDB entry.

The file will be first searched in the local directory. Extensions *.pdb and *.brk will be tried unless explicitly specified. If not found the `s_pdbDir` directory or directories will be looked up according to the `pdbDirStyle` preference. This preference allows file names like pdb1abc.ent recognized by the `read pdb "1abc"` command.

Examples:

```
read pdb "1crn"          # 1crn.brk should be either in the local
                         # directory or in s_pdbDir one

read pdb "2ins.a/"       # load only chain 'a'

read pdb "2ins.a//ca,c,n" # load only the backbone of chain 'a'

read pdb "1crn./4:17"    # load only 4:17 fragment from 1crn.brk
```

read pdb sequence

`read pdb sequence` [`resolution`] [*s_pdbFileNameRoot*]

quickly extract only amino−acid sequence from SEQRES records of a pdb−formatted `file` **without** actually loading molecules. This option does not work with `pdbDirStyleQ` = "PDB ftp−site" or "PDB web−site" .

It is important to understand that sometimes sequence from the SEQRES records **does not match** the sequence extracted from the ATOM records, because some residues in flexible loops and ends are invisible. Option `resolution` appends X−ray resolution to the sequence name (like 9lyz_a19, 19 stands for 1.9 resolution). 'No' is appended for NMR and theoretical structures. It can be used later by the `group sequence unique` command to compile the `representative list` of PDB chains.

PDB is famous for having numerous errors which are never fixed. In SEQRES sometimes the stated number of amino−acids in SEQRES does **not** correspond to the actual number of amino−acids (e.g. 1cty, 1ctz, 1ctz, 2tmn, 1ycc, 2ycc) .

The sequences will be called according to the pdb code and the chain name. In case of one chain without a name, ICM assigns name `"m"` . e.g. 1est_m , 2ins_a , 2ins_b.

Records are converted to lower case. In rare cases, such as `1fnt,` in which there are both upper and lowercase chain names, the lowercase names become uppercase, e.g. `1fnt_a` for the first chain and `1fnt_A` for the 33−rd chain.

Chains with numerical chain identifiers are automatically converted to literal chain IDs in the same way as the `read pdb` procedure does that. Chain `0` becomes `a` , chain `1` becomes `b` , etc.

An example script to detect problems with pdb sequences (you can build the list with the `makeIndexPdb` and `mkUniqPdbSeqs` macros)

```
read sarray s_pdbDir + "pdb.li" name="a"
l_info = no
errorAction = "none"     # otherwise breaks at pdb1aa5.ent
for i=1,Nof(a)
  read pdb sequence s_pdbDir + a[i]
  delete sequence
endfor
Error> no SEQRES records in file  /data/pdb/af/pdb0af1.noc.Z
Error> no SEQRES records in file  /data/pdb/ao/pdb1ao2.ent.Z
Error> no SEQRES records in file  /data/pdb/ao/pdb1ao4.ent.Z
Warning> Sequence of chain  "pdb1ati_c"  starts with 'UNK' and is unknown
Warning> Sequence of chain  "pdb1ati_d"  starts with 'UNK' and is unknown
..
```

read profile

`read profile` [*s_prfFileNameRoot*] [`name=` *s_prfName*]

read ICM−sequence profile from a `file` and create an ICM−shell variable of `profile` type.

read prosite

`read prosite` [*s_prositeFileName*]

read all the patterns from the prosite database (Amos Bairoch, University of Geneva, Switzerland) and create two string arrays: `prositeNames,` and `prositePatterns,` containing names and patterns, respectively. The search may be performed by the `find prosite` command. Check also the `find prosite` command.

Examples:

```
read sequence "zincFing.seq"  # load sequences
 find prosite           # search all 1374 patterns
                        # through the sequence
```

See also: `s_prositeDat` .

read rarray

`read rarray` [*s_rarrayFileNameRoot*] [`name=` *s_RName*]

read `real array` from a file. File `format` is free.

read sarray

`read sarray` [*s_sarrayFileName*] [`name=` *s_SName*]

read any text from a `sar-file` as a bunch of strings separated by carriage returns. Create an ICM-shell variable of `sarray` type.

read segment

`read segment` [*s_fileName*]

reads a simplified description of protein topology from a file. You can append your description to the provided `foldbank.seg` file.

Examples:

```
read segment s_icmhome + "/foldbank"
```

See also: `assign sstructure segment`, `find segment`, `write segment`.

read sequence

`read sequence` [`group` [= *s_groupName*]] [`fasta` | `pir` | `gcg` | `msf`] [*s_seqFile*] : *read *sequence *swiss [field= S_] [*group [= s_groupName]] [s_seqFile]

read amino-acid or DNA sequence from a variety of `sequence file formats` and create an ICM-shell variable of `sequence` type. The GeneBank format is recognized automatically.

Option `group` with optional *s_groupName* creates a sequence group on the fly.

See also: `swissFields`

read sequence database

`read sequence` *T_indexSubset*

read amino−acid or DNA sequence from an `index`ed sequence database. *T_indexSubset* contains the selected entries which can be defined by a `table expression` (e.g. SWISS.ID=="^IL2_*"). The names of the sequences extracted from the database to the ICM memory are stored in the `S_out` system `string array`. `i_out` contains the number of the sequences loaded. These variables are used in automated scripts for bioinformatics (see `searchSeqDb` or `searchPatternDb)` macros.

Examples:

```
 read index s_inxDir+"/SWISS" # load the Swissprot index
 read sequence SWISS[1:20]        # first 20 entries
 show S_out[1], $S_out[1]         # show the 1st name and the sequence
#
 read sequence SWISS.ID=="^IL2_*" SWISS.ID!="*_MOUSE"
 S_seqNames = S_out
 for i=1,Nof(S_seqNames)
   seqName = S_seqNames[i]
   show seqName, Nof(String($seqName),"[KR]") # stat. of positive charge
 endfor
```

read stack

`read stack` [`append`] [*s_stackFileNameRoot*]

read stack of conformations from a `cnf−file`. This command resets the `energy terms` as they were saved in the cnf−file. The terms string is returned in the `s_out` variable.

Both full stacks saved with the `write stack simple` command and compressed stack files (the default) will be recognized. Note that ICM versions before 3.022 could not read or write the compressed format.

read string

`read string` [*s_textFile*] [`name=` *s_sName*]

read any text from either standard input or a *s_textFile*. Place the result into the `s_out` string. Reading string from standard input can be used to get URL−encoded stream generated by the HTML−form. The read string command can also read from `ftp`.

See also: `read unix` command which allows to read in ICM the output of any unix command.

Examples:

```
#Put these lines into _tmp file. See how to precess the HTML−form output.
```

```
 read string     # e.g.: <b>echo "aaa=bbb| icm _tmp</b>
 a=Table(s_out)  # split the input string into two string arrays
                 # a.name and a.value and form table 'a'
 show a          # equivalent to <b>show column a.name a.value </b>
 quit
#
 read string "ftp://ftp.pdb.bnl.gov/index/compound.idx" name="pdbList"
```

In the last example the file will be downloaded from the PDB site and dumped into the pdbList string variable.

read table in ICM or csv/tsv format

ICM−formatted tables `read table` [`database`] [`name=` *s_tableName*] [*s_tableFileName*]

reads internal ICM text format for tables. It has fields for the table headers. ICM needs two lines with the table name and the field names in the following format: (an example):

```
#>T atm
#> name code weight
hydrogen 1    1.008
....
```

CSV or TSV formatted tables `read table separator=`[","|"\t"|":"..] *s_csvtableFileName* [`header`] [`name=`s_tableName] [`comment=` *s_*]

reads tables in portable **csv** (comma−separated−value) or **tsv** (tab−separated−value) formats. Option `header` interprets the first line as the names of the columns. Flanking blanks for each field are trimmed. For example to read the following table from iq.csv file:

```
name,IQ
  Max, 150
 Jack, 150
Peter,  30
```

type:

```
read table separator="," header "iq.csv"  # or
read table separator="," header "iq.csv" name="t" # to rename the table
```

Normally the csv/tsv format does not allow any line comments. ICM supports an extended format in which some lines can bee commented out by a comment string in the beginning of the line, e.g..

```
> cat iq.csv
# this is a list of IQs
name,IQ
Max,  150
Jack, 150
Peter,  30
# Peter is a jerk
> icm
icm/> read table separator="," header "iq.csv" comment="#"
```

See also: `table`, `icm.tab` file.

Examples:

```
 read table s_icmhome+"atm" name="ATOMS"  # atm.tab file by default
 sort ATOMS.weight   # sort according to the weight array
```

`read table mol` [`exact` | `unique`] *s_sdfFileName*

reads an `sdf` file into an ICM table which can be visualized as a chemical spreadsheet. In contrast to the `read mol` command, the `read table mol` command creates only a table and does not create explicit ICM molecular objects Consequently it can read over hundred thousand mol−records into a table without overwhelming ICM. The property fields of the sdf file, e.g.

```
> <logP>
 2.3
> <logD>
 1.8
```

are converted automatically into table columns with appropriate type. The mol−file core which describes atoms and bonds is automatically displayed as a chemical structure by ICM. By default the empty property fields are interpreted as having 0. value, if all non−empty fields are numerical.

Options:

- `unique` : stardardizes the property field names. For example, "Molecular Weight", "MWeight", "Mol_weight" will be translated into "mw". This option may be helpful if you want to merge two sdf files.
- `exact` : keeps columns containing numbers and empty fields as string arrays instead of trying to guess the numerical default value for those columns.

Example:

```
%icm −g
read table mol unique "sigma.sdf"
```

See also the `write table mol` command.

`read column` [`separator=` *s_Separator*] [`group` [`name=` *s_tableName*]] *s_fileName*

read a multicolumn table with strings and numbers and create appropriate arrays. If you add a ruler starting from #> and looking like this

```
#>−name1−−−name2−−−−−−name3−−−−−−−−−name4−−−
```

the arrays will be created with specified names. If ruler is missing, default names (I1, I2 ..., R1, R2,..,S1, S2, .. for iarrays, rarrays and sarrays, respectively) will be created. You may control field formation by `s_fieldDelimiter` variable or by adding **separator**= *s_Separator* explicitly. The list of array names will be stored in `s_out` so you can always say

```
 read column "res"
 show column $s_out
```

Reading comma−separated−value or tab−separated−value formats

To read a table in comma−separated−value (*csv*) or tab−separated−value (*.tsv*) format redefine the `s_fieldDelimiter` value (or use the `separator=","` option), and use the `read column group` command.

```
read column group name="t" "t.csv" separator=","
write t separator=","
```

See also: `write column`, `show column`, `icm.col`.

`read variable` [*s_varFileNameRoot*]

read ICM−molecular object variable values (torsion angles, phase angles, bond angles, bond lengths) from a `var−file`. `vs_out` selection will contain a selection of variables which have been modified by the command. Variables are assigned according to the residue number and the variable name. If residue name is different (i.e. you want to assign phi,psi of an alanine 15 to glycine 15), the program sends a warning. If more than one molecule is present in the current object, matching of molecule names is required. See also `set vs_` command.

`read view` [*s_viewRarrayName*]

read `rarray` of 36 display parameters for window size, scale, view matrices, etc. and set them. See also: `set view`, `View` () function

Examples:

```
 build string "se ala"
 display
 write View( ) "a"
# rotate the image
 read view "a" # restore view
```

`read vrestraint` [*s_rsFileNameRoot*]

read `variable restraints` (often referred to as `rs`) from a `*.rs` file. Do not forget to `read vrestraint type`s first. Option `only` tells the program to delete previous variable restraints.

`read vrestraint type` [*s_rstFileNameRoot*]

read `variable restraint types` from a `*.rst` file. Option `only` tells the program to delete previous variable restraint types.

2.20.63. rename

`rename` *oldName* { *s_newName* | *u_newName* }

rename anything to anything else. More specifically you can rename commands, ICM−shell variables, objects, molecules, residues and atoms. Renaming commands is possible, but then you must not forget to change them in all the standard ICM−scripts. Using `alias`es instead allows you to use both the original

and the translation, however it slows down the ICM−shell interpretation. Be careful with a new name to avoid name conflict.

2.20.64. rename object

`rename` { *os_* [`full`] | *ms_* | *rs_* | *as_* } *s_newName*

change selected names. To change the long name of the object (it can contain space in contrast to a regular object name), use the `full` option.

Examples:

```
rename old   mature         # for elderly
rename sequence[1] ins      # rename the first sequence
rename a_mol1/3/ca "ca1"    # rename an atom
rename a_mol1/3    "alam"   # rename a residue
rename a_mol1      "kuku"   # rename a molecule
rename a_1.        "dna"    # rename an object
       # rename the full name of the object
rename a_1. full "hydroxanthine phosphoribosyl trnasferase"
list a_1.
```

2.20.65. return

`return` [`error`] [*s_message*]

return from a macro before `endmacro` usually under specific conditions. Similar to `exit` command returning from a file to interactive mode. Option `error` will set the error flag which can later (outside the macro) be checked with the `Error`( ) function. The message *s_message* will be stored in the `s_out` string shell variable.

Examples:

```
macro aa
   if(Nof(sequence)==0) return   # a silent return
   .....
 endmacro

 macro aaa as_1
   if(Nof(as_1)==0) return error " aaa> Nothing to do"
   show as_1     # a pretty silly macro
 endmacro

 macro bbb
   if(Nof(object)==0) return error " Error_in_bbb> No objects in the system"
   ....
 endmacro
 bbb             # call this macro
 if(Error) print "something went wrong with macro bbb"
```

2.20.66. rotate

the main `rotate` command. Subtypes of this command include `rotate object`, `rotate view`, `rotate grob`.

rotate object

`rotate` [*os_* | *ms_* | *g_grob*] *M_rotation*

rotate an object (*os_*), one/several molecules (*ms_*) or *g_grob* with the specified rotation matrix.

Examples:

```
rotate a_1. Rot({0. 0. 1.},30.)  # rotate by 30 degrees
                                 # about Z-axis
```

rotate grob

`rotate` *g_grobName M_rotation*

rotate a graphics object.

Examples:

```
read grob "oblate"
display g_oblate magenta
rotate g_oblate Rot({0. 0. 1.},30.)
```

rotate view

`rotate view` *M_rotation*

rotate view in the graphics window with respect to the screen axis X (horizontal), Y (vertical) and Z (perpendicular to the screen). This command is great for creating movies or demos when the graphics should be manipulated from a script.

Example:

```
build "alpha"
read movie "alpha"
display a_//ca,c,n
for i=1,100
  load frame i
  rotate view Rot({0. 1. 0.} , -1.) # rotate around Y by -1 deg.
endfor
```

See also: the `View` () function and the `set view` command.

2.20.67. set family of commands

to change properties of existing icm−objects, e.g.

```
set bfactor a_//c* 20.
```

set area sequence : positional factors for sequence alignment

`set area` *seq_* [{ *R_factors* | *r_factor* }]

sets/resets a property array assigned to a sequence. Each amino acid can be assigned a relative solvent accessibility value for this residue in a three−dimensional model. 0. − fully buried (the highest possible factor), 1. − fully exposed. These values can also be used to influence the alignment (buried residues with accessibilities close to zero will have larger contributions). The exact dependence residue−residue score factor on this value is defined by the `accFunction` array.

`set area` *rs_* [{ *R_areas* | *r_area* }] sets/resets an array or accesible area values (or value) to the residue selection. Note that for the residue areas contain absolute values (e.g. 84., 120., etc.) while for sequences (see above) the area/weight values are relative accessibilities in the range [0.,1.]. The maximal possible accessibilities are returned by the `Area`(*rs_* `type`) function.

Example:

```
show surface area
set area a_/lys Area(a_/lys type) # reset areas to maximal values

set area 1crn_m 0.
set area 1crn_m Random(0. 1. Length(1crn_m))
```

See also: `accFunction` , `Align` (*seq1 seq2* `area`)

set atom

`set` *as_singleAtom* [{ *R_3Dvector* | *as_select* }]

`set` *as_manyAtoms M_XYZ*

With a single atom selection, ICM sets a given atom to the center of gravity of the corresponding molecule (no arguments), given point in space (*R_3Dvector* argument) or center of gravity of selected atoms (*as_select* argument).

If multiple atoms are selected, ICM sets the specified atoms to their new XYZ positions. The XYZ matrix can be returned by the `Xyz` (as_) function.

Examples:

```
build string "se ala his glu"
set a_/3/ca a_//ca  # 3rd Ca to the center of mass of all Ca s
set a_/3/ca {−3., 12., 14.5}

set a_//vt1  # set the first virtual atom to the center of mass
```

```
 randomze a_//vt1 0.1  # randomize the vt1 position in case of singularity
```

For ICM molecular objects, in the most popular operation (set a_1//vt1) the first of the two `virtual` atoms (vt1) attached to the beginning of the selected molecule is set to the center of gravity of the same molecule. The purpose of this action is to simplify molecular rotation and translation via the first six free virtual variables. The tvt2 and tvt3 torsions and avt2 planar angle determine rotation of the whole molecule around the axes passing through the center of gravity. Useful for docking.

Examples:

```
 set a_1//vt1            # now it is easy to rotate the 1st mol.
                         # by changing tvt1
 set a_2//vt1            # now it is easy to rotate the second molecule
 set a_2//vt1 a_2        # equivalent to the previous command
 set a_2//vt1 {1. 1. 1.} # move it to {1. 1. 1.} point
#
# Multiple molecules: let us set vt1 for all water molecules to oxygen
# to fix the first 3 variable and keep the oxygen positions unchanged
 read pdb "2ins"
 convert
 set a_w*//vt1 Xyz(a_w*//o)
 fix v_w*//?vt1
 mc v_w*
```

See also:

command	description
`set a_/* s_secondaryStructure`	to change phi,psi angles according to secondary structure,
`virtual atoms/variables`	information about virtual atoms and variables and the
`move`	command which goes further and actually changes the topology of the ICM−tree.

set bfactor

`set bfactor` *as_* { *r_NewFactor* | *R_NewFactors* } : *set *bfactor rs_ R_NewResidueFactors

set B−factors of selected atoms to a specified real value, respectively. To assign individual b−factors, provide a real array with b−factors for each atom. To assign the individual b−factors at the residue level, provide matching residue selection and *R_NewResidueFactors* array.

Examples:

```
 buildpep "ala his trp"  # also includes N− and C− terminal groups
 set bfactor a_//* 20.
 set bfactor a_//ca {20.,10.,30.}   # individual atomic factors
 set bfactor a_/2:18/ca,c,n 10.
 set bfactor a_/* {10.,20.,30.,20.,10.} # individual residue factors
```

set bond type

`set bond type` *as_class1* [*as_class2*] { *i_type* }

set the bond chemical type (0 − undefined, 1 single, 2 double, 3 triple, 4 aromatic,9 quadruple,10 amid).

`set bond auto` *ms_*

with the `auto` option the command automatically reassigns patterns of single and double bonds. It performs the following operations:

- identify aromatic rings in object os_ from patterns of single and double bonds. Use preference `wireStyle = "chemistry"` (Ctrl−L) to see the bond types. This is done automatically upon reading of objects, mol and mol2 files if logical `l_readMolArom` is set to yes.
- for ICM objects, set ICM bond variable types according to bond chemical type, atom types and distance between them

Example:

```
read pdb "1crn"
display
wireStyle="chemistry"
set bond type a_//c a_//o 2 # double        # standard bonds in a/acids
set bond type a_/phe,tyr,trp/[cn][gdez]* | a_/arg/cz*,nh* 4 # aromatic
set bond type a_/as?/cg*,od,od1 | a_/gl?/cd*,oe,oe1 2
build hydrogen a_/A
```

set charge

`set charge` *as_select* { *r_NewCharge* | `add` *r_Increment* }

sets or increments partial electric charges of selected atoms to or by specified `real` value, respectively.

`set charge` *as_select* { *R_NewChargeArray* | `add` *R_ArrayOfIncrements* }

sets or increments partial electric charges of selected atoms to or by a specified `real array`. The array assignment is useful for saving and restoring the charges.

Examples:

```
set charge a_//* 0.

set charge a_/lys/nz | a_/arg/cz  1.0

set charge a_/asp/od* | a_/glu/oe*  −0.5

oldCrg=Charge(a_//*)
set charge a_//* 0.0
set charge a_/asp/od* | a_/glu/oe*  −0.5
# do something with these simplified charges
set charge a_//* oldCrg
```

See also: `set charge formal`, `set charge mmff` .

set charge formal

`set charge formal` *as_select r_NewFormalCharge*

sets formal partial electric charges of selected atoms to or by a specified `real` value. The charge will be rounded to the nearest value proportional to 1/12th. The following values are common: +−N, +−N/2., +−N/3., +−N/4., +−N/6. Note that the formal charge can not be arbitrarily changed without appropriate changes in the surrounding `bond type`s. The formal charge will be considered by the `Smiles` function.

Example:

```
 set charge formal a_//n −0.333   # a formal charge of −1/3.
```

See also: `set charge`, `set charge mmff` .

set charge mmff

`set charge mmff` *as_select*

set atomic charges according to the rules described in a series of publications on the `Merck Molecular Force Field` abbreviated as MMFF94 or just MMFF.

This command requires the mmff atom types (see the `set type mmff` command). Do not be surprised that the methyl groups have zero partial charges. That is how they are defined in the MMFF algorithm.

Example:

```
 set type mmff       # mmff atom types
 show atom type mmff
 set charge mmff     # charges
#
 rinx MOL3D   # index for small molecule database
 read mol2 MOL3D[23:34]
 for i=2,Nof( object )
   set object a_$i.
   display
   build hydrogen
   convert
   set charge mmff
   display ball
   color a_//* Charge(a_//*)//{−1., 1.} ball
 endfor
```

See also: `set charge`, `set charge mmff` .

set comment

`set comment` [`append`] *os_Object s_comment*

set a text comment string to the specified object. This annotation is preserved in the `read object` and `write object` commands.

Examples:

```
read object "crn"
set comment append a_ "\n The template for modeling\n Energy minimized\n"
```

set a flag of an alternative atom position

`set comment` "A" *as_alterAtoms*

set alternative status to the selected atoms. The alternative flag can be read from a `pdb` file. This flag marks alternative geometrical positions of atoms which are described in the previous ATOM records. For example, the same side−chain or a water molecule can occupy several positions. The symbol of alternative position (usually 'a','b' or 'c' character, since ICM converts the strings to low case) precedes the residue name field. The alternative positions can also be selected with the `a_//A` *alterChar* selection.

Example:

```
read pdb "1cbn" # has alternative positions
show a_//Ab     # show alternative pos. 'b'
set comment a_//Aa "x" # rename 'a' positions to 'x'
#
# example in which we delete all secondary alternatives and
# clear the alternative−flag from the main alternative
#
read pdb "1hyt"
set comment a_//Aa " "  # cleared the main alternative
delete a_//A            # delete atoms with non−space alternative characters, like b,c,2,3 et
```

set comment to a sequence

`set comment` [`append`] *seq_ s_comment*

set comment to a sequence.

Example:

```
a=Sequence("AFSGDHAGSFDSGAHGSDFASGDA")
set comment a "a random test sequence"
```

set comp_matrix: redefine residue comparison matrix.

`set comp_matrix` [`add`] *r_increment* [*s_ijPattern*]

change the numbers in the residue comparison matrix, called `comp_matrix` by a number typically between 0. and 0.2. This may be very important for generating a reasonable alignment for sequences with low sequence similarity. The result is similar to reducing the `gapOpen` parameter by about 0.1.

Examples:

```
 set comp_matrix add 0.05  # try to Align( ) again
 set comp_matrix 10. "CC"  # make C−C alignment really important
 set comp_matrix add 1. "[KR][KR]"
                           # downweight alignment of Gly against
                           # all the residues
 set comp_matrix add −.4 "G?"
 set comp_matrix 0. "[AGS][AGSLI]"
```

set directory

`set directory` *s_newDirectory*

change the *current working directory* from inside the icm−shell. We recommend using: `alias cd set directory "$1"` . In this case you can change directory in the Unix/DOS style.

Example:

```
 make directory "/usr/tmp" # create a new directory
 set directory "/usr/tmp"
 cd ..    # uses alias from _aliases.
# cd .. is equivalent to set directory ".."
 show Path(directory)
```

See also: `make directory`, `delete directory`, `Path`(directory)

set drestraint

`set drestraint` *as_select1 as_select2 i_DrestraintType*

sets distance restraints of specified type between selected sets. Drestraint types (integer numbers) can be either read from a `*.cnt` type file or set directly by the `set drestraint type` command and shown by the `show drestraint type` command.

Examples:

```
 set drestraint a_/15/ca a_/18/ca 5     # distance restraint of type 5
```

set drestraint type

`set drestraint type` *i_DrestraintTypeNumber r_WeightingFactor r_LowerBound r_UpperBound* [`local` *r_Sharpness*]

creates a `distance restraints type`. Drestraint types (integer numbers) can also be read from a `*.cnt` type file and command and shown by the `show drestraint type` command.

Examples:

```
# type 11, weight 10., bounds [1.,3.]A, target dist. 1.5
 set drestraint type 11 10. 1. 3. 1.5

# local type, sharpness 5.
 set drestraint type 12 10. 1. 3. 1.5 local 5.
```

set site

`set site` [`only`] *seq_ I_positions s_siteString* [`type=`"SITE"] : *set *site [*only] seq_ s_swissprotSiteString `set site` [`only`] *ms_ s_siteString* [`type=`"SITE"]

set site to with the specified positions and comment. The default action is `append` . Option `only` erases all site information before setting a new one. Example:

```
read sequence "a.seq"
set site a "FT ACT_SITE 15 15 active site residue"
set site a {10,15,16,17} "active site"
```

See also: `copy site`, `delete site`, showsite{show site} and `color site`.

copy site

`copy site` [`only`] *seq_from* [*ali_*] { *seq_to* | *ms_to* }

transfer (or reassign) `sites` from a sequence or string to a destination sequence *seq_to* or a selection of molecules *ms_to* . Sites are listed in feature tables of swissprot entries and are read by the `read sequence swiss` command.

If alignment is not provided, the sequences will be automatically aligned to find residue−residue correspondences and the reliability of the alignment will be reported. If the source of sites is not provided, the sites will be transferred from the sequences `link`ed to objects. The list of sites and their one−letter codes is given `below`. Normally this command appends to the list of existing sites, unless the `only` option is given in which case the old sites are dismissed. The effort is made to avoid repetition and retain only the unique set of sites.

Alternatively, if the string is specified, create a new site according to the provided legal site string *s_siteString* (e.g. "FT ACT_SITE 15 15 Catalytic residue"). The format of the site string is the same as in the swissprot sequence entries. The list of legal site types is given `in the Glossary`.

The site residues in objects can be delete with the `delete site` command and selected with the `a_/F` *`SiteCodes`* selection, (e.g. a_/FAB selects residues involved in binging and active site).

set site to a residue selection

`set site` [`only`] *rs_ s_sideString*

assign sites to a molecular 3D object (simpler than the previous Swissprot−like definition).

Example:

```
read object s_icmhom+ "crn.ob"
set site a_/10:13 "candidates for mutagenesis"
```

set field

`set field` *selection* { *r_FieldValue* | *R_arrayOfValues* } [`number=` *i_fieldNumber*]

`set field clear` *selection* [`number=` *i_fieldNumber*]

set user−defined values to atoms, residues, molecules or objects selected. Atoms have one user−field, residues have three, molecules and objects have sixteen. To specify which field you need to set, use the `number=` option.

To extract the property use `Field` (*selection*, *i_fieldNumber*) function.

Level	Max.Nof_fields	example
Atom	1	`set field a_//c* Mass(a_//c*)`
Residue	3	`set field a_/trp 1. number=2`
Molecule	16	`set field a_W Random(1.,10.,Nof(a_W)) number=12`
Object	16	`set field a_*. Rarray(Count(Nof(a_*.)))`

User defined fields can further be 2D or 3D averaged with the `Smooth` function and selected by with the `Select` function.

set font

`set font` [`auxiliary`][`bold`][`italic`][`underline`][{ `atom` | `residue` | `variable` | `string` }] *i_Size s_FontName*

set current font for atom−, residue−, variable−, or string− labels in the graphics window. Strings can be displayed in either their main font or the auxiliary one (option `auxiliary`). The following fonts: times, helvetica, courier and symbol, should be available. Default fonts are defined in the `icm.clr` file.

Examples:

```
 set font 28 times        # 'Times' font, size 28
#
 build string "se his"
 atomLabelStyle="[C]"
 display wire atom label
 set font atom 14 bold    # for atom labels
#
 set font auxiliary bold italic helvetica 28
```

set grob coordinates and string label

`set` *g_grobName M_Xyz* : *set g_grobName [*append] s_Label `set` *g_grobName* `reverse` : *set *grob *selection *reverse `set grob selection` [`append`] *s_Label*

Set new coordinates to the vertexes of the specified `graphics object`. The matrix dimensions should correspond to the number of vertices. The initial coordinate matrix can be extracted with the `Xyz` (*grob*) function.

```
 read grob s_icmhome+"beethoven" # try stravinsky if you want
```

```
display
display "DESTRUCTION OF CLASSICAL MUSIC"
xyz= Xyz( beethoven )
fuzz = Random(−0.2,0.2,Nof(xyz),Length(xyz))
xyz = xyz + fuzz
set beethoven xyz
color beethoven Random(Nof( beethoven ),3, 0., 1.)
```

Invert grob normals

`set grob [selection ] reverse`

change direction of vertex plane normals in *all* grobs to change direction of lighting and sign of the `Volume` function. If option `selection` is specified only the GUI−selected grobs are processed.

`set` *g_grobName1 g_grobName2* .. `reverse` # obsolete. *Now* 'grob select'

change direction of normals in *specified* grobs. In some simple grobs the order of vertices defines the normal implicitly. In this case the order is changed.

An example in which we contour a density map, split the grob into outer shell and cavities and measure their volumes:

```
read pdb "1est.m/"
make map potential 1. Box( a_ )
make grob m_atoms 0.2 exact solid
split g_atoms
set grob reverse   # invert normals of all grobs
set g_atoms2 g_atoms3 reverse # invert normals of some grobs
Volume(g_atoms1 )  # outer shell is now illuminated from inside
Volume(g_atoms2 )  # cavities have now positive volume.
  64.865657
```

set key

`set key` *s_keyName s_Command*

binds key to a command. Allowed keys: `F1, .. F12, Ctrl−F1, .. Ctrl−F12, Ctrl−A, ... Ctrl−Z, Alt−A, ... Alt−Z.` Add `"\n"` at the end if you want your command to be automatically executed.

Examples:

```
set key "F1" "set plane 1"
set key "Ctrl−B" "l_easyRotate=!l_easyRotate"
set key "F6" "varLabelStyle=\"nextItem\"\n"
```

set label

`set label` *as_atomForResidueLabels*

assign residue labels to the selected atoms as_atomForResidueLabels .

Examples:

```
build
set label a_/tyr/cb  # move label from Ca's to Cb's for all tyrosines
```

set label distance

`set` [`residue`] `label distance` *rs_* [{ *R_3displVector* | *M_displMatrix* }]

reset the relative displacements of the selected residue labels *rs_* to their default of the specified positions. If vector is specified, all the relative displacements are set to this vector, if a relative displacement matrix Nx3 is given, each selected label is moved to the specified relative position. The default position is the relative displacement of {0. 0. 0.} from the residue label carrying atom (usually the Ca atom for peptides, also see the `set label as_` command). See also: `GRAPHICS.resLabelDrag`

Examples:

```
build string "se tyr tyr glu als his"
set label a_/tyr/cb  # move label from Ca's to Cb's for all tyrosines
display a_*  residue label
GRAPHICS.resLabelDrag=yes  # now drag labels with the MiddleMB
set label distance a_/2:4  # reset labels for residues 2:5
set label distance a_/2:4 {1. 0. 3.}
```

set the current map

`set map` *m_theMapYouWantToWorkWith*

assigns the `current map` status to the specified map.

`set object` [*os_newObjName*]

assigns the `current object` status to the specified object. Switches to the next one by default.

Examples:

```
set object a_crn.   # set it to object crn
set object a_1.     # set it to the first object
set object          # switch to the next or alternative
```

set occupancy

`set occupancy` *as_select r_NewOccupancy*

sets occupancy of selected atoms to or by a specified real value between 0.0 and 1.0

Examples:

```
set occupancy a_/2:5/!ca,c,n,o 0.5

set occupancy a_/2:18/ca,c,n 1.
```

set plane

`set plane` [*i_plane*] [{ `off` | `on` }] [`name=` *s_planeName*]

toggles the specified graphics plane on and off. Up to seven planes can be set. Optional name is assigned to a plane. It is a convenient way to operate with complex composite images. Every image is assigned to a certain graphical "plane" when displayed. Different parts of the image can be assigned to different planes. For example, **plane 1** may contain wire representation of molecule1, **plane 2** its molecular surface ("surface") and **plane 3** molecule2 in "xstick" representation. It can be achieved by pressing "F2" and "F3" (which are `aliased` to **set plane 2** and **set plane 3**, respectively) before displaying surface and xstick respectively. Now by pressing "F1" , "F2" and "F3" one can toggle these three screens (or planes) to display any combination of them. It is much better than `undisplay`ing and `display`ing them directly, especially for representations requiring serious computations like `surface` and `skin` . The main modes of the set plane command:

- set plane 2 : if plane2 is 'off', make current and switch it 'on'; if it is 'on', switch it off.
- set plane 3 on : switch the plane on, but do not change the current plane
- set plane 4 name="homologue" : just assign name to the plane, no switching

Examples:

```
build string "se ala ala"  # create a peptide
set plane 2  # F2 with the cursor in the graphics window
display surface
set plane 3  # F3 with the cursor in the graphics window
display xstick
set plane 2  # switch off the surface
set plane 2  # switch the surface back on
set plane 3  # switch off the xstick
set plane 3  # switch the xstick back on
```

set property

`set property` [`only`] [`on` | `off`] *prop1 prop2* ..

ICM shell objects of the following types: strings, sequences, alignments, profiles, maps, matrixes, tables, grobs, iarrays, rarrays, sarrays have an array of property elements. This elements can be set to `on` and `off` from the shell the they influence visibility, editability and some other properties of a variable in the GUI environment.

Allowed property elements:

bit_name	description
`show`	makes object name invisible in the Workspace, is `off` for system variables
`read`	makes object content unreadable in the Workspace
`delete`	protects from the delete command
`edit`	makes the content of the object un−editable
`field`	makes the content of individual cells of a table un−editable
`index`	indicates that the table is an index table

`factor` indicates that the table is a table of structure factors

`command` indicates that the string contains ICM commands and is a script

Option `only` resets the property mask to 0 before setting the specified bits. Example:

```
ii = {1 2 2 3}
group table t {1 2 3} "a" {3.3 3.3 4.4} "b"
set property t only  # clean up
set property t read off # make it a system table
set property t ii delete edit field off # protect the content
```

set randomize : reset the randomSeed

`set randomize` *i_NewRandomSeed*

resets the random seed to the new value. If you run any procedure or function for the first time, it will show you the value of `randomSeed` . This value can be reset at any time later with the above command.

Example:

```
Random(1,10)
 Info> randomSeed = 1055822291
 4

set randomize 1055822291
Random(1,10)
 4
```

set stereo

`set stereo` [*i_plane*] [{ `off` | `on` }] [`name=` *s_planeName*]

this command allows to reset the stereo mode from a command line or scripts. See also: `GRAPHICS.stereoMode`

set sstructure backbone

`set` *rs_ s_SecStructPattern*

assign the specified local secondary structure to the selected residues of an ICM−type object. Note that this command **changes the conformation** of the selected residues, in contrast to the command `assign sstructure`.

The phi,psi angle values are changed according to the following code:

ss_code	phi,psi angles	description
_	−179.9,179.9	extended conformation
E	−139.0,135.0	antiparallel beta strand
e	−119.0,113.0	parallel beta strand
H	− 62.0,−41.0	alpha−helix

G	− 49.0,−26.0	G−helix (3/10)
I	− 57.0,−70.0	I−helix
P	− 78.0,149.0	poly−proline 2 helix
L	+ 57.0,+47.0	Left−Alpha

Examples:

```
build "all"
display ribbon residue labels
set a_/2:8 "HHHHHHH"
center
set a_/1:12 "HHHHHH__EEEE"
center
set a_/A String("H", Nof(a_/A) )
center
set a_/A String("_", Nof(a_/A) )
center  # ONLY UNFIXED PHI,PSI VARIABLES ARE SET, SO pro IS BENT!
set a_/A String("G", Nof(a_/A) )
center
set a_/A String("E", Nof(a_/A) )
center
```

set sstructure to sequence

`set sstructure` *seq_ s_SSstring*

set secondary structure *s_SSstring* to the specified sequence. If *s_SSstring* is an empty string, the secondary structure definition is removed.

Examples:

```
a=Sequence("LLELGQAPGALHRVPLSRRESLRKKLRAQGQLTELWKSQNL")  # 1st seq.
b=Sequence("PLLEATQIKVPLKKIKSIREVLREKGLLGDFLKNHKPQ")     # homologue
set sstructure a "HHHHHHHHHHH______EEEEEEEE_____HHHHHHHHH__"
l_showSstructure = yes
show Align(a b)
```

set stack energy

`set stack energy` *R_NewEnergies*

resets energy values for conformations stored in the `stack` . It may be useful for the subsequent `sort stack` command.

set symmetry to a torsion

`set symmetry` { *1* | *2* | *3* | *6* | `exact` | `heavy` | `pseudo` } *vs_*

assigns rotational symmetry to selected variables. This symmetry will be used to automatically transform the value of a torsion angle into [−180.0/symmetry , 180.0/symmetry] range.

Options are the following:

- exact − impose exact symmetry (methyl groups=3, xi2_phe=2)
- heavy − impose exact symmetry as if there are no hydrogens
- pseudo− impose pseudo symmetry (no_hydrogens + xi2(his,asn,gln))

set crystallographic symmetry group

`set symmetry` *os_object R_6cell s_symgroup i_NofMolecules*

assigns symmetry and cell parameters to selected object(s).

Information is supposed to be compatible with that provided in **CRYST1** PDB card:

- *R_cell* should be a 6−component real array, containing values of *A, B, C, alpha, beta* and *gamma.*
- *s_symgroup* is a string description of the space group. To check validity of the *s_symgroup*, use the `Symgroup`(*s_symgroup*)} function, which will return a number from 1 to 230 for a valid space group name. Fast Fourier transformations are currently supported for *s_symgroups* "P 1" and "P 21 21 21", but all the other commands (`make map transform` etc.) will work on any space group defined in the International Tables for Crystallography.
- *i_NofMolecules* is the Z−value, the number of polymeric chains in a unit cell.

Examples:

```
build string "se ala ala ala" "z"
     # suppose this is my modified crambin
set symmetry a_z. { 40.96 18.65 22.52  90.0 90.77 90.0 } "P 21"  2
```

set table

`set table` *t_theTableYouWantToWorkWith*

assigns the `current table` status to the specified table (similar to `set object os_` to set the current molecular object).

set energy or penalty terms

`set terms` [`only`] [*s_termsString*]

set `energy and/or penalty terms` for further energy calculations. Each term has a two−character abbreviation. The terms are appended to the string unless option `only` is specified. The final energy−term string is returned in the `s_out` string

Examples:

```
                # vacuum terms, solvation and entropy
set terms only "vw,14,hb,to,el,sf,en"
set terms "tz"  # add tethers to the list
```

set tether

`set tether` [`align` | *ali_*] [`exact`] [`only`] *as_atomsToBePulled* [*as_atomTargets*]

this command sets `tethers` restraining atoms of ICM−object (selection *as_atomsToBePulled)* to corresponding atoms of another object (*as_atomTargets).* The *as_atomTargets* selection may also contain only **one** atom, in which case all *as_atomsToBePulled* will be tethered to a single atom. If the second argument is not specified, all the *as_atomsToBePulled* atoms are tethered to the origin (the {0. 0. 0.} point). Option `only` signals that all previously imposed tethers must be deleted.

In a residue pair the only the backbone atoms such as ca,c,n,o,ha,hn are tethered with the exception of

- identical residues: all atoms are tethered
- F with Y (all but the hydroxyl)
- D with N
- E with Q

The number of imposed tethers is saved in `i_out.`

See also: `superimpose`, `alignment options`, `minimize tether`.

Example (try it as one continuous session):

```
build string "se glu ala"  # a simple object
set tether a_/2            # tether to the origin
display tether wire virtual
minimize v_//?vt* "tz"

delete tether
build string "se gln val" name="gv"  # another object
set tether a_2.//ca,c,n a_1.//ca,c,n exact # tether set to set
display tether wire a_*. only
minimize v_//?vt* "tz"

delete tether
set tether a_2.//ca,c,n a_1./1/ca  # tether to a single atom
display tether wire
minimize v_//?vt* "tz"
```

set atom type

`set type` [`mmff`] [*as_* { *i_type* | *I_type* }]

assigns the specified atom type (see `icm.cod` or `show atom type [mmff]`) to the selected atoms. Both the ICM− and the mmff− atom types may be manually adjusted to correct the automated `set type mmff` command.

set type sequence

`set type` [*seq_* | `sequence` | *ali_*] { `protein` | `nucleotide` }

assigns the specified type to the sequence (*seq_*), all sequences (`sequence`) or sequences from the specified alignment or sequence group (*ali_*). The type can be returned by the `Type`(seq_) function.

Example:

```
aaa = Sequence("AAAAATAAAA")
set type protein aaa

read sequence "f.seq" group="tmp"
set type tmp nucleotide
```

set type mmff

`set` [`atom`] `type` `mmff` [*os_*]

automatic assignment of the MMFF atom types for the selected or the current object of any type. This object can be both ICM−object or a non−ICM object, provided three conditions are satisfied:

1. the bond types are set correctly
2. the formal charges are set correctly
3. the object is complete and has hydrogens (see the `build hydrogen` command)

This command is a prerequisite for the `set charge mmff` command.

set van der Waals radii

`set type` "vw radii" *I_vwTypes R_vwRadii*

reset radii defined in the `icm.vwt` for *I_vwTypes* to the *R_vwRadii* values. The van der Waals radii are used for the surface calculation in the `show surface area`

command

set electrostatic radii

`set type` "vwel radii" *I_vwTypes R_vwRadii*

reset electrostatic radii marked as vwel defined in the `icm.vwt`. The electrostatic radii are used in the boundary element electrostatic calculation.

set 3D view rotation, tranlation and size

`set view` *R_36parameters*

sets all the parameters of the graphics window (position, size, zoom, rotation, etc.) according to a `rarray` of 36 numbers. This array is returned by the `View` () function and can be created, read and written as an ordinary real array. Aren't you disappointed that you still do not know the meaning of these parameters? It is dull, believe me, use the command and take it easy. See also: `View`, `rotate view`.

Example:

```
display a__crn. ribbon  # now move the molecule, resize window ..
write View( ) "a.view"  # write 36 numbers in a file
  # again: rotate, move/resize the window etc., or quit the session
read rarray "a.view"    # read 36 parameters
set view a              # restore the view
```

set vrestraint

`set vrestraint` [`energy`] *rs_* [*s_rsTypeName1 s_rsTypeName2 ...*]

sets variable restraints of specified types to the selected residues `rs_` . Variable restraint type names (strings) can be read from a `*.rst` type file and shown by the `show vrestraint type` command. Option `energy` enforces the "energy" type of vrestraint.

Number of imposed variable restraints is saved in `i_out` .

Examples:

```
set vrestraint a_/*             # assign all zones to relevant residues
set vrestraint a_/ala "aa" "ab" # assign alpha and beta zones to all Ala residues
```

set vrestraint

`set vrestraint` [`only`] [{ `energy` | `fix` }] *vs_ r_1 r_2* [*r_3*] [*R_values*] [`name=` *s_rsName*]

impose a set of `vrestraint`s to the specified variables *vs_*. The zone will be a multidimensional elliptical well *around current values* (default), or the specified *R_values* values, of the selected variables. The shape of the well in each dimension is a *soft square well* . Three types of vrestraints can be imposed, depending on the option:

- **probability** vrestraints (the default). They are marked as "rs" in the `icm.rst` file. Probability vrestraints are used in the BPMC procedure to define the distribution of random steps. The well parameters are as follows:
  - *r_1* : *r_relProbability* , the relative probability of this vrestraint
  - *r_2* : *r_wellRadius*, the well radius

  The relative probability is in arbitrary units, it is only important as a relative number in a *group* of the vrestraints.

- **energy:** "Energy" vrestraints (marked as "rse" in the `icm.rst` file. They allow to form multidimensional wells around groups of variables and are used to softly restrict the variables to certain zones (see the `"rs"` energy term). The well parameters are as follows:
  - *r_1* : *r_energyDepth* (it must be negative for attractive wells)
  - *r_2* : *r_fractionFlat*
  - *r_3* : *r_wellRadius*

  Parameter *r_fractionFlat* (between 0. and 1., default 0.) defines flat fraction of the energy well for the energy vrestraints.

  Note: one can create both **wells** and **bumps** using negative and positive values of *r_energyDepth*, respectively Example:

```
build string "se nter ala ala cooh"
set vrestraint energy v_/3/psi −20., 200., 0.2  # WELL OF DEPTH 20.
set vrestraint energy v_/3/psi  20., 200., 0.2  # BUMP OF HEIGHT 20.
```

An example from the `_dock2mol.icm` script: imposing an individual restraint for the `virtual` bond:

```
               # no penalty for deviations up to 15A
set vrestraint energy v_2//bvt1 only  −50.0 0.5,  30.0
```

- *R_values* contains target values for each angle in the selection *vs_* , e.g. {−120.,60.}, By default the target values are taken from the current values of the selected variables.

- **fix:** Vrestraints on "fixed" variables (marked as "rsr" in the `icm.rst` file). These are used to define switches between different fixed conformations, e.g. alternative conformations of sugar rings, proline rings, switches between L and D amino−acids etc. These switches will be tried in the `montecarlo` procedure if these variables are included in the set of vs_MC variables but not included in the set of the minimization vs_min variables. The parameters are defined as follows:
  - *r_1 r_relEnergy*, relative energy of a conformer
  - *r_2 r_relProbability* .

  The *r_relProbability* is in arbitrary units as for the probability vrestraints.

  Example with L−D transition, through changing the sign of the two phase angles:

```
build string "se ala his trp"
set vrestraint fix V_/3/fha,fcb  Value( V_/3/fha,fcb ) 0. 1. name="l"
set vrestraint fix V_/3/fha,fcb −Value( V_/3/fha,fcb ) 0. 1. name="d"
montecarlo V_/3 v_//*
```

The radius of the vrestraint well (in degrees for angles) is given by the *r_wellRadius.* Option `only` deletes all the previous vrestraints. The name is optional. The names of the "probability" and "fix" vrestraints are be shown in the output of the `montecarlo` procedure. The names need not be unique.

Example: creating a file with equal probability vrestraints around stack conformation angles with 30 deg. radius:

```
read stack "f1"      # read conformational stack
for i=1,Nof(conf)    # go through all the conformations
  load conf i        # load them one by one
  set vrestraint v_/2:5/phi,PSI,xi1  1. 30.
endfor

build string "se ala his trp"
set vrestraint v_/2/phi,xi1,xi2 ,{−60.,−60.,120.} 0.5, 45. name="bb"
set vrestraint v_/2/phi,xi1,xi2 ,{ 60.,−60.,120.} 0.5, 45. name="cc"
montecarlo v_/2/phi,xi1,xi2
```

Note that in the command a special `PSI` torsion specification is used for traditional residue attribution.

set values of internal coordinates

`set` *vs_* [`add`] { *r_value* | *R_arrayOfValues* }

sets specified variables to a given value(s) (for angles the value must be in degrees). If `rarray` *R_arrayOfValues* is specified, its values are assigned sequentially to the variables. It the array is shorter than the selection, the values are applied periodically. Option `add` means increment by the specified value rather than set to this value.

Examples:

```
set v_//phi −60.                 # all phi to −60 degrees
set v_//phi,PSI { −60., −40. }   # make sure that the first
                                 # variable in selection is phi

set v_/1:8/phi Random(−180.,180.,8) # all different random phis
set v_/1:8/phi add 2.0              # increase 8 phi angles by 2 degrees
```

Note that in the second command a special `PSI` torsion specification is used for traditional residue attribution.

set positional variables to place a molecule to polyhedral vertices

`set` *vs_* `grid` *i_vertex i_NofVertices*

(order of arguments is important!) sets specified 2 variables (normally a `virtual` planar angle and torsion angle) to the values such as to put a molecule in the vertices of tetrahedron (i_NofVertices=4), octahedron (6), cube (8), icosahedron (12) or dodecahedron (20). Used to sample uniformly the surface of globular molecules. Values of i_NofVertices other than above are not allowed. The polyhedron is built around the origin. The size of the polyhedron is determined by `v_//bvt1` variable which is a `virtual` bond length from the origin to the first virtual atom (vt1) of the two attached to each molecule. To check how polyhedrons are generated look at this example:

```
read object "complex"
display virtual a_//ca,c,n | a_//vt* only
color molecule
set a_1//vt1       # set vt1 of a_1 to its center of mass
set a_2//vt1       # set vt1 of a_2 to its center of mass
set v_1//bvt1 0.1  # move a_1 to the origin (0.1 to avoid a singularity)
set v_2//bvt1 30.  # offset a_2
                   # this is for a_2 to hop around a_1
for i=1,20
  set v_2//avt1,fvt1 grid i 20
endfor
                   # this is for a_2 to rotate need the same location on a_1
for i=1,12
  for j=1,3
    set v_//avt2,tvt3 grid i 12
    set v_//tvt2 j*120.
  endfor
endfor
```

set size and position of ICM graphics window

`set window` [*i_xLeft i_yDown*] *i_xSize i_ySize* [`margin=` *r_* ...] : *set *window *full [*on | *off]
`set window fix` *i_xSize i_ySize*

sets the position and/or size (only size if 2 arguments are given) of the graphics window without Graphics User Interface (use option `fix` otherwise). Four arguments are in pixels. If you need to display in a fixed size window from a script we recommend to use the set window command first and then the `display` command.

The `full` option will switch into the fullscreen mode (also Ctrl−F and Esc to switch off) This option does now work with GUI.

In the off−screen mode (see the `display off` command) `set window` is accompanied by re−centering of the molecular image with `margin=` *r_* ... and other `center` options.

The `fix` option will change window size for ICM in the GUI mode. In this case the window may become smaller than the actual area in the master GUI window. Option `fix` is used to make video clips with ICM using fixed size frames.

Example:

```
            # square 700x700 window in the upper left corner
 set window 570 30 700 700
 display window
 set window 300 300
 write image window=3*View(window)  # hi-res. image
```

2.20.68. show

show information about specified ICM−shell objects in your shell−window. Show is similar to the `list` command, but it gives you more information, covers a broader range of subjects and allows the user to show constants, subsets and expressions. However, in contrast to the `list` command, `show` does not understand **wildcards.**

Option `full` will show arrays and shell variables which are grouped into tables (the components of tables are hidden by default). The same option `full` temporarily sets `l_showSpecialChar` to `yes` when sarrays are shown.

show site

`show site` [*ms_*] [*seq_1* seq_2..]

show sites assigned to the selected molecules *ms_* or sequences. By default all the sites of the current object are shown. See also: `set site`, `color site` .

show shell variable

`show` *arg1 arg2* ...

show `ICM-shell variable`, `constant`, subsets, or expressions. One needs to separate arguments by comma only if two consequtive arguments are numbers, and the second on is a negative number constant.

Examples:

```
show azurins[3:20]   # show a fragment of the alignment
show a b a*b         # two arrays and their product
show Sin({1. 3. 5.}) # another array
show 2., -3.         # without the comma, it will show -1.
show m_crn           # map (m_crn) header information and
                     # the map sections
```

show key

`show key`

show commands bound to key-strokes. Allowed keys: `F1, .. F12, Ctrl-F1, .. Ctrl-F12, Ctrl-A, ... Ctrl-Z, Alt-A, ... Alt-Z`. See also the `set key` command.

show map

`show` { `map` | *mapName* }

show the current or the specified map in text format. Example:

```
buildpep "AKSD"
make map potential Box(a_) "ge"
display m_ge {1 2 3 0 4 5 6}
show m_ge
m_ge> written in ZYX mode (z-sections). Symmetry group #0
   Box  {sect0,row0,col0, sect,row,col} = {-30,-8,-21, 32,16,28}
   Cell {A,B,C, angles(deg)} = {14.000,8.000,16.000, 90.00,90.00,90.00}
   Nof intervals (at x,y,z)  = {28,16,32}
   Min/max/mean/rms density  = -20.000000, 20.000000, -0.182712, 12.082560
...
::::::::::::::::**##########
::::::::::::::::**##########
::::::::::::.:::**##########
::::*****::.::::**#########
:::***###*:..::::***########
::***####**...:::****#######
:***#####**...:::****######
:***#####*:...:::*****###*
:***##**::.....:::*********
:*****:::.....::::*********
:****:::.....::::::********
::***:::.....::::::********
::***:.....::::::::*******
::***:.....::::::::*******
--- 13 / 32 ---    # shows pages
```

show objects, molecules, residues, atoms and variables

`show` { *os_* | *ms_* | *rs_* | *as_* | *vs_* }

show selected atom(s) `as_` , residue(s) `rs_` , molecule(s) `ms_` , object(s) `os_` , or variable(s) `vs_` , respectively.

Examples:

```
show a_*.     # all objects
show a_*.*    # all molecules of all objects
show a_2.*    # all molecules of the second object
show a_*      # all molecules of the current object
show a_/ala   # all alanines of the current object
show a_1//c*  # carbons of the 1st molecule of the current object
show v_2.a//phi,psi
```

Data fields for **objects** :

```
show object
 # a_objectName.  type    n_Mol  n_Res  n_waters resolution  object_name
  1  a_def.  Type: ICM   Mol: 1 Res: 4   def    <*** the current object
  2  a_1dna. Type: X-Ray Mol: 3 Res: 532 Wat: 216 Resol: 2.20 thymidylate synt..
```

These fields can be accessed with the following functions:

- object name: `Name(` os_)
- object type: `Type(` os_ , `2`) # returns "X−Ray","NMR","ICM",etc.
- number of molecules: `Nof(` ms_), e.g. `Nof( a_2.* )`
- number of residues: `Nof(` rs_), e.g. `Nof( a_2.*/* )`
- resolution: `Resolution(` os_), e.g. `Resolution( a_2. )`
- number of waters: `Nof(` *water_selection*), e.g. `Nof( a_2.w* )`
- full name: `Namex(` os_), e.g. `Namex( a_2. )`

Data fields for **molecules** :

```
read pdb "1a36"
show a_*
    Name     n_residues first_res_name  object_name
-- i Molecule --- N_Res                 Object ---
   1  a            544 ile               1a36
   2  b             22 dpa               1a36
   3  c             22 dpa               1a36
   4  w1             1 hoh               1a36
   5  w2             1 hoh               1a36
...
```

These and other molecule attributes can be accessed with the following functions:

- mol. name: `Name(` ms_)
- mol. type: `Type(` ms_ , `2`) # field not shown Returns. "Nucl","Amino","Hetatm" etc.
- number of residues: `Nof(` rs_), e.g. `Nof( a_2.*/* )`

show alias

`show aliases`

show all currently defined aliases. To show a specific alias, use the

`alias` *aliasName*

command (e.g. `alias cd`).

show alignment

`show alignments` [`color`]

show currently loaded alignments. Option `color` colors residues in the alignment by type.

show area

`show area` { `surface` | `skin` } [`mute`] [*as_1* [*as_12*]]

Calculates the area of the solvent−accessible surface or molecular surface (so called `skin`), respectively. You can specify for which atoms you want to calculate the surface (selection *as_1*).

You can also additionally specify the environment for these selected atoms, i.e. the neighbors which you want to take into account in the surface calculation.

The two most popular modes are the following:

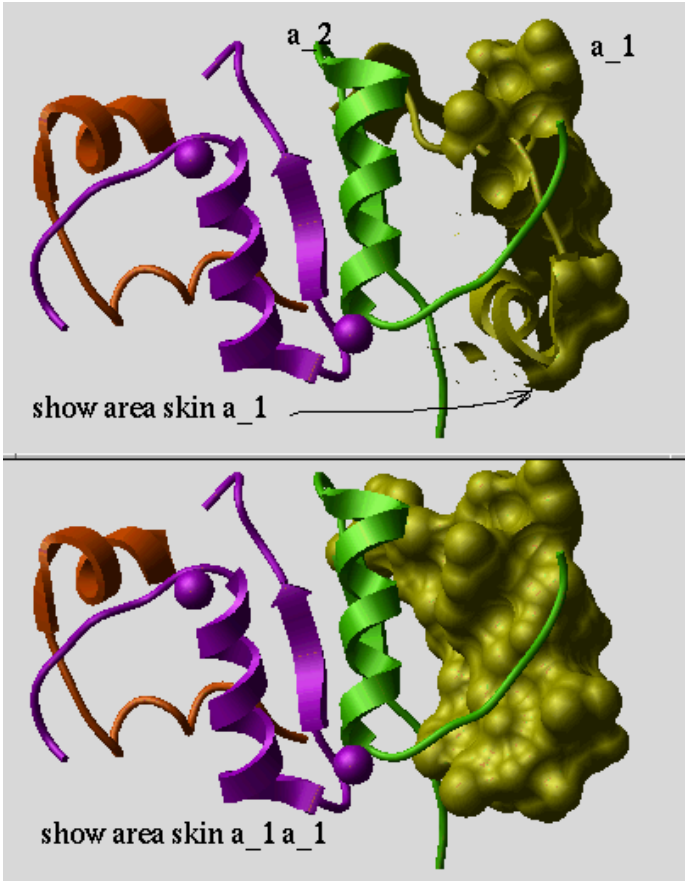
- measuring the surface area of some atoms being a part of the whole system (e,g, `a_1 a_*` or just `a_1` , the top picture)
- measuring the surface area of a group of atoms as if they are the only atoms that exist in space (e.g. `a_1 a_1` the bottom picture).

In essence, two optional selections [*as_1* [*as_12*]] impose a mask on atom pairs, so that only pairs in two selections are considered. If only the first selection is specified, the second one is assumed to be *all atoms* . The two *reasonable* choices for the second selection are *all atoms* (the default), and the *repetition* of the first selection (acts as if not other atoms are present in the system). In all cases, the

second selection must include the atoms of the first one, e.g.

```
show area skin a_1 a_1,2
```

.



The area will be stored in `r_out` and the number of triangles used in the "skin" construction in `i_out` .

show atoms

`show` *as_*

shows properties of the selected atoms. Example:

```
build string "se ala"
show surface area
show a_//c*
 Atom Res    Mol Obj   X      Y      Z    Occ   B  MMFF Code  Xi Chrg formal Grad Area Grp as_
  ca  1  ala  a1 def -2.748  0.000 -2.245 1.00  20.0  1 113 C  1  0.06  0    0.0  0.5    _ a_d
  cb  1  ala  a1 def -2.329 -1.202 -3.093 1.00  20.0  1 113 C  0 -0.09  0    0.0  7.3    _ a_d
  c   1  ala  a1 def -4.247 -0.000 -1.935 1.00  20.0  3 121 C  0  0.45  0    0.0 34.2    c a_d
```

The fields:

Field	Description
Atom	atom name
Res	residue number+[symbol] and name
Mol	molecule name
Obj	object name
X,Y,X	coordinates
Occ	occupancy (from 0. to 1.)
B	B−factor (positive)
MMFF	MMFF atom code
Code	ICM atom code
Xi	chirality number (0,1,2,3)
Chrg	partial charge
formal	formal charge
Area	solvent accessible surface area
Grp	electrostatic group (atoms can not be separated)
as_	selection expression

show atom type

show atom type : *show *atom *type *mmff [{ s_pattern | i_type }]

shows atom types stored in the icm.cod file. The mmff option allows to check the Merck Force Field atom type.

Examples:

```
  show atom type
       # show all ICM types
 ------------- atom codes -------------
 #
 #     icd   vw   hb   hd      wt      sf na
 #
 atcd    0    0    0    0   0.000    0.00 ?
 atcd    1    1    1    0   1.008    0.00 h
 atcd    2    3    1    0   1.008    0.00 h
 ...
  show atom type mmff "*cation*"
       # cations
  show atom type mmff "*iron*ion*"
       # do we have iron ions?
  show atom type mmff "?C=*"
       # what types are connected to doubly−bonded carbon ?
  show atom type mmff "[!C]*ring*"
       # non−carbon types in rings
  show atom type mmff 32
       # some oxygens
 ----------- MMFF atom codes ----------
  Symb.Typ.[V] Description  {formal charge}
```

```
   O2CM 32 [1] oxygen in carboxylate anion
   OXN  32 [1] N-oxide oxygen
   O2N  32 [1] nitro oxygen
   O2NO 32 [1] nitro-group oxygen in nitrate
...
```

show clash

show clash [*as_1* [*as_2*]] [*r_vwReductionRatio*]

shows all the interatomic distances between two atom selections which are shorter than the sum of van der Waals radii multiplied by the *r_vwReductionRatio* parameter (0.8 by default). IMPORTANT: this will work only for the ICM-objects. Use the `show energy "vw"` command (and pay attention to the current fixation) to precalculate interaction lists. The output will show the actual distance and the ratio of this distance and the sum of radii. Mark the two atoms of interest, separated by a logical OR, and paste it into another command if necessary.

See also: `display clash`, `undisplay clash`. Visualize the strained atoms with `show a_//G` or `display a_//G`.

Example:

```
build string "se ala his trp glu"
randomize v_//*
display
show clash a_//c* a_//c*      # clashes between carbons
show clash a_//c* a_//c* 0.7  # more tolerant test
display clash
```

show color list

show color [mute]

shows list of colors defined in the file `icm.clr` and stores the output list in the `S_out` string array. Option `mute` suppresses output to the screen but still saves to the `S_out` array (useful for scripts)

See also: `color` command.

An example:

```
show color
------------- colors -------------
  1 black              #000000
  2 white              #ffffff
  3 grey               #878787
  4 blue               #0065ff
  5 red                #ff0000
...
```

Example of `show color mute` use in a script:

```
if (Exist(view)) then  # check if graphics is active
  show color mute      # saves a list of colors in S_out
```

```
   for i = 1, Nof(S_out)
     color background $S_out[i]
     pause
   endfor
 endif
```

show arrays as parallel vertical columns

`show column` *array1 array2 ....* [*s_fileName*] [`separator=` *s_Separators*] [`comment=` *s_Comment*]

shows several arrays in a multi− `column` format.

See also: `write column`, `show database`, `write database`.

Example:

```
resnam = {"ala" "glu" "arg"}
reschg = { 0., −1., 1.}
show column resnam reschg
show column separator=":" comment="Example table"  resnam reschg
```

show comp_matrix

`show comp_matrix`

shows residue comparison matrix used by the alignment algorithms.

See also: `set comp_matrix`, `read comp_matrix`.

show table in database format

`show database` { *table* | *array1 array2 ....* }

shows several arrays or a table in a database format.

See also: `read database` `show column`, `write database`.

Example:

```
resnam = {"ala" "glu" "arg"}
reschg = { 0., −1., 1.}
show database resnam reschg
```

show drestraint

`show drestraint` [*as_select* [*as_select*]] [`center`] [`mute`] [*r_violation*]

shows distance restraints. Arguments:

- optional *as_select* atom selection arguments specify atom pairs to be considered. **Attention,** the `as_out` selection can not be used as an argument since it is redefined by the command.
- *r_violation* : if the *r_violation* distance is specified, only the restraints deviating from the upper or lower bounds by *r_violation* are shown.
- `center` : If `center` option is specified the violation is measured with respect to the target value of the distance restraint and optionally only the distances greater than *r_violation* are reported.
- `mute` option: allows one to fill out the `as_out` selection and calculate the number of selected drestraints (`i_out`) without actually reporting them. It is useful for scripts.

Output:

- `as_out` atomic selection of all atoms for which the specified criteria have been satisfied
- `i_out` reports the **number** of selected drestraints

See also: `drestraint` and `drestraint type`.

show drestraint type

`show drestraint types`

shows available drestraint types as defined in the `icm.rst` file. The numbered global or local types can be used to impose distance restraints. The other types are fixed and are used to impose disulfide bonds or peptide bonds.

show energy

`show energy` [`mute`] [*s_termString*] [*vs_*] [*as_select1* [*as_select2*]]

calculates and shows values of currently set or explicitly defined in *s_termString* energy terms (e.g. `"vw,el"`). If *vs_* selection is specified, only the selected variables will be unfixed. The initial fixation will be restored after completion. Two additional atom selections may specify a subset of atom pairs that should be considered by the minimization procedure. Note that the contribution from the `"14"` energy term is not displayed separately. It is included in the `"vw"` contribution. If you want to display it separately, use the more straightforward `Energy("14")` function.

Important: the boundary element electrostatics is the most computationally heavy term. It is activated if electrostatic term `el` is switched on and preference `electroMethod` is set to `"boundary` element" . The most demanding part is the calculation of the boundary and its characteristics. Therefore, for multiple calculations with the same boundary we recommend to use `make boundary` and `delete boundary` commands.

show energy gradient

`show gradient`

show gradient calculated by the `minimize` or `show energy` commands.

show hbond

`show hbond` [*r_maxHbondDistance*]

calculates and outputs the list of `hydrogen bonds`. The real argument *r_maxHbondDistance* defines the upper bound of the distance between a hydrogen and a potential hydrogen acceptor to place the pair to the hydrogen bond list. Default value of *r_maxHbondDistance* parameter is 2.5 A. Number of identified hydrogen bonds is saved in `i_out` . To display/undisplay hydrogen bonds, use `display hbond` and `undisplay hbond` commands. Hydrogen bonds can also be calculated by the `minimize` and `show energy` commands provided that the `hydrogen bond term` is switched on.)

show bond exact

`show hbond exact`

calculate the hydrogen bonding energy according to the distributed electron density geometry. Used in virtual screening to evaluate a score.

show table in html format

`show html` *T_* [`link` T_.S_1 *s_linktype1* T_.S_2 *s_linktype2* ...]

show the *T_* table with HTML tags. Interpret web links according to the web link types described in the `WEBLINK.DB` array.

See also:

- `write html` *s_file T_* [`link` ...] − write the html document to a file
- `web` *T_* [`link` ...] − directly show the table in the web browser.

Option `none` suppresses the table title and the copyright notice.

Example:

```
show html SR link SR.NA2 "PDB"
```

show iarray

`show iarrays`

show integer arrays defined in the shell. It shows names, dimensions and the first elements of arrays. The `I_out` array contains the output of some functions and commands and is always in the shell.

```
ii={1 2  3 4 5 6 76}
iii=Count(10)
show iarray
--------------- iarrays ---------------
  I_out[1:1]    { 0, ... }
  ii[1:7]       { 1, ... }
  iii[1:7]      { 1, ... }
```

show integers

`show integers`

show all integer shell variables. Example:

```
show integer
-------------- integers --------------
  a               111
  autoSavePeriod  10
  defSymGroup     1
  i_out           0
  minTetherWindow 20
  mnRemarks       3
  mnSolutions     50
 ...
```

show label

`show labels`

show graphics string labels to find out their number. Then the labels can be addressed as `label 1, label 2` etc.

See also: `display` *string_label*

show library

`show libraries`

show loaded ICM−libraries. It's a lot of stuff, enter 'q' to exit.

show link

`show link`

show links between sequences, alignments and corresponding molecules of 3D objects.

show logical

`show logicals`

shows all logical shell variables in ICM−shell. Example:

```
aa=yes
show logical
-------------- logicals --------------
  aa             yes
  l_alignProfiles yes
  l_antiAlias     yes
  l_antiAliasGLfix no
  l_autoLink      yes
  l_bpmc          yes
```

```
...
```

show mol

`show mol` *as_select*

shows selected atoms in the `mol` file format. See also: `read mol` and `write mol`.

show mol2

`show mol2` *as_select*

shows selected atoms in the `mol2` −file format (file extension .ml2). See also: `read mol2` *"file"* and `write mol2` *"file"* .

show molecule

`show molecules`

shows all molecules of all objects currently in icm−shell. This command is identical to `show a_*.*`

show object

`show objects`

shows all molecular objects currently in icm−shell. This command is identical to `show a_*.`

The same result is achieved with the `list a_*.` command.

show pdb

`show pdb` *as_select*

show selected atoms in the PDB file format.

See also: `read pdb` *"file"*, and `write pdb` *"file"*.

show preferences

`show preference`

shows all icm `preference` variables in icm−shell (e.g. .

```
show preferences
..
 atomSingleStyle  = "tetrahedron"
       1 = "tetrahedron" # current choice
       2 = "cross"
       3 = "dot"
..
```

show profile,rarray,real,sarray,string

show profile | rarray | real | sarray | string

shows all objects of specified type(s) in icm−shell. E.g. E.g.

```
show sarray rarray
```

show residue

show residues

shows all residues in all molecules of all molecular objects. This command is equivalent to

```
show a_*.*/*
```

show residue type

show residue types

show names and characteristics of compounds described in the icm.res and user ICM residue libraries.

show segment

show segment [*ms_*]

show segment representation of 3D structure of a protein for the selected molecules *ms_* (all molecules of the current object by default).

See also assign sstructure segment, ribbonStyle, display ribbon.

show sequence

show sequences [number] [{ fasta | swiss | pir | gcg | msf }]

show all sequences or the specified sequence *seq_* in one of specified formats. The default format is the fasta format. Option number defines if the residue numbers are added.

Three logicals: l_showSstructure, l_showSites, and l_showAccessibility control the display of a corresponding additional information aligned with the sequence.

Example:

```
read sequence "GTPA_HUMAN"
show sequence swiss GTPA_HUMAN

read pdb "1lbd"
show surface area
make sequence
 Info> sequence  1lbd_m  extracted
show 1lbd_m  # you see relative accessibilities in 0−9 scale
```

```
l_showAccessibility = no
show 1lbd_m
```

show stack

show stack [[*i_FromConf*] *i_ToConf*]

show the following parameters of the conformations currently residing in the conformational stack.

- iconf − a slot number
- ener − total energy as calculated before the conformation was stored
- rmsd − the distance (either Cartesian or angular RMSD) between the current conformation of the object and the stack conformation calculated according to the compare command.
- naft − the number of visits AFTER the last improvement of energy
- nvis − the total number of visits to this slot; since new conformation are only compared with the last stack conformation the conformations may drift and cover a large area than described by the vicinity parameter

show table

show *T_table* [database]

shows the specified table . See also: show html *T_* . Database index tables are exceptions, show T_index will show all the entries of the related database. To see members of an index table type the index table name and press TAB.

show terms

show terms [all]

shows the active energy/penalty terms. With option all it shows all the terms available. The result is saved in the s_out string. See also: set terms, delete terms.

show tethers

show tethers [mute] [*as_select*] [*r_minDeviation*]

Shows tethered atoms with deviation larger than *r_minDeviation* (0. by default) and returns these atoms in as_out . Option mute is used when you just want to get a selection (as_out) of strongly deviated atoms.

See also: display tethers.

show version

show version

show characteristics of the current ICM executable. Part of this string containing the version number is returned by the Version( ) function.

show vrestraints

show vrestraint [*vs_*]

shows vrestraints imposed on the internal variables of ICM molecular object.

show vrestraint type

show vrestraint types

shows types of vrestraints. These types are loaded from the icm.rst file.

show volume

show volume { surface | skin } [mute] [*as_1* [*as_2*]]

Calculates the volume confined by the solvent−accessible surface or molecular surface (so called "skin"), respectively . Two optional selections [*as_1* [*as_2*]] impose a mask on atom pairs, only those to be considered. If only the first selection is specified, the second one is assumed to be all atoms. The volume will be stored in r_out and the number of triangles used in the skin construction in i_out .

Examples:

```
read obj "small"
show volume surface              # inside accessible surface
print "volume inside accessible surface = ", r_out
show volume skin                 # inside molecular surface
print "volume inside molecular surface = ", r_out
```

calculate volume of blobs of map density.

show volume [map] [I_indexBox[1:6]] [*r_Threshold*]

Contour electron density map at a given *r_Threshold* and calculate the volume of the high−density blobs. Defaults:

- take the current map;
- contour the whole map;
- use threshold value from the ICM−shell real variable mapSigmaLevel .

Threshold is expressed in the units of standard deviations from the mean map value, i.e. 1. stands one sigma over the mean. The volume will be stored in r_out . See also: make grob *m_* .

Examples:

```
read map "crn"                   # load m_crn map
show volume m_crn 3.             # calculate volume inside the
```

2.20.69. sort

a family of `sort` commands (sort objects, molecules in ojbect, array/arrays or sort tables by their columns).

sort array(s)

`sort` [`reverse`] [`number`] *sort_key_array* [*array2 array3 ...*]

sort one or several integer, real or string arrays. The first array is the sort key. By default ordering is lexicographic for string arrays and by increasing arithmetic value for integer and real arrays.

Options:

- reverse: reverse the sense of comparisons.
- number: enforce sorting according to arithmetic value for string arrays.

Examples:

```
a={3 2 1 5 7 4 6}
b=Sin(a*50.)
c={"three" "two" "one" "Five" "Seven" "four" "Six" }
show column a b c
sort a b c
show column a b c
sort reverse b a c
show column a b c
sort c b a
show column a b c
```

sort molecular objects by mass or a user field

`sort object` [`field` = *i_Field*]

resorts **all** molecular objects by the specified user field (see the `set field` command, and the `Field` function). If the `field` is not specified, the objects are sorted by their mass.

sort molecules in an object by mass or a user field

`sort` *os_ObjectSelection* [`field` = *i_Field*]

resorts the molecules in each of the selected non−ICM objects by the specified user field (see the `set field` command, and the `Field` function). If the `field` is not specified, the molecules are sorted by molecular mass. An ICM object can be stripped, resorted and then converted again.

sort table

`sort` [`reverse`] [`number`] table.keyArray1 [`reverse`] table.keyarray1 [`reverse`] ...

this command sorts all the arrays of the `table` so that all the listed *table.keyArrays* are applied sequentially with descending priority. Each array can be followed by the `reverse` option to change the

sorting order.

Examples:

```
 read table s_icmhome+"res.tab"  # residue properties
 group table RES $s_out  # create an ICM table RES
 sort RES.aa             # resort entries by residue name
 show RES
 sort reverse RES.flexInd RES.aa
 show RES
 sort RES.hPhobInd  RES.flexInd
 show RES
```

`sort stack`

sort conformations in a `stack` according to their energies. New energies can be assigned to the same conformations with the `set stack energy` command.

2.20.70. split

can split grobs or tables into individual components.

split grob

`split` *g_complexGrob* [*s_rootGrobsName*] [*i_maxNofGrobs*] [*r_minNofPointsInGrob*]

divide disconnected parts of a graphics object into a bunch of separate graphics object sorted according to their size (measured as the number of vertices). The maximal number of new grobs is defined either by *i_maxNofGrobs* explicitly or by the MnGrobs parameter. The latter can be redefined in the `icm.cfg` configuration file. The *i_maxNofGrobs* option allows to retain only larger pieces. Grobs will be sorted according to their number of points and named by adding their sequential number to the input grob name or *s_rootGrobsName*, if specified.

The split command is used in protein cavity analysis and other applications where one needs to treat, display, and measure disconnected parts separately. You can also limit the **number of points** of the grobs generated by the command by providing the real argument with the minimal number of vertices you want in a grob.

See also: `Volume`(*g_)*, `Area`(*g_)*, `Xyz`(*g_)*.

Example:

```
 read object "crn"
 make grob skin a_//cb a_//cb
 split g_crn
 display grob smooth # display as one smooth surface
 undisplay g_crn
 color grob unique
 show Volume(g_crn3) Area(g_crn3) # you can also Ctrl-RightClick the grob
 quit
# another session
 read map "crn"
```

```
 make grob
 split g_crn "blob" 30    # create up to 30 largest grobs and
                          # call them "blob1" "blob2"...
# a variant: split g_crn "blob" 40 100.0  # discard grobs smaller than 100. vertices
 delete g_crn
 display grob
 color grob unique
```

`split` [*t_tableName*]

split `table` into individual arrays.

Example:

```
 group table t {1 2 3} "a" {2 3 4} "b"  # t.a t.b arrays
 split t                                # a and b arrays
```

`split` [*tableColumn*] [`separator=` *character*]

takes each string of the specified column and splits it by the separator (comma is the default separator, e.g. `separator=","`) The rows are multiplied accordingly. Example:

```
group table t {1,2} {"a,b,c","d,e"}
t
 #>-A----------B----------
    1           a,b,c
    2           d,e

split t.B separator=","
t
 #>-A----------B----------
   1           a
   2           d
   1           b
   1           c
   2           e
```

Note that extra columns are appended to the original table (that explains somewhat strange order).

Splitting an object into separate molecules

`split object`

There is no such command, but if you want to split a molecular object into separate molecules, you can simply copy the object and delete unwanted molecules in each copy. Example:

```
 copy a_ "b"
 delete a_b.!1  # delete all but the first molecule
 write a_b. "b" # contains only the first molecule
#
 copy a_ "c"
 delete a_c.!2  # delete all but the second molecule
 write a_c. "c" # contains only the second molecule
#etc..
```

2.20.71. sprintf

`sprintf` [`append`] *s_formatString arg1 arg1 arg2 arg3 ...* [`name=` *s_outputStringName*]

Print to the `s_out` string, or the *s_outputStringName* specified after the `name=` option. The same syntax as `printf` command, but the result is not displayed.

Example in which string `outStr` is the destination:

```
sprintf "mncalls = %d\n",mncalls name="outStr"
```

2.20.72. store

store things to internal memory structures.

store conf

`store conf` [*i_slotNumber*] : *store *conf i_slotNumber { r_energy | number= i_nOfVisits }

store current conformation into specified slot of the conformational stack. By default it puts the conformation into the first free slot, or appends it to the end. The energy, by default, is automatically extracted from the previous energy evaluation, or taken from *r_energy* if explicitly provided. The total number of visits (`nvi`) is set to 1 by default, or Example:

```
buildpep "WSD"
montecarlo           # generates a stack
show stack
set v_//omg 180.     # change a conformation
store conf -9.       # add conformation with energy -9.
store conf 3, -9.    # override slot 3 with energy -99.
store conf number=33 # set conf with number of visits=33
```

store conf

`store torsion type` [*vs_*]

store temporary torsion types for new ICMFF potential for a given molecule (not used in the commercial distribution).

2.20.73. ssearch

is a systematic search through torsion space combined with local minimization.

- you may globally optimize any set of energy/penalty terms including electrostatics, solvation, entropy, density correlation etc.
- you may search an arbitrary subset of variables
- you may allow full local minimization after each systematic change
- you may search only through centers of the preferred local `multidimensional zones` (for example `rotamers`) which is more efficient than an even grid sampling

- you may perform both the global search (the full [−180.,180.] range) and the local search (grid search around the current conformation).

`ssearch` [`local`] [*vs_Ssearch* [*vs_minimize*]] [*as_select1* [*as_select2*]]

systematically changes *vs_Ssearch* variables and carries out energy minimization with respect to the *vs_minimize* variables after each systematic conformational change. The lowest energy conformation is loaded from the conformational stack at the end of the procedure. By default every variable from *vs_Ssearch* selection goes through `nSsearchStep` evenly distributed values. The step therefore is 360 deg. over *nSsearchStep*. Option `local` imposes the grid locally around the current values of *vs_Ssearch* variables. In this case the program uses `ssearchStep` parameter.

If you want to prevent the procedure from automatically writing the stack of best conformations to a file set the `autoSavePeriod` variable to zero.

See also `montecarlo` .

Example:

```
read object "crn"  # good old crambin
ssearch v_/14/x*   # place optimally Asn14 side−chain
```

2.20.74. strip

`strip` *os_object* [`virtual`]

strip an ICM−molecular object from its ICM attributes and reduce it into a pdb−object. The latter are still good for graphics, superposition, basic geometric manipulations etc. Also, some chemical operations, e.g. attaching chemical groups are best performed on simpler pdb−objects. Stripping may save you a lot of memory as well.

Option `virtual` tells the command to delete the virtual atoms upon convertion. The virtual atoms (selected as `a_//vt*`) are always present in the ICM object, but are not necessary in the stripped object.

String is also used to perform operations which are not allowed for ICM object, but are allowed for simpler PDB objects (for example dragging individual atoms with a mouse)

These commands include:

- deleting hydrogens
- make bond auto

Example:

```
build smiles "c1ccccc1"
      strip a_ virtual
```

2.20.75. superimpose

`superimpose` [[`align` | *ali_*] [`exact`]] *as_selectStatic as_selectMovable*

`superimpose` *os_static I_atomNumbers1 os_movable I_atomNumbers2*

`superimpose` *as_movableByTethers*

optimally superimpose the second movable object onto the first one using selected atoms or residues as equivalent points. At least one pair of equivalent atoms needs to be provided.

Selections may by of any level: atom selection `as_` residue selection `rs_` molecular selection `ms_` or object selection `os_` . The option defines how the two sets are aligned (the residue alignment may be explicitly provided as the *ali_* argument, and the objects are `link`ed with the alignment):

alignment options:

- Default (no options): Residue alignment: by residue number. Atom alignment: by atom name for pairs of identical residues or pairs of close residues (F with Y; B with D,N; D with N; E with Qor Z, Q with Z), for other residue pairs only the backbone atoms ca,c,n,o,hn,ha are aligned.
- `align` option: *Residue* correspondence is established by *sequence alignment* using the ICM ZEGA alignment Abagyan, Batalov, 1997 *Atom* alignment: by atom name (see the default option).
- `exact` option: Residue matching is ignored. Two atom selections are directly sequentially aligned. Numbers of atoms in two selections must coincide.
- **align exact** option: Residue alignment: Needleman and Wunsch. Inside residue atoms are aligned sequentially and regardless of the name.

Number of equivalent atom pairs is saved in `i_out;` resulting RMSD is saved in `r_out;` a selection of atoms in the "static" object used for superposition is saved in `as_out`, that of "movable" object in `as2_out` .

Virtual atoms. Be default, the first two virtual atoms (`vt1` and `vt2`) are automatically excluded from both selections unless the `virtual` option is explicitly specified.

Note that if the movable object is of ICM−type it is preferable to have all six `virtual` variables unfixed (e.g. `unfix V_movableObj.//?vt*`). Otherwise, if some or all of them (`V_//?vt*`) are fixed, you will get a warning, and only the partial minimization of the RMS distance possible with the given degrees of freedom will be performed.

If the explicit order of atoms is specified and two single object selections are provided, e.g.

```
superimpose a_a. a_b. {3 5 7} {10 3 5}
```

the superposition will be performed in the specified order.

See also: `Rmsd`( ), `Srmsd`( ).

2.20.76. sys (or unix): system command

`sys` *system_shell_command* : *unix unix_shell_command

issues a system shell command from ICM. You may use `sys` or `unix` interchangeably. By default, the ICM process waits until the system shell process has completed. `sys` must be the first word in the command. **Important**: Construction

```
if ( <condition> ) sys system_command
```

is **illegal.** Use

```
if (  <condition> ) then
   sys system_command
 endif
```

instead. For cross−platform compatibility, also use the following portable ICM shell variables instead of non−portable system−specific commands: `s_sysCp` , `s_sysLs` , `s_sysLtt` , `s_sysMv` , `s_sysRm.` Example:

```
sys $s_sysCp   # cross−platform portable list command
sys ls         # non−portable unix only ls command
```

As you might have guessed from the above example, to pass the ICM−shell variables to the *system_shell_command* one may use `integer`, `real` or `string` ICM−shell variables, protected with dollar sign ($) prefix. **Important:** passing ICM−shell variables to the UNIX command is impossible if you use an alias name (e.g. `ux)` instead of the original `unix` command.

Examples:

```
unix grep −i myoglobin /data/pdb/brookdir.doc
unix echo $mncalls $s_pdbDir $dielConst

file="/data/pdb/"+Name(a_1.)     # tricky file name
unix grep ATOM $file | wc −l     # $file will be substituted by
                                 # the value of this ICM−shell
                                 # string variable
```

2.20.77. then

is one of the `ICM flow control` statements, used to perform `conditional statements`.

See also `if`, `elseif`, and `endif` .

2.20.78. transform

transform molecular objects to symmetry related positions.

`transform` {*ms_*|*g_grob*} *R_12transformationVector*

transform molecules (*ms_*) or graphics objects according to the transformation vector.

See also these two examples: (example 1 and example 2).

You can also manually move molecules with respect to each other on the graphics screen by using the `connect` *ms_* command to choose the molecules which can be moved separately.

`transform` [`copy`] *ms_* [*i_number*] [*s_symgroup*] {`box` |*as_selection r_radius*}

transform molecules `ms_` according to the specified transformation. *i_number* is a symmetry operation number in an array of all operators of a space group. The symmetry transformations are defined in a 12*n real array where each chunk of 12 real values defines 3x3 rotation matrix and translation vector {a4,a8,a12}. The complete 4x4 transformation matrix looks like this:

```
a1  a2  a3  | a4
a5  a6  a7  | a8
a9  a10 a11 | a12
------------+----
0.  0.  0.  | 1.
```

If *i_number* exceeds the number of space group symmetry transformations the symmetrical images in up to 26 surrounding cells are created. This operation is only possible, if symmetry information (sym.group name and cell dimensions) is defined for the object. Usually PDB and CSD files contain the above information, it is preserved upon `conversion`. Use the `Cell`( ) or the `Symgroup`( ) functions to find out if the space group is defined. If not, you may assign it to the object with the `set symmetry object` command. In a special case of *i_number=0*, the object is placed in the "primary" subunit of the cell (e.g. in sym.group "P 21 21 21" that is 0<x<a, 0<y<b, 0<z<c/4; currently, the *i_number=0* option is supported only for groups 1 and 19).

Example:

```
read mol2 "ex_mol2"  # several small molecules
display a_4.
build hydrogen a_4.  # added and displayed
```

2.20.79. translate

`translate` { *os_* | *ms_* | *g_grob* } [`add`] [`symmetry`] *R_3translationVector*

translate the center of mass of the specified object(s) (*os_*) or molecule(s) (*ms_*) **to** a specified position, or **by** a *R_3translationVector* vector if option `add` is specified. You can also move molecules/objects interactively with the mouse after the `connect` command.

symmetry option With the `symmetry` option the R_3translationVector should be in **fractional** coordinates. Option `add` translates **by** the specified vector from the current position. Without `add` the program tries to identify a compensating shift to a position in which the center of gravity of the selected molecule(s) has minimal positive fractional coordinates.

Examples:

```
read pdb "1fbi"
delete a_!p,q,y  # get rid of reduncancies
cool a_
```

```
for i=1,10
  translate a_y i*{0., 0., −0.5}  # shift molecule y  by an increment
endfor
```

To calculate a displacement vector, following this example in which we calculate a translation vector for molecule `y` :

```
read pdb "1fbi"
delete a_!p,q,y  # get rid of reduncancies
cool a_
v1 = Rarray( Xyz( a_y/1/ca ) )
connect a_y  # no drag the molecule with the middle button and press Esc
v2 = Rarray( Xyz( a_y/1/ca ) )
v_trans = v2 − v1
```

2.20.80. undisplay

Opposite to `display` . To get rid of the whole graphics window for fast calculations use

```
undisplay window
```

Examples of the undisplay command:

```
undisplay ribbon              # ribbon display not needed any more
undisplay g_icos              # a graphics object not needed any more
undisplay a_/w*,hoh*          # who cares about water molecules ...
undisplay residue labels      # just "labels" will do the same
undisplay string              # see also "delete label" command
undisplay a_//h*              # who cares about hydrogens ...

undisplay hbond a_1./1:29     # ... and, hence, about H−bonds
undisplay tether a_/12:20
undisplay box
undisplay cursor
undisplay origin              # undisplay the coordinate frame
undisplay window              # delete GL graphics window
```

2.20.81. unfix

`unfix` [`only`] *Vs_select*

unfix (set free) specified variables (such as bond lengths, angles and phases or torsions) in an ICM−object. Opposite to `fix` command. This operation can be applied to the `current object` only (use `set object` *`os_newObj`* first).

Important: since it only makes sense to unfix variables which are currently fixed, use `Vs_select` which selects among ALL (both free and fixed) variables, as opposed to `vs_` which selects only from FREE variables.

Examples:

```
      # only this loop has free torsions now
unfix only V_/8:18/phi,PSI,H,M,P
```

Note that PSI torsion references is used for traditional residue attribution

2.20.82. wait

wait for the child ICM processes to finish, quit the child processes

wait

allows to synchronize multiple ICM processes spawned by the fork command.

- for the parent process: wait until all the child processes spawned with the fork command are finished.
- for the child processes: quit the spawned ICM process

See also: iProc , nProc .

2.20.83. web

web *Args* ...

a family of web commands.

web [delete] *u_EntrezRequest*

invoke a web browser call to the WWW page of the Entrez server at NCBI and display your database entries with links. The format of the requests is described at http://www3.ncbi.nlm.nih.gov/Entrez/linking.html. The s_webEntrezLink string defines the location of the link and the webEntrezOption preference defines the type of the Entrez report. The delete option will temporarily set l_confirm=no for this command.

Examples:

```
web sp||GTPA_HUMAN  # Swissprot by ID
web sp|P07497|      # Swissprot by accession
web emb|U01234|     # EMBL by accession
web pdb|1crn|       # PDB by ID (a single chain entry)
web pdb|2ins|a      # PDB by ID and chain character
web 1111111         # NCBI nonredundant database
```

2.20.84. web table: shows an icm table with a web browser

web [delete] [*s_file*] *T_* [link T_.S_1 *s_linktype1* T_.S_2 *s_linktype2* ...]

ICM invokes a web browser call. If you do not have a browser (defined by the s_webViewer string) currently running under your login, the call will fail. The command presents the *T_* table in your web browser window. Optional web links are interpreted according to the web link types described in the WEBLINK.DB array.

See also:

-

`writehtml{write html [s_file] T_ [link ...]}

− write the html document to a file

- `showhtml{show html T_ [link ...] }

− show the table in the icm text window.

Example:

```
 show html SR link SR.NA2 "PDB"
#
 read sequence "GTPA_HUMAN.seq"
 find profile
 show SITES
 web SITES
 web SITES link SITES.AC "AUTO"
```

2.20.85. while

`while`

is one of the `ICM flow control` statements, used to perform a `loop` in the ICM−shell calculations.

See also: `for`, `endwhile` .

2.20.86. write

write stuff to a disk file. Logical variable `l_confirm` defines if you'll be prompted whether to overwrite an existing file with the same name. Use option `delete` to delete (or overwrite) the existing file unconditionally.

For the list of ICM−objects you can write, and formats you can choose, see `read` and `show` commands. Generic syntax:

`write` [`binary`] [`append` | `delete`] { *variable* | *constant* | *expression* } s_fileNameRoot[.ext]

With the `binary` binary option multiple objects or classes of objects can be writtin into a single cross−platform compatible binary file.

See also corresponding `read` commands.

write alignment

`write` [`alignment`] [`msf`] *ali_Name* [*s_fileName*]

write alignment *ali_Name* to a file. Default extension is `.ali` . Note: if alignment is only a group of unaligned sequences, generated by the `group` command, the result will be just a `multiple sequence file`, rather than an `alignment file` (there will be no dashes at the end).

The default ICM format for an alignment looks like this:

```
#>ali sh3
# Consensus       ...#.^.YD%..+~..−#~# K~−.#~##.~~..~WW.#.   ~~.~
Fyn           ----VTLFVALYDYEARTEDDLSFHKGEKFQILNSSEGDWWEARSLTTGET
Spec          DETGKELVLALYDYQEKSPREVTMKKGDILTLLNSTNKDWWKVE−−VNDRQ
Eps8          KTQPKKYAKSKYDFVARNSSELSM−KDDVLELILDDRRQWWKVR−−−NSGD
#Fyn              __EEEE____________________EEEEEEE____EEEEEE_____E

# Consensus   G%#P...#..#.
Fyn           GYIPSNYVAPVDSIQ
Spec          GFVPAAYVKKLD−−−
Eps8          GFVPNNILDIMRTPE
#Fyn          EEEGGGGEEE_____

# nID 7 Lmin 61 ID 11.5 %
```

The lines starting from hash (#) are comments and are not required

The length of each alignment block is controlled by the `sequenceLine` parameter (default value is 60). If you want to save a long alignment as one unwrapped block, increase this value (e.g. `sequenceLine=1000`)

Writing sequences in the alignment order

The sequences can be written in the alignment order with the following commands (they can be store in a little macro)

```
macro wrSeqAli ali_ s_file ("seq.fasta")
 l_showSstructure = no
 seqname = Name(ali_) # Name returns sarray of sequence names
 for i=1,Nof(seqname)
   write sequence fasta append $seqname[i] s_file
 endfor
endmacro
```

Resorting alignment in the order of sequence input.

Upon alignment the source sequences get reordered according to similarity. If you want to keep the original order you may use the `reorderAlignmentSeq` macro described in the `Align`(*ali_ I_newOrder*) section and then write an alignment:

```
read sequence s_icmhome+"zincFing"
group sequence aaa
align aaa
reorderAlignmentSeq aaa
write ali_new    # reordered alignment
```

See also: `String`(*ali_)* function.

write binary

`write` [`binary`] [*class1 class2 ...*] [*obj1 obj2 ...*] [*s_fileName*]

write specified ICM shell objects or all objects of a classes to a single, binary, cross−platform file, or more accurately, database. The following data types are currently supported:

- `table`
- `grob`
- `integer`
- `real`
- `string`
- `iarray`
- `rarray`
- `sarray`

The catalogue of the database can be obtained with the `list binary` command. The default file name is `"icm.icb",` and the default extension is `.icb` (stands for ICm Binary file). The system objects or the objects with property

Examples: ii = {2 3 4} rr = {2. 3.4 5.5} g = Grob("CELL",{1. 1. 1.}) g2 = g*2. # twice as large write binary iarray rarray grob # the default file is icm.icb Info> *4 icm shell objects* icm.icb

list binary # looks at "icm.icb" *1 ii iarray 20* : 2 rr rarray 32 *3 g grob 1788* : 4 g2 grob 1788

delete ii read binary name={"ii"} Info> *1 icm shell objects read from* icm.icb

write binary grob "aaa" Info> *2 icm shell objects* aaa.icb

See also: `list binary`, `read binary`

write iarray

`write` [`iarray`] *I_name* [*s_fileName*]

write rarray

`write` [`rarray`] *R_name* [*s_fileName*]

write sarray

`write` [`sarray`] *S_name* [*s_fileName*]

write matrix

`write` [`matrix`] *M_name* [*s_fileName*]

write an array or a matrix to a disk file. Default file extensions are `.iar, .rar, .sar,` or `.mat,` respectively.

See also: `read iarray`, `read rarray`, `read sarray`, `read matrix`.

write several arrays

`write` [{ `column` | `database`] } *array1 array2* .... [*s_fileName*]

write arrays in the `column` or `database` format to a disk file. Default file extension is `.db`

See also: `read database`.

writing tethers

If you imposed tethers between you current object and another object and you want to quit the session and then restore you setup, you can use the following trick:

first let us create an object a_ly6. tethered to template a_x. read alignment s_icmhome+"sx" read pdb s_icmhome+"x" build model ly6 a_x.m # a new object a_ly6. created and tethered # write string String(a_//T) "tTz.str" # tethered model atoms write string String(a_//Z) "xTz.str" # x−template atoms write object a_x,ly6. "tx.ob" # quit # % icm read object "tx.ob" read string "tTz.str" name="tTz" read string "xTz.str" name="xTz" set tether $xTz $tTz exact # tethers restored

write table

writing ICM table in text format `write` *T_table1* [*T_table2* ..] [`field=` *s_delimiter*] [*s_fileName*]

write the *T_table* `table` to a disk file `*.tab`. It will have two header lines with table name and field name information, followed by the values.

The default extension `.tab` is appended automatically. The ICM text table format has a header which allows to read this table back to icm with the `read table` command

Example:

```
group table t {1 2 3} "a" {"one","two","three"} "b"
t1=t[2:3]
write t t1 "tt"  # write both tables in one file
delete table     # read both tables
```

writing tables in CSV or TSV formats

`write` *T_table1* [`header`] [`separator=` *s_delimiter*] [*s_fileName*]

if the separator or the `s_fieldDelimiter` variable contain just a simple symbol (e.g. comma or tab), ICM will write a comma−separated or tab−separated table with the first line containing the field names, e.g.

```
group table t {1 2 3} "a" {"one","two","three"} "b"
write t header separator="," "t.csv"
unix cat t.csv
a,b
1,one
2,two
3,three

write t separator="," "t.csv"  # without header
unix cat t.csv
1,one
2,two
3,three
```

To read a table in comma−separated format with the headers, use the following commands:

```
read table separator="," header name="t" "t.csv"
```

writing tables in a binary format

`write binary` *T_table1 T_table2 .. s_file* : *write *binary *tables s_file

The most compact and fast format is the binary format. Any object can be saved to and read from a binary project file with `".icb"` (ICM−binary) extension.

See also `write database T` and `write column`.

`write` *table* `mol` *s_sdfFileName*

writes an ICM chemical spreadsheet as a `mol/sdf` file. All the property columns are added as feature records to individual mol−entries.

Example:

```
read table mol "ex_mol.mol" name="t" unique
write table mol t
```

write column

`write column` *array1 array2 ....* [*s_fileName*] [`separator=` *s_Separators*]

write arrays in a multi− `column` format to a disk file.

Examples:

```
read column s_icmhome + "res.tab"    # amino acid properties
write column aa flexInd  "tm.tab"    # two columns
```

If you want to write all the entries of an ICM−table you may do the following.

Examples:

```
read column s_icmhome + "res.tab" # a set of isolated arrays
group table RES $s_out  # create an ICM-table RES (s_out : array names)
write RES               # write in the 'table' layout
write database RES      # write table RES in the 'database' layout
```

Default file extension is `.col`.

See also: `read column`, `show column`. `read table`, `show table`.

write database

`write database` [`html`] { *array1 array2 ....* | *table* } [*s_fileNameRoot*]

write several arrays or a table in a database format to a file (usually tables are written in a multi `column` format). This command can also be used to save a subset of arrays of a table in a specific order. Option `html` writes the table with appropriate HTML tags. See also `read database` `write table`, `show database`.

Example:

```
 resnam = {"ala" "glu" "arg"}
 reschg = { 0., −1., 1.}
 write database resnam reschg "a" # default extension ".db" will be added
#
 group table t resnam reschg
 write database t.reschg t.resnam "a"  # reverse the order</tt>
```

write drestraint

`write` `drestraint` [*as_*] [*s_fileNameRoot*]

write distance restraints of the current object to a file.

See also: `drestraint`s and `drestraint type`s.

write drestraint type

`write` `drestraint types`

write `drestraint type`s to a file. You may define your own types with the `set drestraint type` command or by editing a *.cnt file.

write factor

`write` [`factor`] *factor_Name* [*s_factorFileNameRoot*]

writes crystallographic structure factors to a file.

write grob

`write` [`grob`] [*g_name*] [*s_fileName*] [`append`]

write/append a graphics object `(grob)` to a disk file. If *g_name* is not specified, all `grob`s are written. Default file extension is `.obj`

See also: `write image`, `write postscript`.

write html

`write` `html` *s_htmlFileName T_* [`link` T_.S_1 *s_linktype1* T_.S_2 *s_linktype2* ...]

writes the *T_* table with HTML tags to a file. Interpret web links according to the web link types described in the `WEBLINK.DB` array.

See also:

- `show html T_ [ link ... ]` − show the html formatted table in the text window
- `web T_ [ link ... ]` − directly show the table in the web browser.

Example:

```
write html SR "results.htm" link SR.NA2 "SP"  # link to Swissprot
```

write image

`write image` [{ `png` | `targa` | `gif` | `rgb` }] [`display`] [`print`] [`postscript` [{ `print` | `preview` }]] [`compress`] [`stereo`] [{ `color` | `bw` }] [`window=` *I_xyPixelSizes*] [*s_fileName*]

write the current screen image to a file. The default image file format is `tif` . The png−format is the most compact and is recommended for web−publishing. The default settings are stored in the `IMAGE` table. Some of them can be overridden by the following options:

- `display` − allows to view the saved image or postscript image file. The viewer is defined by the `s_imageViewer` variable for targa, gif, rgb and tif images and by the `s_psViewer` variable for the postscript images.
- `postscript` − write Adobe postscript−bitmap file rather than TIFF−file. See also `write postscript` command which generates **vectorized** scalable high quality postscript files.
- `preview` − add low−resolution preview to postscript file for some EPS−compliant image viewers (i.e. Irix showcase®). Resolution, and therefore the size, of the added preview is defined by the `IMAGE.previewResolution` (default 10).
- `print` − print the postscript file. It will not work for non−postscript images, in which case you may use the display option and print from your image viewing program instead.
- `compress` − use packbits lossless compression standard for **.tif** files. Compression of this kind is currently a standard feature of all baseline `TIFF`−reading programs. Compression is a standard feature of the .gif and .png formats.
- `stereo` − generate stereo image even from the mono display. Tiff−files preserve the image screen dimensions for each image in a stereo−pair. Stereo−base for postscript files is controlled by the `IMAGE.stereoBase` parameter and equals 2.35" (60mm) by default.
- `color` or `bw` − color or black−and−white options surpass `IMAGE.color` logical variable.
- `window=` *I_xyPixelSizes* − generate image of any arbitrarily large resolution (e.g. `window=3*View(window)` to triple the resolution). Suppose that you want to make a poster of 4613 by 2888 pixels. This resolution is not achievable on a 1200x1024 screen. The image area will be divided into many squares and the program will merge them into one image of large resolution. This option will not work with string labels.

  Example:

```
nice "1crn"  # resize the image
delete label
IMAGE.compress = no  #just a plain uncompressed image
write image window={4000,2700} # for slides

write image window=2*View(window) # double the res.
```

`IMAGE.generateAlpha` logical variable controls if the alpha channel information is added to the SGI `rgb` and `tif` image files. This additional channel describes opacity of the image pixels and makes the background transparent. Images generated with alpha channel can be nicely superimposed in the IRIX showcase since their backgrounds are transparent.

Examples:

```
display a__1crn. ribbon
write image "a"              # a.tif image − about 1400 kB
write image "p" compress     # p.tif image − about 88 kB
write image postscript stereo display "aaa.eps"
write image 2*View(window)   # hi−res, may screw up labels
unix lp −c a.eps             # print if you like the result
```

See also: `write grob`, `write image` , `write postscript`.

write index

`write index` [`swiss` | `mol` | `mol2` | `fasta`] [*T_dbDescription*] *s_outFile*

calculate and write index for a database described by the control table *T_dbDescription.* This table contains information about the database file (files) and fields to be indexed. It may have the following components in the header:

- DIR − string directory name
- FI − sarray of database files
- EXT − extension of the database files

After the header there is a string array containing the list of fields. To create this table either define it in a file or use the `group table` command. All text fields (except data) are hashed for fast searching. The `fasta` option allows to index the NCBI nonredundant databases. See also: `makeIndexChemDb` macro to do indexing in one step, `mol`, `mol2` .

Example:

```
group table t {"ID","DE","KW","SQ"} "fd" header "/data/swissprot/" \
      "DIR" {"sprot"} "FI" ".dat" "EXT"
              # we created control table t
write index swiss t "/data/icm/inx/SWISS.inx"  # make index and save to a file
read index "/data/icm/inx/SWISS.inx"           # read index
show SWISS[2:5]
show SWISS.ID=={"12AH_CLOS4","1431_LYCES","B3AT_CHICK"}
read sequence SWISS.DE=="DNA−BINDING"
```

write index blast

`write index sequence` *s_blastRootFileName*

create a set of blast−formatted binary files for searches with the `find database` command. The command will use all the sequences currently loaded into the ICM−shell and will create the following compact binary files (the first three files are the same as those generated by the `setdb` blast command):

- *name.bsq* binary sequences
- *name.atb* pointers
- *name.ahd* sequence headers
- *name.bsa* relative solvent accessibilities for each residue. This information

If you want to do the opposite (i.e. given the three or four blast files, generate one fasta sequence file), use the

`find database write` *s_DBpath* `output=` *s_fastaFile*

command.

Simple example (indexing can also be done with the blast setdb routine):

```
read sequence "aaa.seq" # fasta formatted
write index sequence "./aaa"
delete sequences
a=Sequence("SFDGHASGDFSHGASFDHAGS")
find database a "./dom" 0.001
```

An example in which the sequences+accessibilities are generated from objects:

```
read sarray "domain.list" name="dom"  # e.g. {"1crn","1abc.a/12:115/",..}
for i=1,Nof(dom)
 read object s_icmhome+"data/xpdb/"+dom[i]
 show area surface mute   # calculate the absolute acc. areas
 make sequence a_1        # the relative areas are calculated and assigned to seq.
 delete a_*.
endfor
write index sequence "./dom"  # files .bsq .atb .ahd .bsa created
delete sequences
```

write library

`write library` [`append`] [`auto`] *as_entryAtom* [`exit=` *as_exitAtom*] *s_libFileRoot*

save a selected molecule, residue or a fragment as an `ICM−library entry`. Use `set charge`, `set bond type` and, possibly, `build hydrogens` before writing an entry. We recommend you to do this operation in an interactive session: display your molecule and `Ctrl−Click` the first and last atoms if needed. There are two different situations:

1. the molecule/residue/fragment does not belong to an ICM−type object. For example, you have a pdb−file with a new molecule you would like to create an ICM−library entry from. In this case do NOT use option `auto` and note that the resulting entry will only be a draft, since energy

parameters of atoms (`atom codes` plus related types of van der Waals, hydrogen bondings solvation), as well as parameters of torsions, bond angles, phase angles, and bond lengths will have to be further manually adjusted. Enter the command and you will be prompted for the first and the last atoms of the entry. The purpose of this procedure is to create a regular ICM−tree, create extra bonds if there are cycles and give atoms unique names. Some additional editing of the entry may be required to correct fixed and free torsions suggested by the program. To declare a certain variable free, enter '+' in the appropriate field.

2. the molecule/residue/fragment belongs to an ICM−type object. In this case you may use option `auto` since all the information is there already. The program only needs to extract the molecular subtree according to the specified selection.

Example:

```
 BS nter glu cooh # build glutamic acid residue
 strip   # convert it to a non−ICM object
 write library a_def.a1/1/hg2 "./tm" name ="new" auto  # reroot it
# Now the entry atom is a_//hg2
 build string "se new" library ="./tm"   # read the rerooted residue
 display
```

write map

`write` *m_map* [*s_fileName*]

write specified map to a binary file with specfied file.

`write` { `map` | *m_map1 m_map2 ...* }

write all maps or specified maps to corresponding files (the names for the files are generated from map names, the `m_` prefix is removed from the file names).

`write xplor` *m_map ...* [*s_fileName*]

write the specified map to a Xplor−formatted file.

Example:

```
 make map "ge,gc" potential Box(a_)
 m_gc... done
 Info> Map m_gc created. GridStep=0.50 Dimensions: 16 11 17, Size=2992
 m_ge... done
 Info> Map m_ge created. GridStep=0.50 Dimensions: 16 11 17, Size=2992
 write m_ge m_gc
 Info> 1 map written to file  ge.map
 Info> 1 map written to file  gc.map
```

write model: update or create the loop database file

`write model` [`append`] *s_lpsFile*

writes a compressed representation of the protein structure to the specified loop file (`"def.lps"` by default). To create a large database, read the object list and write a loop over all objects, e.g.

```
# prepare pdbUniq list and ..
 read sarray "pdbUniq.li"
 for i=1,Nof(pdbUniq)
   read object s_xpdbDir+pdbUniq[i]
# add further filters
   write model append "icm.lps"
   delete object
 endfor
```

To make the program use this file , redefine the `LIBRARY.lps` file name to, say `"./icm.lps"`

write mol

`write mol` [`exact`] *as_select* [*s_fileName*]

write selected atoms in the `mol` −file format. By default the formal charges (see the `set charge` command) are saved. Options

- `exact:` preserve the ICM−atom names (like c1, c2).
- `charge:` write the MCHG section containing the atomic real charges.

See also `read mol "file"`, `show mol "file"`.

write mol2

`write mol2` [`exact`] [`formal`] *as_select* [*s_fileName*]

write selected atoms in the `mol2−file` format (extension .ml2). Options:

- `exact` preserves the ICM−atom names (like c1, c2).
- `formal` writes formal atomic charges instead of the real ones. Adds USER_CHARGES (XXXXXX) tag to the header

See also `read mol2 "file"`, `show mol2 "file"`.

write object

`write object` [`options`] [*as_selection*] [*s_fileName* [`rename`]]

write an ICM molecular object (or many selected ICM−objects) in binary `ICM format` to a file. A single object can be renamed in the file according to the *s_fileName,* if option `rename` is specified. **Important**: only **whole** ICM object may be written by this command, and file extension will always be `.ob.`

Options (defaults shown in bold):

- `append` : append to a multiple−object file
- `rename` : rename the single object to *s_fileName* (leave out path and extension) .
- `short` : write a compressed file for non−ICM objects without b−bactors and occupancies.
- `strip` : write a `strip`ped object (i.e. drop information about variables and rigid bodies present in an object of the ICM type).

- auto={yes| no} : if yes the program automatically identifies which atom requisites to save. For example, if molecule is displayed, the view will be saved with the object. Properties such as occupancy and charge are considered essential if the values are not identical for all the atoms.

  If auto=no, the OBJECT table controls the output.

- occupancy={yes|no} : occupancy field
- charge ={ yes|no} : partial atomic charges
- bfactor ={ yes|no} : b−factors
- display ={yes| no} : the current view of your molecular object(s), including graphics planes The written display attributes are automatically restored upon reading of the object.
- library={yes|**no**} : currently not used.

See also: read object, write pdb, OBJECT, strip.

Example:

```
read object "crn"
build string "se ala his" name="AH" # second object named "AH"
write object a_2. "alahis" rename   # rename obj. to "alahis"
display a_1./1:40 ribbon            # display and save with graphics attributes
display a_1./12 cpk
display a_2. xstick
write object a_*. "twoobj" display=yes # both objects in one file
write object a_1. append "twoobj"      # yet another object
```

write object simple

write object simple [*as_selection*] [*s_fileName*]

write a compressed object. The information preserved in the compressed description of the object is limited to 3 coordinates and certain atom names (non−protein atom names will not be preserved and reduced to just one character) plus all residue and molecule requisites. For a PDB−type file, a simple object is the most compact for store and fastest to read. They are used in the compact fold library.

write pdb

write pdb [exact] [charge] [nosort][*as_selection*] [*s_fileName*]

write a molecular (sub)object in PDB format. Normally atoms of each amino acid are sorted in the following order:

```
ATOM     19  N   GLN O   3      −4.565   0.000  −4.592  1.00 20.00
ATOM     20  CA  GLN O   3      −4.712   0.000  −6.037  1.00 20.00
ATOM     21  C   GLN O   3      −6.194   0.000  −6.420  1.00 20.00
ATOM     22  O   GLN O   3      −7.063   0.000  −5.549  1.00 20.00
<i>the rest</i>
```

Also the n−terminal nitrogen and its hydrogens are assigned to the first amino acid. Options are the following:

- charge saves atomic charges instead of occupancies and atomic radii instead of B−factors;

- `exact` keeps the names of hydrogen atoms the same as in ICM objects (i.e. the first character is 'h'). Without this option names of hydrogen atoms are transformed like this:

```
h11 ==> 1H1
h12 ==> 2H1
```

- `nosort` retain the original ICM order of atoms

Default file extension is `.pdb.`

See also: `write object`, `read pdb`.

write postscript

`write postscript` [`display`] [`stereo`] [`preview`] [{ `color` | `bw` | `dash`]} [*i_quality*] [*r_gammaCorrection*] [*s_filename*]

create **vectorized** postscript model of the screen image. Instead of the bitmap snapshot this command generates lines, solid triangles and text strings corresponding to the displayed objects. Since the postscript language is directly interpreted by high−end printers, the printed image may be even higher quality than the displayed image. The final resolution is limited only by the printer since the original image is not pixelized. Warning: there may be inevitable side−effects for some types of solid images at the intersection lines of solid surfaces (i.e. large scale `cpk−representation`, hint: use `display skin` instead).

The default settings are stored in the `IMAGE` table. Some of them can be overridden by the following options and arguments:

- `reverse` − makes white background in the saved postscript file.
- `display` − allows to view the saved postscript file. The viewer is defined by the `s_psViewer` variable.
- `stereo` − generate stereo image even from the mono display. Stereo−base is controlled by the `IMAGE.stereoBase` parameter and is 2.35" (6cm) by default.
- `preview` − generates postscript preview according to the `IMAGE.previewer` command string and the `IMAGE.previewResolution` parameter.
- `color` or `bw` − color or black−and−white options surpass `IMAGE.color` logical variable.
- `dash` − is a great variant of the black−and−white option to generate lines of different width and style. The line colors of your screen image are interpreted according to the following table:
- `gold` − double solid black line
- `pink` − triple solid black line
- `magenta` − dash1
- `orange` − dash2
- `brown` − dotted line
- the rest − solid black line

Examples:

```
 display a__crn.  # display wire model of crambin
 color a_//ca,c,n pink         # triple width backbone
 color a_/arg/!ca,c,n magenta  # dashed lys side chains
# zoom your picture to fill the whole graphics window
 write postscript dash stereo display
```

* *i_quality* (default=3, possible range: 1:100) − defines a parameter in a smoothing procedure. Each side of an elementary triangle is divided into *i_quality* sections and color of all the $i\_quality^2$ smaller triangles is calculated to yield smooth transitions. Optimal value of the parameter depends on an image. Only large scale images may require *i_quality* values above 10. Only in an extreme case of a single triangle on a page with red, blue and green vertexes, one may need *i_quality* of 100.

* *r_gammaCorrection* allows to lighten or darken the image by changing the *gamma* parameter. A gamma value that is greater than 1.0 will lighten printed picture, while a gamma value that is less that 1.0 will darken it. You may adjust your gamma correction parameter for your printer with respect to your display and add this setting to the `_startup` file.

Examples:

```
 display a__crn. brown skin   # molecular surface
                              # Hugh wants to have a look
 write postscript 1 1. "divine_brown" display
                              # change parameters for the printer
 write postscript 5 2. "divine_brown"
                              # and print it
 unix lp −c divine_brown.eps
```

See also: `write image`, `write grob`.

write pov

`write pov` [`image`] [*r_aspectRatio*] [*s_fileName*]

writes a pov−ray object file which can be processed with the pov−ray ray−tracing program.

Example:

```
 buildpdp "ala his trp"
 display cpk
 make grob image
 write pov "x"
% pov−ray x.pov
```

write segment

`write segment` [`append`] [*s_fileName*]

writes a simplified description of protein topology generated by the `assign sstructure segment` command to a file. You can append your description to the provided `foldbank.seg` file.

Examples:

```
 read object "crn"
 assign sstructure segment a_*
 write append segment "myseg"
```

See also: `find segment`, `read segment`.

write sequence

`write` { `sequence` | *seq_* } [{ `fasta` | `swiss` | `pir` | `gcg` | `msf` }] [*s_fileName*]

write all sequences or the specified sequence *seq_* to a file in one of specified formats. The default format is the `fasta` format.

write session

`write session` [*s_fileName*]

write commands from an ICM session to a file. Default file name is "_session.icm". This is a simple text file with icm commands. Feel free to edit the file

Example:

```
..
a=1
history 10
write session
 Info> 4 history lines written to file  _session.icm
```

See also: `history` and `delete session` commands.

write stack

`write stack` [`simple`] [*s_fileName*]

write the current state of the conformational stack to a disk file. Starting from May, 2003, version ICM3.022, the stack file is compressed by default. The stack file is not compressed if the `simple` option is used. Default file extension is `.cnf.`

See also: `show stack`, `delete stack`, `read stack`, `read conf`.

write vs_var

`write` [*vs_variables*][*s_fileName*]

write a variable selection `vs_` to a disk file.

Default file extension is `.var` .

See also: `read variable`.

2.21. Functions

ICM−shell functions are an important part of the ICM−shell environment. They have the following general format: FunctionName **(** arg1, arg2, ... **)** and return an ICM−shell object of one of the following types: `integer`, `real`, `string`, `logical`, `iarray`, `rarray`, `sarray`, `matrix`, `sequence`, `profile.alignments`, `maps`, `graphics objects (grob)` and selections.

The order of the function arguments is fixed in contrast to that of commands. The same function may perform different operations and return ICM−shell constants of different type depending on the arguments types and order. ICM−shell objects returned by functions have no names, they may be parts of algebraic expressions and should be formally considered as 'constants'. Individual 'constants' or expressions can be assigned to a named variable. Function names always start with a capital letter. Example:

```
show Mean(Random(1.,3.,10))
```

2.21.1. Abs

absolute value function.

Abs **(** *real* **)** − returns real absolute value.

Abs **(** *integer* **)** − returns integer absolute value.

Abs **(** *rarray* **)** − returns rarray of absolute values.

Abs **(** *iarray* **)** − returns iarray of absolute values.

Examples:

```
a=Abs(−5.)                 # a=5.
print Abs({−2.,0.1,−3.})   # prints rarray {2., 0.1, 3.}
if (Abs({−3, 1}=={3 1}) print "ok"
```

2.21.2. Acc

accessibility selection function. It returns residues or atoms with relative solvent accessible area greater than certain threshold. **Important:** The surface area must be calculated before this function call. The Acc function just uses surface values, it does not reevaluate them. Therefore, make sure that the show area command (or show energy, minimize , etc. with the "sf" surface term turned on), has been executed before you use the Acc function. If you specify the threshold explicitly, it must range from 0.0 to 1.0, otherwise it is set to 0.25 for residue selections and 0.1 for atom selections.

Acc **(** *rs_* , [*r_Threshold*] **)**

− returns residue selection, containing a subset of specified residues *rs_* for which the ratio of their current accessible surface to the standard exposed surface is greater than the specified or default threshold (0.25 by default). ICM stores the table of standard residue accessibilities in an unfolded state calculated in the extended Gly−X−Gly dipeptide for all amino acid residue types. It can be displayed by the show residue type command, or by calling function Area(*s_residueName*), and the numbers may be modified in the icm.res file.

The actual solvent accessible surface, calculated by a fast dot−surface algorithm, is divided by the standard one and the residue gets selected if it is greater than the specified or default threshold. (*r_Threshold* parameter is 0.25 by default).

Acc **(** as_select, [*r_Threshold*] **)**

− returns atom selection, containing atoms with accessible surface divided by the total surface of the atomic sphere in a standard covalent environment greater than the specified or default threshold (0.1). Accessibility at this level does not make as much sense as at the residue level. The standard surface of the atom was determined for standard amino−acid residues. Note that hydrogens were **NOT** considered in this calculation. Therefore, to assign surface areas to the atoms use

```
show surface area a_//!h* a_//!h*
```

command or the

```
show energy "sf"
```

command.

You may later propagate the accessible atomic layer by applying `Sphere`(as_ , 1.1), where 1.1 is larger than a typical X−H distance but smaller than the distance between two heavy atoms. (the optimal *r_Threshold* at the atomic level used as the default is 0.1, note that it is different from the previous).

Examples:

```
                                  # let us select interface residues
read object s_icmhome+"complex"
                                  # display all surface residues
show surface area
display Acc( a_/* )
                                  # now let us show the interface residues
display a_1,2
color a_1 yellow
color a_2 blue
show surface area a_1 a_1         # calculate surface of
                                  # the first molecule only

                                  # select interface residues
                                  # of the first molecule
color red Sphere(a_2/* a_1/* 4.) Acc(a_1/*)

read object "crn"
show energy "sf"
display
display cpk Acc(a_//* 0.1)   # display accessible atoms

show surface area            # prior to invoking Acc function
                             # surface area should be calculated
color Acc(a_/*) red          # color residues with relative
                             # accessibility > 25% red
```

2.21.3. Acos

arccosine trigonometric function Returns angles in degrees.

`Acos` **(** *real* | *integer* **)** − returns the `real` arccosine of its real or integer argument.

`Acos` **(** *rarray* **)** − returns the `rarray` of arccosines of *rarray* elements.

Examples:

```
print Acos(1.)              # equal to 0.
print Acos(1)               # the same

print Acos({-1., 0., 1.})   # returns {180. 90. 0.}
```

2.21.4. Acosh

inverse hyperbolic cosine function.

`Acosh` **(** *real* | *integer* **)** − returns the `real` inverse hyperbolic cosine of its real or integer argument.

`Acosh` **(** *rarray* **)** − returns the `rarray` of inverse hyperbolic cosines of *rarray* elements.

Examples:

```
print Acosh(1.)              # returns 0
print Acosh(1)               # the same

print Acosh({1., 10., 100.})  # returns {0., 2.993223, 5.298292}
```

2.21.5. Align

aligns two sequences with the Needleman and Wunsch algorithm with zero gap end penalties (`ZEGA`). The ZEGA−statistics of structural significance (Abagyan, Batalov, 1997) is given and can be additionally evaluated with the `Probability` function. The reported pP value is −Log(Probability,10).

`Align` **(** [sequence1, *sequence2* [{ `area` | `distance` | `superimpose` } [*i_window*] [*r_seq_weight*]]] **)** − returns `ZEGA`− `alignment` . If no arguments are given, the function aligns the first two sequences in the sequence list.

Returned variables:

- `i_out` − the number of identical residues in the alingment
- `r_out` − contains `Log(` *Probability_of_structural_dissimilarity*) only for pairwise alignments
- `r_2out` − percent identity of the alignment.

Simple pairwise sequence alignment

`Align` ( )

`Align` **(** *seq1 seq2* **)** − returns an alignment. The `alignMethod` preference allows you to perform two types of pairwise sequence alignments: `"ZEGA"` and `"H−align".` If you skip the arguments, the first two sequence are aligned.

Example:

```
read sequences s_icmhome+"sh3.seq" # read 3 sequences
print Align(Fyn,Spec)              # align two of them
Align( )                           # the first two
```

```
a=Align( sequence[1] sequence[3] ) # 1st and 3rd
if(r_out > 5.) print "Sequences are struct. related"
```

Aligning with custom residue weights or weights according to surface accessible area

`Align` **(** *seq1 seq2* `area` **)**

Option `area` will use relative residue accessibilities to weight the residue−residue substitution values in the course of the alignment (see also `accFunction`).

The weights must be positive and less than 2.37 . Try to be around or less than 1. since relative accessibilities are always in [0.,1.] range. Values larger than `2.37` do not work well anyway with the existing alignment matrices and gap parameters. Use the `Trim` function to adjust the values, e.g. `Trim( myweights , 0.1,2.3 )`).

E.g.

```
read pdb "1lbd"
show surface area
make sequence
 Info> sequence  1lbd_m  extracted
1lbd_m                      # see the relative areas
read pdb sequence "1fm6.a/"  # does not have areas
Info> 1 sequence 1fm6_a  read from /data/pdb/fm/pdb1fm6.ent.Z
ali3d = Align( 1lbd_m 1fm6_a area )
```

This can also be used to assign *custom* weights with the following commands

```
set area seq1 R_weights  # must be > 0. and less than 2.37
Align( seq1 seq2 area )
```

Introducing positional terms into the alignment score.

`Align` **(** *seq1 seq2 M_positionalScores* **)**

If sequence similarity is in the "twilight zone" and the alignment is not obvious, the regular comp_matrix{residue substitution matrix} is not sufficient to produce a correct alignment and additional help is needed. This help may come in a form of the positional information, e.g. histidine 55 in the first sequence must align with histidine 36 in the second sequence, or the predicted alpha−helix in the first sequence preferably aligns with alpha−helix in the second one.

In this case you can prepare a matrix of extra scores for each pair of positions in two sequences, e.g.

```
seq1 = Sequence("WEARSLTTGETGYIPSA")
seq2 = Sequence("WKVEVNDRQGFVPAAY")
Align()
# Consensus   W.#.  .~~.~G%#P^
seq1          WEARSLTTGETGYIPS--
seq2          WKVE--VNDRQGFVPAAY
m = Matrix(17,16,0.)
m[10,4] = 3. # reward alignment of E in seq1[10]  and E in seq2[4]
Align(seq1 seq2 m )
# Consensus   W.#      E    ~G%#P^
```

```
seq1          WEARSLTTGE----TGYIPS--
seq2          WKV------EVNDRQGFVPAAY
```

The `alignSS` macro shows a more elaborate example in which extra scores are prepared to encourage alignments of the same secondary structure elements.

Warning. The alignment procedure is very subtle. Avoid values comparable with gap opening penalty.

Local structural alignment

Two types of structural alignments or mixed sequence/structural alignments can be performed with the `Align` function.

`Align` **(** *seq_1 seq_2* `distance` [*i_window*] [*r_seq_weight*] **)** − performs local structural alignment, using **distance RMSD** as structural fitness criterion. The RMSD is calculated in a window *i_window* and the dynamic programming algorithm combines structural scores with sequence alignment scores if *r_seq_weight>0.*,

`Align` **(** *seq_1 seq_2* `superimpose` [*i_window*] [*r_seq_weight*] **)** − performs local structural alignment, using **superposition followed by coordinate RMSD** calculation as structural fitness criterion. The RMSD is calculated in a window *i_window* and the dynamic programming algorithm combines structural scores with sequence alignment scores if *r_seq_weight>0.*,

In both cases the function uses the dynamic algorithm to find the alignment of the locally structurally similar backbone conformations.

The alignment based on optimal *structural superposition* of two 3D structures may be different from purely sequence alignment

Preconditions:

- sequences must be `link`ed to 3D molecules to access the coordinate information;
- two 3D structures must have a superimposable subsets

The residue−label−carrying atoms (see the `set label a_` command) will be used for structural superpositions. *r_seq_weight* is used to add sequence aminoacid substitution values to the 3D similarity signal.

Extracting pairwise alignment sequences from a multiple alignment

`Align` **(** ali_, seq_1, *seq_2* **)** − returns a pairwise sub− `alignment` of the input alignment *ali_*, reorders of sequences in the alignment according to the order of arguments.

Extracting a multiple alignment of a subset of sequences from a multiple alignment

`Align` **(** ali_, *I_seqNumbers* **)** − returns a reordered and/or partial `alignment` . Sequences are taken in the order specified in *I_seqNumbers.*

Examples:

```
            # 14 sequences
read alignment msf s_icmhome + "azurins"
            # extract a pairwise alignment by names
aa = Align(azurins,Azu2_Metj,Azur_Alcde)
            # reordered sub-alignment extracted by numbers
bb = Align(azurins,{2 5 3 4 10 11 12})
```

Resorting alignment in the order of sequence input with the `Align` (ali_, I_seqNumbers) function.

Load the following macro and apply it to your alignment. Example:

```
macro reorderAlignmentSeq( ali_ )
 nn=Name(ali_)  # names in the alignment order
 ii=Iarray(Nof(nn))
 j=0
 for i=1,Nof(sequence)  # the original order
  ipos = Index( nn, Name(sequence[i] ) )
  if ipos >0 then
    j=j+1
    ii[j] = ipos
  endif
 endfor
 ali_new = Align( ali_ ii )
 keep ali_new
endmacro
```

Deriving an alignment from tethers between two 3D objects

`Align` **(** *ms_* **)** − returns `alignment` between sequences of the specified molecule and the template molecule to which it is tethered. The alignment is deduced from the tethers imposed.

This function may be used to save the alignment after `interactive editing`.

Example:

```
build string "se ala his leu gly trp ala" "a"  # obj. a
build string "se his val gly trp gly ala" "b"  # obj. b
set tether a_2./1:3 a_1./2:4 align                # impose tethers
show Align(a_2.1)         # derive alignment from tethers
write Align(a_2.1) "aa"   # save it to a file
```

2.21.6. Angle

calculates planar angle in degrees. Returns `real` value.

`Angle` **(** *as_atom* **)** − returns the planar angle defined by the specified atom and two previous atoms in the ICM−tree. For example, Angle(a_/5/c) is defined by C−Ca−N atoms of the 5−th residue. You may type:

```
print Angle(  # and then click the atom of interest.
```

`Angle` **(** *as_atom1* , *as_atom2* , *as_atom3* **)** − returns the planar angle defined by three atoms.

`Angle` **(** *R_3point1* , *R_3point2* , *R_3point3* **)** − returns the planar angle defined by the three points.

`Angle ( R_vector1 , R_vector2 )` − returns the planar angle between the two vectors.

Examples:

```
d=Angle( a_/4/c )                          # d equals N−Ca−C angle
print Angle( a_/4/ca a_/5/ca a_/6/ca )    # virtual Ca−Ca−Ca planar angle
```

2.21.7. Area

calculates surface area.

`Area ( grob )` − returns `real` surface area of a solid `graphics object`.

See also: the `Volume`(*grob*) function, the `split` command and How to display and characterize protein cavities section.

`Area ( as_ )` − returns `rarray` of pre−calculated solvent accessible areas for selected atoms *`as_`* .

`Area ( rs_ )` − returns `rarray` of pre−calculated solvent accessible areas for selected residues *`rs_`* . These accessibilities depend on conformation.

`Area ( rs_ type )` − returns `rarray` of maximal standard solvent accessible areas for selected residues *`rs_`* . These accessibilities are calculated for each residue in standard extended conformation surrounded by Gly residues. Those accessibilities depend only on the sequence of the selected residues and do NOT depend on its conformation. To calculate normalized accessibilities, divide `Area(` *rs_*) by `Area(` *rs_* `type`)

Example:

```
read object "1crn"
show surface area
a=Area(a_/* )      # absolute conformation dependent residue accessilities
b=Area(a_/* type ) # maximal residue accessilities in the extended conformation
c = a/b            # relative (normalized) accessibilities
```

2.21.8. Area contact matrix

`Area ( rs_1 rs_2 )` − returns `rarray` of **areas of contact** between selected residues. You can do it for intramolecular residue contacts, in which case both selections should be the same, i.e. Area(a_1/* a_1/*) ; or, alternatively, you can analyze intermolecular residue contacts, for example, Area(a_1/A a_2/A). See also the `Cad` function, and example in `plot area` in which a contact matrix is calculated via interatomic Ca−Ca distances. The table of the pairwise contact area differences is written to the `s_out` string which can later be read into a proper table via: `read column group name="aa" input=s_out` and sorted by the area (see below).

Example:

```
read object "crn"  # good old crambin
s=String(Sequence(a_/A))
PLOT.rainbowStyle="blue/rainbow/red"
plot area Area(a_/A, a_/A) comment=s//s color={−50.,50.} \
```

```
    link transparent={0., 2.} ds

 read object "complex"
 plot area Area(a_1/A, a_2/A) grid color={-50.,50.} \
    link transparent={0., 2.} ds
```

`Area(` *string* `)` − returns the `real` value of solvent accessible area for the specified residue type in the standard "exposed" conformation.

Important : "pre−calculated" above means that before invoking this function, you should calculate the surface by `show area surface` , `show area skin` or `show energy "sf"` commands.

Examples:

```
 build                   # build a molecule according to the sequence
                         # from file def.se (default)
 show area surface       # calculate surface area
 a = Area(a_//o*)        # individual accessibilities of oxygens

 stdarea = Area("lys")   # standard accessibility of lysine

# More curious example
 read object "crn"
 show energy "sf"        # calculate the surface energy contribution
                         # (hence, the accessibilities are
                         # also calculated)

 assign sstructure a_/* "_"
                         # remove current secondary structure assignment
                         # for tube representation
 display ribbon
                         # calculate smoothed relative accessibilities
                         # and color tube representation accordingly
 color ribbon a_/* Smooth(Area(a_/*)/Area(a_/* type) 5)
                         # plot residue accessibility profile
 plot Count(1 Nof(a_/*)) Smooth(Area(a_/*)/Area(a_/* type) 5) display
```

See also: `Acc`( ) function.

2.21.9. Asin

arcsine trigonometric function Returned values are in degrees.

`Asin` (*real* | integer)

− returns the `real` arcsine of its real or integer argument.

`Asin(` *rarray* `)`

− returns the `rarray` of arcsines of *rarray* elements.

Examples:

```
 print Asin(1.)              # equal to 90 degrees
```

```
print Asin(1)                # the same

print Asin({-1., 0., 1.})    # returns {-90., 0., 90.}
```

2.21.10. Asinh

inverse hyperbolic sine function.

`Asinh` (real)

− returns the `real` inverse hyperbolic sine of its real argument.

`Asinh` (rarray)

− returns the `rarray` of inverse hyperbolic sines of *rarray* elements.

Examples:

```
print Asinh(1.)               # returns 0.881374
print Asinh(1)                # the same

print Asinh({-1., 0., 1.})    # returns {-0.881374, 0., 0.881374}
```

2.21.11. Ask

interactive input function. Convenient in macros.

`Ask` **(** s_prompt, *i_default* **)**

− returns entered `integer` or default.

`Ask` **(** s_prompt, *r_default* **)**

− returns entered `real` or default.

`Ask` **(** s_prompt, *l_default* **)**

− returns entered `logical` or default.

`Ask` **(** s_prompt, *s_default* [*simple*] **)**

− returns entered `string` or default. Option `simple` suppressed interpretation of the input and makes quotation marks unnecessary.

Examples:

```
windowSize=Ask("Enter window size",windowSize)
s_mask=Ask("Enter alignment mask","xxx---xxx")

grobName=Ask("Enter grob name","xxx")
display $grobName
```

```
show Ask("Enter string, it will be interpreted by ICM:", "")
        #e.g. Consensus( myAlignm )

show Ask("Enter string:", "As Is",simple)
        #your input taken directly as a string
```

2.21.12. Atan

arctangent trigonometric function Returned values are in degrees.

`Atan` **(** *real* | *integer* **)**

− returns the `real` arctangent of its real or integer argument.

`Atan` **(** *rarray* **)**

− returns the `rarray` of arctangents of *rarray* elements.

Examples:

```
print Atan(1.)                  # equal to 45.
print Atan(1)                   # the same.

print Atan({−1., 0., 1.})       # returns {−45., 0., 45.}
```

2.21.13. Atan2

arctangent trigonometric function. Returned values are in degrees.

`Atan2` **(** r_x, *r_y* **)**

− returns the `real` arctangent of *r_y/r_x* in the range −180. to 180. degrees using the signs of both arguments to determine the quadrant of the returned value.

`Atan2` **(** *R_x R_y* **)**

− returns the `rarray` of arctangents of *R_y/R_x* elements as described above.

Examples:

```
print Atan2(1.,−1.)                       # equal to 135.
print Atan2({−1., 0., 1.},{−0.3, 1., 0.3}) # returns phases {−106.7 0. 73.3}
```

2.21.14. Atanh

inverse hyperbolic tangent function.

`Atanh` **(** *real* **)**

− returns the `real` inverse hyperbolic tangent of its real argument.

`Atanh(` *rarray* `)`

− returns the `rarray` of inverse hyperbolic tangents of *rarray* elements.

Examples:

```
print Atanh(0.)                    # returns 0.
print Atanh(1.)                    # returns error

print Atanh({-0.9999, 0., .9999})  # returns { -4.951719, 0., -4.951719 }
```

2.21.15. Atom

transforms the input selection to atomic level necessary since some of the commands/functions require specific level of selection.

`Atom(` *as_Obj_or_Mol_or_Res_selection* `)`

− returns selection converted to the atomic level.

`Atom(` *vs_* `)`

− returns atom selection (i.e. selection of atomic level) to which the selected variables `vs_` belong.

Examples:

```
asel=Acc(a_2/his)             # select accessible His residues of
                              # the second molecule
show Atom(asel)               # show atoms of these residues
show Atom( v_//phi )          # carbonyl Cs
```

See also: the `Res`, `Mol`, adn `Obj` functions.

2.21.16. Augment

creates augmented affine 4x4 space transformation matrix.

`Augment(` *R_12transformationVector* `)`

− rearranges the transformation vector into an augmented affine 4x4 space transformation `matrix` .

The augmented matrix can be presented as

```
a1  a2  a3  | a4
a5  a6  a7  | a8
a9  a10 a11 | a12
------------+----
0.  0.  0.  | 1.
```

where {a1,a2,...a12} is the *R_12transformationVector* . This matrix is convenient to use because it combines rotation and translation. To find the inverse transformation simply inverse the matrix:

```
M_inv = Power(Augment(R_12direct),−1))
R_12inv = Vector(M_inv)
```

To convert a 4x4 matrix back to a 12−transformation vector, use the `Vector`(M_4x4) function.

See also: `Vector` (the inverse function), `symmetry transformations`, and `transformation vector`.

`Augment` **(** *R_6Cell* **)**

− returns 4x4 `matrix` of oblique transformation for given cell parameters {*a b c alpha beta gamma*}.

This matrix can be used to generate real coordinates from fractional coordinates. It also contains vectors A, B and C. See also `an example`.

Example:

```
display a__crn.         # load and display crambin: P21 group
obl = Augment(Cell( ))  # extract oblique matrix
A = obl[1:3,1]          # vectors A, B, C
B = obl[1:3,2]
C = obl[1:3,3]
g1=Grob("cell",Cell( )) # first cell
g2=g1+ (−A)             # second cell
display g1 g2
```

`Augment` **(** *R_3Vector* **)** − appends 1. to a 3D vector *{x,y,z}* (resulting in *{x,y,z,1.}*) to allow direct arithmetics with augmented 4x4 space transformation matrixes.

`Augment` **(** *M_XYZblock* **)** − adds `{1.,1.,..1.}` column to the *Nx3* matrix of with *{x,y,z}* coordinates to allow direct arithmetics with augmented 4x4 space transformation matrixes.

2.21.17. Axis

calculates rotation/screw axis corresponding to a transformation

`Axis` **(** { *M_33Rot* | *R_12transformation* } **)**

− returns `rarray` with *x,y,z* components of the normalized rotation/screw axis vector. Additional information calculated and returned by the function:

- `r_out` rotation angle (degrees);
- `r_2out` helix rise;
- `R_out` 3−rarray with a point on the axis.

See also: How to find and display rotation/screw transformation axis

2.21.18. Bfactor

crystallographic temperature factors or custom atom parameters.

`Bfactor(` [*as_* | *rs_*] [`simple`]`)` − returns `rarray` of b−factors for the specified selection of atoms or residues. If selection of `residue level` is given, the average residue b−factors are returned. B−factors can also be shown with the command `show pdb`.

Option `simple` returns a normalized b−factor. This option is possible for X−ray objects containing b−factor information. The `read pdb` command calculates the average B−factor for all non−water atoms. The normalized B−factor is calculated as ***(b−b_av)/b_av*** . This is preferable for coloring ribbons by B−factor since these numbers only depend on the ratios to the average. We recommend to use the following commands to color by b−factor:

```
color ribbon a_/ Trim(Bfactor( a_/ simple ),−0.5,3.)//−0.5//3. # or
color a_// Trim(Bfactor( a_// simple ),−0.5,3.)//−0.5//3.  # for atoms
```

This scheme will give you a full sense of how bad a particular part of the structure is.

See also: `set bfactor`.

Examples:

```
avB=Min(Bfactor(a_//ca))     # minimal B−factor of Ca−atoms
show Bfactor(a_//!h*)        # array of B−factors of heavy atoms
color a_//* Bfactor(a_//*)   # color previously displayed atoms
                             # according to their B−factor
color ribbon a_/A Bfactor(a_/A) # color the whole residue by mean B−fac.
```

2.21.19. Boltzmann

returns the `real` Boltzmann constant = 0.001987 kcal/deg.

Example:

```
deltaE = Boltzmann*temperature  # energy
```

2.21.20. Box

the 3D graphics box function. This box can be displayed with the `display box` command or by left−double−clicking on a `grob`, and interactively moved and resized with the mouse. One can select atoms inside a box by this operation: `as_ Box( )`

`Box` ( ) − returns the 6− `rarray` with ***{X_{min} ,Y_{min} ,Z_{min} ,X_{max} ,Y_{max} ,Z_{max} }*** parameters of the graphics box as defined on the screen.

`Box(center)` − returns the 6− `rarray` with *{Xcenter,Ycenter,Zcenter,Xsize,Ysize,Zsize}* parameters of the graphics box as defined on the screen.

`Box(` *as_* [*r_margin*] `)` − returns the 6− `rarray` with *{Xmin,Ymin,Zmin,Xmax,Ymax,Zmax}* parameters of the box surrounding the selected atoms. The boundaries are expanded by *r_margin* (default: `0.0`).

Examples:

```
build string "se ala his"  # a peptide
```

```
display box Box(a_/2 1.2)  # surround the a_/2 by a box with 1.2A margin
color a_//* Box( )
```

`Box(` { *g_* | *m_* } [*r_margin*] `)`

− returns the 6− `rarray` with *{Xmin,Ymin,Zmin,Xmax,Ymax,Zmax}* parameters of the box surrounding the selected grob or map. The boundaries are expanded by *r_margin* (default: `0.0`).

2.21.21. Bracket

bracket the grid potential map by value or by space.

`Bracket(` *m_grid* [*r_vmin r_vmax*] `)`

− returns the truncated `map` . The map will be truncated by value. The values beyond *r_vmin* and *r_vmax* will be set to *r_vmin* and *r_vmax* respectively.

`Bracket(` *m_grid* [*R_6box*] `)`

− returns the modified `map` . All the values beyond the specified box will be set to zero. Example:

```
make map potential "gh,gc,gb,ge,gs" a_1 Box()
m_ge = Bracket(m_ge, Box( a_1/15:18,33:47 )) # redefine m_ge
```

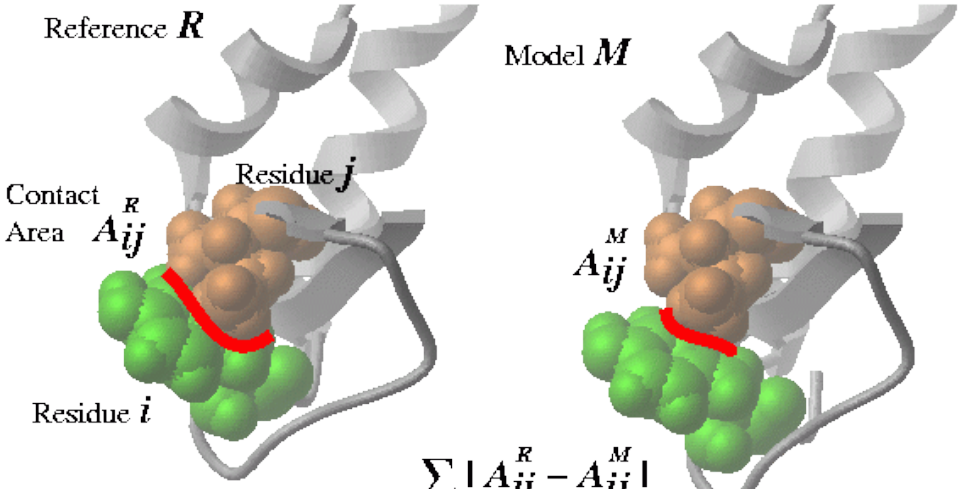
See also: `Rmsd`(map) and `Mean`(map), `Min`(map), `Max`(map) functions.

2.21.22. Cad

Contact Area Difference function to measure geometrical difference between two different conformations of the same molecule. Cad, as opposed to `Rmsd`, is contact based and can measure the difference in a wide range of model accuracies. Roughly speaking it measures the surface weighted fraction of native contacts. Can be used to evaluate the differences between several NMR models, the accuracy of models by homology and the accuracy of docking solutions.

Cad can measure the geometrical difference between two conformations in several different ways:

- between two conformations of the **same** protein based on full atom residue−residue contact area calculation, `Cad`(..)
- between two conformations of the same protein based on Cbeta−Cbeta distance evaluation (`Cad`(.. `distance`) .ICM uses an empirically derived *ContactStrength(Cb−distance*) function.
- between two homologous structures based preservation of the residue contacts through the alignment (`Cad` (.. `alignment`)) . The contact strength in this case is also derived from the interresidue distances.



Comparing two conformations of the same molecule via residue−residue contact conservation.

`Cad(` *rs_A1* [*rs_A2*] *rs_B1* [*rs_B2*] [`distance`]**)**

− returns the `real` contact area difference measure (described in Abagyan and Totrov, 1997) between two conformations A and B of the same set of residue pairs from two different objects. The set of residue pairs in each object (A or B) can be defined in two ways:

- by a single selection *rs_A1* : all pairs between selected residues (is equivalent to *rs_A1 rs_A1*)
- by two residue selections *rs_A1 rs_A2:* cross pairs between two sets of selected residues (e.g. the contacts between two subunits)

The measure is a normalized sum of differences between residue−residue contact areas in two conformations. The measure was calibrated on a set of pairs of conformations. The average distortion due to a noncrystallographic symmetry is about 5%, the average CAD between a pair of models in an NMR entry is 15%. Note that the paper uses an additional factor of 1.8 (i.e. CAD=1.8*Cad()) to bring the scale down to 0:100%, because about 40% of the contacts are trivial contacts between the neighboring residues. However, in evaluation of the docking solutions coefficient 1.8 should not be used. Loops are somewhat intermediate, but still a coefficient of 1.8 is recommended for consistency.

The whole matrix of contact area differences is returned in `M_out` . This matrix can be nicely plotted with the `plot area M_out number ..` command (see example). The full matrix can also be used to calculate the residue profile of the differences.

The table of the pairwise contact area differences is written to the `s_out` string which can later be read into a proper table via: `read column group name="aa" input=s_out` and sorted by the area (see below).

See also `Area`() function which calculates absolute residue−residue contact areas.

Options:

- `distance` option allows to compare approximations of the inter−residue contact areas by the Ca and Cbeta positions. This allows to calculated deformations between two homologous proteins which is not possible in the default mode in which two chemically identical molecules are compared. The residue pairs in two homologues are equivalenced according to the alignments `link`ed to the molecules. Residues deleted in a homologue are considered to have zero contact.

Examples:

```
# Ab initio structure prediction, Overall models by homology
   read pdb "cnf1"   # one conformation of a protein
   read pdb "cnf2"   # another conformation of the same protein
   show 1.8*Cad(a_1. a_2.)   # CAD=0. − identical; =100. different
   show 1.8*Cad(a_1.1 a_2.1) # CAD between the 1st molecules (domains)
   show 1.8*Cad(a_1.1/2:10 a_2.1/2:10) # CAD in a window
   PLOT.rainbowStyle = 2
   plot area grid M_out comment=String(Sequence(a_1,2.1)) link display

# Loop prediction: 0% − identical; ~100% totally different
#    CAD for loop 10:20 and its interactions with the environment
   show 1.8*Cad(a_1.1/10:20 a_1.1/* a_2.1/10:20 a_2.1/*)
#    CAD for loop 10:20 itself
   show 1.8*Cad(a_1.1/10:20 a_1.1/10:20 a_2.1/10:20 a_2.1/10:20)

# Evaluation of docking solutions: 0% − identical; 100% totally different
   read pdb "expr"   # one conformation of a complex
   read pdb "pred"   # another conformation of the same complex
   show Cad(a_1.1 a_1.2 a_2.1 a_2.2)  # CAD between two docking solutions
#
# ANOTHER EXAMPLE: the most changed contacts
   read object "crn"
   copy a_ "crn2"
   randomize v_ 5.
   Cad(a_1. a_2.)
   show s_out
   read column group input= s_out name="cont"
   sort cont.1
   show cont
# the table looks like this (the diffs can be both + and −):
#>T cont
#>−1----------2----------3----------
   −39.        a_crn.m/38  a_crn.m/1
   −36.4       a_crn.m/46  a_crn.m/4
   −32.1       a_crn.m/46  a_crn.m/5
   −29.8       a_crn.m/30  a_crn.m/9
   −25.2       a_crn.m/37  a_crn.m/1
...
   42.5        a_crn.m/43  a_crn.m/5
   45.1        a_crn.m/44  a_crn.m/6
```

```
45.2        a_crn.m/43  a_crn.m/6
55.3        a_crn.m/46  a_crn.m/7
56.         a_crn.m/45  a_crn.m/7
```

Comparing two different, but structurally homologues proteins, via residue−residue contact conservation.

`Cad(` *rs_A1* [*rs_A2*] *rs_B1* [*rs_B2*] `alignment)`

2.21.23. Ceil

rounding function.

`Ceil(` *r_real* [*r_base*] `)`

− returns the smallest `real` multiple of *r_base* exceeding *r_real.*

`Ceil(` *R_real* [*r_base*] `)`

− returns the `rarray` of the smallest multiples of *r_base* exceeding components of the input array *R_real.* Default *r_base*= 1.0 .

See also: `Floor`( ).

2.21.24. Cell

crystallographic cell function.

`Cell(` { *os_* | *m_map* } `)`

− returns the `rarray` with 6 cell parameters {a,b,c,alpha,beta,gamma} which were assigned to the object or the map.

2.21.25. Charge

returns an rarray of partial electric charges of selected atoms, or total charges for residue, molecule or objects, depending on the selection level.

Charges can also be shown with a regular `show` *as_select* command.

`Charge(` { *os_* | *ms_* | *rs_* | *as_* } [`formal` | `mmff`] `)`

− returns `rarray` of elementary or total charges depending on the selection level.

- `formal` : return formal charges
- `mmff` : return *formal* charges calculated according to *mmff* atom types and rules. **Note:** do not confuse this option with a function to return the mmff charges.

Examples:

```
 buildpep "ala his glu lys arg asp"
 show Charge(a_1)      # charge per molecule
 show Charge( a_1/* )  # charge per residue
 show Charge( a_1//* ) # charge per atom

 avC=Charge(a_/15)        # total electric charge of 15th residue
 avC=Sum(Charge(a_/15/*)) # another way to calculate it
 show Charge(a_//o*)      # array of oxygen charges

# to return mmff charges:
 set type mmff
 set charge mmff
 Charge( a_//* )

# to return total charges per molecular object:
 read mol s_icmhome+"ex_mol.mol"
 set type mmff
 set charge mmff
 Charge( a_*. )
```

See also: `set charge`.

2.21.26. Cluster

`Cluster` **(** *I_NxM_NearestNeighb i_M_totalNofNearNeighbors i_minNofCommonNeighbors* **)** −> *I_N_clusterNumbers*

function returns `iarray` of cluster numbers for each or N points.

The input to the first function is an array of M nearest neighbors (defined by the second argument *i_M_totalNofNearNeighbors)* for each of N points. For example for an array for 5 points, and i_M_totalNofNearNeighbors = 3 it can be an array like this: `{3,4,5, 1,3,4 1,2,5 2,3,5 1,2,3}` . The points will be grouped into the same cluster if the number of neighbors they share is larger or equal than *i_minNofCommonNeighbors* . This clustering algorithm is adaptive to the cluster density and does not depend on absolute distance threshold. In other words it will identify both very sparse clusters and very dense ones. The nearest neighbor array can be calculated by the with the `Link` (*I_bitkeys , nBits, nNearestNeighbors*) function.

`Cluster` **(** *M_NxNdist r_maxDist* **)** −> *I_N_clusterNumbers*

This function identifies the *i_totalNofNeighbors* nearest neighbors from the full distance matrix *M_NxNdist* for each point and assembles points sharing the specified number of *common* neighbors in clusters.

All singlets (a single item not in any cluster) are placed in a special cluster number **0** . Other items are assigned to a cluster starting from 1.

Example with a distance matrix:

```
# let us make a distance matrix D
# we will cook it from 5 vectors {0. 0. 0.}
 m=Matrix(5,3)  # initialize 5 vectors
 m[2,1:3]={1. 0. 0.}   # v2
 m[3,1:3]={1. 1. 0.}   # v3
```

```
m[4,1:3]={1. 1. 1.}   # v4
m[5,1:3]={1. 0.1 0.1} # v5 close to v2

D = Distance( m )  # 5x5 distance matrix created

Cluster( D , 0.2 ) # v2 and v5 are assigned to cluster 1
Cluster( D , 0.1 ) # radius too small. All items are singlets
Cluster( D , 2.  ) # radius too large. All items are in cluster 1
```

2.21.27. Color

returns RGB numbers.

`Color` **(** *g_grob* **)** − returns `matrix` of RGB numbers for each vertex of the `g_grob` (dimensions: `Nof` (*g_grob),3).*

See also: color g_ M_

Example:

```
build string "se his"
display xstick
make grob image name="g_"
display g_ only smooth
M_clr = Color( g_ )
for i=1,20    # shineStyle = "color" makes it disappear completely
  color g_ (1.−i/20.)*M_clr
endfor
color g_ M_clr
```

`Color` **(** `background` **)**

− returns `rarray` of three RGB components of the background color.

2.21.28. Consensus

`Consensus` **(** *ali_* **)**

− returns the `string` consensus of alignment *ali_*. The `consensus characters` are these: # hydrophobic; + RK; − DE; ^ ASGS; % FYW; ~ polar. In the `selections by consensus` a letter code (h,o,n,s,p,a) is used.

`Consensus` **(** *ali_* { *i_seq* | *seq_* } **)**

− returns the `string` consensus of alignment *ali_* as projected to the sequence.

Sequence can be specified by its order number in the alignment or by name.

Example displaying conserved residues:

```
read alignment "sx"  # load alignment
read pdb "x"         # structure
```

```
display ribbon
       # multiply rs_ by a mask like "  A C   N  .."
cnrv = a_/A Replace(Consensus(sx cd59),"[.^~#]"," ")
display cnrv red
display residue label cnrv
```

2.21.29. Corr

linear correlation function (Pearson's coefficient **r**)

`Corr` **(** R_array1, *R_array2* **)**

− returns the `real` value of the linear correlation coefficient. Probability of the null hypothesis of zero correlation is stored in `r_out` .

Examples:

```
r=Corr(a,b)                    # two vectors a and b
if (Abs(r_out) < 0.3) print "it is actually as good as no correlation"
```

See also: `LinearFit`( ) function.

2.21.30. Cos

cosine function. Arguments are assumed to be in degrees.

`Cos` **(** { *r_Angle* | *i_Angle* } **)**

− returns the `real` value of cosine of its real or integer argument.

`Cos` **(** *rarray* **)**

− returns `rarray` of cosines of each component of the array.

Examples:

```
show Cos(60.)                          # returns 0.5
show Cos(60)                           # the same

rho={3.2 1.4 2.3}                      # structure factors
phi={60. 30. 180.}                     # phases
show rho phi rho*Cos(phi) rho*Sin(phi)  # show in columns rho, phi,
                                       # Re, Im
```

2.21.31. Cosh

hyperbolic cosine function.

`Cosh` **(** { *r_Angle* | *i_Angle* } **)** − returns the `real` value of hyperbolic cosine of its real or integer argument. ***Cos(x)=0.5(e^{iz} + e^{-iz})***

`Cosh(` *rarray* `)` − returns `rarray` of hyperbolic cosines of each component of the array.

Examples:

```
show Cosh(1.)                          # 1.543081
show Cosh(1)                           # the same

show Cosh({-1., 0., 1.})               # returns {1.543081, 1., 1.543081}
```

2.21.32. Count

function creates an iarray.

`Count(` [i_Min,] *i_Max* `)` − returns `iarray` of numbers growing from *i_Min* to *i_Max.* The default value of *i_Min* is 1.

Examples:

```
show Count(-2,1)         # returns {-2,-1,0,1}
show Count(4)            # returns {1,2,3,4}
```

See also the `Iarray`( ).

`Count(` *array* `)`

− returns `iarray` of numbers growing from 1 to the number of elements in the *array.*

2.21.33. Date

`Date(` [*s_format*] `)` returns `sting` with the current week day, month, year and time in the given format. The default format is `"%m %DD %Y"` which returns something like `"Oct 08 2004"` .

The allowed format specifications are the following:

format	description	example
%D	day, say 1 or 12 or 30	
%DD	day with compulsary two digits, say 01 03 12 etc.	
%M	month (say, 1)	
%MM	see above at %DD (say 01)	
%m	brief month (3 letter), say dec oct etc.	
%mm	full month (december)	
%Y	four letter year	
%YY −		
%y	two letter year (damn with Y3K)	
%W	week day (say, Saturday)	
%w	three letter day (say, sat)	
%z	time zone	

%HH	always aligned by two chars (03)
%H	one or two chars
%hh	the same with in pm/am style,
%h	the same in pm/am style
%pm	the string "pm" or "am", empty otherwise.
%UU	minutes (say 01)
%U	minutes (say 1, 12)
%SS	seconds (say 04)
%S	seconds (say 1, 4,12)

Example:

```
Date()  # uses the default format
Date("%m %DD,%Y %h%pm") # today returns
 Oct 08,2002 5pm
```

2.21.34. Deletion

`Deletion(` rs_Fragment, *ali_Alignment* [, *seq_fromAli*] [, *i_addFlanks*] [{"all"|"nter"|"cter"|"loop"}] **)**

− returns the residue selection which flanks deletion points from the viewpoint of other sequences in the *ali_Alignment.* If argument *seq_fromAli* is given (it must be the name of a sequence from the alignment), all the other sequences in the alignment will be ignored and only the pairwise subalignment of *rs_Fragment* and *seq_fromAli* will be considered. The alignment must be linked to the object. With this function (see also `Insertion` function) one can easily and quickly visualize and/or extract all *indels* in the three−dimensional structure. The default *i_addFlanks* parameter is 1. String options:

- "all" (default: no string option) select deletions of all types
- "nter" select only N−terminal fragments
- "cter" select only C−terminal fragments
- "loop" select only the internal zones of deleted loops

See example coming with the `Insertion`( ) function description.

2.21.35. Det

determinant function.

`Det(` *matrix* **)**

− returns a `real` determinant of specified square *matrix.*

Examples:

```
a=Rot({0. 0. 1.}, 30.)     # Z−rotation matrix by 30 degrees
print Det(a)               # naturally, it is equal to 1.
```

2.21.36. Disgeo

Solves the so called `"DIStance GEOmetry"` problem (finding coordinates from a distance set). This function can be used to visualize in two or three dimensions a distribution of homologous sequences:

```
group sequence se1 se2 se2 se4 mySeqs
align mySeqs
distMatr=Distances(mySeqs)
```

or any objects between which one can somehow define pairwise distances. Since principal coordinates are sorted according to their contribution to the distances and we can hardly visualize distributions in more than three dimensions, the first two or three coordinates give the best representation of how the points are spread in n−1 dimensions. Another application is restoring atomic coordinates from pairwise distances taken from NMR experiments.

`Disgeo` **(** *matrix* **)**

− returns `matrix` *[1:n,1:n]* where the each row consists of n−1 coordinates of point *[i]* sorted according to the eigenvalue (hence, their importance). The first two columns, therefore, contain the two most significant coordinates (say X and Y) for each of *n* points. The last number in each row is the eigenvalue *[i]*. If distances are Euclidean, all the eigenvalues are positive or equal to zero. The eigenvalue represents the "principal coordinate" or "dimension" and the actual value is a fraction of data variation due to the this particular dimension. Negative eigenvalues represent "non−Euclidean error" in the initial distances.

Example:

```
read sequences "zincFinger" # read sequences from the file,
list sequences              # see them, then ...
group sequence alZnFing     # group them, then ...
align alZnFing              # align them, then ...
a=Distance(alZnFing)        # a matrix of pairwise distances
n=Nof(a)                    # number of points
b=Disgeo(a)                 # calculate principal components
corMat=b[1:n,1:n−1]         # coordinate matrix [n,n−1] of n points
eigenV=b[1:n,n]             # vector with n sorted eigenvalues
xplot= corMat[1:n,1]
yplot= corMat[1:n,2]
plot xplot yplot CIRCLE display # call plot a 2D distribution
```

2.21.37. Distance

generic distance function. Calculates distances between two ICM−shell objects or molecular objects, or extracts distances from complex ICM−shell objects.

Distance iarray

`Distance` **(** iarray1, *iarray2* **)**

− returns the `real` **sqrt** of sum of $(I1_i - I2_i)^2$.

Distance rarray

`Distance` **(** R_X, *R_Y* **)** − returns the `real` Cartesian distance between two vectors of the same length. $D = Sum((X_i - Y_i)^2)$

Distance as_

`Distance` **(** as_1, *as_2* **)** − returns the `real` distance in Angstroms between centers of mass of the two specified selections. The interactive usage of this function:

- Display your molecule
- type `Dist` , press TAB
- `Ctrl−RightMB` click on the atom you want (or double click for a residue) and press RETURN

Distance as_ rarray

`Distance` **(** *as_1* , as_2, *rarray* **)** − returns the `rarray` of distances in Angstroms between the two specified selections containing the same number of atoms (1−1, 2−2, 3−3, ...).

Distance matrix

`Distance` **(** *M_coor* **)** − returns the square `matrix` of distances between the rows of the input matrix *M_coor*. Each row contains *m* coordinates (3 in 3D space). For example: `Distance(Xyz(a_//ca))` returns a square matrix of Ca−Ca distances.

Distance matrix

`Distance` **(** *M_coor1 M_coor2* **)** − returns the `matrix` of distances between the rows of the two input matrices. Each matrix row may contain any number of coordinates coordinates (3 in 3D space).

For example: **Distance(Xyz(a_/1:5/ca) Xyz(a_/10:12/ca)** returns a 5 by 3 matrix of distances between Ca−s of the two fragments.

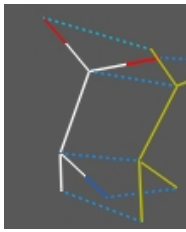
Distance tether

`Distance` **(** *as_* [`r_defaultLength=`−1.] **)**

− returns the `real array` of lengths of tethers for each selected atom or the default value (−1.). The default value can be set to any value. Tethers are assumed to be already set, see command `set tether`. Also note, that the expression `Distance( as_out )` will give the same results if `as_out` selection was not changed by another operation; see also special selections.

Example:

```
read pdb "1crn"
convert tether # keeps tethers to the pdb original
deviations = Distance( a_//!h*,vt* , 9.9)
perResDevs = Group( deviations, a_//!h*,vt* ,"max") # find max.devs per residue
display ribbon
color ribbon a_/* perResDevs

# Another example
 Distance( a_//T ) # selects only tethered atoms
 #>R
   1.677
   1.493
   1.386
   1.435
   1.645
   1.570
   2.165
   1.399
```



Distance Dayhoff

`Distance` **(** sequence1, *sequence2* **)** − returns the `real` measure of similarity between two aligned sequences. Zero distance means 100% identity. The distance is calculated by the following two steps:

1. d1 = 1.0 − (nResidueIdentities/Min(Length(Seq1), Length(Seq2)) (d1 belongs to [0.,1.] range)
2. Distance(Seq1,Seq2) = DayhoffTransformation(d1)

Transformation practically does not change small distances d1, whereas large distances, especially above 0.9 (10% sequence identity) are increased to take occasional reversals into account. Distances d1 within [0.9,1.0] are transformed to [5.17, 10.] range.

Distance alignment

`Distance` **(** *alignment* **)** − returns `matrix` of pairwise sequence−sequence distances in the alignment.

Example:

```
 read alignment msf "azurins"            # read azurins.msf
 NormCoord = Disgeo(Distance(azurins))   # 2D sequence diversity in
```

Distance two alignments

`Distance` **(** *ali_1 ali_2* [`exact`] **)** − returns the `real` distance between two alignments formed by the same sequences.

The distance is defined as a number of non−gap columns identical between two alignments.

Two different normalizations are available:

The default normalization is to the shorter alignment. (`Distance` (*ali_1 ali_2*)). In this case the number of equivalent pairs is calculated and is divided by the total number of aligned pairs in the shorter alignment. *This method detects alignment shifts* but does not penalize un−alignment of previously aligned residue pairs. **D = (La_min − N_commonPairs)/La_min** In the following alignment the residue pairs

which are aligned in *both alignments* are the same, therefore the distance is 0.

```
show a1   # La1 = 3
ABC---XYZ
ABCDEF---
show a2   # La2 = 6
ABCXYZ
ABCDEF
Distance(a1,a2)   # a1 is a subalignment of a2, distance is 0.
0.
```

exact option: normalization to the longer alignment. By *longer* we mean the larger number of aligned pairs regardless of alignment length (the latter includes gaps and ends). **D = (La_max − N_commonPairs)/La_max** Now in the above example, La_max = 6 , while N_commonPairs = 3, the distance is 0.5 (e.g. the alignments are 50% different).

```
Distance(a1,a2,exact)  # returns 0.5 for the above a1 and a2
```

Example showing the influence of gap parameters:

```
read sequence msf "azurins.msf"
gapOpen =2.2
a=Align(Azu2_Metj  Azup_Alcfa)   # the first alignment
gapOpen =1.9                     # smaller gap penalty and ..
b=Align(Azu2_Metj  Azup_Alcfa)   # the alignment changes
show 100*Distance(a b )          # 20% difference
show 100*Distance(a b exact )    # 21.7% difference
show a b
```

2.21.38. Eigen

eigenvalues/eigenvectors function.

`Eigen(`*M_*`)`

− returns the square `matrix` of eigenvector columns of the input *symmetric square* matrix *M_* . Eigenvalues sorted by their values are stored in the `R_out rarray.`

Example:

```
A = Matrix(3, 3, 0.)      # create a zero square matrix...
A[1:3,1] = {1.,-2.,-1.}   # and set its elements
A[2,2] =  4.
for i = 1, 3-1            # the matrix must be symmetric
  for j = i+1, 3
    A[i,j] = A[j,i]
  endfor
endfor
X = Eigen(A)              # calculate eigenvectors...
V = R_out                 # and save eigenvalues in rarray V
printf "eigenvalue 1 eigenvalue 2 eigenvalue 3\n"
printf "%12.3f %12.3f %12.3f\n", V[1], V[2], V[3]
printf "eigenvector1 eigenvector2 eigenvector3\n"
for i = 1, 3
  printf "%12.3f %12.3f %12.3f\n", X[i,1], X[i,2], X[i,3]
```

```
endfor
```

2.21.39. Energy

function.

`Energy` **(** *string* **)**

− returns the `real` sum of **pre−calculated** energy and penalty (i.e. geometrical restraints) `terms` specified by the string.

Important: the terms must be **pre−calculated** by invoking one of the following commands where energy is calculated at least once: `show energy`, `minimize`, `ssearch` command and `montecarlo` command.

Note:

- Allowed terms in the string are `"vw,14,hb,el,to,af,bb,bs,cn,tz,rs,xr,sf";`
- `"func"` stands for the total of all the terms, both energy and penalty;
- `"ener"` is only the energy part (i.e. `"vw,14,hb,3l,to,af,bb,bs,sf"`);
- `"pnlt"` is only the penalty part (i.e. `"cn,tz,rs,xr"`).
- `load conf` and `load frame` commands fill out all the energy/penalty terms, which are stored in both stacks and movies (of course the values also depend on a set of `free variables`). You can get the energy/penalty terms of the loaded conformation without explicitly recalculating them.

Examples:

```
build
show energy
print Energy("vw,14,hb,el,to")  # ECEPP energy

read stack "f1"
load conf 0
print Energy("func")  # extract the best energy without recalculating it
```

`Energy` **(** *rs_* [`simple` | `base` | *s_energyTerms*] **)**

− calculates and returns residue energies in an ICM object. `convert` the object if is not of the ICM type. The energies are calculated according to the current energy terms , and also depend on the fixation of the object. Use `unfix only V_//S` to restore standard fixation.

This function can be used to evaluate normalized residue energies for standard amino−acids to detect local problems in a model.

For normalized energies, use the `simple` option. The `base` option just shifts the energy value to the mean energy for this residue type. If the `simple` or `base` terms are *not* used, the current energy terms are preserved. The energies calculated with the `simple` or `base` option are calculated with the `"vw,14,hb,el,to,en,sf"` terms. The terms are temporarily enforced as well as the `vwMethod` = 2 and `vwSoftMaxEnergy` values, so that the normalization performed with the `simple` option is always correct.

This function will calculate residue energies for all terms and set−ups with the following exceptions:

- electrostatic (`"el"`) term and electroMethod = "boundary element", "MIMEL", or "generalized Born"

The *s_energyTerms* argument allows to refine the energy terms dynamically (see example below).

Example:

```
read pdb "1crn"
delete a_W
convert
set terms "vw,14,hb,el,to,en,sf"
group table t Energy( a_/A ) "energy" Label(a_/A ) "res"
show t
unfix V_//*
group table tBondsAngles Energy( a_/A "bs,bb" ) "covalent" Label(a_/A ) "res"
show tBondsAngles
```

See also: the `calcEnergyStrain` macro.

`Energy` (`conf` i_confNumber)

− returns the `table` of all the energy components for the a given stack conformations.

The table has two arrays:

- `sarray` of the energy term names (.hd) and
- `rarray` of energy values for each energy term (.ey) and

`Energy` ({ `stack` | `conf` })

− returns the `rarray` of total energies of stack conformations. Useful for comparison of spectra from different simulations.

Examples:

```
set terms only "vw,14,hb,el,to"  # set energy terms
show energy v_//xi*              # calculate energy with only
                                 # side chain torsions unfixed
          # energy depends on what variables are fixed since
          # interactions inside rigid bodies are not calculated,
          # and rigid body structure depends on variables

a = Energy("vw,14")      # a is equal to the sum of two terms

electroMethod="MIMEL"    # MIMEL electrostatics
set terms only "el,sf"   # set energy terms
show energy
print Energy("ener")     # total energy
print Energy("sf")       # only the surface part of the solvation energy
print Energy("el")       # electrostatic energy
print r_out              # electrostatic part of the solvation energy
```

2.21.40. Error

function indicates that the previous ICM−shell command has completed with error.

`Error`

− returns `logical yes` if there was an error in a previous command (not necessarily in the last one). After this call the internal error flag is reinstalled to `no.`

`Error(string)`

− returns `string` with the last error message. It also returns integer code of the *last* error in your script in `i_out.` In contrast to the logical `Error()` function, here the internal error code is **not** reinstalled to 0, so that you can use it in expressions like `if( Error ) print Error(string)`.

Examples:

```
read pdb "1mng"  # this file contains strange 28−th residue
if (Error) print "These alternative positions will kill me"

read pdb "1abcd"  # file does not exist
errorMessage = Error(string)
ier = i_out
if ier == 3102  print "What kind of name is that?"
```

See also: `errorAction`, `s_skipMessages`, `l_warn`, `Warning`

`Error(`*r_x* [`reverse`]`)`

− returns `real` complementary error function of real ***x*** : ***erfc(x)=1.−erf(x))*** , defined as

(2/sqrt(pi)) integral{x to infinity} of exp(−t^2) dt

or its inverse function if the option `reverse` is specified. It gives the probability of a normally distributed (with mean 0. and standard deviation 1./Sqrt(2.)) value to be larger than *r_x* or smaller than *−r_x*.

Examples:

```
show 1.−Error(Sqrt(0.5)) # P of being inside +−sigma (about 68%)
show Error(2.*Sqrt(0.5)) # P of being outside +− 2 sigma
```

`Error(`*R_x*`)`

− returns `rarray` of ***erfc(x)=1.−erf(x))*** functions for each element of the real array (see above).

Examples:

```
x=Rarray(1000 0. 5. )
plot display x Error(x ) {0. 5. 1. 1. 0. 1. 0.1 0.2 }
plot display x Log(Error(x ),10.) {0. 5. 1. 1.}
      #NB: can be approximated by a parabola
      #to deduce the appr. inverse function.
```

```
#Used for the Seq.ID probabilities.
```

2.21.41. Exist

function indicates if an ICM−entity exists or not.

`Exist` **(** *s_fileName* **)** − returns `logical yes` if the specified file or directory exists, `no` otherwise.

`Exist` **(** `key` , *s_keyName* **)** − returns `logical yes` if the specified keystoke has been previously defined. See also: `set key` command.

`Exist` **(** `object` **)** − returns `logical yes` if there is at least one molecular object in the shell, `no` otherwise.

`Exist` **(** `view` **)** − returns `logical yes` if the GL − graphics window is activated, `no` otherwise.

`Exist` **(** `gui` **)** − returns `logical yes` if the GRAPHICS USER INTERFACE menus is activated, `no` otherwise.

Examples:

```
if (!Exist("/data/pdb/") then
  unix mkdir /data/pdb
endif

if(!Exist(key,"Ctrl−B")) set key "Ctrl−B" "l_easyRotate=!l_easyRotate"

if !Exist(gui)  gui simple
```

2.21.42. Existenv

function indicating if an UNIX−shell environmental variable exists.

`Existenv` **(** *s_environmentName* **)**

− returns `logical yes` if the specified named environment variable exists.

Example:

```
if(Existenv("ICMPDB")) s_pdb=Getenv("ICMPDB")
```

See also: `Getenv`( ), `Putenv`( ) .

2.21.43. Extension

function.

`Extension` **(** *string* [`dot`] **)**

− returns `string` which would be the extension if the string is a file name. Option `dot` indicates that the dot is excluded from the extension.

`Extension(` *sarray* [`dot`] `)`

− returns `sarray` of extensions. Option `dot` indicates that the dot is excluded from the extensions.

Examples:

```
print Extension("aaa.bbb.dd.eee")   # returns ".eee"
show Extension({"aa.bb","122.22"} dot)         # returns {"bb","22"}
read sarray "filelist"
if (Extension(filelist[4])==".pdb") read pdb filelist[4]
```

2.21.44. Exp

exponential mathematical function (e^x).

`Exp(` *real* `)`

− returns the `real` exponent.

`Exp(` *rarray* `)`

− returns `rarray` of exponents of *rarray* components.

`Exp(` *matrix* `)`

− returns `matrix` of exponents of *matrix* elements.

Examples:

```
print Exp(deltaE/(Boltzmann*temperature))   # probability
print Exp({1. 2.})                          # returns { E, E squared }
```

2.21.45. Field

function.

`Field(` *s_* [*s_precedingString*] *i_fieldNumber* [*s_fieldDelimiter*] `)`

− returns the specified field. Parameter `s_fieldDelimiter` defines the separating characters (space and tabs by default). If the field number is less than zero or more than the actual number of fields in this string, the function returns an empty string.

The s_fieldDelimiter string

Single character delimiter can be specified directly, e.g.

```
Field("a b c",3," ")  # space
```

```
 Field("a:b:c",3,":")  # colon
```

Alternative characters can be specified sequentially, e.g.

```
 Field("a%b:c",3,"%:")  # percent OR colon
```

Multiple occurence of a delimiting character can be specified by *repeating* the same character *two* times, e.g.

```
 Field("a  b   c",3,"  ")    # two==multiple spaces in field delim
 Field("a%b::::c",3,"%::")   # a single percent or multiple colons
```

You can combine a single−character delimiters and multiple delimiters in one *s_fieldDelimiter* string.

More examples:

```
 s=Field("1 ener glu 1.5.",3)    # returns "glu"
 show Field("aaa:bbb",2,":")     # returns "bbb"
 show Field("aaa 12\nbbb 13","bbb",1) # returns "13"
 show Field("aaa 12\nbbb 13 14","bbb",2,"  \n\n") # two spaces and two \n .
# another example
 read object s_icmhome+"all"
       # energies from the object comments, the 1st field after 'vacuum'
 show Rarray(Field(Namex(a_*.),"vacuum",1))
```

`Field(` *S_* , [*s_precedingString*] *i_fieldNumber* [*s_fieldDelimiter*] **)**

− returns an `string array` of fields selected from *S_* string array . `s_fieldDelimiter` is the delimiter. If the field number is less than zero or more than the actual number of fields in this string, an element of the array will be an empty string.

Examples:

```
 show Field({"a:b","d:e"},2,":") # returns {"b","e"}
 s=Field({"aa 2 3.3", "bb 4 1.3", "cc 31a 1.1 3"},2)
         # returns {"2","4","31a"}
 s=Field({"aa 2 3.3", "bb 4 1.3", "cc 31a 1.1 3"},4)
         # returns {"","","3"}
```

See also: `Split`( ).

2.21.46. User field from a selection

`Field(` *as_* **)**

`Field(` { *rs_* | *ms_* | *os_* } [*i_fieldNumber*] **)**

returns `rarray` of user−defined field values of a selection.

Atoms. Only one user defined field can be set to atoms, e.g.

```
set field a_//* Random(0.,1.,Nof(a_//*))
```

```
show Field( a_//* )
```

Residues, molecules and objects.

Three user fields can be defined for each residue and up to 16 for molecules and objects. To extract them specify *i_fieldNumber* . The level of the selection determines if the values are extracted from residues, molecules or objects. Use the selection level functions `Res` `Mol` and `Obj` to reset the level if needed. For example: `Res(Sphere(gg, a_1. 3.))` selects residues of the 1st object which are closer than 3. A to `grob` `gg` . Example:

```
set field 2 a_/A Random(0.,1.,Nof(a_/A)) # set the 2nd field to random values
color a_/* Field( a_/A  2 )              # color by it
```

See also: `set field` , `Smooth` to 2D or 3D averate user fields , `Select` to select by user defined field.

2.21.47. File

function returning file names or attributes of named files.

`File` **(** *os_* **)** returns the name of the source file for this object. If the object was created in ICM or did not come from an object or PDB file, it returns an empty string.

Example:

```
read pdb "/home/nerd/secret/hiv.ob"
File( a_ )
 /home/nerd/secret/hiv.ob
```

`File` **(** *s_file_or_dir_Name* "length" **)**

− returns `integer` file size or −1.

`File` **(** *icm_object* **)**

− returns `string` file name from which this object has been loaded or empty string.

`File` **(** *s_file_or_dir_Name* **)**

− returns `string` with the file or directory attributes separated by space. If file or directory do not exist the function returns **"− − − − 0"** Otherwise, it contains the following 4 characters separated by space and the file size:

1. type character:
   - 'f' − regular file
   - 'd' − directory
   - 'l' − symbolic link
   - 'c' − character special file
   - 'p' − pipe
2. 'r' if you can read the file (or from the directory)
3. 'w' if you can write to this file (or directory)

4. 'x' if you can execute this file (or cd to this directory)
5. file size in bytes

To get a string with any field use Field(File(*s_name), i_fieldNumber)* . To get the size, use Integer(Field(File(*s_name),5)).*

Example:

```
if File("/opt/icm/icm.rst")=="- - - - 0" print "No such file"

if Field(File("PDB.tab"),2)!= "w"  print "can not write"

if ( Indexx( File("/home/bob/icm/") , "d ? w x *" ) ) then
   print "It is indeed a directory to which I can write"
endif
            # Here the Indexx function matched the pattern.

if ( Integer(Field(File(s_name),5)) < 10 ) return error "File is too small"
```

`File ( last )`

returns the file name of the last icm−shell script called by ICM. See also: `Path ( last )`

2.21.48. Find

function searching all fields (arrays) of a table.

`Find (` *table s_searchWords* **)**

− returns `table` containing the entries matching all the words given in the *s_searchWords* string.

If *s_searchWords* is "word1 word2" and table contains arrays a and b this "all text search" is equivalent to the expression :

```
(t.a=="word1" | t.b == "word1") (t.a=="word2" | t.b == "word2").
```

Examples:

```
read database "ref.db"  # database of references
group table ref $s_out  # group created arrays into a table
show Find(ref,"energy profile") ref.authors == "frishman"
```

2.21.49. Floor

rounding function.

`Floor (` *r_real* [*r_base*] **)**

− returns the largest `real` multiple of *r_base* not exceeding *r_real.*

`Floor (` *R_real* [*r_base*] **)**

− returns the `rarray` of the largest multiples of *r_base* not exceeding components of the input array *R_real.*

Default *r_base*= `1.0` .

See also: `Ceil`( ).

2.21.50. Getenv

function returning value for an environment name.

`Getenv` **(** *s_environmentName* **)**

− returns a `string` of the value of the named environment variable.

Example:

```
user = Getenv("USER")      # extract user's name from the environment
if (user=="vogt") print "Hi, Gerhard"
```

See also: `Existenv`( ), `Putenv`( ) .

2.21.51. Gradient

function.

`Gradient` ( )

− returns the `real` value of the root−mean−square gradient over free internal variables.

`Gradient` **(** *vs_var* **)**

− returns the `rarray` of pre−calculated energy derivatives with respect to specified variables.

`Gradient` **(** *as_* | *rs_* **)**

− returns the `rarray` of pre−calculated energy derivatives with respect to atom positions *(G[i] = Sqrt(Gxi*Gxi+Gyi*Gyi+Gzi*Gzi))*

The function returns atom−gradients for atom selection (*as_*) or average gradient per selected residue, if residue selection is specified (*rs_*).

You can display the actual vectors/"forces" *(−Gxi, −Gyi, −Gzi)* by the `display gradient` command.

Important: to use the function, the gradient must be pre−calculated by one of the following commands: `show energy`, `show gradient`, `minimize` .

Examples:

```
show energy               # to calculate the gradient and its components
```

```
if (Gradient( ) > 10.) minimize
show Max(Gradient(a_//c*)  # show maximum "force" applied to the carbon atoms
```

2.21.52. Grob

function to generate graphics objects.

`Grob(` "arrow", { *R_3* | *R_6* } **)**

− returns `grob` containing 3D wire arrow between either `{0.,0.,0.}` and *R_3*, or between *R_6[1:3]* and *R_6[4:6]*.

`Grob(` "ARROW", { *R_3* | *R_6* } **)**

− returns `grob` containing 3D solid arrow. You may specify the number of faces by adding integer to the string: e.g. "ARROW15" (rugged arrow) or "ARROW200" (smooth arrow).

See also: `GROB.relArrowSize`.

Examples:

```
GROB.relArrowSize = 0.1
g_arr = Grob("arrow",Box( ))  # return arrow between corners of displayed box
display g_arr red            # display the arrow

g_arr1 = Grob("ARROW100",{1. 1. 1.})
display g_arr1
```

`Grob(` "cell", { *R_3* | *R_6* } **)**

− returns `grob` containing a wire parallelepiped for a given cell.

If only *R_3* is given, angles `{90.,90.,90.}` are implied.

`Grob(` "CELL", { *R_3* | *R_6* } **)**

− returns `grob` containing a solid parallelepiped for a given cell.

If only *R_3* is given, angles `{90.,90.,90.}` are implied.

Example:

```
read csd "qfuran"
gcell = Grob("CELL",Cell( ) )      # solid cell
display a_//* gcell transparent   # fancy stuff
```

`Grob(` "distance", *as_1* [*as_2*] **)**

− returns `grob` with the distance lines. This grob can be displayed with distance labels (controlled with the `GROB.displayLineLabels` parameter). With one selection it returns all possible interatomic distances within this selection. If two selections are provided, the distances between the atoms of the two sets are

returned. Example:

```
build string "se ala his trp"
g = Grob( "distance", a_/1/ca a_/2/ca )
display g
GRAPHICS.displayLineLabels = no
display new
```

`Grob (` "label", R_3, *s_string* **)**

− returns `grob` containing a point at *R_3* and a string label.

`Grob (` "line", *R_3N* **)**

− returns `grob` containing a polyline *R_3N[1:3]*, R_3N[4:6], ...

Example:

```
display a__crn.//ca,c,n
g = Grob("line",{0.,0.,0.,5.,5.,5.})   # a simple line (just as an example)
display g yellow
gCa = Grob("line",Rarray(Xyz(a_//ca))) # connect Cas with lines
display gCa pink                       # display the grobs
```

`Grob (` "SPHERE", *r_radius i_tesselationNum* **)**

− returns `grob` containing a solid sphere. The *i_tesselationNum* parameter may be 1,2,3.. (do not go too high).

Example:

```
display a__crn.//ca,c,n
              # make grob and translate to a_/5/ca
              # Sum converts Matrix 1x3 into a vector
g=Grob("SPHERE",5.,2)+Sum(Xyz(a_/5/ca))
              # mark it with dblLeftClick and
              # play with Alt-X, Alt-Q and Alt-W
display g red
```

`Grob (` *grob R_6rgbLimits* **)**

returns a `grob` containing selection of vertices of the source grob. The vertices with colors between the RGB values provided in the 6−dim. array of limits will be selected. The array of limits consists of real numbers between 0. and 1. : { *from_R, to_R, from_G, to_G, from_B, to_B* }

If you want a limit to be outside possible rgb values, use negative numbers of numbers larger than 1., e.g. a selection for the red color could be: `{0.9,1.,-0.1,0.1,-0.1,0.1}`

The grob created by this operation has a limited use and will contain only vertices (no edges or triangles). This form of the Grob function can be used to find out which atoms or residues are located to spots of certain color using the `Sphere`(grob as_) function.

Example:

```
buildpep "ADERD" # a peptide
dsRebel a_  no no
g=Grob(g_skin {0.9,1.,−0.1,0.1,−0.1,0.1} )  # red color
display g_skin transparent
display g
show Res(Sphere( g, a_//* 1.5))
```

2.21.53. Group

`Group` **(** *R_atomArray as_atomSelection* "min"|"max"|"avg"|"rms"|"sum"|"first" **)** −> *rarray* : *Group (I_atomArray as_atomSelection "min"|"max"|"avg"|"sum"|"first") −> iarray `Group` **(** *as_atomSelection* "count" **)** −> *iarray*

returns an array of atoms properties aggregated to a per−residue array. One of the following functions can be applied to the atomic values:

- "min" − stores the minimal atomic property for each selected residue
- "max" − stores the maximal atomic property for each selected residue
- "avg" − (syn. "mean") stores the mean of properties for each selected residue
- "rms" − stores the root−mean−square deviation of properties for each selected residue
- "sum" − stores the sum of properties for each selected residue
- "first" − stores the property of the first atom in selected residue
- "count" − stores the number of selected atoms in selected residue

The function name is case−insensitive (you may use "Min" or "MIN").

Example:

```
read pdb "1crn"
show Group( a_A//* "count"  ) # numbers of atoms in residues
show Group( Mass( a_A//* ) , a_A//* "sum"  ) # residue masses
show Group( Mass( a_A//* ) , a_A//* "rms"  ) # residue mass rmsd
```

2.21.54. Histogram

function to create a histogram of an array. Function returns `matrix` [*n,2]*, where *n* is number of cells, the first row contains a number of elements in each cell and the second row contains mid−points of each cell.

`Histogram` (I_inputArray)

− returns `matrix` with a histogram of the input array.

`Histogram` **(** R_inputArray, *i_numberOfCells* [, *R_weights*] **)**

− returns histogram `matrix` [*i_numberOfCells,2]* in which the whole range of the *R_inputArray* array is equally divided in *i_numberOfCells* windows. An array of point weights can be provided.

`Histogram` (R_inputArray, r_cellSize)

− returns `matrix` [*n* ,2], dividing the whole range of *R_inputArray* equally into *r_cellSize* windows.

`Histogram(` R_inputArray, r_from, r_to, *r_cellSize* `)`

− returns `matrix` [*n,2],* dividing into equal cells of *r_cellSize* between minimum value, maximum value.

`Histogram(` R_inputArray, *R_cellRuler* [, *R_weights*] `)`

− returns `matrix` [*n,2],* dividing the range of the input array according to the *R_cellRuler* array, which must be monotonous. An array of R_weights of the same size as the input array can be provided.

Examples:

```
plot display Histogram({ −2, −2, 3, 10, 3, 4, −2, 7, 5, 7, 5}) BAR

a=Random(0. 100. 10000)
u=Histogram(a 50)
s_legend={"Histogram at linear sampling curve" "Random value" "N"}
plot display regression BAR u s_legend

a=Random(0. 100. 10000)
b=.04*(Count(1 50)*Count(1 50))
u=Histogram(a b)
s_legend={"Histogram at square sampling curve" "Random value" "N"}
plot display BAR u s_legend
b=Sqrt(100.*Count(1 100))
s_legend={"Histogram at square root sampling curve" "Random value" "N"}
plot display green BAR Histogram(a b) s_legend
```

2.21.55. Iarray

function to create/declare an empty iarray or transform to an iarray.

`Iarray(` *i_NumberOfElements* [*i_value*] `)`

− returns `iarray` of *i_NumberOfElements* elements set to *i_value* or zero. You can also create an zero−size integer array: `Iarray(0)` .

`Iarray(` *rarray* `)`

− returns `iarray` of integers nearest to real array elements in the direction of the prevailing rounding mode magnitude of the real argument.

`Iarray(` *sarray* `)` − converts *sarray* into an `iarray.`

Examples:

```
a=Iarray(5)                       # returns {0 0 0 0 0}
a=Iarray(5,3)                     # returns {3 3 3 3 3}
b=Iarray({2.1, −4.3, 3.6})        # returns {2, −4, 4}
c=Iarray({"2", "−4.3", "3.6"})    # returns {2, −5, 3}
```

`Iarray(` *iarray* `reverse)`

− converts input real array into an `iarray` with the reversed order of elements. Example:

```
Iarray({1 2 3} reverse)  # returns {3 2 1}
```

See also: `Sarray`(S_ `reverse`), `Rarray`(S_ `reverse`), `String`(0,1,s)

2.21.56. Iarray(as_): relative atom numbers of a selection

− returns `iarray` of relative atom numbers in a single object. This iarray can be saved and later reapplied with the `Select` (*os_ I*) function. If you selection covers more than one object, the function returns an error.

Example:

```
build string "se ala"
ii = Iarray( a_//c* ) # returns {6,8,12}
Select( a_  ii )      # returns three carbons
```

2.21.57. Iarray(stack): numbers of visits for all stack conformations

`Iarray(stack)` − returns the `iarray` of the numbers of visits for each `stack` conformation. This is the same number as shown by the `nvis>` line of the `show stack` command. Example:

```
 show stack
 iconf>       1       2       3       4       5
 ener>    -15.3   -15.1   -14.9   -14.8   -13.3
 rmsd>     84.5    75.3     6.4    37.2   120.8
 naft>        3       0       4       0       2
 nvis>       10       9       8       1       4
Integer(stack)  # returns { 10 9 8 1 4 }
```

2.21.58. IcmSequence

creates a "sequence" for an ICM molecular object. Output is in `icm.se` −file format.

`IcmSequence(` { *sequence* | *string* | *rs_* }, [s_N−Term, s_C−Term] `)`

− returns multiline `string` with full (3−char.) residue names which may be a content of an `icm.se` file. The source of the sequence may be one of the following:

- a sequence, e.g. `IcmSequence(1crn_m)`
- a string, e.g. `"ASDGFRE",` or `"SfGDA;WER"` .
- or residue selection, `rs_` , (e.g. a_2,3/*).

Rules for one−letter coding:

- standard L amino−acids: **upper** case one−letter code (B,J,X,Z are illegal), e.g. ACD
- D−amino acids: **lower** case for a corresponding amino acid (e.g. `AaA` for `ala Dala ala`)
- new molecule: use **semicolon** or **dot** as a chain separator (`;`) (e.g. `AAA;WWW`)

If the source of the icm−sequence is a 3D object, the proline ring puckering is analyzed and residue name `prou` is returned for the up−prolines (the default is `pro`).

The N−terminal and C−terminal groups will be added if their names are explicitly specified or an `oxt` atom is present in the last residue of a chain. Here are the possibilities for automated recognition of C−terminal residue:

```
IcmSequence( a_/* ) # C−terminal residue "cooh" will be added if oxt is found
IcmSequence( a_/* "","" )        # no terminal groups will be added
IcmSequence( a_/* "","@coo−" )    # "coo−" will be added only if oxt is found
IcmSequence( a_/* "nh3+","coo−" ) # "nh3+" and "coo−" will always be added
```

The resulting string can be saved to a ICM mol−sequence file and further edited for unusual amino−acids (see `icm.res`).

Examples:

```
 write IcmSequence(seq1) "seq1.se"      # create a sequence
                                        #  file for build command

 show IcmSequence("FAaSVMRES","nh3+","coo−")  # one peptide with Dala

 show IcmSequence("FAAS.VMRES","nter","cooh") # two peptides
 show IcmSequence("AA;MRES","nter","cooh") # two peptides

 read pdb "2ins"
 write IcmSequence(a_b,c/* ,"nter","@cooh") "b.se" # .se file for b
                                                   # and c chains
```

In the last command the ampersend means that the C−terminal residue will only be added if an `oxt` atom is present in the last residue.

There is a convenient macro called `buildpep` to create a single or multiple chain peptides. Example:

```
 buildpep "SDSRAARESW;KPLKPHYATV"  # two 10−res. peptides
```

See also `icm.se` for a detailed description of the ICM−sequence file format.

2.21.59. Index

function.

`Index(` { *s_source* | *seq_source* }, { *s_pattern* | *seq_pattern* }, [{ `last` | *i_skip*] `)`

− returns `integer` value indicating the position of the pattern substring in the source string, or 0 otherwise. Option `last` returns the index of the last occurence of the substring.

The *i_skip* argument starts search from the specified position in the source string, e.g. `Index("words` words","word",3) returns `7` . If *i_skip* is negative, it specifies the number of characters *from the end of the string* in which the search is performed.

Examples:

```
show Index("asdf","sd")  # returns 2
show Index("asdf" "wer") # return 0
a=Sequence("AGCTTAGACCGCGGAATAAGCCTA")
show Index(a "AATAAA")   # polyadenylation signal
show Index(a "CT" last)  # returns 22
show Index(a "CT" 10)    # starts from position 10. returns 22
show Index(a "CT", -10)  # search only the last 10 positions
```

Another example in which we output all positions of all −"xxx.." stretches in a sequence " xxxx xxxxx xxxx ... xxxx " (must end with space)

```
EX = "xxxx xxxxxx xxxxxxxxxxxxxx xxxxxx  xxx "
sp=0
while(yes)
  x=Index(EX "x" sp)
  if(x==0) break
  sp=Index(EX " " x)
  print x sp-1
endwhile
```

`Index` **(** sarray, *string* **)**

− returns `integer` value indicating the *sarray* element number exactly matching the *string*, or 0 otherwise.

Examples:

```
show Index({"Red Dog","Amstal","Jever"}, "Jever")      # returns 3
show Index({"Red Dog","Amstal","Jever"}, "Bitburger")  # returns 0
```

`Index` **(** `object` **)**

− returns `integer` value of sequential number of the current object in the molecular object list, or 0 if no objects loaded. (Note that here `object` is used as a keyword.)

Examples:

```
l_commands = no
read pdb "1crn"
read object "crn"
printf "The object a_crn. is the %d-nd, while ...\n", Index(object)
set object a_1.
printf "the object a_1crn. is the %d-st.\n", Index(object)
```

2.21.60. Indexx

function to find location of substring pattern.

`Indexx` **(** { *string* | *sequence* }, *s_Pattern* **)**

− returns an `integer` value indicating the position of the *s_Pattern* (see `pattern matching`) in the string, or 0 otherwise. Allowed meta−characters are the following:

- ***** any string including an empty string;
- **?** any single character;
- **[** *string*] any of the enclosed characters;
- **[!** *string*] any but the enclosed characters.
- ^ beginning of a string
- **$** string end

Examples:

```
show Indexx("asdf","s[ed.]")       # returns 2
show Indexx("asdfff","ff$")       # returns 5 (not 4)
show Indexx("asdf" "w?r")          # return 0
```

2.21.61. Insertion

function selecting inserted residues.

`Insertion` **(** rs_Fragment, *ali_Alignment* [, *seq_fromAli*][, *i_addFlanks*] [{"all"|"nter"|"cter"|"loop"}] **)**

− returns the residue selection which form an insertion from the viewpoint of other sequences in the *ali_Alignment.* If argument *seq_fromAli* is given (it must be the name of a sequence from the alignment), all the other sequences in the alignment will be ignored and only the pairwise subalignment of *rs_Fragment* and *seq_fromAli* will be considered. The alignment must be linked to the object. With this function (see also `Deletion`( ) function) one can easily and quickly visualize all indels in the three−dimensional structure. The default *i_addFlanks* parameter is 0.

String options:

- "all" (or no string option) select insertions of all types
- "nter" select only N−terminal fragments
- "cter" select only C−terminal fragments
- "loop" select only the internal loops

Examples:

```
read pdb "1phc.m/"   # read the first molecule form this pdb−file
read pdb "2hpd.a/"   # do the same for the second molecule
make sequences a_*.  # you may also read the sequence and
                     # the alignment from a file
aaa=Align( )         # on−line seq. alignment.
                     # You may read the edited alignment
                     # worm representation
assign sstructure a_*. "_"
display ribbon
link a_*. aaa        # establish connection between sequences and 3D obj.
superimpose a_1. a_2. aaa
display ribbon a_*.
color a_1. ribbon green
color ribbon Insertion(a_1.1 aaa) magenta
```

```
color ribbon Insertion(a_2.1 aaa) red
show aaa
```

2.21.62. Info

function.

`Info(`[`string`]`)`

− returns the `string` with the previous info.

`Info(display)`

− returns the `string` with commands needed to restore the graphics view and the background color. See also: `View` () , `write object auto` or `write object display=yes` .

2.21.63. Integer

function converting to integer type.

`Integer(` *r_toBeRounded* `)`

− returns the `integer` nearest to real *r_toBeRounded* in the direction of the prevailing rounding mode magnitude of the real argument.

`Integer(` *rarray* `)` − see `Iarray` (*rarray*).

`Integer(` *string* `)` − converts string into `integer`, ignores irrelevant tail. Reports error if conversion is impossible.

Examples:

```
show Integer(2.2), Integer(−3.1)      # 2 and −3
jj=Integer("256aaa")                  # jj will be equal to 256
```

See also: `Iarray`( ).

`Integer(` *iarray* `)` transforms integer array containing only one element into an `integer` . You can also convert a one element array into an integer with the `Sum`( ) or the `Mean`( ) functions. If there are more then one elements, the first element is taken.

2.21.64. Integral

function.

`Integral(` *rarray r_xIncrement* `)` − calculates the integral `rarray` of the function represented by *rarray* on the periodically incremented abscissa *x* with the step of *r_xIncrement.*

`Integral(` *rarrayY rarrayX* `)` − calculates the integral `rarray` of the function represented by *rarrayY* on the set of abscissa values *rarrayX*.

Examples:

```
# Let us integrate sqrt(x)

 x=Rarray( 1000 0. 10. )
 plot x Integral( Sqrt(x) 10./1000. ) grid {0.,10.,1.,5.,0.,25.,1.,5.} display

# Let us integrate x*sin(x). Note that Sin expects the argument in degrees

 x=Rarray( 1000 0. 4.*Pi )
# 1000 points in the [0.,4*Pi] interval
 plot x Integral( x*Sin(x*180./Pi) x[2]-x[1] ) \
    {0., 15., 1., 5., -15., 10., 1., 5. } grid display
# x[2]-x[1] is just the increment
```

Let us integrate $3*x^2-1$, determined on the rarray of unevenly spaced *x*. The expected integral function is x^3-x

```
 x=Rarray(100 ,-.9999, .9999 )
 x=x*x*x
 plot display x Integral((3*x*x-1.) x) cross
```

2.21.65. Interrupt

function.

`Interrupt`

− returns `logical yes` if ICM−interrupt (Ctrl−Backslash, ^\) has been received by the program. Useful in scripts and macros.

Examples:

```
 if (Error | Interrupt) return
```

2.21.66. Label

function returning a molecular/grob label string.

`Label(` *g_* `)` => *s*
− returns the `string` label of the grob. See also: `set grob s_label`.

`Label(` *rs_* `)`

− returns `sarray` of residue labels of the selected residues *rs_* composed according to the `resLabelStyle` preference , e.g. −− { "Ala 13","Gly 14"}

See also: `Name` function (returns residue names), and `Sarray`(rs [append|name|residue]) function returning selection strings.

`Label(` *os_objects* `)`

− returns `sarray` of long names of selected objects.

See also: `Name` function which returns the regular object names and the most detailed chemical names of compounds.

`Label(` *vs_var* `)`

− returns `sarray` of labels of selected variables.

Examples:

```
build
resLabelStyle = "Ala 5"  # other styles also available
aa = Label(a_/2:5)       # extract residue name and/or residue number info
show aa                  # show the created string array
```

2.21.67. Length

function.

`Length(` { *string* | *matrix* | *sequence* | *alignment* | *profile* } `)`

− returns `integer` length of specified objects.

`Length(` *sarray* `)`

− returns `iarray` of length of strings elements of the *sarray*.

`Length(` { *iarray* | *rarray* } `)`

− returns the `real` vector length (distance from the origin for a specified vector Sqrt(Sum(I[i]*I[i])) or Sqrt(Sum(R[i]*R[i])), respectively).

Examples:

```
len=Length("asdfg")     # len is equal to 5

a=Matrix(2,4)            # two rows, four columns
nCol=Length(a)           # nCol is 4

read profile "prof"      # read sequence profile
show Length(prof)        # number of residue positions in the profile

vlen=Length({1 1 1})     # returns 1.732051
```

2.21.68. LinearFit

the linear regression function.

`LinearFit(` *R_X* , *R_Y* , [*R_Errors*] `)`

− returns the A,B,StdDev,Corr 4−dimensional array of the parameters of the linear regression for a scatter plot Y(X): ***R_Y = A*R_X + B*** , where the slope ***A*** and the intercept ***B*** are the first and the second elements, respectively. The third element is the standard deviation of the regression, and the fourth is the correlation coefficient. Residuals ***R_Y − (A*R_X + B)*** are stored in the `R_out` array.

You can also provide an array of expected errors of *R_Y* . In this case the weighted sum of squared differences will be optimized. The weights will be calculated as:

$W_i = 1/R\_Errors_i^2$

Example:

```
X = Random(1., 10., 10)
Y = 2.*X + 3. + Random(−0.1, 0.1, 10)
lfit = LinearFit(X Y)
printf "Y = %.2f*X + %.2f\n",     lfit[1],lfit[2]
printf "s.d. = %.2f; r = %.3f\n", lfit[3],lfit[4]
show column X, Y, X*lfit[1]+lfit[2], R_out
```

A more complex linear fit between a target set of Y_i , ***i=1:n*** values and **several** parameters $X_{i,j}$ ***(i=1:n,j=1:m)*** potentially correlating with Y_i is achieved in 3 steps:

```
M1=Transpose(X)*X
M2=Power(M1,−1)
W =(M2*Transpose(X))*Y
```

The result of this operation is vector of weights W for each of m components.

Now you can subtract the predicted variation from the initial vector ($Y_2 = Y - X*W$) and redo the calculation to find W_2 , etc. A proper way of doing it, however, is to calculate the eigenvalues of the covariance matrix.

2.21.69. Link

the linked SWISSPROT sequence names function.

`Link` **(** *ms_* **)** − returns the `sarray` of the swissprot sequence IDs (e.g. {"PHEA_HUMAN"}) referenced by the selected molecules. These references (or links) are read from the pdb entries. If the swissprot name is not found, ICM returns an empty string. Example:

```
read pdb "1avx"
Link(a_1)
 #>S string_array
 TRYP_PIG
rename a_1 Link(a_1)[1]
```

2.21.70. Log

the logarithm function.

`Log` **(** *real* **)** − returns the `real` *natural* logarithm of a specified positive argument.

`Log` (*real* r_realBase) − returns the `real` logarithm of a specified positive argument (e.g. the base 10 logarithm is Log(x, 10)).

`Log` **(** *rarray* **)** − returns an `rarray` of natural logarithms of the array components (they must not be negative, zeroes are treated as the least positive real number, ca. 10^{-38}).

`Log` **(** *rarray r_realBase* **)** − returns an `rarray` of logarithms of the array components (they must not be negative), arbitrary base.

`Log` **(** *matrix* [*r_realBase*] **)** − returns a `matrix` of logarithms of the matrix components (they must not be negative).

Examples:

```
print Log(2.)          # prints 0.693147
print Log(10000, 10)    # decimal logarithm
print Log({1.,3.,9.}, Sqrt(3.)) # {0. 2. 4.}
```

2.21.71. Map

function.

`Map` **(** *m_map* , *I_6box* [`simple`] **)** − returns `map` which is a transformation (expansion or reduction) of the input *m_map* to new *I_6box* box ({ *iMinX,jMinY,kMinZ,iMaxX,jMaxY,kMaxZ}).*

Examples:

```
read object "crn"
read map "crn"
display a_//ca,c,n m_crn
m1 = Map(m_crn, {0 0 0 22 38 38})  # half of the m_crn
m2 = Map(m_crn, {0 0 0 88 38 38})  # double of the m_crn
display m1
display m2
```

2.21.72. Mass

function.

`Mass` **(** *as_* | *rs_* | *ms_* | *os_* **)**

− returns `rarray` of masses of selected atoms, residues, molecules or objects, depending on the selection level.

Examples:

```
buildpep "ala his trp glu"
objmasses = Mass( a_*. )
molmasses = Mass( a_* )
resmasses = Mass( a_/* )

masses=Mass( a_//!?vt* )   # array of masses of nonvirtual atoms
```

```
molweight = Mass( a_1  )   # mol.weight of the 1st molecule
molweight = Sum(Mass( a_1//* )) # another way to calculate 1st mol. weight
```

See also: `Nof`(*sel* `atom`), `Charge`(*sel*)

2.21.73. Matrix

function.

`Matrix` **(** i_NofRows, *i_NofColumns* [*r_value*] **)** − returns `matrix` of specified dimensions. All components are set to zero or *r_value* if specified.

`Matrix` **(** *i_size* [*R_diagonal*] **)** − returns square unity `matrix` of specified size. A matching array of diagonal values can be provided. Example:

```
icm/def> Matrix(3,{1. 2. 3.})
#>M
1. 0. 0.
0. 2. 0.
0. 0. 3.
```

`Matrix` **(** *rarray* [*i_rowLength*] **)** − converts vector[1:n] to one−row `matrix`[1:1,1:n]. If you provide the *i_rowLength* argument, the input *rarray* will be divided into rows, e.g.

```
icm/def> Matrix({1. 2. 3. 4. 5. 6.},3)
#>M
1. 2. 3.
4. 5. 6.
icm/def> Matrix({1. 2. 3. 4. 5. 6.},4)
 Error>  non−matching dimension [4] and vector size [6]
```

`Matrix` **(** *M_square i_rowFrom i_rowTo i_colFrom i_colTo* **)** −> *M* a submatrix of specified dimensions. To select only columns or rows, use zero values, e.g.

```
Matrix( Matrix(3) 0,0,1, 2)  # first two columns
```

`Matrix` **(** *M_square* { `left` | `right` } **)** − generate a symmetrical matrix by duplicating the left or the right triangle of initial square matrix. Example:

```
icm/def> m
#>M m
1. 0. 0.
0. 1. 0.
7. 0. 7.
icm/def> Matrix( m right )
#>M
1. 0. 0.
0. 1. 0.
0. 0. 7.
icm/def> Matrix( m left )
#>M
1. 0. 7.
0. 1. 0.
7. 0. 7.
```

`Matrix` **(** *comp_matrix s_newResOrder* **)** − returns comparison matrix in the specified order. Example in which we extract cystein, alanine and arginine comparison values:

```
icm/def> Matrix(comp_matrix "CAR")
#>M
2.552272 0.110968 −0.488261
0.110968 0.532648 −0.133162
−0.488261 −0.133162 1.043102
```

Tensor product

`Matrix` **(** *R_A R_B* **)**

− returns tensor product of two vectors or arbitrary dimensions: ***M_ij = R_A[i]*R_B[j]***

Examples:

```
mm=Matrix(2,4)          # create empty matrix with 2 rows and 4 columns

mm=Matrix(2,4,−5.)      # as above but all elements are set to −5.

show Matrix(3)          # a unit matrix [1:3,1:3] with diagonal
                        # elements equal to 1.
a=Matrix({1. 3. 5. 6.}) # create one row matrix [1:1,1:4 ]

Matrix({1.,0.},{0.,1.}) # tensor product
#>M
0. 1.
0. 0.
```

`Matrix` **(** *rs_1 rs_2* **)** − returns `matrix` of contact areas. See also: `Cad`, `Area` .

`Matrix` **(** *ali_* **)** − returns a `matrix` of normalized pairwise Dayhoff evolutionary distances between the sequences in alignment *ali_* (for similar sequences it is equal to the fraction mismatches).

`Matrix` **(** ali_, `number` **)** − returns a `matrix` of alignment. It contains reference residue numbers for each sequence in the alignment, or `−1` for the gaps. The first residue has the reference number of 0 (make sure to add 1 to access it from the shell).

`Matrix` **(** *boundary* **)** − returns values generated by the `make boundary` command for each atom.

`Matrix` **(** *R_Xn R_Yn R_ruler* **)** − retuns 2D histrogram of X and Y values. The *R_ruler* array consists of limits for X and Y and step sizes for X and Y : *{xFrom, xTo, yFrom, yTo, [xStep, yStep] }* . Example:

```
icm/def> Matrix(Random(0. 5. 20) Random(0. 5. 20) {0. 5. 0. 5. 1. 1.})
#>M
1. 0. 2. 1. 0.
1. 1. 1. 1. 2.
0. 2. 1. 1. 0.
0. 1. 0. 0. 1.
1. 0. 0. 1. 2.
```

2.21.74. Max

maximum−value function.

`Max` **(** { *rarray* | *map* } **)**

− returns the `real` maximum−value element of a specified object

`Max` **(** *iarray* **)** − returns the `integer` maximum−value element of the iarray.

`Max` **(** *matrix* **)** − returns the `rarray` of maximum−value element of each column of the matrix. To find the maximum value use the function twice (`Max(Max(` m)))

`Max` **(** integer1, integer2, ... **)** − returns the largest `integer` argument.

`Max` **(** real1, real2, ... **)** − returns the largest `real` argument.

`Max` **(** *S s_leadingString* **)** returns the maximal trailing number in array elements consisting of the *s_leadingString* and a number. If there are no numbers, returns `0.` E.g.
`Max({"a1","a3","a5"},"a")` returns `5.`

Max(*grob | *macro | *sequence | *alignment | *profile | *table | *map) −> i

returns the maximal number of shell objects of the specified class. To increase this shell limit, modify the `icm.cfg` file.

`Max` **(** `grob` *s_leadingString* **)** returns the maximal number appended to grob names:

```
g_skin_1
g_skin_2
```

This function is equivalent to Max(Name(grob), s_leadingString) (see the previous function).

Examples:

```
show Max({2. 4. 7. 4.})          # 7. will be shown
```

2.21.75. MaxHKL

an array of three maximal crystallographic h,k,l indices at a given resolution.

`MaxHKL` **(** { *map_* | *os_* | [*R_6CellParameters*] }, *r_minResolution* **)** *=> I3*

the function extracts the cell parameters from *map_* , *os_* object, or reall array of {a,b,c,alpha,beta,gamma}, and calculates an `iarray` of three maximal crystallographic indices { *hMax* , *kMax* , *lMax* } corresponding to the specified *r_minResolution* .

2.21.76. Mean

average−value function.

`Mean` **(** { *rarray* | *map* } **)**

− returns the `real` average−value of elements of the specified ICM−shell objects.

`Mean` **(** *iarray* **)**

− returns the `real` average−value of the elements of the *iarray*.

`Mean` **(** *matrix* **)**

− returns `rarray` [1:m] of average values for each *i−th* column *matrix[1:n,i]*.

`Mean` **(** *R1 R2* **)**

− for two real arrays of the same size returns `rarray` [1:m] of average values for each pair of corresponding elements.

Examples:

```
print Mean({1,2,3})          # returns 2.

show Mean(Xyz(a_2/2:8))      # shows {x y z} vector of geometric
                             # center of the selected atoms
Mean({1. 2. 3.} {2. 3. 4.})
#>R
  1.5
  2.5
  3.5
```

2.21.77. Min

minimum−value function.

`Min` **(** { *rarray* | *map* } **)** − returns the `real` minimum value element of a specified object

`Min` **(** *iarray* **)** − returns the `integer` minimum−value element of the iarray.

`Min` **(** *matrix* **)** − returns the `rarray` of minimum−value element of each column of the matrix. To find the minimum value use the function twice (e.g. `Min(Min(m))`)

`Min` **(** integer1, *integer2* ... **)** − returns the smallest `integer` argument.

`Min` **(** real1, real2, ... **)** − returns the smallest `real` argument.

Examples:

```
show Min({2. 4. 7. 4.})      # 2. will be shown
```

```
show Min(2., 4., 7., 4.)     # 2. will be shown
```

2.21.78. Money

function to print money figures.

`Money` **(** { *i_amount* | *r_amount*}, [*s_format*] **)** − returns a `string` with the traditionally decorated money figure. *s_format* contains the figure format and the accompanying symbols.

- `%m` specification for the rounded integral amount;
- `%.m` specification to add cents after dot. The default is "$%.m", i.e. Money(1222.33) returns $1,222.33.
- `%M` the same as %m but with dot instead of comma in the European style
- `%.M` the same as %.m dot and comma are inverted in the European style

Examples:

```
Money(1452.39)  # returns "$1,452.39"
Money(1452.39,"DM %m")  # returns "DM 1,452"
Money(1452.39,"%.M FF")  # inverts comma and dot "1.452,39 FF"
```

2.21.79. Mod

remainder (module) function. Similar to, but different from `Remainder`() function:

function	description	example
Mod(x,y)	brings x to [0 , y] range	Mod(17.,10.) => 7.
Remainder(x,y)	brings x to [−y/2 , y/2] range	Remainder(17.,10.)=> −3.

`Mod` **(** i_divisor, [*i_divider*] **)** − returns `integer` remainder.

`Mod` **(** r_divisor, [*r_divider*] **)** − returns the `real` remainder r = x − n*y where n is the integer nearest the exact value of x/y; r belongs to [0, |y|] range.

`Mod` **(** iarray, [*i_divider*] **)** − returns the `iarray` of remainders (see the previous definition).

`Mod` **(** rarray, [*r_divider*] **)** − returns the `rarray` of remainders (see the previous definition).

The default divider is 360. (or 360) since we mostly deal with angles.

Examples:

```
phi = Mod(phi)    # transform angle to [0., 360.] range
a   = Mod(17,10)  # returns 7
```

2.21.80. Mol

molecule function.

`Mol` **(** { *os_* | *rs_* | *as_* } **)** − selects molecules related to the specified objects *os_* , residues *rs_* or atoms *as_*, respectively.

Examples:

```
show Mol( Sphere(a_1//* 4.) )
          # molecules within a 4 A vicinity of the first one
          # Sphere function Sphere(as_atoms) selects atoms.
```

See also: `Atom`, `Res`, `Obj` .

2.21.81. Name

generic function returing strings or string arrays with names of things.

`Name` ( ) − returns empty string.

`Name` **(** *s_Path_and_Name* **)** − returns file name sub− `string` if full path is specified

`Name` **(** *s_* [`simple` | `unique`] **)** Opions:

- `simple` : removes non−alpha−numeric simbols from a string and replaces them by underscore.
- `unique` : checks if the name *s_* exists in the ICM−shell. If the name does not exist, it is returned without changes, otherwise a number is appended to the name to guarantee its uniqueness.

Examples:

```
  Name( " %^23 a 2,3 xreno−77−butadien" simple)
23_a_2_3_xreno_77_butadien

  a=1
  Name("a",unique)
a1
```

`Name` **(** { `command` | `function` | `macro` | `integer` | `real` | `string` | `logical` | `iarray` | `rarray` | `sarray` | `matrix` | `map` | `grob` | `alignment` | `table` | `profile` | `sequence` } **)** − returns a string array of object names for the specified class.

`Name` **(** { `iarray` | `rarray` | `sarray` | `matrix` | `map` | `grob` | `alignment` | `table` | `profile` | `sequence` } `selection` **)** − returns a string array of names of **selected** objects for the specified class.

`Name` **(** *as_* **)** − returns `sarray` of names of selected atoms.

`Name` **(** *as_* `sequence` **)** − returns `sarray` of chemical names of the selected atoms according to the icm.cod file (one−letter chemical atom names are low case, e.g. "c", two−letter names start from an upper−case letter, like "Ca"). The names from the periodic table are used in the wrGaussian macro.

`Name` **(** *rs_* **)** − returns `sarray` of names of selected residues. To obtain a one−letter code sequence, use `Sequence( rs_ )` and to convert it to a string use `String( Sequence( rs_ ))` .

`Name` **(** *ms_* **)** − returns `sarray` of names of selected molecules.

`Name ( ms_ sequence )` − returns `sarray` of names of sequence linked to the specified molecules *ms_* or empty strings.

`Name ( ms_ alignment )` − returns `sarray` of names of alignments linked to the specified molecules *ms_* or empty strings

`Name ( ms_ swiss )` − returns `sarray` of names of swissprot names corresponding to the specified molecules *ms_* or empty strings

`Name ( os_ )` − returns `sarray` of names of selected objects. E.g. Name(a_)[1] returns `string` with the name of the current object.

`Name ( vs_ )` − returns `sarray` of names of selected variables.

`Name ( alignment )` − returns `sarray` of constituent sequence names.

`Name ( table )` − returns `sarray` or constituent table ICM−shell object names.

`Name ( sequence )` − returns `string` name of specified sequence.

Examples:

```
 read alignment msf "azurins"        # load alignment
 seqnames = Name(azurins)            # extract sequence names

 show Name( Acc( a_/* ) ) # array of names of exposed residues
```

2.21.82. Namex

comment (or description) function.

`Namex ( os_ )` : *Namex (s_MultiObjectFile)

− returns `sarray` of comments of selected objects *os_* (i.e. a string for each object). This field is set to the chemical compound name by the `read pdb` command. Alternatively, you can set your own comment with the `set comment os_ s_comment` command. If you have a single object and want to convert a string array of one element (corresponding to this one object) to a simple `string`, use this expression, e.g.: `Sum(Namex(a_)).` Other manipulations with a multiline string can be performed with the `Field`, `Integer`, `Real`, `Split` functions (see also `s_fieldDelimiter`).

Example. We stored values in the comment field in annotations like this: "LogP 4.3\n". Now we extract the values following the "LogP" field name:

```
 remarks = Namex( s_icmhome+"all.ob") # get remarks directly without reading
 group table t Rarray(Field(remarks,"vacuum",1,"\n")) "vacuum"
 group table t append Rarray(Field(remarks,"hexadecane",1,"\n")) "hex"
 show t

 read object s_icmhome + "all"  #  read multiple object file
# extract numbers following the 'LogP' word in the object comments
 logPs = Rarray(Namex(a_*.),"LogP",1,"  \n")
```

`Namex` **(** *seq_* **)** − returns `string` of long name ('description' field in Swissprot).

Example:

```
read index s_inxDir+"/SWISS.inx"
read sequence SWISS[2]  # read the 2nd sequence from Swissprot
show Namex( sequence[0] )
```

2.21.83. Next

selection function.

`Next` **(** { *as_* | *rs_* | *ms_* | *os_* } **)**

− selects atom, residue, molecule, or object immediately following the selected one. Next(the_last_element) returns an empty selection.

Examples:

```
show Next( a_/4 ) )      # show residues number 5
phi5=Torsion( a_/5/c )
                         # psi5 formally belongs to the next residue
psi5=Torsion( a_//n & Next(a_/5) )
```

2.21.84. Covalent neighbors of an atom

`Next` **(** *as_* { `bond` | `tree` } **)** − selects atoms forming covalent bonds with the selected single atom. Option `tree` allows to select only atoms **above** a given atom in an icm−tree.

Example:

```
BS his
display
display a_/his/he2 ball red
display Next( a_/his/he2 bond ) ball magenta # show atom preceding he2

cd2_neigh = Next( a_//cd2 bond )
for i=1,Nof(cd2_neigh)
  nei = cd2_neigh[i]
  print "  Distance between a_//cd2 and ",Sum(Name(nei)), " = ", Distance( a_//cd2 nei)
endfor
```

2.21.85. Nof

Number−OF−elements function.

`Nof` **(** { *iarray* | *rarray* | *sarray* } **)** − returns `integer` number of elements in an array

`Nof` **(** *ali_* **)** − returns `integer` number of sequences in the specified alignment *ali_* (see also `Length`(*alignment*)).

`Nof(` *matrix* `)` − returns `integer` number of rows in a matrix (see also `Length(` *matrix)* function which returns number of columns).

`Nof(` *map* `)` − returns `integer` number of grid points in a map.

`Nof(` *grob* `)` − returns `integer` number of points in graphics object.

`Nof(` { *os_* | *ms_* | *rs_* | *as_* | *vs_* } `)` − returns `integer` number of selected objects, molecules, residues, atoms or variables respectively.

`Nof(` { *os_* | *ms_* | *rs_* } [`atom`] `)` − returns an array of the numbers of atoms in each selected unit. This function automatically excludes the 'virtual' atoms added automatically to the ICM−objects (equivalent to the `a_//!vt*` selection). Example:

```
read mol s_icmhome+"ex_mol.mol"
Nof( a_*. atom )
```

`Nof(` { `atoms` | `residues` | `molecules` | `objects` | `conf` | `tether` | `vrestraint` } `)` − returns the total `integer` number of atoms, residues, molecules, objects, stack conformations or tethers, variable restraints, respectively. It is safer than the previous command (e.g. `Nof(a_//*))` since `Nof(atoms)` will work even if object does not exist.

`Nof(` `library` `)` − returns 1 if the force field parameter `library` is loaded and 0 otherwise.

`Nof(` `library` `)` − returns 1 if the `mmff library` is loaded and 0 otherwise.

`Nof(` `plane` `)` − returns the number of active graphical planes

`Nof(` `site` [*ms_*] `)` − returns `integer` number of `site`s in the selected molecule or the `current object`.

`Nof(` { *s_stackFileName* | *s_objFileName* } `)` − returns `integer` number of conformations in the specified

Example:

```
for i=1,Nof("def.cnf",conf)  # stack is NOT loaded
  read conf i
endfor
```

`Nof(` string, *substring* `)` − returns `integer` number of occurrences of *substring* in a *string.* E.g. `Nof("ababab","ba")` returns `2`

`Nof(` string, substring, `pattern` `)` − returns `integer` number of occurrences of regular pattern in a string. E.g. `Nof("ababab","b?")` returns `2`

Example with a strange DNA sequence `dn1:`

```
if(Nof(String(dn1),"[!ACGT]" pattern) > 0.5*Length(dn1)) print " Warning> Bad DNA sequence"
```

`Nof(` { `iarray` | `rarray` | `sarray` | `sequence` | `aselection` | `vselection` | `alignment` | `matrix` | `map` | `grob` | `string` | `object` } [`selection`]`)` − returns `integer` number of ICM−shell variables of specified type. With the `selection` option it returns the number of GUI−selected objects (exceptions: for `aselection, vselection, string , object`).

Examples:

```
nseq = Nof(sequences)         # number of sequences currently loaded
if(Nof(object)==0) return error "No objects loaded"

if ( Nof( sequence select ) == 2 ) a = Align( select )
```

2.21.86. Norm

normalize numbers.

`Norm(` *map* `)` − returns the `map` linearly transformed into the [0.,1.] range.

2.21.87. Obj

object level function.

`Obj(` { *ms_* | *rs_* | *as_* } `)` − selects object(s) related to the specified molecules, residues or atoms, respectively.

Examples:

```
show Obj( a_*./dod )             # show objects containing heavy water
```

See also: `Atom`, `Res`, `Mol` .

2.21.88. Occupancy

function.

`Occupancy(` { *as_* | *rs_* } `)` − returns `rarray` of occupancy for the specified selection. If residue selection is given, average residue occupancies are returned.

See also: `set occupancy`.

Examples:

```
avO=Min(Occupancy(a_//ca))     # minimal occupancy of Ca−atoms
show Occupancy(a_//!h*)        # array of occupancy of heavy atoms
color a_//* Occupancy(a_//*)   # color previously displayed atoms
                               # according to their occupancy
color ribbon a_/A Occupancy(a_/A) # color residues by mean occupancy
```

2.21.89. Path

function.

`Path(` *s_FullFileName* `)` − returns header sub− `string` with the path.

Examples:

```
sPath=Path("/usr/mitnick/hacker.loot") # returns "/usr/mitnick/"
```

See also: `Name`() and `Extension`() functions which return two other components of the full file name.

`Path(preference)`

returns the path to the directory in which the user preferences file `"icm.ini"` is stored. This file is always stored in the `s_icmhome` , but a user can save his or her own preferences in the *s_userDir*`/config/icm.ini` file.

Example:

```
read all Path(preference)+"icm.ini" # restore the settings
```

`Path(unix)`

returns a path to the ICM executable. ICM binary can also be found in the `Version(full)` string.

`Path(directory)`

returns the current working directory.

`Path(last)`

returns the path of the last icm−shell script called by ICM.

2.21.90. Parray

function containing an array of chemical compounds. These compounds can be read from the mol/sdf files into binary chemical representation stored in ICM chem−tables.

Parray `(` *s_smiles* `smiles)` : Parray (s_molFileText *mol)

Example:

```
read table mol "ex_mol.mol" name="t"
sss  = String(t.mol[1]) # sss contains mol/sdf text
t.mol[1] = Parray(sss mol)  # sss is parced and converted
```

2.21.91. Pattern

function.

`Pattern(` { *s_consensus* | *ali_* } [`exact`]`)` − returns `sequence pattern` string which can be searched in a single sequence with the `find pattern` command or in a database with the `find database pattern=s_pattern` command. If ICM−consensus string *s_consensus* is provided as an argument, the string is translated into a regular `pattern` expression (e.g. an expression `"R+. ..^D"` will be translated to `"R[KR]?\{3,6\}[ACGS]D"`). If alignment *ali_* is given as an argument, the pattern is either extracted directly from the alignment, option `exact,` or is converted to consensus first, and only after that translated into a pattern. For example, an alignment position with amino acids `A` and `V` will be transformed into pattern `[AV]` with option `exact` and into pattern `[AFILMPVW]` without the option. Additionally, the `exact` option will retain information about the length of the flanking regions.

Example:

```
read sequence s_icmhome + "zincFing"
group sequence aaa
align aaa
show Pattern("#~???A%  ?P")  # symbols from consensus string
show Pattern(aaa)
show Pattern(aaa exact)
```

`Pattern(` *s_seqPattern* `prosite)` − returns `string` containing the `prosite−formatted` sequence pattern. The input string *s_seqPattern* is an ICM sequence `pattern` .

2.21.92. Pi

function (or rather a reserved name).

`Pi` − returns the `real` value of Pi (`3.14...).`

Examples:

```
print Pi/2. </tt>
```

2.21.93. Potential

function.

`Potential(` *as_targets as_charges* `)` − returns `rarray` of Nof(*as_targets)* real values of electrostatic potentials at *as_targets* atom centers. Electrostatic potential is calculated from the specified charges *as_charges* and the precalculated boundary (see also REBEL, `make boundary` and How to evaluate the pK shift).

Examples:

```
read object "crn"
           # prepare electrostatic boundary descriptions
make boundary
           # potential from oe*, od* at cz of two args
```

```
show Potential(a_/arg/cz a_/glu,asp/o?* )
print 0.5*Charge(a_//*)*Potential(a_//* a_//* )
           # the total electrostatic energy which is
           # actually calculated directly by show energy "el"
```

2.21.94. Power

mathematical function.

`Power` **(** r_base, { *r_exp* | *i_exp*} **)** − returns `real` $r\_base^{r\_exp}$ or $r\_base^{i\_exp}$. Note that *r_base* may be negative if the exponent is an integer, otherwise error will be produced.

`Power` **(** r_base, *R_exp* **)** − returns `rarray` of the *r_base* taken to the *R_exp* powers.

`Power` **(** r_base, *M_exp* **)** − returns `matrix` of the *r_base* taken to the *M_exp* powers.

Example:

```
Power(2.,{1. 2. 3.}) # returns {2.,4.,8.}
```

`Power` **(** rarray, *r_Exponent* **)** − returns `rarray` of elements taken to the specified power.

`Power` **(** matrix, *integer* **)** − for square matrix returns the source matrix taken to the specified power. If the exponent is negative, the function returns the *n−th* power of the **inverse** matrix.

Examples:

```
size=Power(tot_volume,1./3.)        # cubic root

read matrix "LinearEquationsMatrix" # read matrix [1:n,1:n]
read rarray b                       # read the right−hand column [1:n]
x=Power(LinEquationsMat,−1) * b     # solve system of linear equations

a=Rot({0. 1. 0.}, 90.0)
      # create rotation matrix around Y axis by 90 degrees
if (Power(a,−1) != Transpose(a)) print "Wrong rotation matrix"
                            # the inverse should be
                            # equal to the transposed
rotate a_1 Power(a,3)       # a−matrix to the third is
                            # three consecutive rotations
```

2.21.95. Probability

function.

`Probability` **(** *s_seqPattern* **)** − returns the `real` probability of the specified sequence pattern. To get mathematical expectation to find the pattern in a protein of length L, multiply the probability by L−Length(*s_seqPattern).*

Examples:

```
                    # chance to find residues RGD at a given position
```

```
show Probability("RGD")
                  # a more tricky pattern
show Probability("[!P]?[AG]")
```

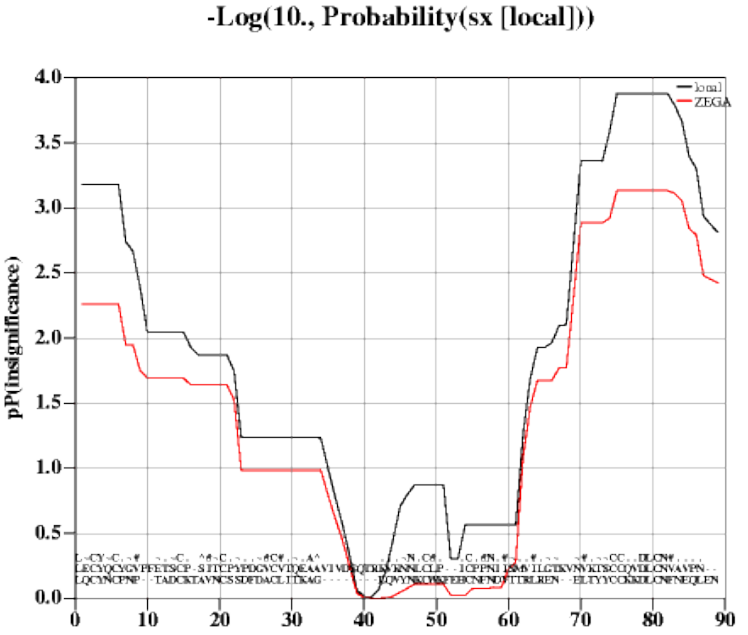
`Probability(` i_minLen, *r_Score* [, { `identity` | `similarity` | `comp_matrix` | `sort` }] `)` − returns the `real` expected probability that a given or higher score (*r_Score)* might occur between structurally unrelated proteins (i.e. it is essentially the probability of an error). This probability can be used to rank the results of database searches aimed at fold recognition. A better score corresponds to a lower probability for a given alignment. The four types of scores

- no argument: alignment score
- `identity:` the number of identical residues * 100 and divided by the minimal sequence length
- `similarity:` alignment score without gap penalties *100. and divided by the minimal sequence length
- `comp_matrix:` alignment score without gap penalties (unnormalized)
- `sort:` an additional score for ranking

are given in the description of the `Score` function. Each score has a different distribution which was carefully derived from all−to−all comparisons of sequence of protein domains.

Example: Probability(150, 30, identity)*55000. is the mathematical expectation of the number of structurally unrelated protein chains of 150 residues with 30% or higher sequence identity which can be found in a search through 55000 sequences. The inverse function is `Score.`

`Probability(` ali_2seq, [*i_windowSize1 w_windowSize2*] [`local`] `)`



− returns the `rarray` of expected probabilities of local insignificance of the pairwise sequence alignment *ali_2seq*. The Karlin and Altschul score probability values (option `local`) or local ZEGA probabilities (see also `Probability`(i_, r_)) are calculated in multiple windows ranging in size from *i_windowSize1* to *w_windowSize2* (default values 5 and 20 residues, respectively). The exact formulae for the Karlin and Altschul probabilities (option `local`) are given in the next section and the ZEGA probabilities are given in the Abagyanpaper. The window with the lowest probability value is chosen in each position. The array returned by this function can be used to color−code the regions of insignificant sequence−structure alignment in modeling by homology. One can use the `Rarray`(R_,ali_,seq_) function to project the array onto selected sequence.

To calculate an array of mean scores for each column of a multiple sequence alignments use the `Rarray`(ali [`exact`]) function.

Example:

```
 read alignment s_icmhome+ "sx"  # 2 seq. alignment
 read pdb  s_icmhome+"x"
 p= −Log(Probability(sx))
 display ribbon a_
 color ribbon a_/A −Rarray(p,sx,cd59)
 # Rarray projects the alignment array to the sequence
```

`Probability(` *seq_1 seq_2* [*i_windowSize1 w_windowSize2*] `)` − returns a dot `matrix` of probabilities of local statistical comparison between the two sequences. This matrix contains local probability values that two continuous sequence fragments of length ranging from *i_windowSize1* to *w_windowSize2* have statistically insignificant alignment score , which means that the match is random. Visualization of this matrix allows to see periodic patterns if sequence is compared with itself as well as identity alternative alignments. The formula is taken from the Karlin and Altschul statistics:

P= 1−exp(−exp(−Lambda*Sum(score in window)/K)), where Lambda and K are coefficients depending on the residue comparison matrix.

This example allows to trace the correct alignment despite an about 100 residue insertion:

```
 read pdb sequence "2mhb"
 read pdb sequence "4mbn"
 m=Probability(2mhb_a 4mbn_m 7 30)
 print " pProbability: Min=" Min(Min(m)) "Max=" Max(Max(m))
 PLOT.rainbowStyle="white/rainbow/red"
# show probability of the chance matching (comparable to the BLAST P−value)
 plot area m display color={.2 0.001} transparent={0.2 1.} link grid
# OR show −Log10(Probability)
 plot area −Log(m,10) display color={0.7 3.} transparent={0. 0.7} link grid
```

2.21.96. Profile

function.

`Profile(` *alignment* `)` − creates `profile` from an alignment

2.21.97. Putenv

function to change or add value to environment.

`Putenv` **(** " *s_environmentName* = *s_environmentValue* " **)** − returns a `logical` `yes` if the named environment variable is created or modified.

Example:

```
show Putenv("aaa=bbb")
     # change/add variable 'aaa' with value 'bbb' to environment
show Getenv("aaa")
     # check if it has been successful
```

See also: `Existenv`( ), `Getenv`( ).

2.21.98. Radius

atomic radii (van der Waals, surface energy, and electrostatic).

`Radius` **(** *as_* **)** − returns the `real array` of van der Waals radii of atoms in the selection.

These radii are used in the construction of the molecular surface `(skin)` and can be found (and possibly redefined) in the `icm.vwt` file.

`Radius` **(** *as_* `surface` **)** − returns the `rarray` of the 'hydration' atomic radii.

These radii are used in construction of the solvent−accessible `(surface)` and can be found (and possibly redefined) in the `icm.hdt` file.

`Radius` **(** *as_* `charge` **)** − returns the `rarray` of the 'electrostatic' atomic radii.

These radii are used for building the skin (analytical molecular surface) for electrostatic dielectric boundary calculation with `electroMethod` = "boundary element". These parameters can be found (and possibly redefined) in the `icm.vwt` file.

2.21.99. Random

evenly distributed random function.

`Random` ( ) − returns a pseudo−random `real` in the range from 0. to 1.

`Random` **(** *i_max* **)** − returns a pseudo−random `integer` distributed in [1, *i_max*]

`Random` **(** *i_min* , *i_max* **)** − returns a pseudo−random `integer` distributed in [*i_min* , *i_max*]

`Random` **(** *r_min* , *r_max* **)** − returns a pseudo−random `real` evenly distributed in [*r_min* , *r_max*]

`Random` **(** *r_min* , *r_max* , *i_n* **)** − returns a `rarray` [1: *i_n*] with pseudo−random real values distributed in [*r_min* , *r_max*]

`Random (` *r_mean* , *r_std* , *i_n* , "gauss" `)` − returns a `rarray` of *i_n* elements with normally distributed pseudo−random values. The mean and standard deviation are provided as the first two arguments

`Random (` *r_min* , *r_max* , *i_nRows* , *i_nColumns* `)` − returns a `matrix` [1: *i_nRows,* 1: *i_nColumns]* with pseudo−random real values distributed in [*r_min* , *r_max]*

`Random (` i_nRows, i_nColumns, r_min, *r_max* `)` − returns a `matrix` [1: *i_nRows,* 1: *i_nColumns]* with pseudo−random real values distributed in [*r_min, r_max*]

`Random (` *sequence* `)` − returns a randomized `sequence` with the same amino−acid composition

Examples:

```
print Random(5)            # one of the following: 1 2 3 4 or 5
print Random(2,5)          # one of the following: 2 3 4 or 5
print Random(2.,5.)        # random real in [2.,5.]
randVec=Random(−1.,1.,3)   # random 3−vector with components in [−1. 1.]
randVec=Random(3,−1.,1.)   # the same as the previous command
randMat=Random(−1.,1.,3,3) # random 3x3 matrix with components in [−1. 1.]
randMat=Random(3,3,−1.,1.) # the same as the previous command
Random(0., 1., 10, "gauss" # normal distribution
a=Random(seq_crn)          # a contains a randomized crambin sequence
```

2.21.100. Rarray

real−array function.

`Rarray (` *i_NofElements* `)` − returns a `rarray;` creates zero−initialized rarray [1: *i_NofElements].* You can also create an zero−size real array: `Rarray(0)` .

`Rarray (` i_NofElements, *r_Value* `)` − returns a `rarray` [1: *i_NofElements*] with all elements set to *r_Value.*

`Rarray (` i_NofElements, r_From, *r_To* `)` − returns a `rarray` [1: *i_NofElements*] with elements ranging from *r_From* to *r_To.*

`Rarray (` r_From, *r_To* , *r_step* `)`

`Rarray (` *iarray* `)` − converts *iarray* into a `rarray.`

`Rarray (` *sarray* `)` − converts *sarray* into a `rarray.`

`Rarray (` *M* [*i_flag*] `)` − extracts different groups of elements of the matrix and casts them into a `rarray.` The possibilities are the following:

1. all elements by rows (the default)
2. all elements by columns
3. the upper triangle,
4. the lower triangle,
5. the diagonal elements
6. the upper triangle without diagonal elements

7. the lower triangle without diagonal elements

Examples:

```
 a=Rarray(54)                     # create 54-th dimensional vector of zeros
 a=Rarray(3,-1.)                  # create vector {-1.,-1.,-1.}
 a=Rarray(5,1.,3.)                # create vector {1., 1.5, 2., 2.5, 3.}
 a=Rarray({1 2 3})                # create vector {1. 2. 3.}
 a=Rarray({"1.5" "2" "-3.91"})    # create vector {1.5, 2., -3.91}
#
 M=Matrix(2)
 M[2,2]=2
 M[1,2]=3
 Rarray( M )
 Rarray( M 1 )
 Rarray( M 2 )
 Rarray( M 3 )
 Rarray( M 4 )
 Rarray( M 5 )
```

rarray sequence projection

`Rarray` **(** *R_ali ali_from* { *seq_* | *i_seqNumber* } **)**

− returns a projected `rarray`. The *R_ali* rarray contains values defined for each position of alignment *ali_from.* The function squeezes out the values which correspond to insertions into sequence *seq_*, that is, in effect, projects the alignment array *R_ali* onto sequence *seq_*.

Projecting from one sequence to another sequence via alignment.

Let us imagine that we have two sequences, *seq1* and *seq2* which take part in multiple sequence alignment *ali* . The transfer of property R1 from *seq1* to *seq2* can be achieved via *two transfers* :

1. *seq1* to *ali* : RA = Rarray(R1 seq1 ali r_gapValues)
2. *ali* to *seq2* : R2 = Rarray(RA ali seq2)

Now R2 has the same dimension as seq2. Values aligned with ~seq1 are transferred by alignment, other values are set to *r_gapValues* .

See also:

`String`(*s_,R_,ali_,seq_*)	function to project strings
`Rarray`(*R_seq seq_ ali_to r_gapDefault*)	function to project *from sequence to alignment*
`Probability`	function

`Rarray` **(** *rarray* `reverse` **)**

− converts input real array into an `rarray` with the reversed order of elements. Example:

```
Rarray({1. 2. 3.} reverse)  # returns {3. 2. 1.}
```

Transfer real sequence properties by alignment

`Rarray` **(** *R_seq* { *seq_* | *i_seqNumber* } *ali_to r_gapDefault* **)**

− projects the input `rarray` from *seq_* to *ali_to* (the previous function does it in the opposite direction). The *R_seq* rarray contains values defined for each position of the sequence *seq_*. The function fills the gap positions in the output array with the *r_gapDefault* values.

Combination of this and the previous functions allow you to project any numerical property of one sequence to another by projecting the r1 property of seq1 first to the alignment and than back to seq2 (e.g. Rarray(Rarray(r1,seq1,a,99.) , a, seq2)).

This function can also be used to determine alignment index corresponding to a sequence index. Example:

```
read alignment s_icmhome+"sh3"
t = Table(sh3)
group table t Count(Nof(t)) "n" append  # add a column with 1,2,3,..
show t  # t looks like this:
 #>T t
 #>−cons−−−−−−−−Fyn−−−−−−−−−Spec−−−−−−−−Eps8−−−−−−−n−−−
    " "         0           1           1           1
    " "         0           2           2           2
    " "         0           3           3           3
    " "         0           4           4           4
    .           1           5           5           5
 ...
t2forFyn =  t.Fyn == 2   # table row for position 2 in seq. Fyn
t2forFyn.n               # corresponding alignment position
```

See also the `String`(*s_,R_,seq_,ali_,s_defChar*) function to project strings.

Assign arbitrary amino−acid property to a sequence

`Rarray` **(** *sequence R_26resProperty* **)**

− returns a `rarray` of residue properties as defined by *R_26resProperty* for 26 residue types (all characters of the alphabet) and assigned according to the amino−acid *sequence*.

Example with a hydrophobicity property vector:

```
 s= Sequence("TTCCPSIVARSNFNVCRLPGTPEAICATYTGCIIIPGATCPGDYAN") # crambin sequence
# 26−dim. hydrophobicity vector for A,B,C,D,E,F,..
 h={1.8,0.,2.5,−3.5,−3.5,2.8,−.4,−3.2,4.5,0.,−3.9,3.8,1.9,−3.5,.0,−1.6,−3.5,−4.5,−.8,−.7,0.,4.
 hs=Rarray(s,h)              # h−array for each sequence position
 hh = Smooth(Rarray(s,h), 5) # window average
```

Calculating array of alignment strength values for each column

`Rarray` **(** *ali_* [`exact` | `simple`] **)**

− returns a `rarray` of conservation values estimated as mean pairwise scores for each position of a pairwise or multiple alignment. The number is calculated as the sum of RESIDUE_COMPARISON_VALUES over `n*(n−1)/2` pairs in each column. The gapped parts of an

alignment are considered equivalent to the 'X' residues and the comparison values are taken from appropriate columns.

Option `exact` uses raw residue substitution values as defined in the comparison matrix These values can be larger than one for the residues the conservation of which is important (e.g. W to W match can be around 3. while A to A match is only about 0.5.

By default (no keyword) the matrix is normalized so that two identical residues contribute the replacement value of 1. and two different amino acid contributed values from about −0.5 to 1. depending on the residue similarity.

If option `simple` is specified, each pair with identical residues contributes 1. while each pair of different amino−acids contributes 0.. The result is divided by `n(n−1)/2` , and the square root is taken. The values returned with the `simple` option are therefore between 0. (all residues are different)

To *project* the resulting array to a specific sequence, use the Rarray(R_ ali_ seq_) function (see above).

To calculate conservation ** with respect to a particular set of residues in a structure, use the `Score`(rs_ [`simple`]) function.

Example:

```
read alignment "sh3"
show Rarray(sh3)
#
a=Rarray(sh3 simple)  # a number for each alignment position
# to project a to a particular sequence, do the following
b=Rarray(a,sh3,Spec)  # a number for each Spec residue
String(Rarray(a, sh3, Spec ))//String(Spec)   # example
```

2.21.101. Real function

generally converts things to a real.

`Real(` *integer* `)` − converts integer to `real` number.

`Real(` *iarray* `)` see `Rarray`(*iarray).*

`Real(` *string* `)` − converts string to `real` number. The conversion routine ignores trailing non−numerical characters.

Examples:

```
 s = "5.3"
 a = Real(s)      # a = 5.3
 s = "5.3abc"     # will ignore 'abc'
 a = Real(s)      # the same, a = 5.3
```

`Real(` *rarray* `)` − returns the first element of the real array. With that trick one can also transform real array with one element into the `real` number. You may also convert a one element array into a real with the `Sum` or the `Mean` functions. If there are more then one elements, the first element is taken. Important

for assignments.

Example:

```
a[2,3]=Real(Value(v_/2/phi))  # a is a matrix, a[2,3] expects a real
```

2.21.102. Remainder function.

Returns the remainder; similar to, but different from the `Mod` function.

function	description	example
Remainder(x,y)	brings x to [−y/2 , y/2] range	Remainder(17.,10.)=> −3.
Mod(x,y)	brings x to [0 , y] range	Mod(17.,10.) => 7.

`Remainder` **(** i_divisor, [*i_divider*] **)** − returns the `integer`

`Remainder` **(** r_divisor, [*r_divider*] **)** − returns the `real` remainder r = x − n*y where n is the integer nearest the exact value of **x**/y; if | *n−x/y|=0.5* then n is even. **r** belongs to [−|*y|/2*, |*y|/2*] range

`Remainder` **(** iarray, [*i_divider*] **)** − returns the `iarray` of remainders (see the previous definition).

`Remainder` **(** rarray, [*r_divider*] **)** − returns the `rarray` of remainders.

The default divider is 360. (real) or 360 (integer) since we mostly deal with angles.

Examples:

```
              # transform angle to the standard
              # [−180., 180.] range. (Period=360 is implied)
phi=Remainder(phi)

              # we assume that you have two objects
              # with different conf. of the same molecule
phiPsiVec1 = Value(v_1.//phi,psi)
phiPsiVec2 = Value(v_2.//phi,psi)
              # average angular
              # deviation
angDev=Mean(Abs(Remainder(phiPsiVec1−phiPsiVec2)))
              # cut and paste these examples into the ICM−shell
print Remainder(13,10 )  Mod(13,10 )
print Remainder(17,10 )  Mod(17,10 )
print Remainder(−13,10 ) Mod(−13,10 )
print Remainder(−17,10 ) Mod(−17,10 )
```

2.21.103. Replace

− text substitution function.

`Replace` **(** *s_source s_regularExpression s_replacement* **)** − returns a `string`, which is a copy of the source *string* with globally substituted substrings matching *s_regularExpression* by the replacement string *s_replacement.*

Example:

```
a=Replace(" 1crn "," ","")  # remove empty space
```

`Replace` **(** *s_source S_fromArray S_toArray* **)** − make several replacements in a row. The size of the two arrays must be the same.

Example which generates a complimentary DNA strand (actually there is a special function `Sequence`(*seq_*, `reverse`) which does it properly).

```
invertedSeq = String(0,1,"GTAAAGGGGTTTTCC")  # result: CCTTT..
complSeq=Replace(invertedSeq,{"A","C","G","T"},{"T","G","C","A"})
# result: GGAAA...
```

`Replace` **(** *s_source S_fromArray s_replacement* **)** − replace several strings by a single other string. If *s_replacement* is empty, the found substrings will be deleted.

Example which generates a complimentary DNA strand:

```
cleanStr=Replace("XXTEXTYYTEXT",{"XX","YY"},"")
```

`Replace` **(** *S_ s_regularExpression s_replacement* **)** − returns a `sarray` with globally substituted elements (the original sarray remains intact).

Examples:

```
aa={"Terra" "Tera" "Teera" "Ttera"}
show column aa Replace(aa "er?" "ERR") Replace(aa "*[tT]" "Shm")
```

`Replace` **(** *S_ S_fromArray S_toArray* **)** − returns a `sarray` with multiple substitutions.

`Replace` **(** *S_ s_regularExpression s_replacement* **)** − returns a `sarray` with multiple substitutions to a single string.

2.21.104. Res

residue selection function.

`Res` **(** { *os_* | *ms_* | *rs_* | *as_* } [`append`] **)** : *Res ({ rs_ [*append])

− selects residue(s) related to the specified objects (*os_)*, molecules (*ms_)* or atoms (*as_)*, respectively. Option `append` extends the selection with the terminal residues (like Nter and Cter in peptides)

Examples:

```
show Res( Sphere(a_1/1/* 4.) )   # show residues within 4 A
                                 # vicinity from the firsts one
```

See also: `Atom` ( ), `Mol` ( ), `Obj` ( ).

`Res(cursor)` − returns residue at which interactive residue cursor is set. See also displaycursor{display cursor}, `color cursor` .

2.21.105. Res(ali ..): from sequence positions in subalignment to residue selection

`Res(` *ali_* { *seq_* | *i_sequence* } `)` − returns residue selection corresponding to the aligned positions of the specified sequence. The sequence can be specified by its order number in the alignment (e.g. `1crn_m` in the example below has number `1`), or by name.

An example in which we find residue selection corresponding to the aligned part of crambin sequence `1crn_m`:

```
read pdb "1crn"
read alignment "bb" # a short sublalignment of 1crn_m
link a_*. bb        # link objects and sequences
show bb
#>ali bb
# Consensus   .C CP~.#A.^.#
1crn_m        TC-CPSIVARSNF------
a             PCGCPDGIAIARIYPFAVG
#1crn_m       EE E__HHHHHHH

# 1crn_m a nID 4 Lmin 46 ID 8.7 % Score 4.75 Sim 15.54 Gap 2.40 nOverlap 12 pP 0.16
#MATGAP gonnet 2.4 0.15

Res(  bb 1  )
- Num  Res. Type ---- SS Molecule ---- Object - sf - sfRatio
    2  thr   Amino    T E  m            1crn     0.0  0.00  .
    3  cys   Amino    C E  m            1crn     0.0  0.00  .
    4  cys   Amino    C E  m            1crn     0.0  0.00  .
    5  pro   Amino    P _  m            1crn     0.0  0.00  .
    6  ser   Amino    S _  m            1crn     0.0  0.00  .
    7  ile   Amino    I H  m            1crn     0.0  0.00  .
    8  val   Amino    V H  m            1crn     0.0  0.00  .
    9  ala   Amino    A H  m            1crn     0.0  0.00  .
   10  arg   Amino    R H  m            1crn     0.0  0.00  .
   11  ser   Amino    S H  m            1crn     0.0  0.00  .
   12  asn   Amino    N H  m            1crn     0.0  0.00  .
   13  phe   Amino    F H  m            1crn     0.0  0.00  .
```

2.21.106. Resolution

− returns the X−ray resolution in Angstroms.

`Resolution` ( ) − returns the `real` resolution of the current object.

`Resolution(` *os_object* `)` − returns the `real` X−ray resolution for the specified object. The resolution is taken from the PDB files.

Examples:

```
res=Resolution(a_1crn.) </tt>
print "PDB structure 1crn: resolution = ", res, " A"
```

`Resolution(` *s_pdbFileName* `pdb)` − returns the `real` resolution of the specified pdb−file. The function returns 9.90 if resolution is not found.

`Resolution(` *T_factors* [*R_6cell*] `)` − returns the `rarray` of X−ray resolution for each reflection of the specified `structure factor table`. The resolution is calculated from h, k, l and cell parameters taken from *R_6cell* or the standard `defCell` shell rarray.

Example:

```
read factor "igd"   # read h,k,l,fo table from a file
read pdb "1igd"     # cell is defined there
defCell = Cell(a_)  # extract the cell parameters from the object
group table append igd Resolution(igd) "res"
show igd
```

2.21.107. Rfactor

crystallographic R−factor.

`Rfactor(` *T_factors* `)` − returns the `real` R−factor residual calculated from the `factor−table` elements *T_factors.fo* and *T_factors.fc*. Reflections marked with *T_factors.free* = 1 are ignored.

2.21.108. Rfree

crystallographic free R−factor.

`Rfree(` *T_factors* `)` − returns the `real` R−factor residual calculated from the `factor−table` elements *T_factors.fo* and *T_factors.fc*. Only reflections marked with *T_factors.free* = 1 will be used.

2.21.109. Rmsd

Root−Mean−Square−Deviation function.

`Rmsd(` { *iarray* | *rarray* | *matrix* | *map* } `)`

− returns the `real` standard deviation (sigma) from the mean for specified sets of numbers

`Rmsd(` *as_tetheredAtoms* `)` `returns the real root−mean−square−deviation of selected atoms` from the atoms to which they are tethered . The distances are calculated **after** optimal superposition according to the equivalences derived from tethers (compare with the `Srmsd`(as_) function which does not perform superposition). This function also returns the transformation in the `R_out` array.

`Rmsd(` *as_select1 as_select2* [{ { `ali_` |*align* } | `exact` }] `)`

− returns the `real` root−mean−square−distance between two aligned sets after these two sets are optimally superimposed using McLachlan's algorithm.

Virtual atoms. Be default, the first two virtual atoms (`vt1` and `vt2`) are automatically excluded from both selections unless the `virtual` option is explicitly specified.

The optional third argument defines how atom−atom alignment is established between two selections (which can actually be of any level atom selection *as_* , residue selection *rs_* , molecular selection *ms_* , or object selection *os_* , see `alignment options`). Number of equivalent atom pairs is saved in `i_out`. Two output selections `as_out` and `as2_out` contain corresponding sets of equivalent atoms. This function also returns the transformation in the `R_out` array.

See also: `superimpose` and `Srmsd` ().

Examples:

```
 read pdb "1mbn"                          # load myoglobin
 read pdb "1pbx"                          # load alpha and beta
                                          # subunits of hemoglobin
 print Rmsd(a_1.1 a_2.1 align)            # myo− versus alpha subunit
                                          # of hemo− all atoms
 print Rmsd(a_1.1//ca a_2.1//ca align)    # myo− versus alpha subunit
                                          # of hemo− Ca−atoms

 print Rmsd(a_1./4,29/ca a_2.1/2,102/cb exact) # exact match
```

2.21.110. Rot

rotation matrix function.

`Rot` **(** *R_12transformVector* **)** − extracts the 3x3 rotation `matrix` from the `transformation vector`.

`Rot` **(** *R_axis* , *r_Angle* **)** − returns `matrix` of rotation around 3−dimensional real vector *R_axis* by angle *r_Angle.*

Examples:

```
        #  rotate molecule by 30 deg. around z−axis
 rotate a_* Rot({0. 0. 1.},30.)
```

`Rot` **(** *R_3pivotPoint R_3axis* , *r_Angle* **)**

− returns `rarray` of `transformation vector` of rotation around 3−dimensional real vector *R_axis* by angle *r_Angle* so that the pivotal point with coordinates *R_3pivotPoint* remains static.

Examples:

```
# rotate by 30 deg. around {0.,1.,0.} axis through the center of mass
 nice "1crn"
 R_pivot = Mean(Xyz(a_//*))
 transform a_* Rot(R_pivot,{0. 1. 0.}, 30.)
```

2.21.111. Sarray

sarray function.

`Sarray` **(** *integer* **)**

− returns empty `sarray` of specified dimension

`Sarray` **(** *integer s_Value* **)** − returns `sarray` of specified dimension initialized with *s_Value*

`Sarray` **(** *string* **)** − converts the input string into a ONE−dimensional `sarray` . To split a string into individual lines, or to split a string into a sarray of characters, use the `Split`() function.

`Sarray` **(** *iarray* **)** − converts input iarray into an `sarray`

`Sarray` **(** *rarray* **)** − converts input rarray into an `sarray`

`Sarray` (*rs_* [{ *append* | *name* | *residue* }]) − converts input residue selection into an `sarray` of residue ranges, e.g.: `{"a_a.b/2:5", "a_a.b/10:15",..}` . Options:

- `append` : will merge residue ranges
- `name` : will return a string array of *residueName residueNumber* records
- `residue` : will return an array of selection strings a*_obj.mol/residueNumber* records

Example:

```
Sarray(a_/2,4:5 name)
 #>S string_array
 def.a1/ala2
 def.a1/trp4
 def.a1/glu5
Sarray(a_/2,4:5 residue)
 #>S string_array
 def.a1/2
 def.a1/4
 def.a1/5
Field(Sarray(a_/2,4:5 name),2,"/") # extract residues
#>S string_array
 ala2
 trp4
 glu5
```

See also `String`(*rs_*) which returns one string and `Label`(*rs_* | *as_*) which will format the output string according to the `resLabelStyle` or `atomLabelStyle` preference.

`Sarray` **(** `stack` , *vs_var* **)** − creates a string representation of all the conformations in the `stack` Variable selection allows to choose the conformational feature you want. Character code:

Backbone (phi,psi pairs):

- 'B': −200 < phi < −80 , 140 < psi < 200
- 'A': −101 < phi < −24 , −81 < psi < 4
- 'g': −169 < phi < −15 , −64 < psi < 54
- 'd': −211 < phi < −5 , 8 < psi < 136
- 'L': 24 < phi < 101 , −4 < psi < 81
- '_': the rest

Sidechain (chi1):

- 'M': −120 <= xi1 < 0
- 'P': 0 <= xi1 < 120
- 'T': 120 <= xi1 < 240

Example:

```
show Sarray(stack,v_/2:10/x*)      # coding of side-chain conformations
show Sarray(stack,v_//phi,psi)     # backbone conformation character coding
show Sarray(stack,v_/2:10/phi,PSI) # character coding of a chain fragment
```

(Note use of special `PSI` torsion in the last example.)

Other examples:

```
ss=Sarray(5)       # create empty sarray of 5 elements
ss[2]="thoughts"   # assign string to the second element of the sarray

sa=Sarray("the first element")

show Sarray(Count(1 100)) # string array of numbers from 1 to 100
```

`Sarray(` *sarray* `reverse)`

− converts input sarray into an `sarray` with the reversed order of elements. Example:

```
Sarray({"one","two"} reverse)  # returns {"two","one"}
```

See also: `Iarray`(I_ `reverse`), `Rarray`(S_ `reverse`), `String`(0,1,s)

`Sarray(` *sarray i_from i_to* `)`

returns `sarray` of substrings from position *i_from* to position *i_to* . If *i_from* is greater than *i_to* the direction of substrings is reversed. Example:

```
a={"123","12345"}
Sarray(a,2,3)
 {"23","23"}
Sarray(a,5,2)
 {"32","5432"}
```

2.21.112. Score

function.

`Score(` R_1, *R_2* `)` − returns the `real` shift between two distributions based on the overlap between the two real arrays. This measure of changes between −1 and 1.. (all values of R_1 are smaller than all values of R_2) and +1. (all values of R_1 are greater than all values of R_2) and may serve as a ranking criterion.

Examples:

```
show Score({1. 2. 5. 3.} {3. 1.5 1.5 5.})  # 0. perfectly overlapping arrays
show Score({2. 5. 3.} {1. 1.5 0.5})        # 1. no overlap R_1 > R_2
```

```
show Score({1. 1.5 0.5} {2. 5. 3.})        # -1. no overlap R_2 > R_1
show 1.-Abs(Score({1. 3. 2.5} {2. 5. 3.})) # relative overlap between R1 and R2
```

Score **(** sequence1, *sequence2* **)**

− returns the real score of the Needleman and Wunsch alignment.

Each pair of aligned residues contributes according to the current residue comparison table, which is normalized so that the average diagonal element is 1. Insertions and deletions reduce the score according to the gapOpen and gapExtension parameters. Approximately, the score is equal to the number of residue identities.

To calculate an array of mean scores for each column of a multiple sequence alignments use the Rarray(ali [exact]) function.

Examples:

```
read sequence "seqs"
a = Score( Azur_Alcde Azur_Alcfa ) # it is around 90.
```

See also: Distance( ).

Score **(** rs, [simple] **)** − returns the rarray of alignment−derived conservation values for the selected residues. For each residue Ri in the residue selection *rs_* the following steps are taken:

- a column is extracted from a linked N−sequence alignment (see the link command)
- Si = Sum(Cij)/N where j=1,..N and Cij is the residue comparison value
- simple mode: Cij = 1. for two identical residues and 0. otherwise
- the default mode: Cij is taken from a **normalized** comp_matrix . Its elements are calculated as Cij_norm = Cij/Sqrt(Cii*Cjj) .

The default mode shows positions with residues of the same type as more conserved than positions with residues of different types.

Example in which we compare conservation on the surface and in the core:

```
read alignment s_icmhome+"sh3.ali"
read pdb "1fyn"
make sequence a_a
group sequence sh3
align sh3
display ribbon
color ribbon a_a/A Score( a_a/A simple )
show surface area
show Mean( Score( Acc(a_a/*) ) )    # conservation score for the surface
show Mean( Score( a_a !Acc(a_/*)))# conservation score for the buried
```

Score **(** ali_, [{ identity | similarity | comp_matrix | sort }] **)**

− returns the real score of the given alignment calculated by different methods:

- *no second argument* : the straight Needleman and Wunsch score: aligned residues score according to the residue comparison table, gaps according to the `gapOpen` and `gapExtension` parameters.
- `identity` the number of identical residues in the alignment divided by the smallest sequence length and multiplied by 100 %.
- `comp_matrix` the alignment score without the gap component. It contains only the total score of the aligned residues calculated from the residue comparison table and does not include penalty term.
- `similarity` the alignment score without the gap component multiplied by 100. and divided by the smallest sequence length.
- `sort` a score occasionally used for ranking/sorting the alignments in fold recognition. Currently it is equal to the **comp_matrix_score** − 1.3***totalGapPenalty**

`Score` **(** i_minLen, *r_Probability* [, { `identity` | `similarity` | `sort` }] **)** − returns the `real` threshold score at a given *r_Probability* level of occurrence of alignment with a protein of unrelated fold. The threshold is related to the corresponding method of the score calculation (see above). For example,

```
Score( 150, 1./55000.,identity)
```

gives you the sequence identity percentage for sequences of 150 residues at which only one false positive is expected in a search through the Swissprot database of 55000 sequences.

See also the inverse function: `Probability` .

2.21.113. Select

Selection of atoms according to their coordinates or properties, transfering selection to another object, or selecting by relative object−specific atom numbers stored in an integer array.

`Select` **(** [`residue` | `molecule` | `object`] **)** − returns either selected (`as_graph`) or displayed atoms (`a_*.//DD`). By providing the argument, you can change the selection level. Example:

```
  display skin Select(residue)
```

`Select` **(** *as_ s_condition* [*r_Value*] **)** − returns a subselection of atom selection *as_* according to the specified condition *s_condition.*

Three example conditions:

`"X >= 2.0" , "Bfactor != 25." , "charge == 0." .` Allowed properties and their aliases (case does not matter, the first character is sufficient) are as follows:

- x,y,z atomic coordinates ("x","y","z")
- bfactor ("bfactor","b","B")
- occupancy ("o")
- charge ("charge","c","q")
- accessible surface area ("area","a")
- user−field ("u") which can be set with `set field` and extracted with the `Field` function.
- residue user−fields: "u","v","w" for the 1st, 2nd and 3rd field, respectively.

Note: do not forget to calculate surface in advance with the `show area` command. Allowed comparisons: (== **!**= > < >= <=). The value can either be specified inside the string or used as a separate argument *r_Value.*

See also the related functions: `Area`, `Bfactor`, `Xyz`, `Charge`, `Field` .

Examples:

```
build string "se glu arg"
show Select(a_//* "charge < 0.")|Select(a_//c* "x> −2.4")
show Select(a_//c* , "x>", −2.4)

show Select(a_/* , "w>3.") # 3rd res. user field greater than 3.
```

Note: atoms with certain Cartesian coordinates can also be selected by multiplying selection to a box specified by 6 real numbers {x,y,z,X,Y,Z}, e.g. `show a_//* {−1.,10.,2.,25.,30.,22.}` or `a_//* Box( ).`

See also: `display box` and the `Box` function.

`Select` **(** *as_sourceSelection os_targetObject* **)**

− returns the source selection *as_sourceSelection* from a source object which is transferred to another object (*os_targetObject*). The two objects must be identical in content. Example:

```
buildpep "ASD"
aa = a_/2/c*          # selection in the current obj a_
copy a_ "b"           # a copy of the source object
bb = Select(aa,a_b.)  # selection aa moved to a_b.
```

`Select` **(** *os_sourceObject I_atomNumbers* **)**

− returns atom selection of relative atom numbers in specified object *os_sourceObject.* The iarray can be generated with the `Iarray` (as_) function. This function allows to pass selections between ICM sessions.

2.21.114. Sequence

function.

`Sequence` **(** *as_select* **)** − returns `sequence` extracted from specified residues.

`Sequence` **(** *string* [`nucleotide` | `protein`] **)** − converts a string (e.g. "ASDFTREW") into an ICM `sequence` object. By default the type is `"protein".` To reset the type use the `set type` *seq* { `nucleotide` | `protein` } command.

Examples:

```
seqA = Sequence( a_1./15:89 )     # create sequence object
                                  # with fragment 15:89

show Align(seq1, Sequence("HFGD−−KLS AREWDDIPYQ")
                                  # non−characters will be squeezed out
```

```
a=Sequence("ACTGGGA", nucleotide)
Type(a , 2)  # returns the type-string :
nucleotide
```

`Sequence` **(** *ali_* **)** − returns a chimeric `sequence` which represents the strongest character in every `alignment` position.

`Sequence` **(** *prf_* **)** − returns a chimeric `sequence` which represents the strongest character in every `profile` position.

2.21.115. reverse complement dna sequence function

`Sequence` **(** *seq_DNAsequence* `reverse` **)** − returns the reverse complement DNA `sequence:`

```
     nucleotide       |complement
______________________|__________
                      |
 A = Adenosine        | T (replace by U for RNA)
 C = Cytidine         | G
 G = Guanosine        | C
 T = Thymidine        | A
 U = Uridine          | A
 R = puRine    (G A)  | Y
 Y = pYrimidine(T C)  | R
 K = Keto      (G T)  | M
 M = aMino     (A C)  | K
 S = Strong    (G C)  | S
 W = Weak      (A T)  | W
 B = !A      (G T C)  | V
 D = !C      (G A T)  | H
 H = !G      (A C T)  | D
 V = !T      (G C A)  | B
 N = aNy              | N
```

2.21.116. Sign

transfer−of−sign function. It returns the value (or values) of sign { *−1.|0.|+1.}* of its argument.

`Sign` **(** *real* **)** − returns `real` sign of the argument.

`Sign` **(** *integer* **)** − returns `integer` .

`Sign` **(** *iarray* **)** − returns `iarray.`

`Sign` **(** *rarray* **)** − returns `rarray.`

Examples:

```
Sign(-23)
-1
Sign(-23.3)
-1.
Sign({-23,13})
{-1,1}
```

```
Sign({-23.0,13.1})
{-1.,1.}
```

2.21.117. Sin

sine trigonometric function. Arguments are assumed to be in degrees.

`Sin` ({ *real* | *integer* }) − returns the `real` sine of its real or integer argument.

`Sin` **(** *rarray* **)** − returns the `rarray` of sines of *rarray* elements.

Examples:

```
print Sin(90.)                  # equal to 1
print Sin(90)                   # the same

print Sin({-90., 0., 90.})      # returns {-1., 0., 1.}
```

2.21.118. Sinh

hyperbolic sine function.

`Sinh` **(** { *real* | *integer* } **)** − returns the `real` hyperbolic sine of its real or integer argument.
$\boldsymbol{Sinh(x)=0.5(\ e^{iz} - e^{-iz}\ )}$

`Sinh` **(** *rarray* **)** − returns the `rarray` of hyperbolic sines of *rarray* elements.

Examples:

```
print Sinh(1.)                  # equal to 1.175201
print Sinh(1)                   # the same
print Sinh({-1., 0., 1.})       # returns {-1.175201, 0., 1.175201}
```

2.21.119. Site

`site` selection function

`Site` (*s_siteID* [*ms_*]) − returns the `iarray` of the site numbers in the selected molecule. The default is all the molecules of the current object.

Example:

```
nice "1est"  # contains some sites
delete site a_1 Site("CONFLICT",a_1)
```

2.21.120. Smiles

convert chemical structure into a Smiles string.

`Smiles` **(** *as_* **)** − returns the `smiles- string` with the coded representation of the chemical structure of selected fragment.

See also: `build smiles`, `String`(*as_*) − chemical formula.

2.21.121. Smooth

sliding window averaging, convolution, 3D−gaussian smoothing, map smoothing and function derivatives.

Smooth

`Smooth` **(** R_source, [*i_windowSize*] **)** − returns the window−averaged `rarray`. The array is of the same dimension as the *R_source* and *i_windowSize* is set to `windowSize` by default. An average value is assigned to the middle element of the window. *i_windowSize* must be an odd number. At the array boundaries the number of averaged elements is gradually reduced to one element, i.e. if *i_windowSize=5*, the 3rd element of the smoothed array will get the mean of R1,R2,R3,R4,R5, the second element will get the mean of R1,R2 and R3, and the first element will be set to R1.

`Smooth` **(** R_source, *R_weightArray* **)** − returns the `rarray` of the same dimension as the *R_source*, performs convolution of these two arrays. If *R_weightArray* contains equal numbers of 1./ *i_windowSize*, it is equivalent to the previous option. For averaging, elements of *R_weightArray* are automatically normalized so that the sum of all elements in the window is 1.0.

Normalization is not applied if the sum of elements in the *R_weightArray* is zero. Convolution with such an array may help you to get the derivatives of the *R_source* array. Use:

```
{−1.,1.}/Xstep            # for the first derivative
{1.,−2.,1.}/(Xstep*Xstep)  # for the second derivative
{−1.,3.,−3.,1.}/(Xstep*Xstep*Xstep)  # for the third derivative
#  ... etc.
```

Examples:

```
gauss=Exp( −Power(Rarray(31,−1.,1.) , 2) )   # N(0.,1.) distribution on a grid
x = Rarray(361,−180.,180.)                   # x−array grows from 0. to 180.
a = Sin(x) + Random(−0.1,0.1,361)            # noisy sine

b = Smooth(a,gauss)          # gauss averaging
                             # see how noise and smooth signals look
plot x//x a//b display {−180.,180.,30.,10.}
                             # take the first derivative of Sin(x)
c = Smooth(Sin(x),{−1., 1.}) * 180.0 / Pi
                             # plot the derivative
plot x c display {"X","d(Sin(X))/dX","Derivative"}
```

Smooth: three−dimensional averaging of residue properties

`Smooth` **(** rs_, R_property, *r_smoothRadius* **)** − gaussian averaging of property array *R_property* of residues *rs_* . The averaging is performed according to the spatial distance between residue Ca atoms. The function returns the `rarray` of the residue property AVERAGED in 3D using spherical gaussian with sigma of *r_smoothRadius.* Each residue contributes to the smoothed property with the weight of $\exp(-\text{Dist\_i\_j}^2 / \text{r\_smoothRadius}^2)$.

The interresidue distances Dist_i_j are calculated between atoms carrying the residue label (normally a_//ca). These atoms can be changed with the `set label` command. Array R_1 is normalized so that the

mean value is not changed.

The distances are calculated between

Examples:

```
nice "1tet"   # it is a macro displaying ribbon++
R = Bfactor(a_/A ) # an array we will be 3D−averaging
color ribbon a_/A Smooth(a_/A R 1.)//5.//30.  # averaging with 1A radius
color ribbon a_/A Smooth(a_/A R 5.)//5.//30.  # with 5A radius
color ribbon a_/A Smooth(a_/A R 10.)//5.//30. # with 10A radius
 # 5.//30. are appended for color scaling from 5. (blue) to 30.(red)
 # rather than automated rescaling to the current range

set field a_/A Smooth(a_/A R 5.)
show Select( a_/A "u>30." ) # select residues with 1st field > 30.
```

Smooth: expanding alignment gaps

`Smooth` **(** ali_, [*i_gapExpansionSize*] **)** − returns a transformation of the initial `alignment` in which every gap is widened by the *i_gapExpansionSize* residues. This transformation is useful in modeling by homology since the residue pairs flanking gaps usually deviate from the template positions.

The default *i_gapExpansionSize* is 1 (the gaps are expanded by one residue)

Smooth: transforming three−dimensional map functions.

`Smooth` **(** *map_* , ["expand"] **)**

weighted 3D−window averaging

`Smooth` **(** *map_* **)** − returns `map` with averaged map function values. By default the value in each grid node is averaged with the six immediate neighbors (analogous to one−dimensional averaging by Smooth(R,{1.,2.,1.}) . By applying `Smooth` several times you may effectively increase the window. This operation may be applied to "ge","gb","gs" and electron density maps

low−values propagation

`Smooth` **(** *map_* "expand" **)** − returns `map` in which the low values were propagated in three dimensions to the neighboring nodes. This trick allows to generate more permission van der Waals maps.

This operation may be applied to "gh","gc" and electron density maps.

Examples:

```
m_gc = Smooth(Smooth(m_gc "expand"), "expand" )
```

See also: `map` .

2.21.122. Sql

functions to connect to a MySql server and run SQL queries. This function has the following properties:

- it supports one connection at a time
- requires a running MySql server (see `www.mysql.com`) with a database
- the record columns from the database are converted into the ICM sarrays, rarrays and iarrays with one exception. The mysql BIGINT values can not be converted into iarray and are stored as a string array (sarray).

`Sql(connect` *s_host s_loginName s_password s_dbName* `)` − returns the `logical` status of connection to the specified server. The arguments are the following:

- *s_host* (default `"localhost"`) − the host name
- *s_loginName* (default `"root"`)
- *s_password* − the database password
- *s_dbName* − the database name

`Sql(` *s_SQLquery* `)` − returns the `table` of the selected records. Some SQL commands are not really queries and do not return records, but rather perform certain operations (e.g. insert or update records, shows statistics). In this case an empty table is returned. An example:

```
 if !Sql( connect "localhost","john","secret","swiss") print "Error"
 id=24
 T =Sql( "SELECT * FROM swissprothits  WHERE featureid="+id )
 sort T.featureid
 web T
# Another example
 tusers = Sql("select * from user where User=" + s_usrName )
 Sql(off)
```

`Sql(off)` − disconnects from the database server and returns the `logical` status.

2.21.123. Sqrt

square root function.

`Sqrt(` *real* `)` − returns the `real` square root of its real argument

`Sqrt(` *rarray* `)` − returns `rarray` of square roots of the *rarray* elements.

`Sqrt(` *matrix* `)` − returns `matrix` of square roots of the *matrix* elements.

Examples:

```
 show Sqrt(4.)                # 2.
 show Sqrt({4. 6.25})         # {2. 2.5}
```

2.21.124. Sphere

sphere selection function. It returns a selection containing atoms, residues or molecules within a certain radius around the initial selection. It returns atom selection which can be then converted into residue and molecules with the Res and Mol functions respectively. The default value is defined by the `selectSphereRadius` . ICM−shell variable which is equal to 5.0 A by default.

`Sphere` **(** { *as_source* | *g_* | *R_xyz*| *M_xyz* } [*as_whereToSelect*] [{ *i_Radius* | *r_Radius*}] **)** this function always returns a selection of **atoms** in a certain vicinity of the following:

- a group of atoms (*as_)*
- any vertex point of a `grob` (*g_)*
- a point in space (*R_xyz)*
- a group of points in space (*M_xyz)* (e.g. see the `Xyz` function)

The atoms will be searched in the specified selection *as_whereToSelect* if the second selection is explicitly specified. If only one atom selection is specified, the atoms will be selected from the same object.

Use the selection level functions (`Res` , `Mol` , and `Obj` to convert the atom selection into residues, molecules or objects, respectively (e.g. `Res(Sphere(a_/15,4.))`). For example, selection

```
show Sphere( a_subA/14:15/ca,c,n,o , 5.2)
Res(Sphere( a_1.2 a_2.)) # residues of a_2. around ligand a_1.2
```

2.21.125. Split

function.

`Split` **(** s_multiFieldString, [*s_Separators*] **)** − returns `sarray` of fields separated by *s_Separators.* By default *s_Separators* is set to `s_fieldDelimiter.` Multiple spaces are treated as one space, while all other multiple separators lead to empty fields between them. If *s_Separator* is an empty string (""), the line will be split into individual characters. To split a multi−line string into individual lines, use Split(s_, "\n").

Examples:

```
lines=Split("a 1 \n 2","\n")  # returns 2−array of {"a 1" " 2 "}
flds =Split("a b c")          # returns 3−array of {"a" "b" "c"}
flds =Split("a b:::c",":")    # returns 4−array of {"a b","","","c"}
resi =Split("ACDFTYRWAS","")  # splits into individual characters
                              # {"A","C","D","F",...}
```

See also: `Field`( ).

2.21.126. Srmsd

"static" root−mean−square deviation function.

`Srmsd` **(** *as_select1 as_select2* [{ { `align` | *ali_* } | `exact` }] **)** − returns `real` value of root−mean−square deviation. Similar to function `Rmsd`, but works without optimal superposition, i.e. atomic coordinates are compared as they are without modification. Number of equivalent atom pairs is

saved in `i_out` (see `alignment options`).

Virtual atoms. Be default, the first two virtual atoms (`vt1` and `vt2`) are automatically excluded from both selections unless the `virtual` option is explicitly specified.

Examples:

```
superimpose a_1.1 a_2.1            # two similar objects, each
                                   # containing two molecules
print Srmsd(a_1.2//ca a_2.2//ca)   # compare how second molecule
                                   # deviates if first superimposed
```

`Srmsd` **(** *as_select* **)** − returns `real` root−mean−square length of absolute distance restraints (so called, tethers) for the tethered atoms in ICM−object.

Equivalent to

`Sqrt(Energy("tz")/Nof(tether))` after `show energy "tz" .`

2.21.127. String

function.

`String` **(** *sequence* **)** − converts sequence into a `string`

`String` **(** *integer* **)** − converts integer into a `string`

`String` **(** *real* [*i_nOfDecimals*] **)** − converts real into a `string` . It also allows to round a real number to a given number of digits after decimal point.

`String` **(** string, *i_NofRepeats* **)** − repeat specified `string` *i_NofRepeats* times

`String` **(** string, `all` **)** − adds flanking quotes and extra escape symbols to write this string in a form interpretable in shell in $string expression.

`String` **(** s_input, *s_default* **)** − if the input `s_input` string is empty returns the *s_default*, otherwise returns the *s_input* string

`String` **(** string, i_offset, *i_length* **)** − returns `substring` of length *i_length.* If *i_length* is negative returns substring from the offset to the end.

`String` **(** *sarray* **)** − extracts the first `string` from the array

`String` **(** { *iarray* | *rarray* | *matrix* } [*s_translateString*] **)** − converts numbers into a `string` or ascii characters (the "Ascii art", i.e. 12345 −> "..:*#").

The range between the minimal and maximal values is equally divided into equal subranges for each character in the string. This function is useful for ascii visualization of arrays and matrices. The default `translation string` is ".:*0#". Another popular choice is "0123456789".

Examples:

```
file=s_tempDir//String(Energy("ener"))   # tricky file name
show Index(String(seq),"AGST")             # use Index to find seq. pattern
tenX = String("X",10)                      # generate "XXXXXXXXXX"

read matrix
show String(def," ..:*#")
```

See also: `show map`.

`String (` i_from, i_to, *string* **)** − returns `substring` starting from *i_from* and ending at ~i_to. If *i_from* is less than *i_to* the *string* is **inverted.** Zero value is automatically replaced by the string length, −1 is the last but one element etc.

Examples:

```
String(1,3,"12345")  # returns substring "123"
String(4,2,"12345")  # returns substring "432"
String(1,0,"12345")  # returns "12345"
String(0,1,"12345")  # returns INVERTED string "54321"
String(−1,1,"12345") # returns "4321"
```

`String (` *ali_* **)** − converts the alignment into a multiline `string` . You can further split it into individual lines like "−−NSGDG" with the `Split(String(ali_))` command. The offset in a specific sequence and its number can be found as follows.

Examples:

```
read alignment s_icmhome+"sh3"
offs=Mod(Indexx(String(sh3),"−−NSGDG"),Length(sh3)+1)
        # extract alignment into a string, (+1 to account for '\n')
iSeq = 1 + Indexx(String(sh3),"−−NSGDG")/(Length(sh3)+1)
        # identify which sequence contains the pattern
```

`String (` *ali_* `tree` **)** − returns a Newick tree `string` describing the topology of the evolutionary tree. The format is described at
`http://evolution.genetics.washington.edu/phylip/newicktree.html` .

Example:

```
read alignment s_icmhome+"sh3"
show String(sh3 tree)
```

Projecting properties from alignment to a member sequence.

`String (` *s_ali ali_from* { *seq_* | *i_seqNumber* } **)**

− returns a projected `string` . The *s_ali* string contains characters defined for each position of alignment *ali_from.* The function squeezes out the characters which correspond to insertions into sequence *seq_* . This operation, in effect, projects the alignment string *s_ali* onto sequence *seq_*.

See also the `Rarray`(R_,ali_,seq_) function to project rarrays.

Example (projection of the consensus string onto a sequence):

```
read alignment s_icmhome+"sh3"  # 3 seq.
cc = Consensus(sh3)
show String(Spec)//String(cc,sh3,Spec)
```

Projecting properties from member sequence to alignment

`String` **(** *s_seq* { *seq_* | *i_seqNumber* } *ali_to s_gapDefChar* **)** − projects the input `string` from *seq_* to *ali_to* (the previous function does it in the opposite direction). The *R_seq* string contains characters defined for each position of the sequence *seq_*. The function fills the gap positions in the output with the *r_gapDefChar* character. Combination of this and the previous functions allow you to project any string s1 from one sequence to another by projecting the s1 of seq1 first to the alignment and than back to seq2 (e.g. String(String(s1,seq1,a,"X") , a, seq2)).

See also the `Rarray`(*R_,seq_,ali_,r_gapDefault*) function to project real arrays.

Example (transfer of the secondary structure from one sequence to another):

```
read alignment s_icmhome+"sh3"  # 3 seq.
ssFyn = Sstructure(Fyn)
set sstructure Spec String(String(ssFyn,Fyn,sh3,"_"),sh3,Spec)
show Spec
```

String(selection): converting selections into the text form

`String` **(** { *os_* | *ms_* | *rs_* | *as_* } [*i_number*] **)** converts a selection into a compact string form. Continuous blocks of selected elements in different molecules or objects are separated by vertical bar (|) which means logical *or* (e.g. `a_a.1:4|a_b.2,14`) You can also divide this selection info a string array with the `Split` function.

Option *i_number* allows to print only *i−th* element of the selection. It is convinient in scripts. For atom selections it will also show full information about each atom, rather than only the ranges of atom numbers.

This string form is convenient used for several purposes:

- to store selections in tables and arrays.
- to transfer selections from object to object and from session to session (see also the `Select` function)

An example in which we generate text selection of the Crn leucine neighbors :

```
nice "1crn"
nei = String( Res(Sphere( a_/leu a_/!leu , 4.)) )
show nei
a_1crn.m/14:17,19:20
display xstick $nei
```

Another example with a loop over atom selection of carbon atoms:

```
read pdb "2ins"
for i=1, Nof( a_//c* )
   print String( a_//c* i )
endfor
```

Chemical formula

`String(` *as_* { `dot` | `all` | `smiles` | `sln` } `)`

− returns `string` with the following chemical information:

option	description	example
all	chemical formula	e.g. `C2H6O`
dot	chemical formula with dot−separated molecules	e.g. `C2H6O.C3H8`
smiles	smiles string	e.g. `[CH3][CH2][OH]`
sln	sln notation	e.g. `CH3CH2OH`

Molecules with a certain chemical formula (calculated without hydrogens) can be selected by the a*_formula1,formula2..* `selection` . See also: `Smiles` , `smiles` , `selections` by molecule.

Example:

```
build string "se ala"     # alanine
show String(a_//!h* all ) # returns no hydrogen chemical formula: C3NO
show String(a_//* all )   # returns chemical formula: C3H5NO
show String(a_//* sln )   # returns SLN notation: NHCH(CH3)C=O
show String(a_//* smiles) # returns SMILES string: [NH][CH]([CH3])C=O
```

2.21.128. Sstructure

secondary structure function.

`Sstructure(` *rs_* `)` − returns `string` of secondary structure characters ("H","E","_", etc.) extracted from specified residues *rs_* .

`Sstructure(` { *rs_* | *s_seqStructure* } `compress)` − returns the compressed `string` of secondary structure characters, one character per secondary structure segment, e.g. HHE means helix, helix, strand. Use the `Replace` function to change B to '_' and G helices to H helices, or simply all non H,S residues to coil (e.g. Sstructure(Replace(ss,"[!EH]","_"),compress))

Example:

```
 show Sstructure("HHHHHHH_____EEEEE",compress)  # returns string "HE"
#
 read object "crn"
 show Sstructure( a_/A , compress)  # returns string "EHHEB"
```

`Sstructure(` { *seq_* | *s_sequenceString* } `)` − returns `string` of secondary structure characters ("H","E","_"). If this string has already been assigned to the sequence *seq_* with the `set sstructure` command or the `make sequence ms_` command, the function will return the existing secondary structure string. To get rid of it, use the `delete sstructure` command.

Alternatively, if the secondary structure is not already defined, the `Sstructure` function will predict the secondary structure of the *seq_* sequence with the Frishman and Argos method.

If the specified sequence is not a part of any `alignment of sequence group` only a single sequence prediction will be effected (*vide infra*). Otherwise, a group or an alignment will be identified and a true multiple sequence prediction algorithm is applied. The multiple sequence prediction by this method reaches the record of 75% prediction accuracy on average for a standard selection of 560 protein chains under rigorous jack−knife conditions. The larger the sequence set the better the prediction. Prediction accuracy for a single sequence is about 68%. To collect a set perform the **fasta** search (Pearson and Lipman, 1988) with `ktup=1` and generate a file with all the sequences in a fasta format.

Method used for derivation of single sequence propensities.

Seven secondary−structure related propensities are combined to produce the final prediction string. Three are based on long−range interactions involving potential hydrogen bonded residues in anti−parallel and parallel beta sheet and alpha−helices. Other three propensities for helix, strand and coil, respectively, are predicted by the "nearest neighbor" approach (Zhang et al., 1992), in which short fragments with known secondary structure stored in the database (icmdssp.dat) and sufficient similarity to the target sequence contribute to the prediction. Finally, a statistically based turn propensity (also available separately via the `Turn`(*sequence)* function), is employed over the 4−residue window as described by Hutchinson and Thornton (1994). The function also returns four real arrays in the `M_out matrix` [4, *seqLength]*. There arrays are:

- M_out[1] : alpha−helix propensity [0., 1.]
- M_out[2] : beta−sheet propensity [0., 1.]
- M_out[3] : coil propensity [0., 1.]
- M_out[4] : prediction reliability [0., 1.]

Note that these propensities are not directly related to the prediction. Usually the reliability level of 0.8 guaranties prediction accuracy of about 90%. Do not be surprised if the propensities are all zero for a fragment. It may just mean that the statistics is too scarce for a reliable estimate.

Examples:

```
show Index(Sstructure(a_1crn.,"HHHHHH"))  # first occurrence of
                                          # helix in crambin

read sequence "sh3"    # load 3 sequences (the full name is s_icmhome+"sh3")
show Sstructure(Spec)  # secondary structure prediction for one of them
show Sstructure("AAAAAAAAAAAAA")  # sec. structure prediction for polyAla

read sequence "fasta_results.seq"
group sequences a unique 0.05     # remove redundant sequences
show Sstructure(my_seq_name)      # the actual prediction, be patient
plot number M_out display         # plot 3 propensities and reliability
```

2.21.129. Sum

function.

`Sum` **(** *iarray* **)** − returns the `integer` sum of iarray elements.

`Sum` ({ *rarray* | *map* }) − returns the `real` sum of elements.

`Sum` **(** *matrix* **)** − returns the `rarray` of sums in all the columns.

`Sum` **(** *sarray* [*s_separator*] **)** − returns `string` of **concatenated** components of a sarray separated by the specified *s_separator* or blank spaces by default. See also the opposite function: `Split` .

Examples:

```
show Sum({4 1 3})                    # 8
show Sum(Mass(a_1//*))               # mass of the first molecule
show Sum({"bla" "blu" "bli"})        # "bla blu bli" string
show Sum({"bla" "blu" "bli"},"\t")   # separate words by TAB
show Sum({"bla" "blu" "bli"},"\n")   # create a multiple line string
```

2.21.130. Symgroup

function.

`Symgroup` **(** { *s_groupName* | *os_object* | *m_map* } **)** − returns the `integer` number of one of 230 named space groups defined in ICM.

`Symgroup` **(** { *i_groupNumber* | *os_object* | *m_map* } `string` **)** − returns the `string` name of one of 230 space groups defined in ICM.

`Symgroup` **(** *i_groupNumber* **)** − returns the `rarray` of transformation matrices (12 numbers each) describing symmetry operations of a given space group.

Examples:

```
iGroup = Symgroup("P212121")  # find the group number=19
print "N_mol. in the cell =", Nof(Symgroup(iGroup))/12
```

2.21.131. Table

generic function return a table.

`Table` **(** *s_URL_encoded_String* [`crypt`] **)**

− returns the `table` of "name" and "value" pairs organized in two `string arrays`. The URL−encoding is a format in which the HTML browser sends the HTML−form input to the server either through standard input or an environmental variable. The URL−encoded string consists of a number of the "name=value pairs separated by ampersand (**&**). Additionally, all the spaces are replaced by plus signs and special characters are encoded as hexadecimals with the following format %NN. The Table function decodes the string and creates two string arrays united in a table.

Option `crypt` allows to interpret doubly encoded strings (e.g. ' ' is translated to '+' which then converted into a hexadecimal form). Frequently the problem can be eliminated by specifying the correct port. Example: you need to set a="b c" and d="<%>". Normal server will convert it to `a=b+c> Double encoding leads to a=b%2bcE. To parse the last string, use the crypt`

option.

To see all the hidden symbols (special attention to '\r'), set l_showSpecialChar =yes.

Examples:

```
 read string       # read from stdin in to the ICM s_out string
 a=Table(s_out)    # create table a with arrays a.name and a.value
 show a            # show the table
 for i=1,Nof(a)    # just a loop accessing the array elements
   print a.name[i] a.value[i]
 endfor
```

See also: Getenv( ).

2.21.132. Converting alignment into a table

Table(*ali_* [number]) − returns the table of relative amino acid positions for each of the sequence in alignment *ali_*. Gaps are marked by zero. The first column of the table, .cons , contains sarray of consensus characters. All the other arrays are named according to the sequence names by default, or by the sequential number of a sequence in the alignment, if option number is specified. The table may be used to project numbers from one sequence to another. See also the Rarray(R_, ali_, seq_) function. This table may look like this:

```
#>T pos
#>-cons----seq1-----seq2-------
   " "       0        1
   " "       0        2
   C         1        3
   " "       2        0
   ~         3        4
   C         4        5
   " "       0        6
# for the following alignment:
# Consensus    C ~C
seq1         --CYQC-
seq2         LQC-NCP
```

To calculate an array of mean scores for each column of a multiple sequence alignments use the Rarray(ali [exact]) function. This array can be appended to the table.

Example:

```
 read alignment "sh3"
 t = Table(sh3 number)  # arrays t.1 t.2 t.3
 t = Table(sh3)         # arrays t.cons t.Fyn t.Spec t.Eps8
#
 cc = t.cons ~ "[A-Z]"  # all the conserved positions
 show cc                # show aa numbers at all conserved positions
 show t.Fyn>=10 t.Fyn<=20 # numbers of other sequences in this range
```

2.21.133. Extracting parameters of stack conformations

`Table(stack[ vs_ ])`

− return `table` of parameters for each conformation in a `stack` . If a variable selection argument is provided, the values of the specified variables are returned as well.

```
% icm
 buildpep "ala his trp"
 montecarlo
 show stack
 iconf>       1       2       3       4       5       6       7
 ener>    -15.1   -14.6   -14.6   -14.2   -13.9   -11.4    -1.7
 rmsd>      0.3    39.2    48.0    44.1    27.4    56.6    39.3
 naft>        1       0       0       1       1       1       0
 nvis>        4       1       1       4       4       4       1
t= Table(stack)
show t
 #>T t
 #>-i--ener--------rmsd--------naft--------nvis-------
    1  -15.126552  0.295555    1           4
    2  -14.639667  39.197378   0           1
    3  -14.572973  47.996203   0           1
    4  -14.220515  44.058755   1           4
    5  -13.879041  27.435388   1           4
    6  -11.438268  56.636246   1           4
    7  -1.654792   39.265912   0           1
t1= Table(stack v_//phi,psi)  # show also five phi-psi angles
 #>T
 #>-ener----rmsd--naft-nvis------v1------v2------v3------v4-------v5-----
    1 -15.12   0.29   1   4     -79.10  155.59  -75.30  146.99  -141.13
    2 -14.63  39.19   0   1    -157.22  163.56  -78.25  139.51  -137.30
    3 -14.57  47.99   0   1    -157.26  166.87  -85.08   92.55   -84.74
    4 -14.22  44.05   1   4     -67.65   80.43  -76.67  103.05   -81.85
    5 -13.87  27.43   1   4     -82.72  155.86  -85.02   93.11   -81.46
    6 -11.43  56.63   1   4     -78.28  152.80 -154.79   66.26   -77.61
    7  -1.65  39.26   0   1     -78.17  169.41 -133.89   96.39   -96.03
```

See also: `Iarray(stack)` function

2.21.134. Tan

tangent trigonometric function. Arguments are assumed to be in degrees.

`Tan(` { *r_Angle* | *i_Angle* } `)` − returns the `real` value of the tangent of its real or integer argument.

`Tan(` *rarray* `)` − returns `rarray` of the tangents of each component of the array.

Examples:

```
 show Tan(45.)               # 1.
 show Tan(45)                # the same

 show Tan({-30., 0. 60.})    # returns {-0.57735, 0., 1.732051}
```

2.21.135. Tanh

hyperbolic tangent function.

`Tanh` ({ *r_Angle* | *i_Angle* }) − returns the `real` value of the hyperbolic tangent of its real or integer argument.

`Tanh` **(** *rarray* **)** − returns `rarray` of the hyperbolic tangents of each component of the array.

Examples:

```
show Tanh(1)                 # returns 0.761594
show Tanh({−2., 0., 2.})     # returns −0.964028, 0., 0.964028
```

2.21.136. Tensor

function the second moments for a multidimensional distribution.

`Tensor` (M_)

− returns the square `matrix` of second moments of ***K*** points in ***N*** −dimensional space, M_{ki} ***(k=1,K,i=1,N)*** . The matrix ***NxN*** is calculated as

$< X_i >< X_j > - < X_i X_j >$, where < .. > is averaging over a column ***k=1,K,*** and ***i,j=1,N.***

If xyz is a coordinate matrix Nx3, the Tensor function is identical to

```
Transpose( xyz ) * xyz / Nof(xyz)
```

- In one−dimensional case, ***N=1,*** when ***M_*** is just one column ***(k=1,K; i=1,1)*** the function returns a one by one matrix with the mean−square−deviation of the vector (which is equal to Rmsd(R_)*Rmsd(R_)).
- ***N=2,*** ***x*** and ***y*** dimensions; In this case the function returns the 2 by 2 matrix: with $<x>^2-<x^2>$ and $<y>^2-<y^2>$ on the diagonal and $<x><y>-<xy>$ off−diagonal elements.
- In three−dimensional case the function returns three by three **tensor of inertia** (it was too tiring to type the formula in html). This matrix is useful for superposition of bodies or molecules on the basis of shape, since three principal coordinates can be easily derived from the tensor using the `Eigen` or `Disgeo` functions. This trick used in the _dockScan script.

  Example: buildpep "AAA" # a long molecules xyz = Xyz(a_//c*) # a coordinate matrix of carbons # you can also do it with grobs: xyz = Xyz(g_myGrob) a=Tensor(xyz) # compute 3 by 3 matrix of the second moments b=Eigen(a) # returns 3 axis vectors ax1= b[?,1] # this is the longest half axis ax2= b[?,2] # this is the second half axis ax3= b[?,3] # this is the shortest half axis len1 = Length(ax1) # long axis length len2 = Length(ax2) # mid axis length len3 = Length(ax3) # short axis length r = Matrix(3,3) # to make the rotation matrix from b normalize the axes r[?,1] = ax1 / Length(ax1) r[?,2] = ax2 / Length(ax2) r[?,3] = Vector(r[?,1], r[?,2]) rotate a_ Transpose(r) # rotates the principal axes to x,y,z # x the longest

This commands are assembled in the `calcEllipsoid M_xyz` macro which returns `ellipseRotMatrix` , and three vectors: `ellipseAxis1` , `ellipseAxis2` and `ellipseAxis3`

See also: `Rot`, `rotate`, `transform`

Example to orient the principal axes of the molecule along X,Y and Z (the longest axis along X, etc.).

```
build string "se ala ala ala ala"  # let is define the ellipsoid
display virtual
a = Tensor(Xyz(a_//!h*))  # Xyz returns matrix K by 3
b=Eigen(a)                # 3x3 matrix of 3 eigenvectors
b[?,1] = b[?,1] / Length(  b[?,1] ) # normalize V1 in place
b[?,2] = b[?,2] / Length(  b[?,2] ) # normalize V2
b[?,3] = Vector( b[?,1], b[?,2] )   # V3 is a vector product V1 x V2
rotate a_ Transpose( b )  # b is the rotation matrix now
 # Transpose(b) is the inverse rotation
set view  # set default X Y Z view
```

2.21.137. Temperature

function returning the oligonucleotide duplex melting temperature.

`Temperature` **(** { *s_DNA_sequence* | *seq_DNA_sequence* } [*r_DNA_concentration_nM* [*r_Salt concentration_mM*]] **)**

− returns the `real` melting temperature of a DNA duplex at given concentration of oligonucleotides and salt. The temperature is calculated with the Rychlik, Spencer and Roads formula (Nucleic Acids Research, v. **18,** pp. 6409−6412) based upon the dunucleotide parameters provided in Breslauer, Frank, Bloecker, and Markey, Proc. Natl. Acad. Sci. USA, v. 83, pp. 3746−3750. The following formula is used:

`Tm=DH/(DS + R ln(C/4)) −273.15 + 16.6 log[K+]`

where DH and DS are the enthalpy and entropy for helix formation, respectively, R is the molar gas constant and `C` is the total molar concentration of the annealing oligonucleotides when oligonucleotides are not self−complementary. The default concentrations are C=0.25 nM and `[K+]=` 50 mM. This formula can be used to select PCR primers and to select probes for chip design. Usually in primer design the temperatures do not differ from 60. by more than several degrees.

2.21.138. Time

function returning time spent in ICM.

`Time` **(** *string* **)** − returns the `string` of time (e.g. `00:12:45`) spent in ICM.

`Time` ( ) − returns the `real` time in seconds spent in ICM.

Examples:

```
if (Time( ) > 3660.) print "Tired after " Time(string) " of work?"
```

2.21.139. Tolower

convert to the lowercase.

`Tolower(` *string* `)` − returns the `string` converted to the lowercase. The original string is not changed

`Tolower(` *sarray* `)` − returns the `sarray` converted to the lowercase. The original sarray is not changed.

Examples:

```
show Tolower("HUMILIATION")

read sarray "text.tx"  #create sarray 'text' (file extension is ignored)
text1 = Tolower(text)
```

See also: `Toupper`( ).

2.21.140. Torsion

angle function.

`Torsion(` *as_* `)` − returns the `real` torsion angle defined by the specified atom `as_` and the three previous atoms in the ICM−tree. For example, Torsion(a_/5/c) is defined by `{ a_/5/c , a_/5/ca , a_/5/n , a_/4/c }` atoms. You may type: `print Torsion(` and then click the atom of interest, or use GUI to calculate the angle.

`Torsion(` as_atom1, as_atom2, as_atom3, *as_atom4* `)` − returns the `real` torsion angle defined by four specified atoms.

Examples:

```
d=Torsion( a_/4/c )                    # d equals C−Ca−N−C angle

print Torsion(a_/4/ca a_/5/ca a_/6/ca a_/7/ca)  # virtual Ca−Ca−Ca−Ca
                                                # torsion angle
```

2.21.141. Toupper

convert to the uppercase.

`Toupper(` *string* `)` − returns the `string` converted to the uppercase. The original string is not changed

`Toupper(` *sarray* `)` − returns the `sarray` converted to the uppercase. The original sarray is not changed.

Examples:

```
show Toupper("promotion")

read sarray "text.tx"
text1 = Toupper(text)
```

See also: `Tolower`( ).

2.21.142. Tr123

translate one−character sequence to three−character notation.

`Tr123` **(** *sequence* **)** − returns `string` like "ala glu pro".

Examples:

```
show Tr123(seq1)
```

See also: `Tr321`( ). `IcmSequence`( ).

2.21.143. Tr321

translate three−character sequence to one−character notation.

`Tr321` **(** *s_* **)** − returns `sequence` from a string like this: "ala glu pro". This function is complementary to function `Tr123`( ). Unrecognized triplets will be translated into 'X'.

Examples:

```
show Tr123("ala his hyp trp")  # returns AHXT
```

2.21.144. Trace

matrix function.

`Trace` **(** *matrix* **)** − returns the `real` trace (sum of diagonal elements) of a square matrix.

Examples:

```
show Trace(Matrix(3))     # Trace of the unity matrix [3,3] is 3.
```

2.21.145. Trans

translation function. 3D translation vector or DNA sequence translation.

`Trans` **(** *R_12transformationVector* **)** − extracts the `R_3` vector of translation from the `transformation vector`.

`Trans` **(** *seq_DnaOrRnaSequence* **)**

− returns the translated DNA or RNA sequence ('−' for a Stop codon, 'X' for an ambiguous codon) using the standard genetic code. See also: `Sequence`(*seq_* `reverse`) for the reverse complement DNA/RNA sequence.

Example (6 reading frames):

```
w=Sequence("CGGATGCG>>AAATGATGCTGTGGCTCTTAAAAAAGCAGATATTGGAG")
show Trans(w), Trans(w[2:999]),Trans(w[3:999])
```

```
c=Sequence(w,reverse)
show Trans(c), Trans(c[2:999]),Trans(c[3:999])
```

`Trans` **(** *seq_DnaOrRnaSequence* { `all` | `frame` } [*i_minLen*] [*s_startCodons*] **)**

return a `table` of identified open reading frames in DNA sequence not shorter than *i_minLen* . The function was designed for very large finished sequences from the genome projects. Currently the Standard Genetic code is used. Option *s_startCodons* allows to provide a comma−separated list of starting codons; if omitted, the default is `"ATG"` , another example would be `"ATG,TTG"` (for S.aureus).

Option `frame` indicates that both start and stop codons need to be found. If they is not found or the fragment is too short, the table will be empty.

Option `all` allows to translate ALL POTENTIAL peptides by assuming that the start and/or stop codons may be beyond the sequence fragment. In this case, initially all 6 frames are produces. Later, some of them can be filtered out by the *i_minLen* threshold. The unfinished end codons will be marked by 'X'.

The table has the following structure:

- frame − integer 1 2 3 for the direct chain, or −1, −2, −3 for the complementary chain, respectively
- left − translation offset in the direct strand (even if translation occurred in the complementary chain)
- right − translation offset in the direct strand.
- dir − direction (+1 for the direct, −1 for the complementary)
- len − fragment length
- seq − sequence string

For example, if the fragment is in the complementary strand it may have the following parameters:

```
#>−frame−−−−−−−left−−−−−−−−right−−−−−−−dir−−−−−−−−−len−−−−−−−−−seq−−−−−−−−
   −1          22          57          −1          12          XCVXVAAESVAS
```

In this case translation follows the reverse strand (frame=−1), starts in position 57 of the original direct sequence and proceeds to position 22.

Example:

```
dna=Sequence("TTAAGGGTAA TATAAAATAT AAAGTTCGAA CAATACCTCA CTAGTATCAC AACGCATATA")
T=Trans(dna frame 10)
sort T.left
show T
```

2.21.146. Transpose

matrix function.

`Transpose` **(** *matrix* **)** − converts the argument *matrix[n,m]* into the transposed `matrix` [m,n]

`Transpose` **(** *rarray* **)** − converts real vector [n] into a one−column `matrix` [n,1]

Examples:

```
Transpose(a)              # least squares fit
Transpose({1. 2. 3.})     # [3,1] matrix
```

2.21.147. Trim

function to trim array/matrix/string.

`Trim` **(** *I_iarray i_lower i_upper* **)** − returns `iarray` clamped into the specified range. Values smaller than *i_lower* are replaced with *i_lower*, and values greater than *i_upper* are replaced with *i_upper*.

`Trim` **(** *R_rarray r_lower r_upper* **)** − returns `rarray` clamped into the specified range.

`Trim` **(** *i_ i_lower i_upper* **)** − returns `integer` clamped into the specified range (e.g. Trim(6,1,3) returns 3).

`Trim` **(** *r_ r_lower r_upper* **)** − returns `real` clamped into the specified range.

`Trim` **(** *M_matrix r_lower r_upper* **)** − returns `matrix` clamped into the specified range.

`Trim` **(** *s_string* [`all`] **)** − returns `string` with removed trailing blanks and carriage returns. If option `all` is specified, both leading and trailing blank characters will be removed.

`Trim` **(** *s_iarray s_list_of_allowed_characters* **)** − returns `string` with all characters except for the listed in the second argument are removed. Example:

```
Trim("as123d","abcds")
 asd
```

`Trim` **(** *s_string i_maxLength* **)** − returns `string` which is truncated if it is longer than the *i_maxLength* argument.

`Trim` **(** *S_sarray* [`all`] **)** − returns `sarray` of strings with removed trailing blanks. With option `all` it removes white space characters from both ends.

2.21.148. Turn

beta−turn prediction function.

`Turn` **(** { *seq_* | *rs_* } **)** − returns `rarray` containing beta−turn prediction index. The index is derived from propensities for i,i+1,i+2,i+3 positions for each amino−acid. Pi = pi+pi1+pi2+pi3, then high Pi values are assigned to the next three residues. The propensities are taken from Hutchinson and Thornton (1994).

Examples:

```
s =  Sequence("SITCPYPDGVCVTQEAAVIVGSQTRKVKNNLCL")
plot comment=String(s) number Turn(s) display # plot Turn prediction
```

See also the `predictSeq` macro.

2.21.149. Type

generic function returning type.

`Type` **(** *icm_object_or_keyword* **)** − returns a `string` containing the object type (e.g. `Type(4.32)` and `Type(tzWeight)` return string `"real"`). The function returns one of the following types: `"integer", "real", "string", "logical", "iarray", "rarray", "sarray", "aselection","vselection","sequence",` "alignment", "profile", "matrix", "map", "grob", "command", "macro", "unknown".

`Type` **(** *as_* , `1` **)** − returns a `string` containing the level of the selection ("atom","residue","molecule","object").

`Type` **(** *os_object* , `2` **)** − returns a `string` containing the *os_object* (or `current` by default) molecular object type. Defined types follow the `EXPDTA` (experimenal data) card of PDB file with some exceptions, see below:

`"ICM"`	ready for energy calculations. Those objects are either built in ICM or `converted` to the ICM−type.
`"X−Ray"`	determined by X−ray diffraction
`"NMR"`	determined by NMR
`"Model"`	theoretical model (watch out!)
`"Electron"`	determined by electron diffraction
`"Fiber"`	determined by fiber diffraction
`"Fluorescence"`	determined by fluorescence transfer
`"Neutron"`	determined by neutron diffraction
`"Ca−trace"`	upon reading a pdb, ICM determines if an object is just a Ca−trace.
`"Simplified"`	special object type for protein folding games.

The non−ICM types can be converted to `"ICM"` with the `convert` command or `convertObject` macro.

`Type` **(** { *ms_* | *rs_* }, `2` **)** − returns the `string` type of the specified molecule or residue. Legal types are "Amino", "Hetatm", "Nucl", "Sugar", "Lipid", "empty". Residues of the "Amino" type can be selected with the 'A' character (e.g. a_/A). See also a one−letter code for the type which is used in selections, (e.g. `a_A,H`). Examples:

```
if (Type(a_1.1)!="Amino") goto skip:      # deal only with proteins
if (Type( ) == "NMR") print "Oh, yes!"
```

`Type` **(** *as_* { `atom` | `mmff` } **)** − returns an `iarray` containing the ICM or MMFF atom types. Example:

```
buildpep "his ala"
show Type(a_//!vt* atom )  # icm types for non−virtual atoms
```

`Type` **(** *as_1 as_2* **)** − returns an `integer` containing the covalent bond type between the selected atoms.

`Type` **(** *seq_* , *2* **)** − returns the `string` type of the sequence. Two types are recognized: `"protein"` and `"nucleotide"` . An example in which we rename and delete all DNA sequences from the session:

```
 read pdb sequence "1dnk"
 Type( 1dnk_b, 2)
 nucleotide
```

read pdb sequence "1dnk" Type(1dnk_b, 2) nucleotide

```
for i=1,Nof(sequence)
  if Type(sequence[i],2) == "nucleotide"  rename sequence[i] "dna"+i
endfor
delete sequence "dna*"
```

2.21.150. Unix

the output of a UNIX command.

`Unix` **(** *s_unix_command* **)** − returns the `string` output of the specified unix command. This output is also copied to the `s_out` string. This function is quite similar to the `unix` command. However, the function, as opposed to the command, can be used in an expression.

Examples:

```
 show Unix("which netscape")  # equivalent to 'unix which netscape'
#
 if ( Nof(Unix("ls"),"\n") <= 1 ) print "Directory is empty"
```

2.21.151. Value

values of bond lengths, bond angles, phase and torsion angles.

`Value` **(** *vs_var* **)** − returns `rarray` of selected parameters. The function considers variables only in the `current object`.

Examples:

```
 ang=Value(a_/14:50/phi,PSI)          # array of phi−psi values
 hbonds=Value(a_//bh*)                # array of lengths for all H−X bonds
```

(Note use of special torsion `PSI` in the first example.)

2.21.152. Vector

vector product between two 3D−vectors.

Vector product

`Vector` **(** *R_vector1 R_vector2* **)** − returns `rarray` [1:3], which is the vector product with components

{ v1[2]*v2[3] − v2[2]*v1[3], v1[3]*v2[1] − v2[3]*v1[1], v1[1]*v2[2] − v2[1]*v1[2] }

Vector symmetry transformation

`Vector` **(** *M_matrix* **)** − transforms an augmented affine 4x4 space transformation `matrix` into a `transformation vector`.

See also: `Augment`( ) function.

2.21.153. Version

information about version of the current executable.

`Version` **(** [`full`] **)** − returns `string` containing the current ICM version. The second field in the string specifies the operating system: "UNIX" or "WIN". At the end there is a list of one−letter specifications of the licensed modules separated by spaces (e.g. `" G B R "`).

Option `full` adds a few fields:

- The compilation date of the executable, e.g. `[Mar 18 2002 14:48]`
- the path of the current executable
- the names of the licensed modules spelled explicitly

See also: `show version`.

Example:

```
 show Version( )  # it returns a string
 if (Real(Version( )) < 2.6) print "YOUR VERSION IS TOO OLD"

 if (Field(Version( ),2) == "UNIX") unix rm tm.dat
 if (Field(Version( ),2) == "WIN") unix del C:\tm\tm.dat
 if Version() == " D " print " Info> the Docking module license is ok"
```

`Version` **(** *s_binaryFile* [`binary` | `gui`] **)** − returns either `string` version of the binary file (`binary` option) or the version of the ICM executable used to save the file (`gui` option).

```
Version("tmp.icb" gui) # returns string
 3.025j
if( Integer(Version("tmp.icb" binary ))> 6 ) print "OK"
```

2.21.154. Volume

volumes of grobs, spheres, residues and cells.

`Volume` **(** *grob* **)** − returns `real` volume of a solid `graphics object` (would not work on dotted or chicken wire grobs). ICM uses the Gauss theorem for calculate the volume confined by a closed surface:

V = 1/3 * Sum(A * **n** * **R**)

where A is a surface area of a triangle, **n** a normal vector, and **R** is is a vector from an arbitrary origin to any vertex of the triangle. It is important that the grob is closed, otherwise, strictly speaking, the volume is not defined. However, small surface defects will not affect substantially the calculation. ICM minimizes

possible error by rational choice of the origin, which is mathematically unimportant for an ideal case. To define directions of the normals the program either takes the explicit normals (i.e. they may be present in an input Wavefront file) or uses the order of points in a triangle. ICM−generated grobs created by the `make grob [ potential | matrix | map]` command have the correct vertex order (the corkscrew rule), while the `make grob skin` command calculates explicit normals. The best way to make sure that everything is all right is to `display grob solid` and check the lighting. If a grob is lighted from the outside, the normals point outwords, and the grob volume will be positive. If a grob is lighted from the inside (as for cavities), the normals point inwords and the volume will be negative. If the lighting, and therefore normals, are inconsistent you are in trouble, since Mr Gauss will be seriously disappointed, but he will issue a fair warning from the grave. The surface area is calculated free of charge and is stored in `r_out` .

Example:

```
read grob "swissCheese"
                # divide one grob it into several grobs
split g_swissCheese
for i=3,Nof(grob)
                # see, all the holes have negative volume
 print "CAVITY" i, Volume(g_swissCheese$i)
endfor
```

See also: the `Area`(*grob*)} function, the `split` command and How to display and characterize protein cavities section.

`Volume` **(** *r_radius* **)** − returns `real` volume of a sphere, **(4/3)Pi*R^3**

`Volume` **(** *s_aminoAcids* **)** − returns `real` total van der Waals volume of specified amino−acids.

`Volume` **(** *R_unitCellParameters* **)** − returns `real` volume of a cell with parameters {a,b,c} for a parallelepiped or {a, b, c, alpha, beta, gamma} in a general case.

`Volume` **(** *g_grob* **)** − returns `real` volume confined by a grob.

Examples:

```
vol=Volume(1.)                        # 4*Pi/3 volume of unit sphere
vol=Volume("APPGGASDDDEWQSSR")        # van der Waals volume of the sequence
vol=Volume({2.3,2.,5.,80.,90.,40.})   # volume of an oblique cell
```

2.21.155. View

parameters of the graphics window and graphics view.

`View` **(** [`window`] **)** − returns `rarray` of 36 parameters of the graphics window and view. With the **window** option the function returns only *WindowWidth* and *WindowHeight* .

- first 16 numbers: rotation matrix and perspective.
  - ♦ V[1] V[5] V[9] screen X−axis (from left to right)
  - ♦ V[2] V[6] V[10] screen Y−axis (from bottom to top)
  - ♦ V[3] V[7] V[11] screen Z−axis (outwords into the screen)

- V[17:32] (next 16 numbers): the model view matrix, view point, scale and cliping planes
- V[33:34] XleftPos YupperPos
- V[35:36] WindowWidth WindowHeight. Size is given in pixels, Y is measured from the top down.

See also `set view` and `set view`. `Info(display)`

Example (how to save the image with 3 times larger resolution):

```
nice "1crn"  # resize window
write image window=2*View(window) # 2−times larger image
```

`View (` R_36_FromView, R_36_ToView, *r_factor* **)**

− returns `rarray` of the **interpolated view** between the from and to view at the intermediate point 0 *r_factor1*. If *r_factor* is out of the [0,1] range, the operation becomes extrapolation and should be used with caution. The camera view is changed in such a manner that the physical space is not distorted (the principal rotation is determined and interpolated, as are translation and zoom)

Example:

```
nice "1crn" # manually rotate and zoom
r1= View()  # save the current view
# INTERACTIVELY CREATE ANOTHER VIEW
r2= View()  # save the new view
for i=1,100 # INTERPOLATION
  set view View(r1,r2,i*0.01)
endfor
```

See also `View` (), `set view` and `set view`.

`View (` { "x"|"X"|"y"|"Y"|"z"|"Z" } **)** − returns `rarray` of 3 coordinates of the specified axis of the screen coordinate system.

Example:

```
build string "se ala"
display    # rotate it now
show View("x")
g1=Grob("ARROW",3.*View("x"))
display g1
```

2.21.156. Warning : the ICM warning message

indicates that the previous ICM−shell command has completed with warning.
`Warning` ()
− returns `logical yes` if there was an warning in a previous command (not necessarily in the last one). After this call the internal warning flag is reinstalled to `no.`
`Warning (string)`
− returns `string` with the last warning message. In contrast to the logical `Warning()` function, here the internal warning code is **not** reinstalled to 0, so that you can use it in expressions like `if Warning() print Warning(string)`.

Example:

```
read pdb "2ins" # has many warnings
if Warning() s_mess =  Warning(string) # the LAST warning only
print s_mess
```

2.21.157. Xyz : atom coordinates and surface points

function returning a matrix of x,y,z coordinates.

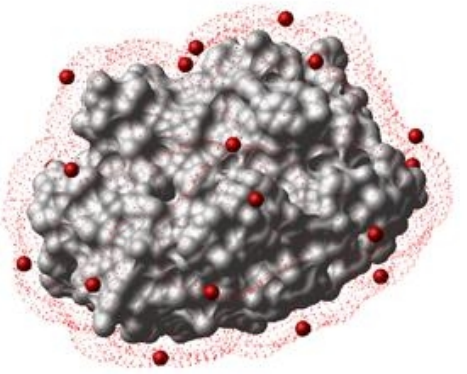
`Xyz` **(** *as_* **)**

− returns `matrix` [*number_of_selected_atoms* , 3] in which each row contains x,y,z of the selected atoms.

Examples:

```
coord=Xyz(a_//ca)          # matrix of Ca−coordinates
show coord[i]              # 3−vector x,y,z of i−th atom
show Mean(Xyz(a_//ca))     # show the centroid of Ca−atoms
```

`Xyz` **(** *as_ r_interPointDistance* `surface` **)**



− returns a subset of representative points at the accessible `surface` which are spaced out at approximately *r_interPointDistance* distance. This distance from the van der Waals surface (or `skin`) is controlled by the `vwExpand` parameter.

Example:

```
buildpep "ala his trp"
vwExpand = 3.
mxyz = Xyz( a_ 5. surface )
display skin white
dsXyz mxyz
color a_dots. red
```

2.22. Macros

`Macros` provide you with a great mechanism to create and develop your ICM environment and adjust it to your own needs (see also How do I customize my ICM environment.). Very often a repeated series of ICM commands is used for dealing with routine tasks. It is wise not to retype all these commands each time, but rather to combine them into a bunch for submission as a single command. Several examples follow.

2.22.1. buildpep: Building peptides from a sequence

`buildpep` *s_seq*

creates a new ICM object from an input sequence. This macro recognizes if you specified the sequence in one−letter upper−case letters or lower−case `three−letter code` and adds uncharged N− and C− termini. Use semicolon (`;`) to separate molecules. If you want to use different termini, or build a non−peptide molecule apply the `build` command directly or modify the macro.

For a multimolecular object you can also create separate objects and then `move` them together.

Examples:

```
buildpep "ala his trp glu"   # one tetrapeptide: nter and cooh added
buildpep "ala his ; trp glu" # two di−peptides
buildpep "one ; one"         # two oxygens

buildpep "YTGSNVKVAV"            # decapeptide
buildpep "AQSVPYGVSQ;IKAPALHSQG" # two decapeptides
```

2.22.2. calcBindingEnergy: estimates electrostatic, hydrophobic and entropic binding terms

`calcBindingEnergy` *ms_1 ms_2 s_terms* (`"el,sf,en"`)

evaluates energy of binding of two complexed molecules *ms_1* and *ms_2 s_terms* for the given set of energy terms *s_terms.* This macro uses the boundary element algorithm to solve the Poisson equation. The parameters for this macro have been derived in the Schapira, M., Totrov, M., and Abagyan, R. (1999) paper.

Example:

```
read object s_icmhome+"complex"
cool a_
calcBindingEnergy a_1  a_2  "el,sf,en"
```

2.22.3. calcDihedral4atoms: calculate a torsion angle defined by four atoms

`calcDihedral4atoms` *as_1 as_2 as_3 as_4*

calculates an angle between the two planes specified by any four atoms, *as_1 as_2 as_3 as_4.* Usually these are four consequtive covalently bound atoms.

Example:

```
buildpep "ala his his"
display atom label
calcDihedral4atoms a_/3/nd1 a_/3/cg a_/3/cd2 a_/3/ne2
Angle=  −0.06781 deg. (also saved in r_out) # it is almost flat
```

2.22.4. calcDihedralAngle: calculate an angle between two planes in a molecule

`calcDihedralAngle` *as_plane1 as_plane2*

calculates an angle between the two planes specified by two triplets of atoms, specified by the *as_plane1* and *as_plane2* selections

An example in which we measure an angle between planes of two histidines:

```
buildpep "ala his his"  # we use another macro here
display atom labels
calcDihedralAngle a_/2/cg,nd1,cd2 a_/3/cg,nd1,cd2
Angle=  131.432612  deg. (in r_out).
```

2.22.5. calcEnsembleAver: Boltzmann average the energies of the stack conformations

`calcEnsembleAver` *r_temperature s_parameter*

a macro showing an example of how to calculate a Boltzmann−weighted average given a conformational stack of conformation representatives. The `stack` may be formed as a result of a Monte Carlo simulation or created manually. The *s_parameter* string contains any expression returning the parameter to be averaged (e.g. `"Value(v_/2/phi)"` or `"Distance(a_/2/ca a_/4/ca)"`).

Example:

```
buildpep "ala his his"
set vrestraint a_/*  # impose rotamer probabilities
mncallsMC = 5000
montecarlo           # a stack is formed with energies
calcEnsembleAver 300. "Value(v_/2/phi)"
```

See also macro `helicity`.

2.22.6. calcMaps: calculate five energy maps and write them to files

`calcMaps` *s_fileNameRoot* (`"rec"`) *R_box* **(** `Box` (*a_* 5.) **)** *r_gridSize* (`0.5`)

calculates five energy grid `maps` for the current object with the grid size `r_gridSize` in the 3D box volume defined by the `R_box` . The maps are saved to files with names *s_fileNameRoot_gc.map s_fileNameRoot_gh.map* etc. and are deleted upon return from the macro. Be careful with selecting a box. You may focus the box on the area of interest (e.g. `Box( a_/55,66 , 7.)`). To use the maps read them in, rename to m_gc m_gh, etc. and `set terms "gc,gh,ge,gb,gs"` . If you determined the `box` interactively you may just use the `Box` () function without arguments (it returns the parameters of the graphical box).

Example:

```
read object s_icmhome+"crn"
```

```
 calcMaps "crn" Box( a_/15 4. ) 0.6
 read map "crn_ge"
 rename m_crn_ge m_ge
 display m_ge {1 2 3 0 4 5 6}
# the maps can be used in another session
```

2.22.7. calcPepHelicity: calculate average helicity of a peptide from movie frames

`calcPepHelicity` *s_movieName r_temperature* (`300.`)

a macro showing an example of how to calculate the helicity of a peptide structure given an ICM movie of the conformations accepted during a Monte Carlo run. A simulation using `montecarlo movie` option is a prerequisite for this macro. A good script prototype can be found in the `$ICMHOME/_folding` file. The `movie` option saves each accepted conformation to a `movie` file. The secondary structure of all transient conformations is assigned with the `assign sstructure` command.

Example:

```
% _folding  # run the _folding script with the movie option.
% icm
 read object "mypep"  # the name of your peptide object
 calcPepHelicity "mypep" 600.
```

See also macro `calcEnsembleAver`

2.22.8. calcProtUnfoldingEnergy: rough estimate of solvation energy change upon unfolding

`calcProtUnfoldingEnergy` *ms_* **(** *a_1* **)** *i_mncalls* **(** *100* **)**

calculates an octanol/water transfer solvation energy for the given # conformation as compared to an extended chain conformation.

2.22.9. calcRmsd: calculate three types of Rmsd between protein conformations

`calcRmsd` *rs_1* (`a_1.1/*`) *rs_2* (`a_2.1/*`)

calculates Ca−atom, backbone−atom, and heavy−atom RMSD for two input residue selections. The main effort in this macro is to take the internal symmetry of amino−acid sidechains into account.

For example, two phenylalanines related by the 180 degrees rotation of the `xi2` angle are identical, but will have a non−zero `Rmsd(a_1./phe a_2./phe)` because cd1 and ce1 of one selection lay on top of cd2 and ce2 atoms of the second selection, respectively. To calculate this `Rmsd` correctly, we need to find the rotation The following residues have internal symmetry (or pseudo−symmetry):
`leu,tyr,phe,asp,glu,arg,val.`

2.22.10. calcSeqContent

calcSeqContent *s_seqNamePattern* ("*")

analyzes amino acid composition of the input sequence or sequences. Specify quoted sequence name, pattern (e.g. "*_HUMAN") or "*" for all sequences.

Example:

```
read sequence s_icmhome+"seqs"
calcSeqContent "*"   # matches names of all sequences
 ..
 Statistics for 3 sequence(s): Azur_Alcde Azur_Alcfa Azur_Alcsp
 AA   N   %   Expected
 A   42 10.34   7.85
 C    9  2.22   2.55
 ...

calcSeqContent "*de"  # sequences ending with 'de'
 Statistics for 1 sequence(s): Azur_Alcde
 Res  N   %   Expected
 A   20 13.42   7.85
 C    3  2.01   2.55
 D    8  5.37   5.17
 E    6  4.03   6.95
```

The columns are as follows:

1. One−letter amino−acid code
2. The total occurrence of the amino acid
3. Relative percentage occurrence in the given set of sequences
4. Expected mean occurrence of the amino acid in proteins

convertObject auto *ms_* (a_) *l_delete_water* (yes) *l_optimize_hydrogens* (no) *l_replace_the_original* (no) *l_display* (no)

converts a non−ICM object into and ICM object and performs some additional refinements. The macro returns r_residialRmsd value containing the Rmsd of the model atoms from the equivalent template atoms (the same value is returned by the convert command in r_out). If this residual is greater than 0.5 , it usually means some problems with the conversion (e.g. unusual residues, missing parts, etc.).

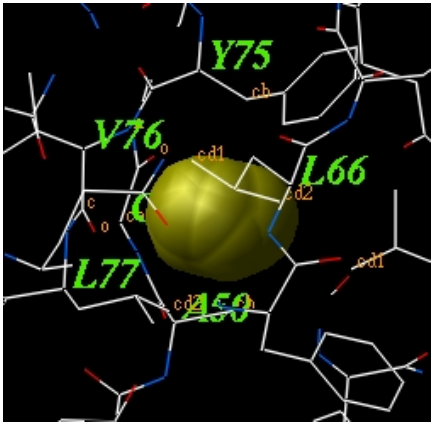
clusterChem *s_inObjects* ("*.ob") *s_outObject* ("clustered.ob")

performs clustering based on chemical similarity

2.22.11. icmCavityFinder: analyze and display cavities

icmCavityFinder *as_* **(** *a_1* **)** *l_interactive* (no) *r_minVolume* **(** 3. **)**

calculates and displays cavities in a molecular structure. These



cavities are sorted by size, and displayed. The *l_interactive* argument allows cavities to be displayed one by one interactively. To display the transparent outer shell edit the macro and activate this feature.

The *r_minVolume* parameters defines the volume of the smallest retained cavity. Increase it if you want only large cavities.

For each cavity this macro calculates volume `V` (in square Angstoms), area `A` and an effective radius `R` (compare it with the radius of a water molecule of 1.4A).

The icmCavityFinder macro uses two powerful features of ICM−shell:

- a grob with analytical molecular surface (a.k.a. `skin`) of the selected atoms can be built using the `make grob skin as_ as_ "g_skin"` command.
- this grob can be divided into the separate grobs with the outer shell and all the inner cavities with the `split g_skin` command.
- icmCavityFinder also uses the `Volume(g)` and `Area(g)` functions to measure volume and area of the cavities, as well as the `Sphere( g_ r_radius )` function to select atoms and residues around any grob.

Example:

```
read object s_icmhome+"1qoc"
delete a_w*  # remove water molecules
icmCavityFinder a_1 yes 4.
  3 icm-objects deleted
 Info> finished surface search, n_of surface atoms = 744
 Surface ..................................................
 Info> finished basic surface element calculations
 Info> Estimated vertex number = 335800, actual = 184896
 Info> packing vertices... sorted... done!
 Info> skin grob "g_skin" created (solid model: 32197 point
 Info> 3 grobs  g_skin1 ... g_skin3  created
Shell  1: V=11039.291805 A=4525.876702
 Warning> Volume(g_skin2) may be improperly calculated: env
CAVITY 2: V=25.253718 A=44.282805 R~1.710848 --------------
- Num  Res. Type ---- SS Molecule ---- Object - sf - sfRati
   26  ile   Amino    I H  m            1qoc     0.0  0.00
   53  leu   Amino    L E  m            1qoc     0.0  0.00
   58  val   Amino    V _  m            1qoc     0.0  0.00
   76  val   Amino    V E  m            1qoc     0.0  0.00
   87  val   Amino    V E  m            1qoc     0.0  0.00
   89  ile   Amino    I E  m            1qoc     0.0  0.00
```

...

2.22.12. dsCellBox: displays crystallographic unit cell

dsCellBox *os_*

displays unit crystal cell box for the specified object *os_* generated according to crystal symmetry parameters. This tiny macro extracts the cell from the object using the `Cell` function and makes a grob out of this array with the `Grob` function.

```
macro dsCellBox os_ (a_)
  gCell = Grob ("cell" Cell(os_))
  display gCell magenta
  keep gCell
endmacro
```

See also: `findSymNeighbors`

2.22.13. findSymNeighbors: cell and crystallographic neighbors

findSymNeighbors *as_* **(** *as_graph* **)** *r_radius* (`7.`) *l_makeObjects* (`yes`) *l_merge* (`no`) *l_display* (`yes`)

finds and builds symmetry related molecules around the input selection.

2.22.14. dsCharge: one of many ways to show charge residues

dsCharge

displays CPK representation of positively and negatively charged amino acid residues in red and blue colors, respectively. See also macro `undsCharge`

```
macro dsCharge
  display a_*./asp,glu/o?* cpk red
  display a_*./lys,arg/nz,n?* cpk blue
endmacro
```

2.22.15. dsChem : chemical style display

`dsChem` *as_* (`a_`)

3D display of the input atom selection in chemical style and on white background.

If you want to 'flatten' the molecule you can perform a procedure from the following example:

```
buildpep "trp"      # you need an ICM object
tzMethod = "z_only" # tether to the z-plane
set tether a_       # each atom is tethered to z=0
minimize "tz"       # keep the cov. geometry
```

2.22.16. dsCustom: extended display and property−coloring

`dsCustom` *as_* (`a_//*`) *s_dsMode* (`"wire"`) *s_colorBy* (`"atom"`) *l_color_only* (`no`)

Displays the specified representation (`"wire", "cpk", "ball", "stick", "xstick", "surface", "ribbon"`) of a molecular selection and colors the selection according to the following series of features:

- atom type (s_coloringType="atom"),
- residue type ("residue"),
- unique molecules ("molecule"),
- secondary structure type ("sstructure"),
- N−to−C−terminal chain course (NtoC""),
- B−factors ("bfactor"),
- electric charges ("charge"),
- solvent accessibility ("accessibility"),
- residue polarity ("polarity"),
- residue hydrophobicity ("hydrophobicity")

2.22.17. dsCustomFull macro for molecular display

`dsCustomFull` *as_* (`a_//*`) *s_display_mode* (`"wire"`) *s_color_by* (`"atom"`) *l_noWater* (`yes`) *l_areaSelfMode* (`no`) *l_color_only* (`no`)

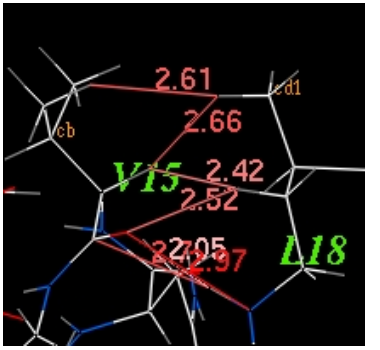
an extension of the previous `dsCustom` macro which, in addition, allows to color by an external `rarray` of 26 elements for each character. This user−defined array may contain any residue property information.

Flag *l_areaSelfMode* determines if the surface area is calculated for the selection in the context of all the atoms of the object (`no`) or only the selection itself, as if no other atoms existed (the *self* mode)

2.22.18. dsDistance: display distances between two selections

`dsDistance` *as_1 as_2 r_lowerLimit* (`0.`) *r_upperLimit* (`3.`)

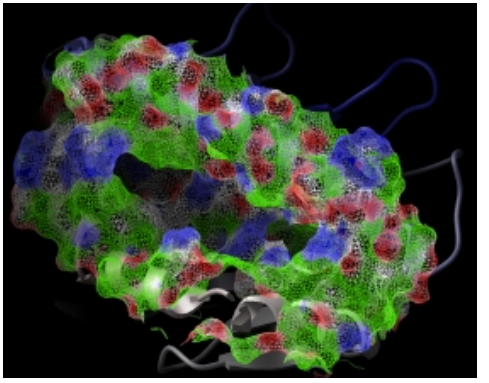
displays distances in a specified range between atoms of two input atom selections. This macro saves atom names and distances in `T_dist` table. This table can later be resorted and analyzed.



Example:

```
read object s_icmhome + "crn"
dsDistance a_/15 a_/18 0. 10.
show T_dist
```

2.22.19. dsPropertySkin: display molecular surfaces colored by properties essential for binding



`dsPropertySkin` *as_sel* (`a_`) *l_wire* (`yes`)

displays essential properties of molecular surfaces which are essential for binding small ligands, peptides or other proteins.

The first argument is a selection of atoms involved in the surface calculation. The second argument allows you to display the surface as:

- skin (`l_wire=no`), or
- wire (`l_wire=yes`)

The color code:

- white − neutral surface
- green − hydrophobic surface
- red − hydrogen bonding acceptor potential
- blue − hydrogen bonding donor potential

Example shown:

```
read pdb "1a9e"
delete a_w*
convert    # convert to ICM for map calculations
  # select receptor atoms 9. away from the peptide with Sphere
cool a_    # display ribbon
dsPropertySkin Sphere( a_3 a_1 9. ) yes
  # adjust clipping planes for better effect
write image png
```

Interactive surface display under GUI The same can be performed interactively on ICM objects with the popup−menu:

1. display your ICM object
2. switch selection level to **residue** (R)
3. select region with selection box or lasso
4. click on the right mouse button over one of the selected residues
5. selected `Display` and then `Property Skin`
6. it creates grob `g_recSkin` which can then be undisplayed and further manipulated

2.22.20. calcEnergyStrain: analyzing energy strain in proteins

`calcEnergyStrain` *rs_* (`a_/A`)

calculates relative energy of each residue for residue selection *rs_* ; and colors the selected residues by strain (if logical *l_colorByStrain* is `"yes"`). The *R_limits* argument determines the range represented by the color gradient (i.e. residues strained beyond 5. will still be shown in red).

This macro uses statistics obtained in the Maiorov, Abagyan, 1998 paper.

Example:

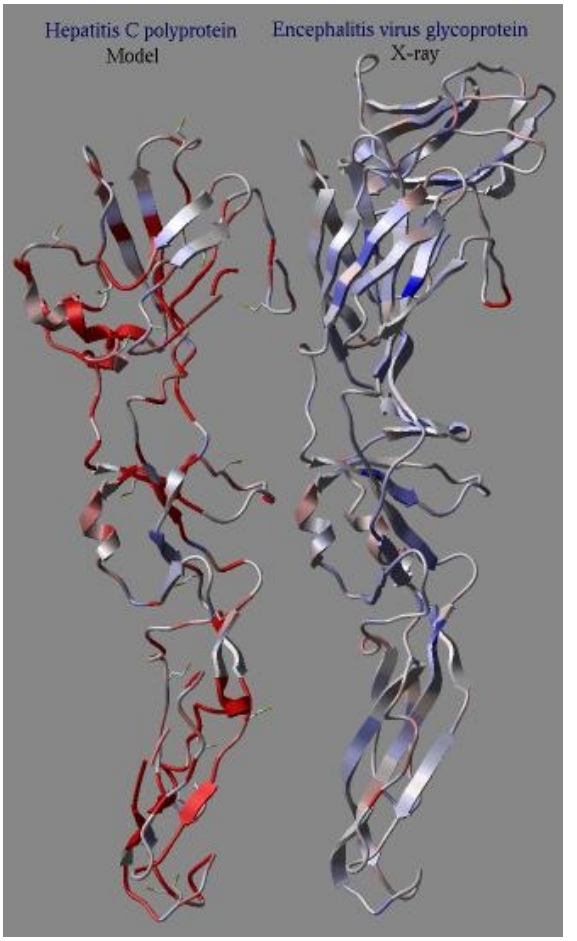
```
read object s_icmhome + "crn" # an ICM object
calcEnergyStrain  a_/A
show ENERGY_STRAIN
```

2.22.21. icmPmfProfile

`macro icmPmfProfile` *os_* **(** *a_* **)**
l_accessibilityCorrection (`yes`) *l_display* **(** *no* **)**

calculates a statistical energy of mean−force for each residue of a provided object. This energy is calculated with the "mf" parameters defined in the `icm.pmf` file. The residue energies are then normalized to the expected mean and standard deviation of the same residue in real high resolution structures. The mean energy value can be calculated as a function of its solvent accessibility if *l_accessibilityCorrection* is set to `yes.`

The calculated table contains residue energies and accessibilites. These values can be used to color residues of the molecule according to those values. In an example shown here we build a model (using the `build model` command of HCV protein on the basis of another viral coat protein. Then the profile was calculated for the model and the original structure. The calculation clearly shows the problematic regions of the model (the red parts) while the source structure looks quite reasonable.



2.22.22. dsPrositePdb

`dsPrositePdb` *ms_* (`a_*`) *r_prositeScoreThreshold* (`0.7`) *l_reDisplay* (`no`) *l_dsResLabels* (`yes`)

Finds all PROSITE pattern−related fragments in the current object and displays/colors the found fragments and residue labels.

2.22.23. dsRebel: surface electrostatic potential

`dsRebel` *ms_ l_assignSimpleCharges l_wire* (`no`)

generates the skin representation of the molecular surface colored according to the electrostatic potential calculated by the REBEL method (hydrogen atoms are ignored). The coloring is controlled by the `maxColorPotential` parameter. This macro uses a simplified charge scheme (a_/lys/nz : 1.0, a_/arg/nh* : 0.5 , a_/asp,glu/oe*,od* : −0.5) and uses only the heavy atoms for the calculations for the sake of speed. A full atom version of this macro is `dsRebel` .

2.22.24. dsSeqPdbOutput : visualize the sequence similarity search results

`dsSeqPdbOutput` *s_searchSeqPdbOutput* (`"tm.ou"`)

Goes through a list of PDB hits resulting in `find database` command and displays alignment(s) of the input sequence(s) with the found PDB structures and SWISSPROT annotations.

2.22.25. dsSkinLabel

`dsSkinLabel` *rs_ s_color* (`"magenta"`)

For all residues specified by the input residue selector, `rs_,` displays residue labels shifted toward the user to make the labels visible when skin representation is used.

2.22.26. dsSkinPocket and dsSkinPocketIcm

`dsSkinPocket` *ms_ligand* (`a_2`) *ms_receptor* (`a_`) *r_radius* (`7.`) : *dsSkinPocketIcm ms_ligand (a_2) ms_receptor (a_1) r_radius (7.)

display the receptor pocket around the selected ligand *ms_ligand.* Only the largest contiguous pocket surrounding the ligand is retained for clarity. The `dsSkinPocketIcm` macro also colors the molecular surface by hydrogen bonding potential and hydrophobicity. Best used with the ligand shown in cpk, if the ligand is small.

These macros can also be used to show the protein−protein interface.

Example:

```
read object s_icmhome+"complex"
cool a_
dsSkinPocket a_1 a_2 7.  # shows the surface of a_1
```

2.22.27. dsStackConf

`dsStackConf` *as_*

displays superimposed set of conformations from a conformational stack for given selection *as_*.

2.22.28. dsVarLabels

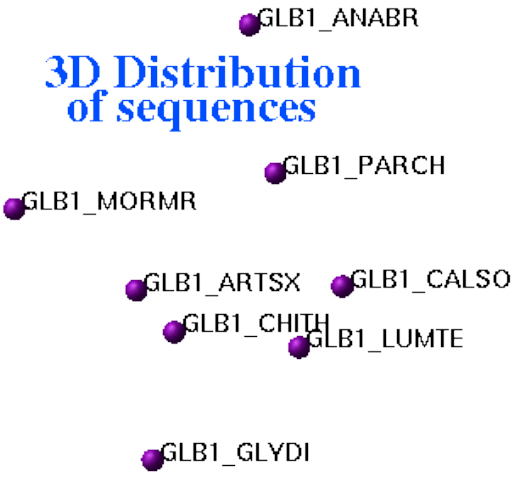
`dsVarLabels`

displays color labels for different types of torsion variables.

2.22.29. ds3D

`ds3D` *M_interObjectDistances* [*S_names*]

display 3D coordinates corresponding to an input square distance data matrix. Relative errors (in percent) of embedding to 3D space are in R_out: first entry is for the total error, next three are for X, Y and Z coordinates.



Representation of inter−sequence evolutionary distances in three−dimensional space

2.22.30. dsWorm

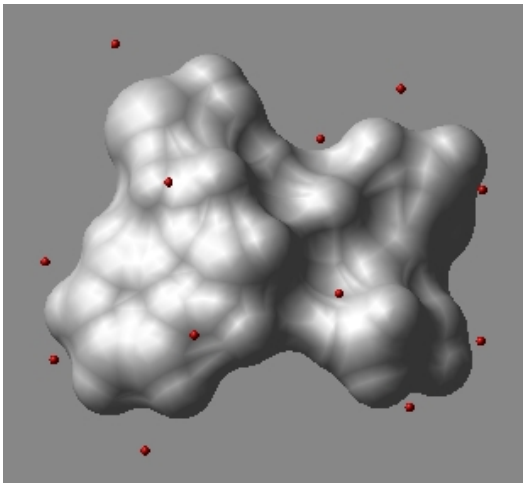
`dsWorm` *ms_*

displays "worm" (or "tube") representation of selected molecule(s). Residue colors are smoothly changed from blue (at N−terminus) to red (at C−terminus).

2.22.31. dsXyz : display

`dsXyz` *M_xyz_coordinates*

displays points from the *N_atoms* x 3 matrix of *M_xyz_coordinates* in 3D space as blue balls. The origin of the Nx3 matrix is not important. The macro creates an object called `a_dots.` In this object each dot is a one−atom residue called `'dot'.` The atom type is arbitrarily assigned to oxygen, and the atom names are 'o'.



One can further manipulate this object, e.g. `color a_/12:15/o green` .

An example in which we generate sparse surface points at vwExpand distance around a molecule and display them.

```
buildpep "ala his trp"
mxyz = Xyz( a_ 5. surface )
display skin white
dsXyz mxyz
color a_dots. red
```

2.22.32. findFuncMin

`findFuncMin` *s_Function_of_x* (`"Sin(x)x −1."`) *r_xMin* (`−1.`) *r_xMax* (`2.`) *r_eps* (`0.00001`)

minimizes one−dimensional functions provided as a string with the function expression. The macro uses successive subdivision method, and assumes that the function derivative is smooth and has only one solution in the interval

Example:

```
findFuncMin "Sin(x)*x−1." , −1. 2. 0.00001
 −1.000000 < x < 0.500000
 −0.250000 < x < 0.500000
 −0.062500 < x < 0.125000
 ....
 −0.000004 < x < 0.000008
 −0.000004 < x < 0.000002
```

2.22.33. findFuncZero

`findFuncZero` *s_Function_of_x* (`"Cos(x)x "`) *r_xMin* (`1.`) *r_xMax* (`100.`) *r_eps* (`0.00001`)

finds a root of the provided function of one variable with specified brackets with iterations. E.g.

```
findFuncZero "x*x*x-3.*x*x" 1. 33. 0.00001
 => x=17.000000  F=4046.000000
 => x=9.000000  F=486.000000
 => x=5.000000  F=50.000000
 => x=3.000000  F=0.000000
```

2.22.34. nice

`nice` *s_PdbFileName* (`"1crn"`) *l_wormStyle* (`no`)

reads and displays a PDB structure in ribbon representation; colors each molecule of the structure by colors smoothly changing from blue (at N−terminus) to red (at C−terminus).

Example:

```
nice "365d"  # new DNA drug prototype
nice "334d"  # lexitropsin, derivative of netropsin
```

2.22.35. cool

`cool` *auto rs_sel* (`a_`)

similar to the macro `nice` above, but refers to a residue selection.

2.22.36. homodel

`homodel` *ali_ l_quick* (`yes`)

homology modeling macro. The first sequence in the input alignment should contain the sequence of a PDB template to which the modeling will be performed. If flag `l_quick` is on, only an approximate geometrical model building is performed. You can also use the `build model` command directly.

2.22.37. makeIndexChemDb

`makeIndexChemDb` *s_dbFile* (`"/data/acd/acd.mol"`) *s_dbIndex* (`"/inx/acd"`) *s_dbType* (`"mol"`) *S_dbFields* (`{"ID"}`)

Creates and saves an `index` to a small compound database existing in standard `mol` or `mol2` formats (specified by the `s_dbType` parameter). `s_dbIndex` defines full−path root name of several index−related files. `String array S_dbFields` specifies fields of the input database which are indexed by the macro.

An example in which we index the `cdi.sdf` file and generate the `cdi.inx` file in a different directory:

```
% icm
makeIndexChemDb "/data/chem/chemdiv/cdi.sdf" "/data/icm/inx/cdi" "mol" {"ID"}
```

2.22.38. makeIndexSwiss

`makeIndexSwiss` *s_swiss* (`"/data/swissprot/fseq.dat"`) *s_indexName* (`s_inxDir+"/SWISS.inx"`)

Creates and saves an `index` to the SWISSPROT sequence database (datafile `s_swiss`). `s_indexName` defines the root name of several index−related files with respect to ICM user directory, `s_userDir`.

2.22.39. makePdbFromStereo: restore 3D coordinates from a stereo picture

transforms two stereo sets of two−dimensional coordinates in arbitrary scale into 3D coordinates. See also: How to reconstruct a structure from a published stereo picture .

2.22.40. mkUniqPdbSequences

`mkUniqPdbSequences` *i_percentDifference* (5) *s_seq_dir s_pdb_dir* (`s_pdbDir+""`) *l_replace* (`no`)

Creates a collection of PDB sequences with specified degree of mutual dissimilarity, `i_percentDifference`. Replace old dataset if `l_replace` is on.

2.22.41. plot2DSeq

`plot2DSeq` *ali_*

generates a 2D representation of "distances" between each pair of sequences from the input alignment.

2.22.42. plotSeqDotMatrix

`plotSeqDotMatrix` *seq_1 seq_2 s_seqName1* (`"Sequence1"`) *s_seqName2* (`"Sequence2"`) *i_mi* (5) *i_mx* (`20`)

generates an EPS file in which local sequence similarities between two sequences are shown in the form of a two−dimensional dot−matrix plot. Significance of local sequence similarities is shown by logarithm of the probability values and is calculated in multiple windows from i_mi to i_mx. The log−probability values are color−coded as follows: light blue: 0.7, red 1.0.

2.22.43. plotSeqDotMatrix2

`plotSeqDotMatrix2` *seq_1 seq_2 s_seqName1* (`"Sequence1"`) *s_seqName2* (`"Sequence2"`) *i_mi* (5) *i_mx* (`20`)

generates an EPS file in which local sequence similarities between two sequences are shown in the form of a two−dimensional dot−matrix plot. Significance of local sequence similarities is shown by (`1. − Probability`(..)) values and is calculated in multiple windows from i_mi to i_mx. The `( 1 − P )` values are color−coded as follows: light blue: 0.7, red 0.99.

2.22.44. plotBestEnergy

`plotBestEnergy` *s_McOutputFile* (`"f1,f2"`) *r_energyWindow* (`50.`)

plots profile of energy improvement during an ICM Monte Carlo simulation. Data are taken from the MC output log file or files, s_McOutputFile. You can specify a single output file (e.g. `"f1.results"),` or several files, e.g. `"f1.ou,f2.ou",` or drop the default `".ou"` extension, e.g. `"f1,f2,f2".`

This macro gives you an idea about the convergence between several runs.

2.22.45. plotOldEnergy

`plotOldEnergy` *s_McOutputFile* (`"f1.ou"`) *r_energyWindow* (`50.`)

plots profile of energy changes during an ICM Monte Carlo simulation. Data are taken from the MC output log file, s_McOutputFile.

2.22.46. plotFlexibility

`plotFlexibility` *seq_ i_windowSize* (7)

calculates and plots flexibility profile for input sequence *seq_* and smooths the profile with *i_windowSize* residue window.

2.22.47. plotCluster

`plotCluster` *M_distances S_names* (`{""}`) *s_plotArgs* (`"CIRCLE display {\"Title\" \"X\" \"Y\"}"`)

plot distribution of clusters. Arguments:

- a square matrix of distances between n objects. For arrays it may be calculated with the `Distance ( )` function (e.g. Distance(Xyz(a_//ca))). For angular RMSD the distance can be calculated from a matrix **v** of values of torsion angles for many conformations:

```
for i=1,n-1
  di[i,i]=0.
  for j=i+1,n
            # takes care of -179 and 181, base 360 is the default
     dif=Remainder(v[i]-v[j])
            # angular RMSD
     di[i,j]=Sqrt(Mean(dif*dif))
     di[j,i]=di[i,j]
  endfor
endfor
di[n,n]=0.
```

- sarray of names for each of n points . Possibilities:
  - the empty sarray: {""}. No name tags will be attached to each point
  - Sarray(Count(n)) generates names like this: {"1" "2" "3" ... }
  - user-defined: e.g. Name(a_*.) if each point correspond to an object

- manual: e.g. {"A" "compound X" "c"}
- See also: arguments for the `plot` command.

2.22.48. plotMatrix

`plotMatrix` *M_data s_longXstring S_titles* (`{"Title","X","Y"}`) *s_fileName* (`"tm.eps"`) *i_numPerLine* (`10`) *i_orientation* (1)

generates combined X−Y plot of several Ys (2nd, 3rd , etc. rows of the input matrix `M_data)` versus the one X−coordinate, assumed to be the first row of the matrix. `i_numberPerLine` parameter defines the size of the plotted block size if the number of data points is greater then `i_numberPerLine.` `i_orientation` equal to 1 defines portrait orientation of the output plot, landscape otherwise.

2.22.49. plotRama

`plotRama` *rs_ l_show_residue_label* (`no`) *l_shaded_boundaries* (`yes`)

generates a *phi−psi* Ramachandran plot of an *rs_* residue selection. If logical *l_show_residue_label* is on, the macro marks the residue labels. If *l_shaded_boundaries* is on, the allowed (more exactly, core) regions are shown as shaded areas; otherwise the contours of the core regions are drawn.

2.22.50. plotRose

`plotRose` *i_prime* (`13`) *r_radius* (`1.`)

just a nice example of a simple macro generating "rose" plot.

2.22.51. plotSeqProperty

`plotSeqProperty` *R_property s_seqString S_3titles* {"Y property","Position","Y"} *s_fileName* (`"tm.eps"`) *i_numPerLine* (`30`) *s_orientation* (`"portrait"`)

a generic macro to plot local sequence properties. Modify it for your convenience. Here is an example in which we plot residue b−factors along with the crambin sequence. `s_seqString` could be the sequence (e.g. `String(1crn_m)`) or secondary structure, (e.g. `Sstructure(1crn_m)`) or any other string of the same length as the sequence.

```
read pdb "1crn"
make sequence
b = Bfactor( a_/* )
plotSeqProperty b String(1crn_m ) {"" "" ""} "tm.eps" 20 "portrait"
```

2.22.52. predictSeq

`predictSeq` *s_seq s_fileName l_predictSecStr*

calculates and plots hydrophobicity and flexibility profiles and secondary structure diagrams for the given sequence *s_seq* (this is a string with the sequence name) and saves the results in *s_fileName* PostScript file.

2.22.53. prepSwiss

`prepSwiss` *s_IDpattern* (`"VPR_*"`) *l_exclude* (`yes`) *s_file* (`"tm"`)

extracts all sequences from the SWISSPROT database which exclude (`l_exclude=` yes) or include (`l_exclude=` no) the specified sequence pattern, `s_IDpattern` and creates a set of database files with the rootname `s_file` intended to use in the command `find database`.

2.22.54. printFast

`printFast` *s_ofPrinterName* (`"graphic"`)

writes current content of the graphic window to a PostScript file and calls unix `'lp'` command to send the resulting PostScript file to the specified printer, `s_ofPrinterName` .

2.22.55. printMatrix

`printMatrix` *s_format* (`" %4.1f"`) *M_matrix* (`def`)

prints matrix *M_matrix* according to the input format *s_format.*

2.22.56. printPostScript

`printPostScript` *s_ofPrinterName* (`"grants"`)

converts the current content of the graphics window to a PostScript file and directs it to the *s_ofPrinterName* printer.

2.22.57. printTorsions

`printTorsions` *rs_*

outputs all torsion angles of the input residue selection.

2.22.58. refineModel: globally optimize side−chains and anneal the backbone

`refineModel` *i_numberOfAnnealingIters* (5) *l_sideChainSampling* (`no`)

This macro can be used to improve any ICM model. The model can come from the `build model` command or the `convert` command or `regul` macro, etc. It performs

- side−chain sampling using `montecarlo fast`
- interative annealing with tethers you have provided
- second side−chain sampling to resolve the new problems resulting from the second step

To perform only the side−chain refinement, set the *i_numberOfAnnealingIters* argument to `0` .

2.22.59. regul

`regul` *rs_* (`a_/A`) *s_regObjName* (`"regobj"`) *s_ngroup* (`"nh3+"`) *s_cgroup* (`"coo−"`) *l_newIcmSeq* (`yes`) *l_displayRegul* (`yes`) *l_freeMin* (`no`)

creates a `regularized` ICM−model of an input residue selection (`rs_`) under the name `s_regObjName.` If `l_newIcmSeq` is set to `yes` , the macro will create sequence from that of the input residue selection, optionally modified by the N− and C−terminal groups (`s_ngroup` and `s_cgroup,` empty `""` strings are allowed); otherwise the macro will use an ICM−sequence file, **s_regObjName**.se The protocol course may be displayed if `l_displayRegul` set to `yes` . The resulting ICM model will be written to file `s_regObjName.ob.` If `l_freeMin` set to *yes*, the resulting model will be additionally minimized, now without tethers, and be written to file `s_regObjNamef.ob.` The summary of the macro's work will be saved to file `s_regObjName.log` .

2.22.60. rdBlastOutput

`rdBlastOutput` *S_giArray*

reads a set of sequences defined in a BLAST's output file, `S_giArray` from the NCBI database.

2.22.61. rdSeqTab

`rdSeqTab` *s_dbase* (`"NCBI"`)

reads a set of sequences listed in the `ICM−table` `SR,` an output of `find database` command, from the database defined by `s_dbase.`

2.22.62. readPdbList

`readPdbList` *S_list_of_pdb_codes*

reads a series of PDB files specified in the input string array and creates sequences for all loaded structures.

2.22.63. remarkObj

`remarkObj`

allows editing an `annotation (comment)` of the current object. Existing comment (if any) is read in an `editor` and after modification assigned to the object.

2.22.64. searchPatternDb

`searchPatternDb` *s_pattern* (`"?CCC?"`) *s_dbase* (`"SWISS"`)

searches for the pattern in the sequences of the specified `indexed` database `s_dbase.`

2.22.65. searchPatternPdb

`searchPatternPdb` *s_pattern*

searches for the specified pattern in pdb sequences taken from the `foldbank.db` file.

Example (first hydrophobic residue, then from 115 to 128 of any residues, non−proline and alanine at the C−terminus):

```
searchPatternPdb "^[LIVAFM]?\{115,128\}[!P]A$"
```

2.22.66. searchObjSegment

`searchObjSegment` *ms_ i_MinNofMatchingResidues* (`20`) *r_RMSD* (`5.`)

for given molecule *ms_* finds all examples of similar 3D motifs not shorter than *i_MinNofMatchingResidues* residues with the accuracy *r_RMSD* A in the ICM protein fold database.

2.22.67. searchSeqDb

`searchSeqDb` *s_projName* (`"sw1"`) *S_seqNames* (`{""}`) *r_probability* (`0.00001`) *l_appendProj* (`no`) *s_dbase* (`"SWISS"`)

search the database `s_dbase` using query sequence(s) specified in `S_seqNames.` Found hits and their specs are collected in the output table file `s_projName.tab.` If logical flag `l_appendProj` is on data will be appended to the existing table. Similarity of hits to the query sequence(s) is controlled by parameter `r_probability` (see `Probability`()).

2.22.68. searchSeqPdb

`searchSeqPdb` *s_projName* (`"pdb1"`) *r_probability* (`0.01`) *l_appendProj* (`no`)

sequence search of all currently loaded sequences in the sequences of the proteins from the `fold bank collection`. Found hits and their specs are collected in the output table file `s_projName.` If logical flag `l_appendProj` is on data will be appended to the existing table. Similarity of hits to the query sequence(s) is controlled by parameter `r_probability` (see `Probability`()).

2.22.69. searchSeqPdb

`searchSeqPdb` *s_projName* (`"pdb1"`) *r_probability* (`0.01`) *l_appendProj* (`no`)

sequence search of all currently loaded sequences through all proteins from the collection s_pdbDir+"/derived_data/pdb_seqres.txt.Z", a subset of PDB sequences with given degree of mutual dissimilarity. Found hits and their specs are collected in the output table file `s_projName.` If logical flag `l_appendProj` is on data will be appended to the existing table. Similarity of hits to the query sequence(s) is controlled by parameter `r_probability` (see `Probability`()).

2.22.70. searchSeqSwiss

`searchSeqSwiss` *seq_*

Searches for homologues of the query sequence `seq_` in the SWISSPROT database.

2.22.71. setResLabel

`setResLabel`

moves displayed atom labels to the atoms specific to each residue type.

2.22.72. sortSeq

`sortSeq`

sort sequences by their length and suggest outliers.

2.22.73. undsCharge

`undsCharge`

color display of the charged residues.

2.22.74. makeSimpleModel

`makeSimpleModel` *seq_ ali_ os_*

This macro rapidly builds a model by homology using simplified residues described in the residue library. Input data are the sequence of the model, `seq_` and alignment `ali_` of the model's sequence with the template object `os_` .

2.22.75. makeSimpleDockObj

`makeSimpleDockObj` [*os_object*] [*s_newObjName*]

This macro builds an ICM object from simplified residues described in the residue library. The goal is to convert an all−atom molecular object into an object in simplified representation for fast docking calculations.

2.22.76. searchSeqProsite

`searchSeqProsite` *seq_*

compares input sequence against all sequence patterns collected in the PROSITE database.

Examples:

```
 read sequence "zincFing.seq" # load sequences
 find prosite 2drp_d            # search all < 1000 patterns
                                # through the sequence
 find profile 2drp_d            # search profile from prosite database
```

See also:

`find pattern`, `find database pattern=s_pattrn`, `find prosite`.

2.23. Files

2.23.1. _macro. A collection of ICM macros.

This `file` contains a set of ICM macros. You can use them, modify them, or browse them to develop your own macros. _macro is downloaded by the `call _macro` command.

2.23.2. _startup. ICM startup file

This ICM script contains a set of commands issued automatically upon invoking ICM. The file will be searched for in the directory defined by the UNIX environmental variable `ICMHOME.` This location may be different from the `$ICMHOME` directory. It allows users to share the ICM executable but have their individual _startup files. **Important**: edit this file to customize your environment. A template to modify follows.

```
 s_pdbDir     = "/data/pdb/" # set it to the place where PDB lives
 pdbDirStyle  = "pdb1abc.ent" # style currently distributed by PDB
 s_helpEngine = "icm"        # reasonable default, HTML-help is
                             # an alternative

                             # you may have your own PROSITE updated file
 s_prositeDat = Getenv("ICMHOME")+"/prosite.dat"

                             # xpsview may be more standard
 s_psViewer   = "/usr/opt/bin/gs -q"

                             # better be accessible only for you
 s_tempDir = "/usr/tmp/"
#
 read libraries              # they will be read from $ICMHOME

 call _aliases               # by default it will be taken
                             # from the directory defined by
                             # environmental variable $ICMHOME
 call _macro                 # by default it will be taken
                             # from the directory defined by
                             # environmental variable $ICMHOME

 print "...ICM startup file executed..."
```

2.23.3. _startCheck script

This script checks the presence of and access to the directories and files used by ICM and specified by some ICM-shell `string variables`. This script is recommended during `customization` of the

ICM.

2.23.4. foldbank.db

Bank of assigned secondary structures (foldbank.db) This text file may be created by `_mkSegmentLib` script and contains secondary structures for a nonredundant set of protein chains. Description of fields:

- NA − chain name ('m' usually stands for main or 'NO chain identifier')
- RZ − resolution. NMR entries get 9.99 (they may be actually worse than that).
- ER − all−atom RMSD−error upon PDB−>ICM conversion. Beware of entries with ER > 0.5!!
- SE − amino acid sequence as extracted from the structure (not SEQRES)
- SX − authors' secondary structure assignment, all _____ if not provided (as in 1knt.m).
- SS − automatically assigned by ICM secondary structure using modified Kabsh and Sander algorithm.
-

The commented field contains a serial number.

Example two entries:

```
...
...
## 355
NA 4tpi.i
RZ 2.20
ER 0.027
SE RPDFCLEPPYTGPCRARIIRYFYNAKAGLCQTFVYGGCRAKRNNFKSAEDCMRTCGGA
SX _________________EEEEEEEEEE__EEEEEEEE__________HHHHHHHHHH__
SS ___GGG___________EEEEEE____EEEEEE_________B__HHHHHHHH___
...
...
## 364
NA 1knt.m
RZ 1.60
ER 0.015
SE TDICKLPKDEGTCRDFILKWYYDPNTKSCARFWYGGCGGNENKFGSQKECEKVCA
SX ____________________________________________________________
SS _GGGG______B____EEEEEEE____EEEEEEE__B______B__HHHHHHHH_
...
...
```

2.23.5. Bank of protein folds (foldbank.seg)

This text file contains descriptions of `segment` (or vector) representations of protein three−dimensional structures.

Example:

sis.m scorpion insectotoxin i5a _E_H_E_E_ 1 1 2 3 6 8 4 4 1 5 3 −1 2.50 1.11 −0.95 3.95 2.97 −3.10 5.41 −3.20 −10.98 13.48 −0.74 −12.05 11.31 4.10 −3.08 13.56 0.33 −0.05 5.08 −8.21 −5.66 4.15 −7.57 −8.58 8.77 −1.09 2.21 6.15 0.21 7.04

Each molecule is represented by a single line containing the following fields:

- sis.m : molecular selection (note 'm' is used as a chain identifier if the pdb−file has no chain information).
- scorpion insectotoxin i5a : long name (up to the 30th position)
- _E_H_E_E_ : secondary structure of ('_' coil, 'E' extended, 'H' helix)
- 1 1 2 3 6 8 4 4 1 5 3 −1 : a segment list; the first integer indicates the format for the segment list, the last −1 is a terminator. There are two formats, indicated by numbers 1 and 0.
- 1 : concise : *ResNumberOffset 1st_SegmentLength 2nd_Segment_Length 3rd_Segment_Length ...*
- 0 : full format (e.g. 0 74b 4 78b 8 86b 4 90b 5 −1) : *1st_Res_Number/char 1st_Segment_Length 2nd_Res_Number/char 2nd_Segment_Length ...*

* 2.50 1.11 −0.95 ... : x,y,z for all reference points. The full format allows more complex residue numbering which may frequently be found in the pdb−entries (i.e. 4 5 6 8 9 9a 9b 9c 10 12 ..). The concise format is used for the regularly numbered molecules.

2.23.6. Atom codes (icm.cod)

This text file contains description of (1) *atom types* and references to (2) MMFF types, (3) van der Waals types, (type 0 or 9 to ignore) (4) hydrogen bonding types, (type 1 means no H−bonds) and (5) hydration types (0 to ignore). The real numbers are atomic mass (6) and surface (7). The character (8) is used to define atom color. Free−format. Two example lines:

```
#      (1)  (2)  (3)  (4)  (5) (6)     (7)   (8)  *  Comment
#>     cd   mmff vw   hb   hd     wt    sf    na  comment
cod    63    6   18    6    6  16.000  40.77 o    * o in r−c−oh (thr,ser)
cod    71   32   19    6    8  16.000  36.79 o    * o− in carboxylate ion
cod    92   12   61    1    1  35.453 133.8  Cl   *    (MMFF)
cod   223   38   13    4    3  14.007  61.16 n    * pyridin nitrogen (MMFF)
```

2.23.7. Bond angle bending and improper torsion deformation parameters (icm.bbt)

This text file contains a factor (kcal/mole) and an equilibrium angle in degrees for the bond angle bending deformation energy for different types of angles.

```
#   Type   Factor  OptAngle(a0).   E=Factor*(a−a0)<sup>2</sup>
#
bbt    1  160.7000  115.0000  ca−c#−n
bbt    2  128.2000  120.5000  ca−c#=o
...
```

2.23.8. Bond stretching parameters (icm.bst)

This text file contains a factor (kcal/mole) and an equilibrium bond length in Angstroms for the bond stretching energy for different types of bonds.

```
#     E=Factor*(b−b0)<sup>2</sup>
#     Type   Factor  BondLength(b0).
#>    ity    eybs      eqbl     bt   comment
#
bst     1  500.0       1.4530  1 cn  n−ca
bst     2 1150.0       1.3250  1 cn  c#−n
bst     3  460.0       1.5300  1 cc  ca−c#
```

```
bst     4  430.0       1.5300  1 cc  ca-cb
...
```

2.23.9. Conformational stack (*.cnf)

This binary file contains descriptions of several conformations of the same molecule. You can not edit this file. The stack is automatically generated and saved in the course of Monte Carlo, or systematic search procedures. Alternatively the stack may be created directly by the `store conf` command. To read/write a stack use: `read stack [s_StackName]` `write stack [s_StackName]`

2.23.10. Distance restraint types (icm.cnt or *.cnt)

The file describes legal types of drestraints to impose attraction or repulsion between atom pairs (e.g. NOE distance restraints derived from NMR data). This penalty term is called `"cn"`. The system icm.cnt can be edited, however, user files (e.g. mydist.cnt) of the same format can be created and loaded with the `read drestraint type` command. The file contains:

```
#      type    weight    lower     upper  sharpness
#                                            4 special types for S-S bonds
ssSS1         10.0       2.04      2.04     10.0 # Sharp well for S-S dist.
ssSS2          2.0       2.04      2.04      1.0 # Wide well  for S-S dist.
ssSC           5.0       3.052     3.052    10.0 # S -Cb distance
ssCC           3.0       3.855     3.855    10.0 # Cb-Cb distance
global    1    1.0       0.0       3.0           # a global drestraint
global    2    1.0       2.0       4.0           # a global drestraint
local    12    1.0       2.5       2.8       1.0 # a local drestraint
```

Both local distance restraints and global ones force two atoms to stay between the upper and lower boundaries, however, the local restraints diminish at large distances (similar to van der Waals interactions), whereas the global restraints grow bi-quadratically as deviation from the target distance range increases. You can have and read several *.cnt files. If the type numbers overlap the previous types are redefined.

See also related commands: `read drestraint type`, `show drestraint type`, `set drestraint type`, `make drestraint type`.

2.23.11. Distance restraints (*.cn)

Contains list of atom pairs for which interatomic distances should be restrained according to specified types defined in a separate `icm.cnt` file. The .cn files are created by the user. Supplied icm.cn file is just an example.

```
#  ml1  re1   at1   ml2 re2   at2  cn_type
cn crn 1 val  hg22   * 1 val  ca      1
cn  *  1 val  hg23   * 1 val  cg1     1
cn  *  2 gln  ca     * 1 val  hg11    1
cn  *  2 gln  ca     * 1 val  ha      1
```

Molecule name and residue number (e.g. 14, 25A, etc.) are normally used to find an atom. An asterisk instead of the molecule name means that only the residue number should be matched. See also: `read drestraint`, `show drestraint`, `set drestraint`, and `make drestraint (un)display drestraint`

2.23.12. Graphics objects (*.gro)

This text file contains streams of POINT coordinates (i.e. a triple of floats in one line, preceded by an integer reference number), LINE descriptors (i.e. pair of integer numbers of recently described POINTS in one line) and/or TRIPLES (or TRIANGLES, i.e. triples of integer numbers of POINTS). The order of streams is arbitrary, provided that referenced POINTS are already described. Either LINES or TRIPLES can be omitted. Graphics objects can be read, written, displayed , or made from a 3D map.

```
1 1.00 −1.00 0.00
2 1.00  1.00 1.00
3 0.00  2.00 0.50
 1 2
 1 3
 2 3
1 2 3
```

Check content of other .gro files in you icm directory. ICM also understands the Wavefront obj−format (files *.obj). You can create your own dot, wire or solid graphics objects either manually or automatically.

2.23.13. ICM HTML help file (icm.htm)

contains this manual

2.23.14. Hydrogen bonding types (icm.hbt)

A and *B* parameters for the $A/r^{12} - B/r^{10}$ potential between HB donors and acceptors. See Nemethy et al. for reference.

Example lines:

```
#     i  j     B        A        E      r0
#
hbt   2  4   8244.0   32897.0  0.550   2.190      * n−h...n
hbt   3  4   8244.0   32897.0  0.550   2.190      * o−h...n
```

2.23.15. Hydration parameters (icm.hdt)

Parameters to calculate solvation energy based on atomic solvent−accessible surfaces (see solvation term). The file contains several sets (e.g. Eisenberg and McLachlan (1986), Wesson and Eisenberg (1992)) although only one of them is not commented out.

Example lines:

```
rwater  1.4000  # water radius used to roll around the molecule
#
#       1      2          3      4     5
#
hdt     4   −0.0500    1.7000  0.0016  n+
```

1. reference type number
2. solvation energy density from vacuum−water transfer experiments for a given hydration type

3. solvation energy density from octanol−water transfer experiments for a given hydration type
4. radius used to calculate accessible surface
5. comment

2.23.16. Configuration file (icm.cfg)

This file contains limits and memory requirements for ICM. It will be searched in the **current** directory (`./`) first and, if not found, in the directory defined by the UNIX environmental variable $ICMHOME or `$HOME/.icm/config/` directory ($USERPROFILE/.icm/config/ for Windows), if present.

You may edit the file and change the limits.

```
# ICM configuration file. Free format
# Mn stands for "Maximal Number of"
# Mx stands for "Maximal Size of"
BufferSpace 2097152 # ICM will not let you decrease BufferSpace less than 131072
MnResidueTypes  200
MnSequences   20000
MnAlignments   1500
MnProfiles       40
MnGrobs         200
MnMaps           40
MnMacros        400
XTermFont  *−fixed−medium−*−*−*−24−* # to set font in the terminal window
Xterm      xwsh                      # default for SGI
# Xterm    xterm                     # default for Linux and other UN*Xes
```

2.23.17. Colors (icm.clr)

file contains default color and font settings. The default `icm.clr` file resides in the `$ICMHOME` directory. The `LIBRARY.clr` variable defines the default path and name of the `icm.clr` file.

Keep your own color and graphics controls file in `~/.icm` directory. Example of `~/.icm/user_startup.icm` file (`$USERPROFILE/user_startup.icm` under Windows):

```
LIBRARY.clr = Getenv("HOME")+"/.icm/icm.clr"
read color    # load your custom settings
```

Modify the file if needed. The following lines are recognized (free format):

```
# CONFIGURABLE GRAPHICS.mode translation table
#   Use keywords Left Mid Right, Shift Ctrl Alt Dbl, At
#   TopNN LeftNN RightNN BottomNN, where NN is a percentage of the zone
#   Modes 0,3,4,5,14,15 require a hit in 'At' = (atom | grob)
#   otherwise control falls through to next best appropriate action
#   Some modes have submode switches listed in parentheses ()
#   Users are encouraged to modify bindings to their needs
# ---mode--combination------------ # equivalent GRAPHICS.mode preference
mode   0  Right−At                # popup (in GUI only)
mode   1  (Shift)−Left            # Rotation
mode   2  (Shift)−Mid             # Translation
mode   3  (Ctrl)−Shift−Right−At   # Label atoms
mode   4  (Ctrl)−Dbl−Right−At     # Label residues
mode   5  (Shift)−Ctrl−Left−At    # Change torsion angles
```

```
mode   6  (Shift)-Bottom5-Left      # Rotation of the view
mode   7  (Shift)-Top5-Left         # Z-axis rotation
mode   8  Left5-Mid                 # Zoom
mode   9  Alt-Mid                   # Move rear clipping plane
mode  10  Ctrl-Mid                  # Move front clipping plane
mode  11  Ctrl-Alt-Mid              # Slab
mode  12  (Shift)-Right             # Rectangular selection
mode  13  (Shift)-Ctrl-Left         # Lasso selection
mode  14  (Shift)-Ctrl-Alt-Right-At # Connect to molecule
mode  15  Shift-Ctrl-Dbl-Right-At   # Set alignment cursor
mode  16  Ctrl-Mid-At               # Drag atoms
mode  17  Right5-Mid                # Z-translate

#-------------- Colors --------------
# -----color-----------RRGGBB--A_real_if_not_1
....
color lightgreen        # 80ff80
color rita              # ff1b00  0.3
color darkseagreen      # 8fbc8f
...
#--------  Atom/Grob/Font Colors  ----------
atom c grey  # c is the first character of chemical element.
background    black
#             color    font      size bold italic underline
atomFont      rose       times     12  0   0    0
varFont       yellow     symbol    12  0   0    0
residueFont   green      helvetica 18  0   0    0
grobFont      green      helvetica 18  0   0    0
stringFont    green      times     24  0   0    0
auxiliaryFont green      symbol    28  0   0    0
fixedFont     green      courier   12  0   0    0
#
alphaRibbon red
piRibbon    blue
threetenRibbon magenta
betaRibbon  green
coilRibbon  yellow
#- 0:127 rainbow colors (address them by number: color 15.5) -------
# ---------i-color----
rainbow     0  # 0000ff
rainbow    63  # ffffff
rainbow   127  # ff0000
....
```

2.23.18. Electron density map (*.map)

This binary file contains a complete description of the electron density map, compatible with the format devised by Phil Evans. Maps are stored as a 3−dimensional array preceded by a header which contains all the necessary information about the map. See "The CCP4 Suite" manual for details.

2.23.19. MC simulation movie (*.mov)

This binary file contains a description of a set of geometric parameters (free variables, usually torsions and overall rotation/translation variables), participating in MC simulation, followed by a stream of their values for each conformation accepted during the simulation, together with the energy of each accepted conformation. Movies can be created or appended during MC simulation runs, and then played in any

direction with optional smoothing, superimposition (to the initial conformation) and/or centering. These files tend to be large, watch them carefully and do not create them without a need. See also: `display movie`.

2.23.20. ICM−object (*.ob)

a binary noneditable file describing one or several molecules forming an ICM−object. In addition to information available in a PDB−file it contains a description of atomic charges, tree−like connectivity, detailed atom codes, information about which internal coordinates are constrained, references to energy parameters, secondary structure, etc. The object can be read and written.

2.23.21. Residue library (icm.res or *.res)

The main residue library, describing all "residues" and molecules which can constitute a legal ICM−object. You can create your own entry either manually or using the `write library` command and add the entry to the `icm.res` file. You can also keep it in a separate file and append the file to the `LIBRARY.res` sarray (i.e. `LIBRARY.res=LIBRARY.res//"usr"` followed by the `read library` command). A example of an entry for a *pro* residue:

```
#  resName 1−ch Type AccSurf Eentropy LongName
nare  pro   P  AMINO    150  0.0  proline
rem
rem         _________atom_________    _dihedral_angles    __bond_angles__    _bond_lengths
rem       /                       \ /                 \ /               \ /             \
rem    at na    cd lwat   qu    gu na  fe   vuva   ey na  fe  vuva   ey na  fe  vuva ey qfm
#    Fields:
#       1 2      3    4      5   6 7    8        9 10 11  12 13      14 15  16    17 18  19
#
atre    1 n    216    0 −0.285   0 psi  +  180.000  2 an   . 118.000  1 bn   . 1.340 31
atre    2 ca   113    1  0.050   0 omgp +  180.000 24 aca  . 121.000  1 bca  . 1.465  1
atre    3 ha     1    2  0.040   0 fha  .  116.800  0 aha  . 110.200  1 bha  . 1.090  0
atre    4 cb   112    2 −0.025   0 fcb  . −120.850  0 acb  . 103.700 37 bcb  . 1.530  4
atre    5 hb1    1    4  0.015   0 fhb1 .  120.200  0 ahb1 . 111.600  1 bhb1 . 1.090  0
atre    6 hb2    1    4  0.015   0 fhb2 . −120.200  0 ahb2 . 111.600  1 bhb2 . 1.090  0
atre    7 cg   112    4 −0.050   0 xi1  .   27.400 21 acg  . 103.700  1 bcg  . 1.502  4
atre    8 hg1    1    7  0.025   0 fhg1 .  120.450  0 ahg1 . 111.200  1 bhg1 . 1.090  0
atre    9 hg2    1    7  0.025   0 fhg2 . −120.450  0 ahg2 . 111.200  1 bhg2 . 1.090  0
atre   10 cd   114    7  0.100   0 xi2  .  −35.600 21 acd  . 105.300 39 bcd  . 1.501  4
atre   11 hd1    5   10  0.010   0 fhd1 . −119.730  0 ahd1 . 111.600  1 bhd1 . 1.090  0
atre   12 hd2    5   10  0.010   0 xi3  .  −90.760 21 ahd2 . 111.600  1 bhd2 . 1.090  0
atre   13 c    121    2  0.455   1 phip .  −68.800 19 ac   . 112.300  3 bc   . 1.520  3
atre   14 o     81   13 −0.385   1 fo   .  180.000  0 ao   . 120.500  1 bo   . 1.230  5
#    F 20
lwat   13
#       F 21
exbo    1   10
```

Eentropy is the entropic contribution to the free energy for a fully accessible residue divided by the solvent accessible surface of this residue (in gly gly X gly gly environment) and multiplied by a factor of 1000.

Fields:

1. relative atom number
2. atom name

3. main atom code (see `icm.cod` file). It in turn refers to other codes such as hydrogen bonding code, van der Waals code and hydration code.
4. previous atom in a connectivity graph of the directed ICM−tree.
5. electric charge
6. groups of close charges (they should not be separated due to cutoffs distance in interaction lists)
7. torsion name
8. fixation status (+ free variable, . fixed)
9. torsion angle (degrees)
10. torsion energy type (see `icm.tot` file).
11. bond angle name
12. bond angle fixation status
13. bond angle value (degrees).
14. bond angle deformation energy type (see `icm.bbt` file).
15. bond length name
16. bond fixation status
17. bond length (Angstroms)
18. bond stretching energy type (see `icm.bst` file).
19. (qfm) formal charge (may be +1, −1/3, −1/2 etc.), if any
20. (lwat) exit atom of the residue
21. (exbo) additional (non−tree) covalent bonds (atom1 atom2). Normal ICM−tree bonds form regular directed graph without cycles, therefore all the remaining bonds should be declared separately.

See also: `LIBRARY.res` .

2.23.22. Object Variables (*.var)

Text file containing either a subset or a complete set of internal coordinates (variables). Usually created by the `write vs_var` command. It may also be typed manually. In contrast to an object file (*.ob) which is a complete description of an object, icm.var may contain any selection of variables. These variables can be read and automatically assigned to a molecule according to molecule name, residue number and variable name.

Examples:

```
rem Va fx Atom  Residue  Mol Obj VaType Symm  Value
va psi  + n       3  gln  mol dl   2    1   180.00
va phi  + c       3  gln  mol dl   1    1   −60.00
va psi  + n       4  met  mol dl   2    1   120.00
va phi  + c       4  met  mol dl   1    1   180.00
```

2.23.23. Multidimensional variable restraint types (icm.rst or *.rst)

define generic attraction zones in internal coordinate space (usually torsion space) in terms of residue name pattern (* for any residue type), relative residue number, and variable names. After the types are loaded, you may use them to assign specific vrestraints using the `set vrestraint` command. Three example restraint types (the third one marked with 'rse' will be used as a penalty term, the first two will be used for BPMC steps):

```
------------------------------------ Two−variable vrestraint
rs  aa      −3.300     0.700     0.542
```

```
va ala* 1 phi    −63.200    22.500
va    * 2 psi    −38.540    25.500
----------------------------------- One−variable vrestraint
rs  vt      −3.511     0.700     0.670
va val* 1 xi1    174.690    29.225
-------------------------------------
rse fmr     −3.267     0.700     0.525
va phe* 1 xi1    −66.780    29.700
va    * 1 xi2     98.680    75.100
```

Explanation of fields:

- **aa** − rs−name (not longer than 4 characters). Usually the first character is a 1−char residue name, and the second is the zone character (a − alpha, b−beta, g−gamma,d−delta,t−trans,p−plus 60, m−minus 60,n−null)
- **−3.300** − well depth (should be negative)
- **0.700** − flat fraction of the well
- **0.542** − occupancy (probability) of the well with respect to other wells which could be assigned to the same set of variables.
- **ala*** − residue name pattern
- **1** − relative residue number
- **phi** − variable name
- **−63.2** − center of the well for 1 phi
- **22.5** − size of the well (well is −63.2 +− 22.5)
- *** 2 psi** − residue name pattern (* means any), relative residue number (psi formally belongs to C atom of the next residue, that is why the relative number is 2) and variable name

WARNING: remember that the outer borders of the two−dimensional restraints are ellipses, rather than rectangles (the same for the multidimensional ones). To create a sloped surface for all variables involved in the restraint, the well sizes for these variables should be greater than 180.*sqrt(number of angles in the rs) (255.0 for 2 angles).

2.23.24. Multidimensional variable restraints (*.rs)

This file has similar format to the `icm.rst` file. The differences are:

- `rse` and `rs` fields indicate whether the zone will be used for energy or probability, respectively.
- .rs file contains specific residue numbers rather than the relative ones.
- instead of the residue name pattern the file should contain molecule name or "*".

Example:

```
----------------------------------- Two−variable vrestraint
rs  aa      −3.300     0.700     0.542
va 1crn 1 phi    −63.200    22.500
va 1crn 2 psi    −38.540    25.500
----------------------------------- One−variable vrestraint
rse vt      −3.511     0.700     0.670
va    * 3 xi1    174.690    29.225
-------------------------------------
rs  fmr     −3.267     0.700     0.525
va 1crn 4 xi1    −66.780    29.700
va 1crn 4 xi2     98.680    75.100
```

2.23.25. A sample *.col file

The file shows an example of a multicolumn file which can be read with the `read column` command. Arrays *r, e s* and *ent* will be created.

```
# Entropies of several amino acids
#>-r---e------s--------ent---
arg 2.13 184.920211 11.5181
asn 0.81 99.516352 8.1393
asp 0.61 89.629773 6.8057
cys 1.14 85.947233 13.263
gln 2.02 129.68481 15.576
glu 1.65 119.957333 13.75
his 0.99 121.124577 8.173
ile 0.75 132.717054 5.651
```

2.23.26. A sample *.tab file

The file shows an example of a .tab file which can be read with the `read table`. It is similar to the previous file but additionally command. Table t consisting of header string t.titl and arrays *t.r, t.e t.s* and *t.ent* will be created.

```
#>s t.titl
 Entropies of several amino acids
#>T t
#>-r---e------s--------ent---
arg 2.13 184.920211 11.5181
asn 0.81 99.516352 8.1393
asp 0.61 89.629773 6.8057
```

2.23.27. Torsion parameters (icm.tot)

The file contains torsion parameters according to Momany et al., 1975. Parameters for type 21 for pro taken from Venkatachalam et al., (1974), Macromolecules, 7, 212, parameters for types 22−23 for cooh taken from Karplus et al., J.Comp.Chem., (1983),4,187−217, DNA parameters are from Veal and Wilson, 1991. We added extra terms and modified the original Momany et al. parameters (psi and xi3 of Met). The format is free.

```
#                              +----symmetry-----+
#        maxEner sign fold exact heavy Pseudo selChar phase
#
tot   0    0.00    0    0    1    1     1 -  0.  # fixed dihedrals
tot   2    0.25    1    1    1    1     1 S  90. # psi
tot  44    0.50    1    1    1    1     1 S  90. # psi : removing the ECEPP alpha bias
tot   3   10.00   -1    2    1    1     1 S  0.  # omg
tot   4    1.35    1    3    1    1     1 H  0.  # xi CH2-CH2
tot   8    0.90    1    3    3    3     3 M  0.  # nh3 term.group of lys,lysn
tot  14    0.00    0    2    1    1     2 H  0.  # xi2 of his (+-90)
tot   5    1.00    1    3    1    1     1 H  0.   # xi3 met
tot   5    1.17   -1    1    1    1     1 H  0.   # xi3 met additional torsion
```

Torsion energy is calculated as: maxEner*(1 + sign*Cos(fold * torsion_angle)) Symmetry is a rotational symmetry in different situations: **Exact** is the exact symmetry (implies presence of all atoms, including hydrogens), **Heavy** implies presence of only the heavy atoms (no hydrogens) but uniqueness of different

atom types. **Pseudo** implies that all heavy atoms are equivalent, and hydrogens are ignored. The last character is a short reference name which can be used in vs_var. For example: v_//M specifies all the torsions rotating terminal hydrogen atoms with symmetry higher than 1, v_//H side−chain torsions rotating heavy atoms, etc.

2.23.28. Van der Waals parameters (icm.vwt)

The file contains ECEPP/2 parameters for peptides (Momany et al., 1975, Nemethy et al., 1983), parameters for DNA atoms: Veal and Wilson, 1991 and other parameters (unpublished).

Example lines:

```
#    type pzat   n_el  energy   Deq     Rvw   Rvwel electroRadii
#
vwt   1   0.42   0.85  0.0370   2.92    1.200 1.200 * h aliphatic
vwt   2   0.42   0.85  0.0610   2.68    1.200 0.808 * h amide,amine
vwt   7   1.51   5.20  0.1400   3.74    1.700 1.700 * c carbonyl
vwt  39   0.00   0.00  0.55     5.911   2.631 2.631 * pseudo atom
```

Each line contains:

1. type reference number (see icm.cod file)
2. atomic polarizability $*10^{24}$ (cm cubed);
3. effective number of electrons
4. −e(kk), kcal/mol − depth of energy minimum at the optimal interatomic distance
5. r(kk), a − equilibrium (optimal) distance between two atoms of the same type
6. van der Waals radius (used in graphics,electrostatics,etc)
7. electrostatic radii, used to calculate geometrical surface boundary in boundary element method and MIMEL calculations

Normally van der Waals parameters *A* and *B* are calculated from polarizability and effective number of electrons (fields 2 and 3). However, if these two fields contain zeros, parameters *A* and *B* are calculated directly from the energy depth and equilibrium distance (e.g. for type 39).

2.23.29. Protein databank file (or *.ent)

Protein Data Bank formatted files consist of x,y,z coordinates, occupancies, and B−factors.

Examples:

```
ATOM    1  N   THR     1      17.047  14.099   3.625  1.00 13.79
ATOM    2  CA  THR     1      16.967  12.784   4.338  1.00 10.80
ATOM    3  C   THR     1      15.685  12.755   5.133  1.00  9.19
```

This file does not provide a complete and unambiguous description of a molecular object. Therefore an object resulting from the `read pdb` command has a special type and needs conversion in order to become a full−scale ICM−object for which energy calculations are possible.

See also: `convert` and `minimize tether` commands .

2.23.30. Sequence (*.seq *.pir *.gcg *.msf *.gb)

Acceptable formats of sequence files:

- ***FASTA and ICM format*** (*.seq the simplest and the most natural):

```
> Name1 comment1 comment2
AGFDSTREMNH−FQW
> Name2
RTPIYQWSCCVANMKL
```

- ***PIR format:*** (*.pir)

```
>P1;Azur_Pses4
    Length: 80
AECSVDIQGN DQMQFSTNAI TVDKACKTFT VNLSHPGSLP KNVMGHNWVL TTAADMQGVV
TDGMAAGLDK NYVKDGDTRV*
//
>P2;Azur_Pses3
    Length: 50
AECSVDIQGN DQMQFSTNAI TVDKACKTFT VNLSHPGSLP KNVMGHNWVL*
```

- ***GCG format*** (difficult to generate and impossible to edit because of the CheckSum):

```
Azur_Alcfa  Length: 69  Check: 4484  ..

       1  ACDVSIEGND AMQFNTKSIV VDKTCKEFTI NLKHTGKLPK AAMGHNVVVS
      51  DGMKAGLNND YVKAGDERV
```

- ***MSF format*** − obsolete multiple sequence format for alignments. Noneditable, contains CheckSums.

- ***GB−Gene Bank format*** − Gene Bank format. Entries start with field names followed by a tabulation and the value. NCBI allows to save in this format.

```
LOCUS     (entry code)
.........(other fields) ...
ORIGIN ...(then the sequence)
        1 tctaaataag ttttacacaa aataagttat ..
//
```

2.23.31. ICM−sequence file (*.se)

contains molecular names and sequences. A simple example with two peptides:

```
ml a
se gly ala ser pro tyr his
se phe trp tyr
ml b
se ala ala ser asn
```

A more advanced example with numbering, N− and C−termini and D−amino acids:

```
ml sub1
```

```
se 0 nter 1 gly 2 ala 2A Dglu 4 asp cooh
ml water
se 18 hoh
```

`ml` field followed by molecule name signals that a new molecule is started. `se` field indicates sequence lines (free format). Residue names should correspond to entries in the `icm.res` residue library. Residue numbers (if any) may be arbitrary, negative and may contain additional characters (e.g. 15A, 15B, etc.). Terminal modifiers (*nter, nh3+, cooh, coo−, conh,* etc.) may be explicitly specified.

2.23.32. ICM−alignment file

ICM−format for sequence alignments. The consensus string contains the following symbols:

symbol	description
space	gap in at least one of the sequences
character	this amino acid is conserved in all the sequences
+	positively charged amino acids (R,K)
−	negatively charged amino acids (D,E)
^	small amino acids: (A,S,G,S)
%	aromatic residues (F,Y,W)
#	hydrophobic amino acid (F,I,L,M,P,V,W)
~	polar amino acid (C,D,E,G,H,N,Q,S,T,Y)
dot	the rest (no consensus, no gap)

The file looks like this:

```
# comments
# Consensus:                        .C~.~I.^ND.MQ.~.K~#.V~K~CK~FT#~LKH.GK#.K..MG
Azur_Alcde   MLAKATLAIVLSAASLPVLAAQCEATIESNDAMQYNLKEMVVDKSCKQFTVHLKHVGKMAKVAMG
Azur_Alcfa   ----------------------ACDVSIEGNDSMQFNTKSIVVDKTCKEFTINLKHTGKLPKAAMG
Azur_Alcsp   --------------------AECSVDIAGNDQMQFDKKEITVSKSCKQFTVNLKHPGKLAKNVMG

# Consensus: FCSFPGH#^#MKG.#
Azur_Alcde   FCSFPGHWAMMKGTLKLSN
Azur_Alcfa   FCSFPGHWSIMKGTIELGS
Azur_Alcsp   FCSFPGHFALMKGVL----
```

Residues can be colored by consensus with the `color alignment rs_` command.

2.23.33. ICM all−file: a file with multiple icm objects.

a file containing several ICM−shell objects divided by the following separators:

```
#> type1  ICM-shell-object-name1
.... obj1.....
.... obj1.....
..............
#> type2  ICM-shell-object-name2
.... obj2.....
.... obj2.....
..............
```

```
etc.
```

Legal separators:

- #>i `integer_name`
- #>r `real_name`
- #>s `string_name`
- #>l `logical_name`
- #>p `preference_name`
- #>I `iarray_name`
- #>R `rarray_name`
- #>S `sarray_name`
- #>M `matrix_name`
- #>seq `sequence_name`
- #>prf `profile_name`
- #>ali `alignment_name`
- #>m `map_name`
- #>g `grob_name`
- #>T `table_name` # the column layout
- #>col `table_name`

  # the column layout

- #>db `table_name`

  # the database layout

- #> `brk` # a protein−data−bank file content
- #> `var` # internal variables (torsions, angles, bonds) for the current ICM−object

A sample file `a.all` containing an integer, real, logical, real array, a pdb−file and a table. You can `read all` this from a file or simply mark the lines and paste them into your ICM−session after the command: `read all unix cat` followed by `Ctrl−D.`

```
#>i numberOffset
  0
#>r lineWidth
  1.00
#>l logo
  yes
#>R boxx
 0. 0. 1. 1.
#>brk
ATOM      1  n   leu m   1       2.602 −12.770  −6.750  1.00 20.00
ATOM      2  ca  leu m   1       2.423 −11.442  −7.311  1.00 20.00
ATOM      3  cb  leu m   1       0.947 −11.187  −7.625  1.00 20.00
ATOM      4  cg  leu m   1       0.758 −11.068  −9.138  1.00 20.00
ATOM      5  cd1 leu m   1       1.487  −9.824  −9.649  1.00 20.00
ATOM      6  cd2 leu m   1       1.335 −12.309  −9.822  1.00 20.00
#>s tt.h
this is a header string of table tt. The arrays follow.
#>i tt.i
15
```

```
#>T tt
#> a b c d
1 2. bla  13
3 5. bli  13
```

2.23.34. Residue comparison table (icm.cmp or *.cmp)

A triangular matrix with relative residue exchange frequences (see actual file). The amino acid character line serves as a ruler. Use your favorite comparison matrix.

2.23.35. Protein profiles (*.prf)

A profile table contains residue preferences for each residue type in each sequence position. The preferences may be derived from a multiple sequence alignment or from three−dimensional structure.

Examples:

```
Cons A    B    C    D    E    F  etc.   Z  Gap Len ..
C   35  −32  143  −42  −52  −12  etc. −62  100  100
P   55   17    6   17   17  −71  etc.  26  100
```

2.23.36. Integer array (*.iar)

File looking like this (free−format):

```
# everything which is not a number will be skipped
1 2 4
  9
numbers may be in a row, or column or be in an arbitrary order.
 −14  9
```

2.23.37. String array (*.sar)

Actually any text file. Each line will be a separate element of a `string array`

2.23.38. Matrix (*.mat)

File looking like this:

```
1 0 0
0 1 0
0 1 1
```

or like that

```
# my matrix
0. 1. 1. 2.2
1. 0. blu  1. 2. # text will be skipped
# 1. 1. 0. 3.      this line is commented out
```

In the latter case the result of `read matrix` command is a matrix of two rows `{0. 1. 1. 2.2 }` and `{1. 0. 1. 2.}` . Lines can be commented out with # sign. All the fields which do not look like

numbers are skipped. If you matrix is symmetric, you may specify only the upper left or the lower right triangle like this:

```
1.
1. 2
1. 2 −1.
1. 2  3. 5.
```

2.23.39. Numerical data (real arrays) (*.rar)

File may contain arbitrarily mixed numbers and strings. Strings will be skipped and numbers will form an array. A hash sign # at the beginning of a line comments this line out.

Examples:

```
# 1.2
1.4
1.8
rem 2.2
```

This array will lead to `{1.4 1.8 2.2}` array.

3. User's guide

This section of the ICM manual contains answers to some popular questions and example scripts for different tasks. We assume that you now understand the basic syntax and concepts of the ICM−shell and elementary molecular operations.

3.1. ICM−shell

3.1.1. How to get help

This entire book can be searched from the command line. You may just type `help` and use */searchString* to find what you want, or use **help commands** or **help functions** to find out about the syntax. If you want help on a multi−word term, e.g. `read pdb`, merge the words, e.g. `help readpdb` . The web version of this book with links is also available (`man.tar.gz` file contains about 2000 html files). See also: `help`, `help commands`, `help functions`.

3.1.2. Customization

There are several mechanisms of helping you to customize your ICM environment:

ICMHOME

Define UNIX environmental variable `ICMHOME` in your `.cshrc` file, e.g.

```
setenv ICMHOME /opt/icm/
```

This will be the directory from which ICM program takes all necessary libraries, databases, etc.

USER environment: $HOME/.icm and $HOME/icmprojects files and directories

In contrast to `$ICMHOME` directory which may be installed under `root` for several users, the `$HOME/.icm` directory contains files which can be changed by a user. Under Windows the directory is `$USERPROFILE/.icm` . The icm−user directory contains the following files and directories:

dir/file	description
`blastdb/`	contains blast−formatted files for ICM sequence searches (see also `s_blastdbDir`)
`config/`	contains `icm.cfg` and `icm.rc` files with startup preferences.
`../icmprojects/`	contains subdirectories with icm files for saved project (see also `s_projectsDir`).
`inx/`	default location for database index files (see also `s_inxDir`)
`log/`	contains session logs, (see also `s_logDir`)
`_startup`	if present, overrides the global _startup in $ICMHOME.
`user_startup.icm`	user startup files. Executed **in addition** to `_startup`

Notice that the `icmprojects` is a subdirectory of the user `$HOME` directory rather than the `$HOME/.icm` directory. As a result, the whole `$HOME/.icm` directory can be removed and automatically

recreated with the default settings by `icm` without loosing any of the project information.

general _startup

Adjust `_startup` file to your needs. Define directories, PostScript viewer, help engine, database directories, etc.

Examples are given below.

```
 s_pdbDir     = "/data/pdb/" # set it to the place where PDB lives
 s_helpEngine = "icm"        # default, web-browser is an alternative
 s_prositeDat = s_icmhome+"prosite.dat" # you may have your own updated file
 s_psViewer   = "/usr/opt/bin/gs -q"    # xpsview may be more standard
 s_tempDir = "/tmp"       # better be accessible only for you
```

Set $BLASTDB system environment variable for searches in the blast−preprocessed sequence databases (see the `find database` command).

individual user_startup.icm , gui−controls and menus :

additional **personal custom commands** can be stored in $HOME/.icm/user_startup.icm file under UNIX and `$USERPROFILE/.icm/user_startup.icm` under Windows . This allows to have your own additional setup which follows a general $ICMSCRIPTDIR/_startup[.icm] file execution. We also recommend that you create a `.icm` directory in your home directory and store all additional files, such as your personal `icm.clr` , GUI−setup and color file, and other custom files. Example personal `user_startup.icm` file in which we use personal GUI files:

```
LIBRARY.clr = Getenv("HOME")+"/.icm/icm.clr"  # USERPROFILE under Windows
LIBRARY.men = Getenv("HOME")+"/.icm/icm.gui"  # now gui will invoke your file
read color   # updates your GUI−control and color setup
```

aliases :

Define `aliases` convenient for you.

hotkeys :

Use, define new or modify old keystrokes. `Set key` command allows you to create efficient keystrokes to control graphics

macros:

Create `macro`s for all frequently used interactive operations and their combinations.

3.1.3. How to write a nice demo with menus to impress the boss

See example in the description of the `menu` command and the _demo family of scripts.

3.1.4. How to boost learning process while reading the ICM manual

- Start ICM, mark (copy) all the example lines from the manual with the mouse and paste them to the ICM−shell text window. Try each line as you read it! You will immediately see the result and will be able to play around. Note: in principle you may mark several lines, but sometimes the buffer gets overflown. In this case paste lines in smaller chunks or one by one.
- Use HTML cross−references.
- Write to support@molsoft.com if you have questions or need an ICM−shrink.
- Always use TAB key while typing the command.

3.1.5. How to get the list of the command words

Use `list command` to see the whole list of valid ICM words. If you need a list of all available ICM functions, use `list function` command instead.

`help commands` and `help functions` will give all the syntax lines too.

3.2. ICM graphics

3.2.1. How to learn the ICM molecular graphics in 30 seconds

To master ICM graphics you only need to know the following words: **commands:** `display`, `undisplay`, `color`, `center`, `delete`, `connect` ;

nouns: `wire`, `cpk`, `ball`, `stick`, `xstick`, `surface`, `skin`, `ribbon`, `label`, `residue`, `atom` ;

`selection`: e.g.

```
a_1.       # the first object
a_1.1      # the first molecule
a_1.1/5:10 # residues from 5 to 10
a_1.1//ca,c,n          # the backbone atoms
Sphere(a_1.1 a_2. 10.) # atoms around a_1.1 in a_2.
```

colors: white, black, blue, green, etc. (see file `icm.clr`).

output image formats: png , tif (default) , targa, gif , rgb .

Now start from the command word and type what you need, and use `controls` to `rotate`, `translate`, label, zoom, mark and color.

Example:

```
read pdb "1crn"
display ribbon
color ribbon a_/4:8 blue
display xstick a_1.1/10 green
center a_/6:12
display residue label a_/6:12
display string "Crambin" 36 red
write image rgb "crn"  # use IRIX imgview to check the image
```

```
write image window=2*View(window) # hi-res picture
```

More advanced topics: `connect` , `graphics objects` .

3.2.2. How to make a nice high−resolution image

So called *computational biology* is primarily about generating nice pictures. Here are a few tips.

1) **image display.** Display your molecule or molecule the way you like. Running the `nice` macro (e.g. nice "1est") is a good start.

2) **background.** Change **background** color with `Ctrl−E` and `Ctrl−Q` to your liking.

3) **fog.** It is a great visual effect. Use it! Switch on the depth−cueing effect, i.e. fog with `Ctrl−D` (depth). Move the bright front clipping planes with `Ctrl−MidMB` and move the back clipping plane closer with vertical movements with `MidMB` at the right margin of your graphics window (the mapping of the mouse controls to effects is defined by the icm.clr file).

You may color the **fog** with `color volume` *color* command and modify `fogStart` to increase or decrease the unfogged slice of the molecule.

4) **grobs.** Make them smooth with `select g_..` and pressing `Ctrl−X` and unselecting with the `Esc` button. To shine light from outside sometimes you need to say `display reverse` .

5) **quality** of graphic elements. set `IMAGE.quality=12` or `15.` This parameter determines the number of triangles in shapes like spheres and cylinders. The default value is only 5. because at routine interactive work you prefer speed to quality.

6) **image resolution.** Let us count pixels. Your screen window is usually about 600x600 pixels which corresponds to 2x2inch picture at 300dpi resolution, or 1x1 inch at 600dpi. Therefore, if you want to `generate image` at high resolution use two tricks: (i) make your window as large as possible; (ii) use the `write image` command with option `window=` and select a factor 2 or 3 to generate 2 or 3 times large image respecively, e.g.

```
write image png window= 2 * View(window)
```

Be careful, the `window` option will not save the text labels. It is preferable to add text labels outside ICM anyway.

7) The picture is ready. Enjoy the attention.

3.2.3. How to rotate one molecule around its own center of mass

First, you need to move the molecule of interest to the center of the screen: `center` to this molecule and use the `connect` a_*molselection* command to 'connect' your mouse to just this molecule and leave everything else unchanged. You will see that E.g.

```
read pdb "2ins"
center a_b
connect a_b    # use mouse LB to rotate and translate
```

3.2.4. How to rotate or translate one or several molecules with respect to the rest.

You can rotate/translate/zoom the whole scene with all molecules (see the `set view` command), or rotate/translate a selection of molecules with respect to the rest.

To achieve the second goal from a script, learn about these elementary operations

Memorizing and resetting position of an ICM object

To memorize rotation and translation of an object or a group of molecules in an object, use the Value function and memorize the values of six positional variables for each molecule which have names `tvt1,avt1,bvt1,tvt2,avt2,tvt3` and can be selected as v_*molecules*//?vt* .

```
buildpep "AAA;GGG;WERR"  # (or read pdb and convertObject )
      v1 = Value( v_1,2//?vt* )# MEMORIZE 6-var per molecule.
      connect a_1,2            # move the connected 2 molecules around
      set v_1,2//?vt* v1       # RESET the values
```

Translating the selected molecules

```
buildpep "AAA;GGG;WEGG"
      translate a_1,2 add {0., 0., 1.}
      for i=1,10
        translate a_1,2 add i*{0.,0.,0.2}  # incremental translation
      endfor
```

Calculating translation vectors

Follow these steps:

- choose one representative atom (e.g. the first virtual atom `a_1//vt1 )`)
- memorize its coordinates using the `Xyz` function (e.g. `r1 = Xyz( a_1//vt1 )`)
- set you molecules to another position (e.g. `connect`)
- memorize the position again (e.g. `r2 = Xyz( a_1//vt1 )`)
- calculate the difference: `vtr = Rarray( r2 - r1 )` . The `Rarray` function will convert a 3x1 matrix to a 3-dim. vector

Now one can translate the first molecule only with respect to the rest. It can be done iteratively like this:

```
buildpep "AAA;GGG;WEGG"
      for i=1,10
        translate a_1 0.1*i*vtr
      endfor
```

Rotating selected molecules around specified axes.

First one needs to do the following:

- find the rotation axis with the `Rmsd` function (described in a section below)
- find the rotation matrix with the `Rot(R_center,R_axis,r_angle)` function.

- apply the `rotate` command.

Making grob gradually disappear in the backround

One needs to use `Color` (grob) function. See examples in the description of the `color grob` command.

3.2.5. How to annotate a molecular image in the graphics window

Simply use `display string` command allowing to place a string into the graphics screen. The string can be dragged later to any location with the middle mouse button. You can set font, color and positions you like. Obsolete strings can also be `undisplayed` or removed by the command `delete label`, or by the `BACKSPACE` key when the cursor is in the graphics window (see `keyboard and mouse controls`).

3.2.6. How to save and print the generated image

Save the image using `write image` command, preview it with the IRIX `imgview,` convert it to the PostScript format and print it. You may also save image directly in PostScript format, either as a bitmap snapshot or as a vectorized high−quality model of linear, triangular and string primitives, as they are rendered on your display. See

`write image`

and

`write postscript`

for details.

3.2.7. How to change the color of the graphics window background

Command `color background` allows to set any color from those specified in the file `icm.clr`, for example

```
  color background white              # or
  color background black              # or
  color background aquamarine
```

Note that numeric values may also be used, for example:

```
display string "background\ncolor test" 0.4, 0.9
ncolor = 127
for icolor = 1, ncolor, 1
  color background icolor
  display string "color number " + String (icolor)
  delete label 2
endfor
delete label
display string "the end"
color background black
```

See also `icm.clr` file.

3.2.8. How to return a molecule to the center of the graphics window

Use the `center` command.

3.2.9. How to color atoms according to their B−factors

Command `color` can use any real array as a set of individual color numerical specifications. The smallest number corresponds to the red color, the largest number to the blue one. Function `Bfactor(` *as_* `)` returns the real array of B−values for each selected atom.

Examples:

```
read pdb "1crn"
color a_1crn.//* Bfactor(a_1crn.//*)
```

3.2.10. How to color residues according to their hydrophobicities

It is very simple:

```
read object "4pti"
display a_//!h* white
display surface a_1.1 a_1.1
s_method = "surface"   # s_method = "xstick" or "cpk" is also possible
                                    # hydrophobic
color $s_method yellow a_/ala,val,phe,ile,leu,pro,met/!c,n,o,hn
                                    # polar
color $s_method pink   a_/ser,thr,tyr,cys,asn,gln,his,trp,gly
                                    # charged (+)
color $s_method blue   a_/lys,arg/nz,hz*,nh*,hh*
                                    # charged (−)
color $s_method red    a_/asp,glu/oe*,od*
display string yellow  "hydrophobic: yellow" 25, −0.9, 0.9
display string pink    "polar: pink"         25, −0.9, 0.6
display string blue    "charged(−)"          25, −0.9, 0.8
display string red     "charged(+)"          25, −0.9, 0.7
```

See also How to color atoms according to their charges.

3.2.11. How to color residues according to their accessibilities

Function `Area` is required.

Example:

```
read object "crn"
show surface area   # calculate the surface energy contribution
                    # (hence, the accessibilities are also calculated)

assign sstructure a_/* "_"
                    # remove current secondary structure assignment
                    # for "tube" representation
```

```
display ribbon
                    # calculate smoothed relative accessibilities
                    # and color the tube according
                    # to the accessibilities of the residues
color ribbon a_/* Smooth(Area(a_/*)/Area(a_/* type) 5)
                    # plot residue accessibility profile
plot Count(1 Nof(a_/*)) Smooth(Area(a_/*)/Area(a_/* type) 5) display
```

3.2.12. How to color atoms according to their charges

Use function `Charge` . For example:

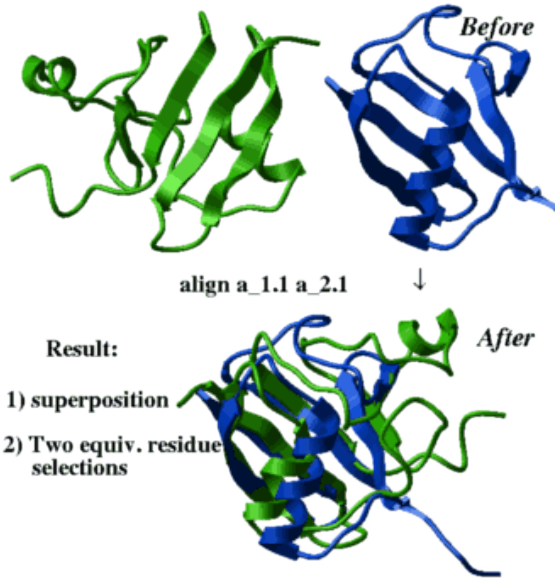
```
read object "crn"
display surface
color a_//* Charge(a_//*)
```

Another example is selected residues coloring:

```
display a_*./asp,glu/o?* cpk red
display a_*./lys,arg/nz,n?* cpk blue
```

3.3. Structure analysis

3.3.1. How to optimally superimpose two 3D structures



Optimal superposition implies optimization of the Ca−RMSD upon rigid body superposition of the *equivalent* residues/atoms. This set of equivalent positions can be predefined, or determined by sequence alignment, or automatically derived from structure. In the latter case the optimized value is the RMSD of a trial alignment is corrected by the alignment length to reward longer alignment with slightly worse RMSD.

There are several different algorithms which can be applied:

- superimpose by known residue or atom equivalences (see the `superimpose` command)

- superimpose by sequence alignment which is calculated on the fly:

```
superimpose a_1.1 a_2.1 align  # the sequences are generated on the fly
```

  This procedure fails if two structures have no significant sequence similarity
- `align ..` command to find *global structural* alignment (returned by the `ali_out` variable) and superimpose accordingly. Here we do not rely on sequence alignement (although it can be added to the optimized scoring function with a certain weight).

```
align a_1.1 a_2.1
```

- Align(.. distance) for local structural alignment

Use `superimpose` command. It performs an optimal rotation and translation of one structure onto the other. If necessary, a sequence alignment may be done prior to superposition by specifying `align` option in the command line.

Example:

```
read pdb "3znf"
display a_1.1//n,ca,c magenta
make sequence a_1.1
read pdb "1ard"
display a_2.1//n,ca,c blue
make sequence a_2.1
show sequence
                # somewhat different sequences of two Zn-fingers
                # sequence alignment is required
superimpose a_1. a_2. align
```

Note, in this particular example, the whole structural similarity is not so high. However, better fit may be obtained if only portions of the structures are superimposed, for example:

```
superimpose a_1.1/16:27/n,ca,c a_2.1/116:127/n,ca,c align
```

See also: `Rmsd( )` and `Srmsd( )`.

3.3.2. How to optimally superimpose without the residue alignment

The core of this procedure is the

`align` *ms_molecule1 ms_molecule2*

command. There are two variants: a fast superposition using dynamic programming algorithm `align [distance]` *ms_1 ms_2* or a more rigorous, but somewhat less stable and slow `align heavy` *ms_1 ms_2* ... command. This first command is well described above and identifies only the best superposition. The initial superposition is then refined similarly to the `find alignment` command.

The second algorithm (option `heavy`) identifies a number of possible superpositions (solutions) based on the Ca atom coordinates only. The first solution is the best hit. See also `load solution` command.

Examples:

```
read pdb "4fxc"
read pdb "1ubq"
display a_*.//ca,c,n
color molecule a_*.
align a_1.1 a_2.1
center
color red  as_out
color blue as2_out
show ali_out
```

3.3.3. How to make a Ramachandran plot

Use macro `plotRama` . The macro is invoked by

`plotRama` *rs_selection l_addLabel l_addBoundaries*

Important: if a PDB structure is analyzed, `convert` it first to get a proper ICM−object (true ICM−molecular object does not require prior preparation for building Ramachandran plot).

Example:

```
read pdb "1crn"
convert a_1.               # Note, one more object appeared in addition
                           # to the original (PDB) object 1crn
l_addLabel = yes           # add residue labels to the plot
l_shadedBoundaries = yes   # add allowed regions to the plot

plotRama a_2. l_addLabel l_shadedBoundaries
quit
```

3.3.4. How to display hydrogen bonds

A list of `hydrogen bonds` may be calculated and displayed for an ICM−objects or non−ICM object with hydrogens. If you are dealing with a PDB structure without hydrogens, `convert` it first. The command `show hbond` prints list of hydrogen bonds in the text window. After that they can be `display`ed. (Hydrogen bonds can also be calculated by `minimize` and `show energy` commands provided that the `hydrogen bond energy term` is switched on.)

The `display hbond` command allows to show the deviation angle of the hydroben bond from linearity (see the `GRAPHICS.hbondStyle` preference).

Examples:

```
read object "crn"      # already converted
show energy
display
show hbond 2.5 a_/1:15  # list of H−bonds with H−X distance < 2.5 A
                        # appears in the text window
display hbond 1.9       # H−bonds shorter than 1.9 A are shown
GRAPHICS.hbondStyle = 3
display hbond
```

See also: GRAPHICS.hbondStyle

3.3.5. How to identify atoms or residues at the molecular interface

When two or more parts of the polypeptide chain(s) are near each other in space, they are referred to as a molecular interface. What "interface" is can be defined more specifically in the context of a particular study, so here only an example is given to illustrate how interface may be identified and displayed. Two ICM functions are to be used for that, viz. Sphere and Acc . Suppose, you analyze 3D structure of a complex of two molecules, and would like to see what residues are at the interface. It can be done by the following:

```
read object "complex"
display a_1,2//!h*         # display both molecules
                           # without hydrogens

color a_1 yellow
color a_2 green

show area surface a_1//!h* a_1//!h*      # calculate surface of
                                         # the 1st molecule only

color red Sphere(a_2//* a_1//* 4.) Acc(a_1/*)# interface residue atoms
                                             # of the 1st molecule
                                             # in 4 A radius vicinity
                                             # of the 2nd molecule

show area surface a_2//!h* a_2//!h*      # calculate surface of
                                             # the 2nd molecule only

color blue Sphere(a_1//* a_2/* 4.)# interface residue atoms
                                             # of the 2nd molecule
                                             # in 4 A radius vicinity
                                             # of the 1st molecule
```

If, instead, you need to mark **residues,** convert the selection of the interface atoms to residues with the Res () command:

```
....                                         # same as above.
....
resAtInterf =  Res( Sphere(a_2//* a_1//* 4.)) Acc(a_1/*)
display residue label resAtInterf
```

Note that in the Sphere command it does not matter if you specify the atom selection or a residue selection as an argument, since the function operates at the atom level anyway. The difference in the specification of the ICM selection in these two examples (usage of **two** slashes for atom selection, and **one** slash for residue selection):

Sphere(a_1.1/* 4.) *versus* Sphere(a_1.2//* 4.) and also Acc(a_1.1/*) *versus* Acc(a_1.2//*) for specifying residues and atoms, respectively.

Important: when calculating surface, be sure that you properly specify the selection arguments in the show area surface command.

3.3.6. How to select accessible, buried, hydrophobic, residues.

Selecting exposed residues. Here is one way to compile a list of exposed residues. Use the `Acc` (*rs_* [*r_threshold*]) function. It will return all residues for which relative residue solvent accessibility is larger than certain limit (by default it is 25% of its fully accessible surface). To use the function you need to get rid of water molecules and use the `show surface are` command. Follow this example:

```
read pdb "1crn"
delete a_W                # delete water molecules
show surface area         # compute exposed surface areas for each residue
show Acc( a_/* , 0.25 )   # show all residues exposed more than 25%)
show !Acc(a_/* , 0.25 )   # show buried residues
```

Converting the selection into other formats

You can also show the selection in a different format, e.g.

```
  String( Acc( a_/* ))  # or
a_1crn.m/1,5:8,11:12,14:15,17:20,22:25,28:29,31,33:34,36:46
       Label(  Acc(a_/*))
#>S string_array
T1
P5
S6
I7
V8
S11
...
```

Identifying buried polar residues

About 50% of all residues have relative accessibility less than 25%. Polar residues typically do not like to be buried. The charged residues like it even less, and if they are buried they usually form a salt bridge. Example:

```
read pdb "1qau" # neuronal nitric oxide synthase
display
display xstick a_/62,121 # buried asp and arg form a bridge
```

To identify buried charged residues, use combine the previous selection of the buried residues with specific residue type selection, e.g.:

```
read pdb "1qau"
delete a_W
show surface area
show a_/asp,glu,arg,lys ! Acc( a_/* 0.15 )
```

Here we used a more conservative threshold of `0.15` as the burial threshold. Feel free to modify the selection of residue types above to find other buried residues.

Identifying exposed hydrophobic patches

A similar technique can be used to identify hydrophobic patches:

```
read pdb "1qau"
delete a_W
show surface area
show a_/leu,ile,val,met,trp ! Acc( a_/* )  # buried ones
show Acc( a_/leu,ile,val,met,trp )           # exposed hydrophobs
```

To find clusters of exposed hydrophobic residues, use the `Sphere` function. The Sphere function returns atoms, and they need to be converted to residues with the `Res` function.

```
exposed_hres =  Acc( a_/leu,ile,val,met,trp )
for i=1,Nof(exposed_hres )
  nbrs = Res(Sphere( exposed_hres[i] exposed_hres , 5.0 ))
 if Nof( nbrs ) >= 2 show nbrs   # show pairs of exposed hydrophobs
endfor
```

3.3.7. How to identify torsions at the molecular interface

Identification of the torsions belonging to residues at the molecular interface is a necessary and non−trivial step in many tasks of the molecular modeling. An example below shows how this identification may be done in ICM. The same as above ICM−object "complex" is considered.

```
read object "complex"
display a_1.1,2//!h*                  # display both molecules
                                      # of the complex w/o hydrogens
color a_1.1 yellow
color a_1.2 green

show area surface a_1.1//!h* a_1.1//!h*   # calculate surface of
                                          # the 1st molecule only
a1=Sphere(a_1.2//* 7.) Acc(a_1.1//*) # define the 1st molecule atoms
                                      # belonging to the interface
                                      # of the 1st molecule
                                      # in 7 A radius vicinity

v1=V_1.1//S a1                       # identify standard geometry
                                      # torsions of the 1st molecule
                                      # belonging to the interface

color red Atom(v1)                    # color atoms which torsions
                                      # belong to

                                      # similar for the 2nd molecule
show area surface a_1.2//!h* a_1.2//!h*

a2=Sphere(a_1.1//* 7.) Acc(a_1.2//*)
v2=V_1.2//S a2
color blue Atom(v2)
```

3.3.8. How to calculate packing density

The packing density analysis requires understanding of two types of surfaces: the `skin` (molecular surface) and solvent−accessible `surface` of water probe **centers** (which is one water radius away from the `skin`). The following is an example of how it may be done for a fragment of a protein.

```
read object s_icmhome+"crn"
asel = a_/5:15
show volume skin asel asel
rskin = r_out
vwExpand = 0.
show volume surface asel asel
rsurf = r_out
print "skin volume = ", rskin, "; vw volume = ", rsurf
print "packing density = ", rskin/rsurf
```

3.3.9. How to perform a principal component analysis

For a set of objects with given measure of similarity between each two of them, one can easily perform the principal component analysis or to solve a `distance geometry` problem by using `Disgeo` function. The following example shows how to get a two−dimensional distribution of amino acid sequences of a series of Zn−fingers given the distance between sequences is defined by `Distance`(*sequence1 sequence2*) function. This distance is essentially a measure of sequence similarity: the distance is 0. for two identical sequences, it is propotional to percent identity divided by 100. for very similar sequences and goes above one at about 30% sequence identity, tending to infinity for very small seq. identity numbers.

```
read sequences s_icmhome+"zincFing" # read sequences from file,
list sequences              # see them, then ...
group sequence alZnFing     # group them, then ...
align alZnFing              # align them, then ...
a = Distance(alZnFing)      # calculate a matrix of pairwise
                            # distances among them
n=Nof(a)                    # number of points
b=Disgeo(a)                 # calculate principal components
corMat = b[1:n,1:n−1]       # coordinate matrix [n,n−1] of n points
eigenV = b[1:n,n]           # vector with n sorted eigenvalues
xplot  = corMat[1:n,1]
yplot  = corMat[1:n,2]
                            # plot 2D distribution
plot xplot yplot CIRCLE display
```

3.3.10. How to calculate a dihedral angle

Normal dihedral angles like torsion angles describing conformation are directly available through the `Value`( ) function. You need to `convert` an object into the ICM type if necessary.

Example:

```
read pdb "1crn"        # read it in
convert                # quickly convert into ICM−object
show v_//phi,psi       # just show all phi,psi's
show v_/3:17/xi*       # show chi angles of residues from 3 to 17
a = Value(v_//phi,psi) # create a real array of values of spec. torsions
```

You can calculate a dihedral angle between any two planes defined by three atoms (for example two Phe rings) with the `calcDihedralAngle` macro. If this macro is loaded, you can do the following:

```
read object "crn"
as_1 = a_/1/n,ca,c
as_2 = a_/3/n,ca,c
display a_//n,ca,c blue
color as_1 magenta
color as_2 green
calcDihedralAngle as_1 as_2
print "dihedral angle 1(n,ca,c) and 3(n,ca,c) (deg) = ", r_out
```

Note that the order of atoms in the selections *as_1* and *as_2* is determined only by the ICM−molecular tree (will be the same for a_//n,c or a_//c,n). Thus, any changes in the selections *as_1* and *as_2* not changing their content has no effect on the resulting dihedral angle:

```
as_1 = a_/1/ca,c,n
as_2 = a_/3/ca,c,n
calcDihedralAngle as_1 as_2
print "dihedral angle 1(n,ca,c) and 3(n,ca,c) (deg) = ", r_out
```

See also: `Acos( )`, `Length( )`, `Sum( )`, `Vector( )`.

3.3.11. How to print a table of the torsion angles

The simplest list can be generated by:

```
show V_//*               # or
show V_//phi*,psi*,omg*  # or
show V_//xi*             # side chain torsions
```

A nicer formatted output (one line per residue) may be generated with macro `printTorsions,` for example:

```
read pdb "1crn"
convert
printTorsions a_/2:15
```

Note, that you do not need to convert your molecular object if it is an ICM−object.

3.3.12. How to build a hydrophobicity profile

First, define a hydrophobicity scale, for example that from Kyte and Doolittle, 1982 or use your favorite one. (Note, there should be 26 entries in the hydrophobicity parameters list *hPhobInd* corresponding to the 26 letters of the alphabet. Non−participating letters B,J,O,U,X,Z are marked by zero values.)

```
                # define a hydrophobicity scale
hPhobInd = { 1.8,  0.0,  2.5, −3.5, −3.5,  2.8, −0.4, \
            −3.2,  4.5,  0.0, −3.9,  3.8,  1.9, −3.5, \
             0.0, −1.6, −3.5, −4.5, −0.8, −0.7,  0.0, \
             4.2, −0.9,  0.0, −1.3,  0.0}

                                # make a macro
```

```
 macro hPhobProfile seq_ i_windowSize
   if (Type(i_windowSize)=="unknown") then
     i_windowSize = Ask("Enter window size",windowSize)
   endif
   R_window = Rarray(i_windowSize,1./i_windowSize)
   R_hphob  = Smooth (Rarray(seq_,hPhobInd),  R_window)
   R_ruler  = {0.,0.,10.,10.,0.,0.,0.,0.}
   R_ruler[2] = Real(Length(seq_))
   r_tic = 1./Sqrt(Real(i_windowSize))
   r_tic = Integer(r_tic*100.0)/100.
   R_ruler[5] = -7.*r_tic
   R_ruler[6] =  7.*r_tic
   R_ruler[7] = r_tic
   R_ruler[8] = r_tic
   print R_ruler
   s_legend = {"Hydrophobicity plot","Sequence","Hydrophobicity"}
   xplot = Count(1 Length(seq_))
   yplot = R_hphob
   psfilename = "hphob"
   plot xplot yplot R_ruler s_legend grid="xy" display psfilename
   delete R_window R_ruler r_tic
 endmacro
                                  # now, an example
 read object "crn"
 s = Sequence(a_)
 hPhobProfile s 7
```

3.3.13. How to display and characterize protein cavities

ICM offers fast, elegant and mathematically accurate way to identify, display, and measure protein cavities. An example session which displays all cavities with their surroundings, and calculates their volumes and surface areas:

Examples:

```
 read object "crn"  # or whatever
 make grob skin "g_skin"
 split g_skin
 nShells = i_out
 display wire residue labels
 for i=1,nShells
   v = Volume(g_skin$i)   # actually its surface is returned in r_out
   s = r_out              # there is no need to use the explicit Area(g_skin$i)
   if(v > 0.) then        # note that cavities have negative volume!
     display transparent smooth g_skin$i
     printf "Shell  %d: V=%f A=%f\n", i, v, s
   else
     display reverse smooth yellow g_skin$i
     center g_skin$i
     printf "CAVITY %d: V=%f A=%f R~%f\n", i, -v, s, -3.*v/s
   endif
# add pause here for an interactive session
 endfor
```

3.4. Sequence, searches and alignments

3.4.1. How to search all Prosite patterns in your sequence

Use macro `searchSeqProsite.` For example:

```
  read pdb "2dhf"
  make sequence a_1.1        # sequence of a PDB structure
  show sequence
  find prosite 2dhf_a        # 2dhf_a is the sequence of the protein
```

See also `find prosite`, `find pattern` and `read prosite`.

3.4.2. How to find a fragment in the PDB database (obsolete)

First, make sure that you have a library of representative icm−objects. String variable `s_qsearchDir` should contain the relative path of this directory with respect to the `s_dataDir` directory. The library may be created and updated with the provided `_mkQsearchLib` script. Use `qsearch` or `iqsearch` macros. Load the object and type qsearch or iqsearch + arguments. You will be prompted for the forgotten arguments.

To understand the meaning of the arguments, see the `find pdb` command.

Examples:

```
 read object s_icmhome+"crn"
 call s_icmhome+"_qsearch"
                # no graphics, just the list of solutions
# qsearch a_/2:6,14:18
                # interactive
 iqsearch a_1crn./2:6,14:18 "xxxxx------xxxxxx" "*" "*" .7
```

3.4.3. How to identify binding pockets

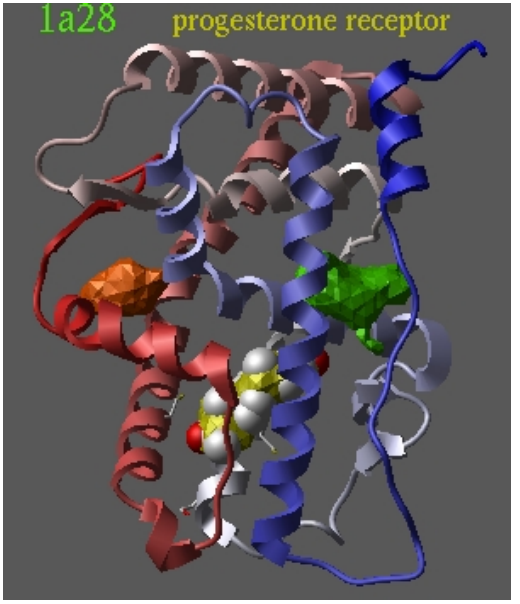
There are three algorithms (A, B, and C) with ICM which can identify pockets:

option	target	macro
A	closed pockets	`icmCavityFinder`
B	almost closed pockets	`make map potential` , etc., see below
C	pockets with good ligand−binding potential	`icmPocketFinder`

For the areas of space attracting ligands (option C), use two macros:

Example:

```
read pdb "1a28"
delete a_!1,2
convert
delete a_2
icmPocketFinder a_ 3.
```



In the following example we find an **almost closed pocket** which can not be identified with icmCavityFinder .

```
read pdb "1fm6"  # read the 'a' chain of RXR
delete a_!1,9    # keep the RXR and its ligand only
make map potential a_1 Box( a_ 1. ) 1.  # grid size 1.5 A
make grob m_atoms exact 0.1 solid
split g_atoms
cool a_
display g_atoms2 reverse
```

If you have problems with identifying pockets, change the grid size, the threshold level for `make grop m_atoms` , or try to `convert` object to the ICM type (the conversion will add hydrogens and make the object more dense).

3.4.4. How to find a similar fold or topological motif in the PDB database

Use macro `searchObjSegment,` for example:

```
read object s_icmhome+"crn"
searchObjSegment a_1.1 30 3.
# or
read pdb "1pxt"
delete a_!1
convert
searchObjSegment a_1.1 24 6.
```

You may need to adjust the seed fragment length and the RMSD parameters for a cleaner list.

The database `foldbank.seg` is provided and may be recompiled, customized and updated by the supplied `_mkSegmentLib` script.

See also `segment`, `find segment`, `write segment`, `foldbank.seg`, How to extract a diverse set of PDB entries How to compile a database of protein secondary structures and their folds .

3.4.5. How to generate a non−redundant list of PDB sequences

The following script is a skeleton of the provided script _mkUniqPdbSeqs which is somewhat more automated.

```
 l_commands=no
 errorAction="none"        # if something goes wrong do not
                           # interrupt the loop
 s_pdbDir = "/data/pdb/"   # make sure you have correct path
 pdbDirStyle = 4           #
 read sarray s_pdbDir+"/derived_data/index/source.idx"
                          # you need a list of all pdb−entries
                          # (4 char. code per line will do)
 source = Tolower(Trim(Field(source,1)))
 n=Nof(source)
 for i=1,n
   read pdb sequence resolution source[i]
        # append resolution to the chain name (like 9lyz_a19)
 endfor
 group sequence "*" uniqSeqs unique 0.1
        # cutoff inter−sequence
        # distance 0.1 (dissimilar by more than 10%)
#
# Other possibilities
#
#  group sequence uniqSeqs unique 5     # if two seqs differ by more
#                                       # than 5 mutations
#  group sequence uniqSeqs unique       # throw away only identical
#                                       # sequences
#
 delete sequences                     # get rid of sequences not
                                      # included in uniqSeqs

 write sequence s_inxDir + "/pdb1.seq"
                              # actual sequences for searches
 write Name(uniqSeqs) "chainList"
                              # list of protein chains if you need it
 quit
```

3.4.6. How to merge several pdb files

The simplest way to merge two pdb files is to read them as separate objects and the use the `move a_1. a_2.` command. Example:

```
 read pdb "1crn"
 read pdb "1d48"
 move a_2. a_1.        # merges objects
```

```
write pdb a_1. "both" # saves both files in pdb format
write object a_1.     # saves merged object in compact binary form
```

Before or after merging, the objects can also be edited, `translated` to a new position, `rename` chains, `change residue numbers` etc. Example:

```
read pdb "1d48"
delete a_w*
delete a_2       # delete the second chain
read pdb "1crn"
delete a_/33:99  # delete a C−term. part of crambin
move a_1. a_2.   # merge the remains
write object a_
```

If you want to re−engineer a polypeptide chain of a protein, using two pdb−files, e.g. to transplant one part of a protein to another and restore the bonding connectivity, you may use the `modify` command:

```
read pdb "1crn"  # one pdb
read pdb "1cbn"  # similar protein
modify a_1./20:25 a_2./20:25
  # translants a loop from 2nd object to the 1st one
write pdb a_1. "combo"
```

3.4.7. How to compile a database of protein secondary structures and their folds

The following script uses the previously compiled list of unique pdb chains and creates two files: `foldbank.db` containing sequences, resolutions, the deposited and the automatically assigned secondary structures of the nonredundant set and `foldbank.seg` containing quantitative topology descriptions of the folds. The GAP (which stands for Gly−Ala−Pro) library allows to build only the backbones necessary for the secondary structure prediction algorithm and speeds up the PDB−>ICM conversion. The `foldbank.db` is in the ICM `database` format, so that you can create an ICM `table` shell−object. This allows to `sort` entries and perform searches to create subsets.

```
l_commands    =no
l_info        =no
l_confirm     =no
errorAction="none"
segMinLength  =3
mncalls       =300
s_icmhome     ="./"
s_reslib      ="icmGAP" # Gly−Ala−Pro residue library
read library
      # ...getting the representative list of chains...
read sequences s_pdbDir+"/derived_data/pdb_seqres.txt"
      #make sure to have  _mkUniqPdbSeqs  executed recently
li=Name(sequence)
delete sequences
      #...you may modify the method or create your own list...
if (Error) quit

unix mv foldbank.db  foldbank.db.OLD
unix mv foldbank.seg foldbank.seg.OLD
for i=1,Nof(li)
  lii=Tolower(li[i])
```

```
  read pdb lii[1:4]+"."+lii[6]+"/"
  delete !Mol(a_*/A)                    # delete HET-molecules
  convert
  er=r_out
  rz=Resolution(a_1.)
  if(rz < 0.01)rz=9.99
  sx=Sstructure(a_*)
  assign sstructure
                    # uncomment the following line, if you'd like
                    # to save GAP objects. requires GAP subdirectory
                    # write object "GAP/"+lii[1:4]+lii[6]
  sprintf "# %d\nNA %s.%s\nRZ %.2f\nER %.3f\nSE %s\nSX %s\nSS %s\n" \
          i lii[1:4] lii[6] rz er String(Sequence(a_*)) sx Sstructure(a_*)
  write append s_out "foldbank.db"
  assign sstructure segment
  rename a_2. lii[1:4]  # restore the original pdb-name
  write append segment "foldbank.seg"
  delete a_*.
endfor
quit
```

3.4.8. How to search headers of the PDB entries

There is an PDB.tab file which contains one line header descriptions of all the entries. Now you have three ways of doing it:

- In unix:

  grep -i kinase PDB.tab

- From ICM: you have more possibilities:

```
read table s_icmhome+"data/inx/PDB.tab"  # or in s_userDir+"inx/"
show PDB.head ~ "kinase"   # or
show PDB.head ~ "*kinase*" # or
show PDB.comp ~ "kinase*"  # regular expressions
# You can also
a=PDB.head~"kinase"
for i=1,Nof(a)
  nice PDB.ID
  pause
  delete a_*.
endfor
```

- Use the gui (Find.In PDB.By Keyword..)

3.5. Energetics and electrostatics

3.5.1. How to plot the distance dependence of a van der Waals interaction

The following script will plot three energy-interatomic distance plots for three possible van der Waals terms defined by the `vwMethod` preference ("exact"-black,"soft"-blue and "old soft"-red). Simply mark and paste the following lines into your ICM session:

```
 buildpep "one;one"  # two oxygens
 set term "vw" only
 set a_2//o Sum(Xyz(a_1//o ))+{.0 .0001 .0}
 n=200
 a=Rarray(n)
 b=a
 c=a
 r=Rarray( n .03 3.)
 vwSoftMaxEnergy = 14.5
 for i=1,n
   translate a_2 add {0.03 0. 0.}
#
   vwMethod="exact"
   r[i]=Distance( a_2//o  a_1//o ) # use Sum(Distance(..)) for the old version
   show ey mute
   a[i]=Energy("vw")
#
   vwMethod="old soft"
   show ey mute
   b[i]=Energy("vw")

   vwMethod="soft"
   show ey mute
   c[i]=Energy("vw")
 endfor
 s=Sarray(3*n)
 s[n+1]="_red line"
 s[2*n+1]="_blue line"
 plot ds r//r//r a//b//c s {0. 6.01 1. 1. ,-1. 17. 1. 1.}
```

3.5.2. How to calculate the electrostatic free energy by the REBEL−method

This short script solves the Poisson equation by the "Rapid−Exact− Boundary ELement (REBEL) method for crambin.

Examples:

```
 electroMethod="boundary element"
 read object "crn"
 delete a_w*       # get rid of water molecules
 show energy "el"
 show Energy("el")-r_out, r_out # Coulomb and solvation components
```

3.5.3. How to evaluate the pK shift

Suppose we mutate a surface Asp into Ala and want to evaluate how the pK of the neighboring His is changed. The pK shift may be evaluated as the difference of potential at Nd1 His and Ne2 His nitrogens due to the mutation. Since Ala may be considered as uncharged, the shift is simply the potential at the nitrogens due to the Asp charge.

Example (pKshift of His34 from Asp22):

```
 read object "rinsr" # load insulin
                     # we assume that the positive charge is
                     # equally distributed between the two nitrogens
```

```
make boundary
pKshift=Sum({0.5, 0.5}*Potential(a_/his/nd1,ne2 a_/22/*))/ \
        (Boltzmann*300.*Log(10.))
```

3.5.4. How to evaluate the binding energy

There are many different approaches to the evaluation of binding energy. One of the reasonable approximations has the following features:

- van der Waals/hydrogen bonding interaction is excluded since it has close magnitudes for protein−protein and for protein−solvent interactions;
- electrostatic free energy change is calculated by the REBEL method (see also the section "How to calculate the electrostatic free energy ... ") above);
- side−chain entropy change is calculated by standard ICM `entropic term` based on exposed surface area of flexible side−chains;
- hydrophobic energy change is calculated using `surface term` with constant surface tension of 20. cal/Angstrom.

Example:

```
electroMethod="boundary element"
surfaceMethod="constant tension"
surfaceTension=0.020
dielConst = 12.7
set terms "sf,el,en"
read object s_icmhome+"2ptc"
show energy a_1 a_1 mute
e1  =Energy("el,sf,en")
show energy a_2 a_2 mute
e2  =Energy("el,sf,en")
show energy mute
e12 =Energy("el,sf,en")
print "Binding energy = ", e12 − e1 − e2
```

3.5.5. How to calculate an ensemble average

The following is an example of calculating the average of an interatomic distance over a set of conformations collected in the conformational stack. This calculation is written as a macro. Feel free to change it. You may also use `movie` and `load frame` instead of `stack` and `load conf`, respectively.

```
                                # first, define the macro
macro ensembleAverage r_temperature
 l_commands = no
 l_info = no

 load conf 0                     # extract the lowest energy
 e0 = Energy("func")

 ansAver = 0.                    # the statistical sum initialization
 statsum = 0.
 r_temperature = r_temperature * Boltzmann

 for i = 1,Nof(conf)             # loop through all the stack
                                 # conformations
```

```
   load conf i
   prob = Exp((e0-Energy("func"))/r_temperature)

                                  # averaging distance between two ca
                                  # is just an example
   ansAver = ansAver + Distance(a_/2/ca a_/4/ca)*prob
   statsum = statsum+ prob
 endfor
 r_out = ansAver/statsum
 print " Ensemble average is: ", r_out
endmacro
                                # Now you can calculate your average

read object "my_peptide"
read stack                     # stack file is assumed to have
                               # the same name
ensembleAverage 600.           # sometimes you may use the elevated
                               # temperature to account for relaxation
```

3.5.6. How to evaluate helicity of a peptide from the BPMC simulation

1. Run the `_folding` script first. Make sure the procedure converges by running several simulations (say _f1 _f2 _f3) from different random starting conformations. E.g.:

   ```
   cp $ICMHOME/_folding _f1      # adjust the script
   icm _f1 > f1.ou cp _f1 _f2
   icm _f2 > f2.ou cp _f2 _f3
   icm _f3 > f3.ou
   ```

2. You can evaluate helicity for each simulation. If they converge the result will be about the same.

3. Helicity is just the ensemble average of the parameter which can be calculated as the relative number of the helical residues. Therefore you need to assign secondary structure for a particular movie frame or stack conformation and count number of helical residues. See macro _helicity averaging helicity over the movie frames.

   ```
   macro helicity s_movieName r_temperature
   # attention: 'temperature' is extremely important.
   # You may use elevated temperature to account for relaxation.
    l_commands=no
    l_info=no
    read conf 0 s_movieName
    e0=Energy("func") # the lowest energy
    av=0.
    ssum = 0.
    r_temperature = r_temperature * Boltzmann
    res = Real(Nof(a_/*))
    read movie s_movieName
    for i=1,Nof(frame)
       load frame i s_movieName
       assign sstructure
       prob = Exp((e0-Energy("func"))/r_temperature)
       av = av + prob*Nof(Sstructure(a_1/*),"H")/res
       ssum= ssum+prob
    endfor
    print " The best E=", e0, "  Helicity= " av*100./ssum
   ```

```
endmacro
```

3.5.7. How to merge and compress several conformational stacks

You may run several `montecarlo` simulations and accumulate several conformational stacks (`*.cnf` files). To unite them it is essential that they have been created with the same energy function, because the compression algorithm takes the energy into account to decide which structure is more valuable. If it is not the case, you can always recalculate energies for the stack conformations by the following procedure:

```
read object "f"
read stack "f1"
read stack "f2" append # the second stack will be appended
for i=1,Nof(conf)
  load conf i
  show energy s_correctTerms  # say, "vw,14,to,el,sf,en"
  store conf i
endfor
```

Now, to unite all the stacks and compress them you may do the following (just the idea):

```
read object "f"
delete stack
read stack "f1"        # first simulation
read stack "f2" append # second simulation
read stack "f3" append # third simulation
show stack             # look at what you have now
compare v_//phi,psi  # use the comparison criterion from the simulation script
                     # compose a new one, see also the compare command
vicinity = 40.       # you may redefine the vicinity parameter
compress stack
show stack           # look at the compressed stack
write stack "f4"     # save the result
```

3.6. Manipulations with molecules

3.6.1. How to build new object from a sequence

The easiest way to build an object with one of several peptides is to use the `buildpep` macro. There you can use a one letter code (upper case characters) or three−letter code and separate sequences of different chains by a semicolon. Examples:

```
buildpep "AAAAA"       # penta−alanine
buildpep "ASFHGD;EQWR" # two chains
```

To create a DNA duplex or a compound, use GUI.

For a more flexible building procedure, follow the following steps:

1. Create the `ICM sequence file` either manually or using `IcmSequence` function, e.g.:

   ```
   write IcmSequence( "FAASVRES", "nh3+", "coo−") "file.se"

   read sequence "memb.seq" # creates the ICM sequence memb
   ```

```
write IcmSequence( memb , "nh3+", "coo−") "myseq.se"
build "myseq"
```

You can also build sequence directly without creating a file with the `build string`. See the `build` command and `IcmSequence`( ) function.

2. Change the default conformation using the available information. Possibilities:
   - ♦ You have a template pdb file with all the coordinates. Use `regul` macro.
   - ♦ Set particular dihedral angles with the `set` *vs_variableSelection R_arrayOfValues* or

     `set` *vs_variableSelection r_theValue* command.

   - ♦ you can use `minimize`, `montecarlo` and `ssearch` commands to find a low−energy conformation.

Examples:

```
build string "se nh3+ ala his leu trp coo−"
set v_/3/xi1 −60.
minimize
```

3.6.2. How to quickly convert a pdb file into an ICM−object

Sometimes it is necessary to have a PDB file in the form of an ICM molecular object. For example, it's a convenient way to list and/or to change a torsion angle (or a series of them). All what you need is to use `convert` command. One more ICM−format object will be created (use `show object` command to see the list of currently loaded molecular objects). The above method is good only for a limited set of tasks mostly related to structure analysis. If you want to perform further conformational sampling by energy optimization it is better to `regularize` the pdb−object (see the next section)

We recommend to use the `convertObject` macro which optimizes hydrogens and can do some necessary cleanup.

See also `strip`.

3.6.3. How to prepare a PDB structure for energy calculations (regularization)

`Regularization` is a sophisticated multi−step procedure. It consists of the following six steps.

- Preparation of a file with the amino acid sequence.
- Creating full−atom ICM−model (geometrical approximation).
- Rotational positioning of methyl groups.
- Iterative optimization of geometry and energy of the whole structure.
- Adjustment of polar hydrogen positions.
- Free minimization to check the consistency of the resulting structure.

See macro `regul` .

3.6.4. How to create a new molecule or a residue for the ICM residue library

Let us assume that your input is a pdb file with a new small organic molecule and you want to create a proper ICM object from this molecule. What is currently missing in the description may be the following:

- proper chemical bond types (single, double, triple, aromatic). To see them press `Ctrl-W` to switch to wireStyle="chemistry".
- hydrogen atoms (you need proper bond types to add hydrogens)
- proper atom types
- partial atomic charges
- directed graph (ICM−tree) imposed on all the atoms. This graph defines torsion angles and will be built by the write library command. In an ICM object the graph can be displayed if wireStyle="tree".

Identify the molecule or residue you would like to transform into the ICM−residue entry. To build all the above descriptions, perform the following procedures:

- read pdb "ligand" # molecule has no hydrogens

  display

- set bond type 1 a_//* # initialize all bond types by 1, the default is 0

  # 0 type means that the convert command will try to guess the type

- set bond type 2 a_//o2 a_//p1 # type 'set bond type 2' and `Ctrl-rightClick` two atoms

  # set all other non single bonds: 1−single, 2−double, 3−triple, 4 aromatic.

- set bond type 4 a_//c1,c2,c3,c4,c5,c6 # an example of setting aromatic type for a ring
- build hydrogen # use 'delete hydrogen as_' if things go wrong

- set type mmff
- set charge mmff `write library` command to save the residue entry file or append it to the `icm.res` or create you own library file.

3.6.5. How to modify an ICM−object: some standard modifications.

`Methylation`, `hydroxylation`, `glycosylation`, `sulfation`, `amidation`, `phosphorylation`, `disulfide bond formation`, `peptide cyclization/bond`,

ICM allows to perform most of the common chemical modifications of peptides and other biological molecules. It is easy to build a linear chain of amino acids and add N− and C− termini. D−amino acids can be introduced by adding capital D in front of the residue name (i.e. Dala). To make further modifications we will use the `modify` and the `make [disulfide | peptide] bond` commands. Let us consider the main categories, using the nh3−DCSTVYHCK−coo peptide as an example. Start you session with

```
build string "se nh3+ asp cys ser thr val tyr his cys lys gly coo-"
```

Now, if you like to see the results of your operations, display the molecule and do the following:

- type **modify** in the command window;
- `Ctrl-RightClick` on the atom of interest (the selection will appear in the command window);
- and, finally, enter the quoted chemical group name and press Enter.

The popular modifications:

- **Methylation:**

  ...−NH−... + CH_3 −>...−N−CH_3 + H

  ```
  modify a_/val/hn "ch3"
  ```

- **Hydroxylation:**

  ...R−CH_2... + OH −>...R−CHOH... + H

  where **R** belongs to side−chain of Lys or Pro.

  Examples:

  ```
                     # 5-hydroxylysine (Hyl) in collagen
     modify a_/lys/hd2 "oh"
                     # 4-hydroxyproline (Hyp) in collagen
     modify a_/pro/hg2 "oh"
  ```

- **Glycosylation:**

  1. O−glycosylation:

  ...−R−OH + O−CH− *Carb* −>...−R−O−CH− *Carb* + OH

  where **R** is a side−chain radical of `Ser` or `Thr` and *Carb* is an O−capped carbohydrate. Groups available for O−glycosylation are "acgl", "xyl", "agal", "bgal". You can further modify these groups.

  Examples:

  ```
  modify a_/ser/og  "acgl" # beta-D-N-acetylglucosaminide
  modify a_/thr/og1 "xyl"  # xylose
  ```

  2. N−glycosylation:

  ...−R−NH_2 + O−CH− *Carb* −>...−R−NH−CH− *Carb* + OH

  where **R** is a side−chain radical of Asn. *Carb* is an O−capped carbohydrate (see O−glycosylation above). The following example illustrates an alternative way of modification when a part of the attached group is disregarded.

  ```
          # It is assumed that the modified object (a_1.) is already built.
  ```

```
        # Now build the second object including only one aclg residues.
build string "se acgl" "modgroup"
display a_ red
set object a_1.
modify a_/asn/hd21 a_2.1/1/c1   # o1 atom of the acgl is disregarded, and
                                # asn's Nd and acgl's c1 is directly connected.
delete a_2.                     # Remove obsolete second object
```

If glycosylation follows hydroxylation, you explicitly do the same by N−glycosylation:

```
modify a_/lys/hd2 "oh"
modify a_/lys/o_a "bgal"  # o_a is the new unique name for the oxygen
```

Alternatively (and preferably) replace hydrogen directly:

```
  modify a_/lys/hd2 "bgal"
```

- **Sulfation:**

  ...−R−OH + SO_4 −>...−R−O−SO_3 + OH where **R** belongs to Tyr.

```
modify a_/tyr/oh "sul" # tyrosine−O−sulfate in fibrinogen
```

- **Amidation of the C−terminal glycine:**

  Build the peptide with the last `gly` replaced by the `conh` C−terminal residue. Tether it to the previous object and minimize tethers.

- **Phosphorylation:**

  ...−R−OH + O−PO_2−OH −>...−R−O−PO_2−OH + OH where **R** belongs to Ser, Thr, Tyr

  or

  ...−R−H + O−PO_2−OH −>...−R−O−PO_2−OH + H where **R** belongs to Lys, His

  or

  ...−R−O + O−PO_2−OH −>...−R−O−PO_2−OH + O where **R** belongs to Asp.

```
modify a_/ser/og  "pho"  # skip if you have already modified this residue
modify a_/thr/og1 "pho"
modify a_/tyr/oh  "pho"
modify a_/lys/hz2 "pho"
modify a_/his/hd1 "pho"
modify a_/asp/od2 "pho"
```

- **Disulfide bond formation:**

  ...(cys)−S−H + H−S−(cys)... −>...(cyss)−S−S−(cyss)... + H_2

  (note that names of the residues are changed upon bond formation (see `disulfide bond`).

```
   #ds extended ICM model of the sequence
display
    # set only one SS-bond, disregard all previous
make disulfide bond a_/3 a_/9 only
    # MC search for plausible conformations
montecarlo
```

- **Peptide cyclization and peptide bond:**

...COO + NH_3... ->...-CO-NH-... + H_2O

```
build string "se nh3+ gly gly gly gly his coo-"
display
make peptide bond a_/nh3*/n a_/his/c       # form a cyclic peptide
display drestraint
minimize "ss"
minimize "vw,14,hb,el,to,ss"
```

The following example shows how to build a cyclic peptide **cyclosporin A**:

```
#  read pdb "1csa"
#  make bond a_1csa.m/1/n a_1csa.m/11/c
#  write library "cs" a_/1
#  display grey
 build string  "se thr thr gly leu val leu ala Dala leu leu val"
 modify a_/2/og1 a_/2/hb
 modify a_/3/hn "ch3"
 modify a_/4/hn "ch3"
 modify a_/6/hn "ch3"
 modify a_/9/hn "ch3"
 modify a_/10/hn "ch3"
 modify a_/11/hn "ch3"
 rename a_/1  "bmt" # actually, the residue BMT is more complex
 rename a_/2  "aba"
 rename a_/3  "sar"
 rename a_/4  "mle"
 rename a_/6  "mle"
 rename a_/9  "mle"
 rename a_/10 "mle"
 rename a_/11 "mva"
 display
 make peptide bond a_/11/c a_/1/n
 minimize "vw,14,to,hb,el,ss"
 montecarlo "vw,14,to,hb,el,ss"
```

3.6.6. How to merge two ICM-objects

(the **move** command). It may be necessary to **merge** two or several ICM-objects or molecules to one, For example, if you are dealing with a docking problem and have prepared two molecular objects separately. The ICM command `move` allows you to do that. Technically, it rearranges `virtual` connections in the ICM molecular tree responsible for the description of the molecules in one ICM-object or in several ones.

```
 read object "complex"    # load a two-molecule ICM-object
 display virtual a_//!h*  # display molecules with virtual bonds
 color molecule
 show object              # one ICM-object loaded
```

```
read object "crn"        # load one more ICM-object
display virtual
color a_2. magenta
show object              # two ICM-objects loaded
move a_2.* a_1.          # merge two ICM-objects to one
                         # with virtuals connected to the origin

show object              # now two loaded ICM-objects becomes one

connect a_1.3            # you can move newly incorporated molecule
                         # w/respect to the original complex.
                         # do not forget to press ESC key in the
                         # graphics window to complete the command

                         # and / or you can save the new
                         # three-molecule object to a new file
write object "super_complex"
```

(See `connect` to learn more about the command.)

If, on the contrary, you would like to have one or several molecules from an ICM−object as an independent ICM−object, you should simply `delete` unnecessary molecules and to save the remaining one(s) as a new ICM object, for example:

```
read obj "super_complex" # suppose you saved "supercomplex"
                         # from above example, then...

delete a_1.1             # all what you need is a_1.2 and a_1.3,
show molecule            # right?
write object "remains_of_super"
                         # new ICM-object file "remains_of_super.ob"
                         # contains the 2nd and the 3rd molecules
```

3.6.7. How to make a hybrid model from several pdb files

To swap parts between several pdb files, read all of them to icm, and rename the chain which are you going to graft into the template, so that the template and the graft have the same name. Sometimes the two structures need to be superimposed. So, what is important for 'graftability' is

1. the graft has the same chain name (see `rename`)
2. the graft has residue numbers consistent with the template (see `align number`)
3. the graft has consistent coordinates (see `superimpose`)

Example:

```
read pdb "1crn"
read pdb "1cbn"
rename a_2.1 "m"
    # or rename a_2.1 Name(a_1.1)[1]  to do it automatically
superimpose a_1.1 a_2.1 align   # see more specific
```

The second concern is residue numbers. They need to be unique. This can be performed with the `align number` command, e.g.

```
align number a_2.1/21:28 22   # renumber the loop starting from 22
```

Now you can write the pieces to a file and after you read it back the pieces will become one molecule.

```
write pdb a_1.1/1:20  "hyb"
write pdb a_2.1/21:28 "hyb" append
write pdb a_1.1/29:99 "hyb" append

read pdb "hyb"   # read the hybrid in
cool a_          # display it
```

These operations are combined in the `mergePdb` macro, e.g.:

```
mergePdb a_2./20:25  a_1./300:308 # creates hybrid.pdb file
```

3.6.8. How to generate a series of intermediates between the two given structures

The following procedure will solve the problem:

```
read pdb "bj1bb"       # first structure
read pdb "bj2bb"       # second structure
strt = Xyz(a_1.//*)    # matrix (3, N_of_atoms) of the first ...
fnsh = Xyz(a_2.//*)    # ... and of the second
display a_1. red       # to see what is going on if you need it
display a_2. blue
nn = 300               # to generate 300 intermediate conformations
x = 1./nn
for i = 1, nn
  set a_1.//* strt*(1.-x*i) + fnsh*x*i
  write pdb a_1. "x"+i
               # uncomment the above line if you need
               # to save intermediates in x1.pdb, x2.pdb, etc.
endfor
quit
```

3.6.9. How to reconstruct a structure from a published stereo picture

Follow these steps:

- Scan the picture and create arrays of arbitrarily scaled coordinates xLeft xRight and Y for the Ca atoms.
- When you have the coordinates in your ICM session call the makePdbFromStereo macro.
- mark the PDB−formatted lines and paste it after the read pdb unix cat command.
- inspect the results, possibly return to step 1 and correct the coordinates or use stereoAngle = −6.
- to build all−atom model, create sequence file and use the macro `regul` .

Example:

```
read column "xxy"  # 3 numbers in each line + a header: #> xl xr y
makePdbFromStereo xl xr y 6.
read pdb unix cat
ATOM ....
ATOM ....
```

```
          # Ctrl-D
 display
```

3.7. Animation

3.7.1. How to rotate and zoom in a script

The simplest script will use the `View(v1,v2,r)` function to interpolate between views with different rotation and zoom. Example:

```
 buildpep "ACDF" # tetrapeptide
   # zoom out and create a small remote view
 v1=View()  # the 1st view
   # zoom in and rotate
 v2=View()  # the last view
 for i=1,100
   set view View(v1,v2,i*0.01) # interpolation
 endfor
```

Now you can add a specific display (`cpk, skin` or anything else) and add the `write image` command after −− set view.

The following script and macro make a .mov file for a specified molecule.

```
# makemovie −f qt −o tamox.mov −c qt_anim −r 15 `ls −tr ../f*.tif`
 print "DO NOT FORGET icmt −24;  set view 10 10 640 480"
 macro molkino i_tZoom (20) i_tRotate (20) l_preview (yes) R_startView R_endView s_Files ("/ic
  GRAPHICS.ballQuality = 15
  nfr=30
  for i=0,i_tZoom*nfr
    set view View(R_startView ,R_endView, 0.5−0.5*Cos(180.*i/Real(i_tZoom*nfr)))
    if(!l_preview) write image s_Files + i
  endfor
  B = 0.
  for i=0,i_tRotate*nfr
    A = 360./Real(nfr*i_tRotate) * i
    A = 180. − 180.*Cos(A/2.)
    rotate view Rot({0. 1. 0.} A−B)
    B = A
    if(!l_preview) write image s_Files + (i_tZoom*nfr+ i)
  endfor
 endmacro
#read object "tamoxifen"
 read object "propecia.ob"
 set window 10 10 640 480
 GRAPHICS.ballRadius=0.4
 display xstick
 color a_//c* green
 color a_//h* white
 read rarray "v0"
 read rarray "v1"
 set view v0
```

3.7.2. How to make a molecular movie from a Monte Carlo trajectory

We assume that you have a `Monte Carlo` trajectory saved as an ICM `movie file`. Displaying this movie interactively on your graphical screen is the simplest form of animation. You just load the object, the ICM movie and run the `display movie` command. Adjust your window and view and the allowed types of representation. This method will not work in two situations.

- First, `skin` and `surface` are not automatically recalculated and redisplayed upon the conformational change.
- Second, if you would like to display computationally heavy forms of graphical representation the interactive movie may become too slow.

In these two situations you may resort to external tools generating movie from individual image files.

In this case, the process of making a molecular movie animating the trajectory can be split into two steps.

The first step is a preparation of a series of images stored as separate disk files. Watch the ICM movie by the `display movie` command and select a range of frames you are going to include to the movie. There are two ways how a series of the molecular graphics images can be saved as `tif` or `rgb` formatted files.

Image collection (type I)

The following molecular representations are allowed in this case: `wire`, `cpk`, `ball`, `stick`, `xstick` and `ribbon` . The `image` option of the ICM `display movie` command is required. An example:

```
 build       "alpha"
 read movie  "alpha"
 display ribbon
 color ribbon a_/1:9   magenta
 color ribbon a_/10:18 green
 print "Adjust the view, press ENTER to continue"
 pause             # Pause to adjust a view of the molecule
                   # start of the collection of the image disk files
                   # (note, tif files are to be saved)
 nframe = Nof(frame)
 print "Total number of frames = ", nframe
                   # specify the range you need, for example:
 ifrom = 10
 ito   = 20
                   # otherwise, for all frames:
#  ifrom = 1
#  ito   = nframe

 display movie ifrom ito image
```

Computationally more expensive `skin` and `surface` molecular representations (or a combination of any of these two with those mentioned above) require an ICM script, as in the following example.

Image collection (type II)

```
 build       "alpha"
 read movie  "alpha"
 display xstick a_//n,ca,c
```

```
 set window 600 30 640 480  # good to convert it later into NTSC format
# change   640 480  to appropriate dimensions for PAL
 lineWidth = 3.
 print "Adjust the view, press ENTER to continue"
 pause

 nframe = Nof(frame)
 print "Total number of frames = ", nframe
 ifrom = 10
 ito   = 20
 icount = 0
 l_confirm = no
 IMAGE.compress = yes
 for iframe = ifrom, ito
   load frame iframe
   icount = icount + 1
   imgname = s_tempDir + "alpha_" + String(icount-1)
   display xstick a_//n,ca,c green
   display surface a_/7:12/!n,ca,c a_/7:12/!n,ca,c magenta
   write image imgname
   undisplay surface       # should be removed and redisplayed at the next step
 endfor
```

Whatever protocol you make use of, a series of files should appear in the `s_tempDir` directory. List their names in a file, for example, **alpha.lst:**

```
/usr/tmp/alpha_0.tif
/usr/tmp/alpha_1.tif
/usr/tmp/alpha_2.tif
/usr/tmp/alpha_3.tif
/usr/tmp/alpha_4.tif
/usr/tmp/alpha_5.tif
/usr/tmp/alpha_6.tif
/usr/tmp/alpha_7.tif
/usr/tmp/alpha_8.tif
/usr/tmp/alpha_9.tif
```

(Note, image numbers are started from zero, and "_" (underscore) is inserted before the current frame number.) Now, you can put these image files into a movie file. We suggest to use the **makemovie** command for Silicon Graphics machines. The following is a sample UNIX−shell command line which should be entered to make a non−interlaced MPEG−formatted movie with the frame size 640 by 480 saved in the Apple QuickTime movie file **alpha.qt:**

```
makemovie −f qt −o alpha.qt −c qt_anim −s 640,480 −r 30 ` cat alpha.lst`
```

Upon completion, use the **movieplayer** IRIX command to see the movie. UNIX **man** on−line help should allow you to learn more about these (and other) helpful commands. And let us give you several **helpful hints:**

- While the collection of the image disk files is in progress, do not hide any portion or the whole area of the graphics window by opening another window which can cover the first one, and do not move the mouse cursor through the graphics window area. This procedure typically requires quite a time, so be ready to be off your terminal/workstation for the whole time required for the image collection to complete.
- Do not forget to deactivate your screen saver before you start!

- Make sure you have enough disk storage. All images are assumed to be stored in the directory specified by `s_tempDir` string variable. The easiest way to estimate the required disk storage is to store the content of a single image by the `write image` command, and multiply the size of the resulting `tif` or `rgb` file by the number of frames. You could do it without leaving your ICM−session. For example, if you have a molecular image in the graphics window, then:

```
write image "testsize"
unix ls −l testsize.tif | awk '{print $5}' > testsize.rar
read rarray "testsize.rar"
sizeValue = testsize[1]
nFrame = 0
nFrame = Ask("Number of frames?", nFrame)
printf "Required storage for %d frames is %8.3f Mbytes\n", \
        nFrame, Real(nFrame)*sizeValue/1048576.
unix rm testsize.tif testsize.rar
delete sizeValue testsize nFrames
```

(Note that in the above example the file is stored in the current directory, not in that defined by the `s_tempDir` variable).

3.8. Transformations and symmetry

This section describes geometrical transformations of molecular objects and manipulations with crystallographic symmetry.

3.8.1. Main concepts and functions

Molecular objects and 3D density `maps` may contain symmetry information. This information allows to generate symmetry related parts of the density or molecular objects.

An elementary space transformation is defined by a `rarray` where values {a1,a2,...,a12} define 3x3 rotation matrix and translation vector {a4,a8,a12}. The complete augmented affine 4x4 transformation matrix in direct space can be presented as:

```
a1  a2  a3  | a4
a5  a6  a7  | a8
a9  a10 a11 | a12
------------+----
0.  0.  0.  | 1.
```

The related commands and functions (transformation vector will be referred to as *R_tv):*

command/function	description
`Axis` (*R_tv*)	calculates the rotation axis R_3 of the transformation. Rotation angle is returned in `r_out` .
`Augment` (*R_tv)*	converts 12−membered transformation vector into the augmented transformation matrix 4x4.
`Cell` (*os_*)	returns {a,b,c,alpha,beta,gamma} of the unit cell

`Rmsd` (*as_1 as_2* [`exact`])	returns *R_tv* in `R_out`
`Rot` (*R_tv*)	extracts the 3x3 rotation matrix
`Rot` (*R_center R_axis r_angle*)	returns rotation matrix for the `rotate` command
`rotate` ms_ M_rotationMatrix	rotates selected molecules
`superimpose` *as_1 as_2 ...*	returns *R_tv* in `R_out`
`Symgroup` (*i_spaceGroupNumber*)	returns a chain (R_[1:12*n]) of all n transformation vectors composing the specified space group.
`Symgroup` (s_groupName)	returns the *i_spaceGroupNumber* from which the transformations can be determined.
`transform` *ms_ R_tv*	applies transformation to an object.
`Trans` (*R_tv*)	extracts the translation 3−vector which is applied after rotation

3.8.2. How to generate symmetry related molecules

There are three steps:

- define symmetry
- find elementary transformation
- apply the transformation with the `transform` command.

Objects read with the `read pdb` or `read csd` commands grab the symmetry information from the files. Otherwise assign the symmetry with the `set symmetry os_` *`s_spaceGroupName R_6cell i_NofMolecules`* command. This way you may define your own set of symmetry transformations. Finally, loop through all the transformations and aplly the `transform` command.

Example: see example in the `transform` command or paste the following lines into your ICM session:

```
read csd "qfuran"
for i=2,Nof(Symgroup(Symgroup(a_)))/12 * 2 # 2 elem.cells will be filled
  copy a_1. "a"+i
  transform a_a$i. i-1
  display
  center
endfor
color ml a_*.
gcell=Grob("cell",Cell( ))
obl=Augment(Cell( ))          # this will work also for any oblique matrix
g1 = gcell + (-1)*obl[1:3,2]  # shift cell by a-vector
g2 = g1 + obl[1:3,3]
display gcell g1 g2
print " cell=" Cell( ) "\n Symgroup=" Symgroup(a_) \
      "Nof.sym.=" Nof(Symgroup(Symgroup(a_)))/12
```

3.8.3. How to find and display rotation/screw transformation axis

Steps:

- find the transformation with the `Rmsd(` *as_sub1 as_sub2* `exact)` function. It returns the transformation vector in the `R_out` system variable.
- find the axis with the `Axis(` *R_out)* function. This function also return the a point at the axis in `R_out` and the rotation angle in `r_out`
- display the axis with the `Grob( "arrow",` *R_6*) function.

Examples:

```
 read obj "crn"  # let us display an axis of the alpha helix 7:17
 ds a_/7:17
 R1=Mean(Xyz(a_/7:17/ca))  # this point will be projected onto the axis
 show Rmsd(a_/7:16/ca a_/8:17/ca exact ) # find the transformation
 vv=R_out
 aa=Axis(vv) # now R_out contains xyz of a point at the axis
 print "The rotation angle is ",r_out
 # grob + V3 translates grob by V3
 gg=Grob("arrow",aa )*10.+ Sum((R1-R_out)*aa)*aa+R_out # projection of R1 on aa
 display gg
 center
 pause

#Symmetry of an extended fragment
 delete object
 build string "se ala ala ala ala ala ala ala ala ala ala ala ala"
 R1=Mean(Xyz(a_/*/ca))    # this point will be projected onto the axis
 show Rmsd(a_/2:12/ca a_/1:11/ca exact )
 vv=R_out
 aa=Axis(vv)
 print "The rotation angle is ",r_out
 gg=Grob("arrow",aa )*10.+ Sum((R1-R_out)*aa)*aa+R_out # projection of R1 on aa
 display gg
 center
```

Now you can rotate your selection of molecules around the axis `aa` with the `rotate` command and the `Rot(` R_center R_axis r_angle) function, e.g.

```
 for i=0,360,30
  rotate a_1 Rot( R1 aa Real(i) )
 endfor
```

3.8.4. How to combine several transformations

To combine several transformations simply multiply their augmented matrices.

Examples:

```
 tv = Symgroup(19)   # 12*4 vector of the P212121 symmetry group
 tv1 = tv[13:24]     # grab the second transformation of the symmetry group
                     # the first is the identity transformation
 tv2 = tv[37:48]     # grab the last transformation of the symmetry group
 tvComb = Vector(Augment(tv1)*Augment(tv2))      # self-explanatory
 show tvComb         # you can apply it now with the transform command
```

3.8.5. How to build a helix from the two contacting monomers

Two steps:

- find the transformation from the two coordinate sets
- apply the transformation as many times as you need

The transformation may be helical or (a degenerate case) a rotational.

Example:

```
read pdb s_icmhome + "chq" # download two molecules related by a rot. symmetry
display a_*.
R1=Mean(Xyz(a_/*/ca))      # this point will be projected onto the axis
show Rmsd( a_2 a_1 exact)  # we assume that molecules are the same
tv = R_out                 # this is the transformation 12-vector
ha = r_out                 # rotation angle  (just FYI)
delete a_2                 # we will regenerate the 2nd molecule anyway
rename a_1. "s1"
for i=1,4                  # build a helix with 4 new elements
  j=i+1
  copy a_s$i. "s"+j        # names for a new subunits: s2,s3,s4,s5,s6
  transform a_s$j. tv      # apply tv to the last copied object
endfor
aa=Axis(tv)
print "The rotation angle is ",r_out
g_ax=Grob("arrow",aa )*10.+ Sum((R1-R_out)*aa)*aa+R_out
                           # projection of R1 on aa
display a_*. g_ax
color a_*. Count(Nof(a_*.))
```

3.9. Maps and factors

3.9.1. How to manipulate with structure factors

The basic description of `structure factors` is given in the `Glossary`.

3.9.2. How to calculate phases of reflections given a 3D model and a cell

Basic steps:

- define crystallographic cell, map gridstep, and resolution (i.e. max h,k and l)
- build electron density map with the specified parameters
- calculate structure factors

Example:

```
read pdb "1igd"                       # use your PDB name here
myCell   = Cell(a_1.)
gridstep = 0.5
                                      # map dimensions
maxHKL = Iarray(0.45 * myCell[1:3]/gridstep)
defSymGroup = 19  # P212121 group
```

```
make map gridstep
make factor maxHKL "mySF"
fcalc = Sqrt( mySF.ac * mySF.ac + mySF.bc * mySF.bc )
phase = Atan2(mySF.bc , mySF.ac)
group table mySF phase
show mySF
```

In order to compare calculated phases I would recommend using the same factor table when calculating the _second_ set of phases. Then "ac" and "bc" columns will be simply replaced by the new calculated data, and new "phase2" column would be right next to the "phase" column, relating to the original object. In addition to the previous script:

```
read pdb "1igd"                       # use your PDB name here
myCell   = Cell(a_1.)
gridstep = 0.5
maxHKL = Iarray(0.45 * myCell[1:3]/gridstep)
defSymGroup = 19 # Symgroup("P 21 21 21")
make map "myMap" gridstep
make factor maxHKL "mySF"
phase = Atan2(mySF.bc , mySF.ac)
                           # ... now the 2nd object ...
read pdb "1crn"            # the second PDB, not 1crn, of course
superimpose a_1. a_2.
  # you may need an alignment, see superimpose
make map "myMap" gridstep myCell     # to have the same cell!
make factor maxHKL "mySF"
phase2 = Atan2(mySF.bc , mySF.ac)
delta = Remainder(phase2-phase , 360.0)
group table mySF phase phase2 delta  # maybe something else
show mySF
```

3.9.3. How to automatically place a fragment into density

This section needs to be written. Make maps, set GRID.margin to about the size of the ligand and run montecarlo.

3.10. How to plot

3.10.1. How to make a simple plot *y*=F(*x*)

If your function is determined on an uneven set of abscissa values, stored in array *x*, then use:

```
plot display x y
```

If your function is determined on a regular 1D−grid of values varying from *x0* to *x1*, and is stored in the array *y*, use:

```
plot display Rarray(Nof(y), x0, x1) y
```

Use on−line help:

```
help plot
```

or to see the concise list of arguments

```
help command plot
```

3.10.2. How to plot a histogram

Function `Histogram` returns the *2*N* matrix which may be used on the fly with a command like

```
   plot display BAR red Histogram(a 50)
```

More examples:

```
a=Random(0. 100. 10000)
b=.04*(Count(1 50)*Count(1 50))
annot = {"Histogram with quadratic ruler" "Random value" "N"}
plot display BAR red Histogram(a b) annot

b=Sqrt(100.*Count(1 100))
annot = {"Histogram with square root ruler" "Random value" "N"}
plot display green BAR Histogram(a b) annot
```

3.10.3. How to make a 3D−surface plot of a 2D−function

In the most common case you may have a matrix *N*M my_matrix* representing a two−dimensional function of *x* and *y* `real arrays`. First create a `graphics object`, then display it and save as a picture if you wish:

```
read matrix "ram"
                          # let's try a "wire" representation first
x=Rarray(Nof(ram),−180.,180.)  #this scale may be nonlinear
y=x
make grob "matwire" ram x y # scales for x,y. Def. z−scale=1.
display matwire
                          # now let's have a look at a solid surface
make grob solid "matsolid" ram x y 0.9 # scales for x,y and z
display matsolid solid
                          # adjust the view by rotating/translating
#   connect matsolid      # you may move them with respect to each other
                          # and save image
write image rgb "img_matsolid"
```

3.10.4. How to create a new graphics object of a specific shape

First, use one of the provided `graphics objects`, stored in `*.gro` files to try these kind of ICM non−molecular objects. You can scale graphics objects (by multiplicating them by a real number) and/or adjust their positions either by `translate` or `rotate` commands or by `connecting` to the selected `grob` and dragging/rotating them with the mouse in the graphics window, for example:

```
read grob "icos"
my_icos = g_icos*0.2
display my_icos g_icos
translate add my_icos {5. 15. 0.}
```

You may also create a new or edit an existing graphics objects (see provided `*.gro` files to learn about format).

3.10.5. Flexible peptide docking

Let us consider a problem of flexible peptide docking to a receptor. The peptide may be completely free or constrained (e.g. have a helical fragment in the middle), and the receptor will be assumed to have a fixed conformation. We will be going through a series of interactive or non−interactive steps. Feel free to put the commands below into several scripts and run them sequentially.

We will follow a particular example through all the steps. In this example we will be docking a constrained 11−residue alpha−helical peptide to a Bcl−XL molecule. It is a good idea to create a separate directory for the project, say, `projectX`, to keep all the files in one place.

Preparing the receptor binding surface for peptide docking.

First, we need to get the receptor model as an ICM object. It may come from several sources. The most common one is a pdb−structure converted with the `convertObject` macro, or the `build model` command which builds a model by homology, followed by regularization and refinement with the `refineModel` macro.

We will create two objects:

`a_1.` the original pdb object with receptor with some other peptide
`a_2.` converted receptor (without the peptide)
Example:

```
% cd projectX
% icmgl −G
 nice "1g5j"  # an open form of the receptor
 delete a_w*  # delete waters but keep bound peptide
 copy a_ "rec"
 delete a_rec.2  # keep only the main chain
 undisplay window
 convertObject a_rec. yes yes yes no # also optimizes hydrogens
#
 display box Box( a_1.2 4. )  # display a box around the peptide
```

Now you may rotate the scene and adjust the box size by pulling a box corner with the leftMouseClick. The box needs to cover the receptor surface you need to include in the simulation, but needs to be minimized to reduce the computational burden and memory use.

Sometimes the orientation of the box with respect to the receptor surface is not favorable. In that case, use `connect a_*.` and rotate the objects with the respect to the origin (use `axisLength = 15.` and `display origin` to to see the axis in addition to seeing the box). If you change the absolute position of the receptor model, you may want to save the new orientation of the pdb object (e.g. `write pdb a_1. "template"`)

The result
Now we have two objects: (i) a pdb object in which we deleted the unnecessary molecules, but kept the

peptide for comparison and convenience in the box definition; and (ii) an ICM−object with a receptor for which we will be calculating the grid maps.

Create grid potential maps

Now calculate five grid potentials with the make map command:

```
make map potential "gc,gh,ge,gs,gb" Box() 0.5
```

This command uses *all* molecules in the *current object* as a source for the map calculations. The Box() function will return the box you see on your screen. Alternatively you can just provide the 6 numbers defining that box.

0.5 is the grid size. Even though the ICM grid potential is extremely fast compared to other programs, for large boxes you may need to increase the grid cell size. We do not advise to go beyond 0.7A, however.

The result of this step is five grid maps around the docking surface of interest.

Building the peptide

The peptide of interest can be build with the following simple command:

```
buildpep "ECLKRIGDELD"   # peptide sequence from Bax
rename a_ "pep"
set a_/* "HHHHHHHHHHH"
superimpose a_1.2/310:320/ca a_/1:11/ca align
```

Saving the results

Let us now save both the objects and the maps for future use.

```
write m_gc m_gh m_ge m_gs m_gb # gc.map .. files are created
write object a_*. "all"  # write 3 objects in one multi−object file
```

Running a simple simulation from one starting conformation

The actual simulation does not need to be run interactively. An ICM script file _dockpep is described below. Run the script by

```
% _dockpep >! f1.out  # the output file
```

The file contains the following commands:

```
#!/usr/local/bin/icmng
read libraries
read object "all"  # contains a_
set object a_pep.  # the peptide is the current object
fix v_/3:10/phi,psi,omg       # fix some backbone angles
nvar = Nof( v_//phi,psi,H,P ) # number of essential variables
  # let us choose iteration limits depending on nvar
mncallsMC    = 10000 + Integer(0.008*nvar*nvar*nvar*nvar*nvar)
mncalls      = 170+nvar*3
```

```
print mncallsMC mncalls
  # make sure that these two numbers are not insane
  # or set smaller mncallsMC and mncalls (e.g. 10000 and 100) as a test
temperature  = 600   # optimal temperature for the simulation
tolGrad      = 0.001 # exit minimization when gradient is < 0.001
mnhighEnergy = 15 + nvar/2   #
set vrestraints a_/* # load preferred backbone and side-chain angle zones
#
vicinity = 2.5
compare a_pep. static  # use sRmsd of the peptide
set terms "vw,14,hb,el,to,en,gc,gh,ge,gb,gs"
minimizeMethod = "conjugate"
#
# maps
read map "gc,gh,ge,gb,gs"
GRID.margin = Distance( a_pep./1/ca a_pep./11/ca )
#
# run montecarlo from a single start
# the reverse option will make more reasonables moves
#
# impose tethers ?
montecarlo reverse movie

# run montecarlo from multiple starts and merge the stacks
 for i=1,Nof(<starting conditions>)
  montecarlo reverse movie append
 endfor
```

This simulation created several files:

`f1.cnf` a stack file with `mnconf` (or less) best non−redundant conformations
`f1.mov` a trajectory file with all accepted conformations (if you used the `movie` option)
`f1.ou` the file with the text output of the script
The output file `f1.ou` contains information about every accepted conformation of the simulation, e.g.

```
...
 __ __      300   5   asp BPMC   db   da   da    −32.42    −23.66  100   1.29 97810
 DY Visi    300   1   phe BPMC   fb   fb   fb    −32.42    −32.42  101   0.57 97911
 __ __      300   4   ser BPMC   sa   sg   sd    −32.42    −24.45   88   0.06 97999
 DY Visi    300   5   asp BPMC  dmn  dmn  dmn    −32.42    −32.43   49   0.08 98048
...
```

Analyzing the results of a single simulation

Energy profile: Is the simulation long enough

The energies can be plotted to analyze the progression of the global energy optimization.

```
plotEnergy "f1.ou" 50.
plotBestEnergy "f1.ou" 50. "display append"
```

The first macro plots energies of each conformation generated and accepted in the course of the ICM stochastic global energy optimization. Due to the nature of the procedure, the energy may go up and down. The second macro plots (and appends the plot to the previously generated `def.eps` file) only the lowest energy achieved by a given iteration. This plot shows if and when a better conformation is found.

Naturally, the energy can not be improved after the global minimum is found.

However, having a long flat plateau does not guarantee that the global minimum is found since a new drop of energy may come after a very long simulation. The time required for finding the global minimum in general depends on the number of variables, number of atoms (the cost of a single energy calculation) and complexity of the potential energy surface.

The best empirical way to make sure that the minimum is found is to compare the lowest energies found from completely different starting conformations (read about multiple start simulations below).

We use a window of 50 kcals/mole from the lowest energy. It helps to avoid the dependence of the scale on the initial energy which may be quite high.

To analyze the improvements only use `plotBestEnergy` .

Graphical analysis of the results

You can generate all stack conformations as independent ICM objects with the `mkStackConf` macro,e.g.:

```
read object "all"  # three objects, the peptide is the current object
mkStackConf 1 10   # make ICM objects from 10 best energy structures
```

The objects will be called `a_pep1. , a_pep2.` , etc. Now these objects can be displayed simultaneously or separately and further analyzed, e.g.

```
display a_pep*.
color a_pep?*. Energy( stack ) # in case you extracted all confs
```

You can loop through the conformations interactively either with the original stack, e.g.

```
# create some view you like
for i=1,10 # or Nof(conf)
  load conf i
  pause   # rotate and zoom, hit Return
endfor
```

, or use the objects you created with the `mkStackConf` macro.

Running a multiple start simulation

You can figure it out yourself :−) .

convergence analysis

The key question we would like to ask is if at least two independent simulations from random starting conformations identified a nearly identical conformation with a similar energy as the lowest energy conformation. A low−tech example with just two simulations `f1` and `f2` :

```
read object "all"
load conf 0 "f1"  # 0 is the lowest energy conformaiton.
load conf 0 "f2"
```

You can also plot the best energy (see above) and compare the plots, as well as perform graphical analysis to see if the best conformations are similar.

Analyzing the results of a multiple start simulation

merging stacks

Use the `read stack append` command to merge all stack conformations together. Now you can redefine the `compare` command and the `vicinity` parameter depending on how you want to further compare and filter out the accumulated conformations. The `compress` command performs the compression.

3.11. How−to: Docking and Virtual Ligand Screening

by Max Totrov and Ruben Abagyan

3.11.1. Docking and virtual ligand screening. Overview.

This section concerns with predictions of interactions of drugs or small biological substrates (less than about 600−700 dalton) to pockets of larger, more rigid, receptors (typically, protein molecules, DNA or RNA). There are five major steps in docking and screening.

Where to dock. Building Receptor and Pocket Model

The **goal** here is to have an adequate three−dimensional model of the receptor pocket you are planning to dock ligands to. And the **pitfalls** are that your model is not accurate overall, or does not reflect the induced fit, or alternative conformations of the receptor binding pocket are missed.

Receptor from PDB

If you have only a single entry with your receptor, convert the protein with `convertObject yes yes no no` , after deleting water molecules and irrelevant chains (e.g. `delete a_!1`), or use menus as in the `ligand docking section`.

However, if you have a choice between several templates, take the following into account:

- X−ray structure is preferable to an NMR structure
- high resolution X−ray structure (less than 2.1A) is much better than, say 2.5A .
- watch out for **high−B−factor** regions and avoid them; sometimes crystallographers deposit fantasy coordinates with high−B−factors. Use:

  ```
  color a_//* Bfactor( a_//* )  # from command line
  ```

  or `Color/B-factor` from the Gui−menu .
- place polar hydrogens and choose correct form of `histidine` (`convertObject yes yes no no` takes care of that)
- a **bound** conformation of the receptor is preferable, however if you use an apo−model, an NMR structure or a model by homology, the side−chains in a pocket may be incorrect. Frequently they **stick out** and prevent a ligand from binding. Those stubborn side−chains can be 'tamed', (i)

manually; (ii) by a side chain simulation with elevated `surfaceTension;` or (iii) by an explicit flexible docking calculation with a known ligand.

Receptor from homology modeling

A model by homology can be built with the `build model` command (menu `Homology/Build_Model)` followed macro `refineModel`.

Identifying pockets

If a binding pocket is not known in advance, use `icmPocketFinder` or `icmCavityFinder` (for closed pockets) macros. `icmPocketFinder` can also be accessed from menu `Docking/Receptor Setup` , submenu `Identify_Binding_Sites`

What to dock. Ligand, ligands, a database or a library.

Usually a good start is to try to dock the known ligand(s) to the receptor model. You may also want to dock a library of compounds in order to identify lead candidates. In this case the main **pitfall** is that the library is too restricted, molecules are not chemically feasible or not drug−like.

Ligand from PDB

Then to dock a ligand from pdb, go through the procedure described in the `ligand docking section`.

Ligand(s) from a mol/mol2− file, or SMILES strings.

The main prerequisite is that the formal charges and the bond types are correct. If they are not correct, you need to process each molecule manually as described in the `ligand docking section`. From a command line you may use the `build smiles` or `convert2Dto3D` macro.

Flexible docking considerations.

After the receptor maps are built, you will start a docking simulation. The goal of the flexible docking calculation is prediction of correct binding geometry for each binder. ICM stochastic global optimization algorithm attempts to find the global minimum of the energy function which includes five grid potentials describing interaction of the flexible ligand with the receptor and internal conformational energy of the ligand. During this process a stack of alternative low energy conformations is saved (one of the choices in the `Docking` menu). Some facts about ICM docking:

- an average docking time is 1 − 3 minutes per ligand per processor
- ICM docking is probably the most accurate predictive tool of the binding geometry today.
- the time per ligand was chosen to be the smallest possible to allow screening of very large data sets. To increase the time spent per ligand, change the `Docking_thoroughness` parameter from the `Docking.Small Set Docking Batch` menu to 3. or 5., or supply this parameter to the `rundock` script directly.

Pitfalls. Inaccurate receptor model, or incorrectly converted ligands, or insufficient optimization effort may lead to incorrect predictions.

Scoring

The goal of scoring in `virtual ligand screening` is to ensure **maximal separation between binders and non−binders** , and **not** to rank a small number of binders according to their binding energies. The **vls** module allows you to access a good scoring function.

3.11.2. How−to: Ligand docking simulations.

Introduction and pre−requisites

ICM ligand docking procedure performs docking of the fully flexible small−molecule ligand to a known receptor 3D structure. Before setting up the docking project, ICM object of the receptor has to be created. In most cases, x−ray structure of the receptor is initially in the PDB format. Thus, it has to be converted to the ICM format. This process involves addition of the hydrogen atoms, assignment of atom types and charges from the residue templates (icm.res) and imposition of internal coordinates tree (icm−tree) on the original pdb coordinates. The easiest way to convert pdb structure into icm object is through GUI as follows:

1. load pdb file into icm (menu `File/Read Molecule/PDB`)
2. convert loaded structure into icm object (menu `MolMechanics/ICM−convert/Protein`).

It is recommended that "optimize hydrogens" option is selected. To accelerate the procedure, disable the 3D graphics window (side menu `Clear/No Graphics`) When the procedure finishes, converted object is the 'current' object in icm. You can check the results by displaying the converted structure.

Docking project setup

Start project setup by defining the project name (menu `Docking/Set project name`). Avoid spaces and leading digits in the name. All files related to the docking project will be stored under names, which start from the project name. Most customized parameters will be saved in the table file under the project name as well:

```
DOCK1.tab     # control table
DOCK1_gb.map  # 3D potential grids, or 'maps'
DOCK1_gc.map
DOCK1_ge.map
DOCK1_gh.map
DOCK1_gs.map
DOCK1_rec.ob  # receptor object
```

etc..

The next step is to set up the receptor (menu `Docking/Receptor setup`). Select the receptor molecules, in most cases a_* will do − all molecules in the current object will be included. Define binding site residues, either manually e.g. a_/123,144,152 for selection by residue numbers, or graphically using

lasso tool (don't forget to set selection level to residue). This selection is used solely to define boundaries of the docking search and the size of the grids and doesn't have to be complete, selecting some 4 residues delimiting the binding site is sufficient. Receptor setup dialog also lets you run binding site identification routine to quickly locate putative binding sites on your receptor.

After the receptor setup is complete, the program normally displays the receptor with the selected binding site residues highlighted in yellow xstick representation. Ligand setup offers a number of ways (submenu `docking/ligand setup`) to define the ligand, depending on the source of the ligand structure(s).

Converting a chemical from pdb.

The Protein data bank, due to unprecedented ignorance, for the last 15 years has not been storing any information about covalent bond types and formal charges of the chemical compounds interacting with proteins! This oversight makes it *impossible* to *automatically* convert those molecules to anything sensible and requires your manual interactive assignment of bond types and formal charges for each compound in a pdb−entry. Therefore, if you apply the `convert` command to a pdb−entry with ligands, the ligands will just become some crippled incomplete molecules which can not be further conformationally optimized.

Follow these steps to convert a chemical properly from a pdb form to an a correct icm object.

- display the molecule, set `wireStyle=2` (or via top−left gui−menu), and selection type to `GRAPHICS.selectionMode=1` (the first item of the gui−selection−mode menu)
- invoke `MolMechanics.Structure.SetBondType` menu item
- graphically select groups of atoms (e.g. a ring) and set appropriate bond type
- invoke the next menu item, `MolMechanics.Structure.SetFormalCharge` and set formal charges
- proceed to the `MolMechanics.ICM−Convert.Chemical` menu (see below)

Setting up a ligand or a set of ligands

Let's now consider the situation when icm object of the ligand loaded. ICM object of the ligand can also be prepared, for instance, by reading structure from SD file (menu `File/Read Molecule/Mol/SDF`) and converting it to ICM (menu `MolMechanics/ICM−Convert/Chemical`).

Once the icm object of the ligand is ready, proceed to docking ligand setup (menu `Docking/Ligand Setup/From Loaded ICM object`). The ligand setup procedure will first display the grid box, allowing you to adjust the box dimensions, and then the 'probe' which defines the initial positioning of the ligand's center of mass and long/short axis. The probe can be moved/rotated. While its positioning has only minor influence on the results as long as it remains inside the binding site, it may help the procedure to find the correct docked orientation more reliably and/or in shorter time.

Ligand setup procedure can be ran repeatedly to change the ligand within the same docking project. Also box size and probe position can be changed later (menu `Review/Adjust ligand/box`). At this point, the project is ready for the calculation of maps (menu `docking/Make receptor maps`). The calculations generally take several minutes to prepare the maps. While the dialog allows changing the grid step, we do not recommend altering the default value of 0.5 which was found optimal for a large number of test cases. With the map calculations completed, everything is ready to start the actual docking simulation. A larger set of ligands in a mol file can be considered as a **database** and indexed with the ICM indexing tool (menu `Docking/Tools/Index Mol,Mol2 Database`) for fast access. Ligand structures from mol/mol2 file can be converted to ICM on the fly and do not require manual preparations necessary in the

case of PDB structures.

Running docking simulations

Use menu `docking/Small Set Docking Batch` to start docking of one or few ligands in the background. You can also view the process interactively (menu `docking/Interactive Docking`) although it is much slower due to the time spent on drawing the molecules. The results of the batch docking job are saved in the

```
PROJECTNAME_answers*.ob  #icm-object file with best solutions for each ligand
PROJECTNAME_*.cnf        # icm conformational stack files with multiple docked conf.
PROJECTNAME_*.ou         # output file were various messages are stored.
```

Multiple conformations accumulated during the docking of the ligand can be visualized and browsed in ICM (menu `Docking/Browse Stack Conformations`). Use menu `Docking/Display/Preferences` to change default graphic representation of ligand/receptor.

Rundock UNIX shell script

Docking batch jobs should be started from the UNIX command line using rundock shell script. The syntax is as follows:

```
rundock <options> <project name>
 options: -f <ligand entry from>" # if using multiple ligand input file
       -t <ligand entry to>"      # range of ligands to dock can be selected
       -L <list of ligands>       # comma-separated list of ligand numbers from database
       -l <thoroughness>          # change the length of MC docking, default is 1.
       -n <scanName>              # change the run name in the output files
       -a                # force docking and saving of all compounds
       -s                # save stack conformations
       -S                # evaluate score for all stack conformations (slow)
       -o                # redirect output to <project name>_from-to.ou
       -c <output file>  # continue interrupted job with <output file>
```

Example:

```
 rundock -f 3 -t 5 -l 3. -s MYPROJECT
```

will thoroughly (3 times longer simulation than default) dock ligands 3 to 5 and save conformational stacks for each one of them.

Template constrained docking

It is possible to use a template object to tether part of the ligand structure to a preferred position during the docking simulation. Prepare an object file containing the group of atoms to be tethered to. Edit the .tab docking setup file, setting the s_templateObj field to the name of the template object file (it is 'none' by default). The variable l_superByName controls the way correspondence is established between the ligand and template atoms. If it is 'no', chemical substructure search is performed and tethers imposed according to the substructure match. If l_superByName is 'yes', simple matching according to atom names is performed. Tethers can be individually weighted by assigning b-factor values to the template atoms. Weights are

reversely proportional to b−factor, default b−factor of 20. corresponds to the weight of 1.

3.11.3. How−to: Virtual Ligand Screening

Introduction

Virtual Ligand Screening (VLS) in ICM is performed via docking of each ligand in the database to the receptor structure, with subsequent evaluation of the docked conformation with a binding−score function. Best−scoring ligands are then stored in the multiple icm−object file. The set−up of the VLS is largely identical to the set−up of the docking simulation (see How−to: Ligand Docking Simulations). In most cases the ligand input file will be an SDF or MOL2 file. These files need to be indexed by ICM before they can be used in VLS runs. The index is used to allow fast access to an arbitrary molecular record in a large file. Use menu `Docking/Tools/Index Mol/Mol2 File/Database` to generate the index, then set up the SDF/MOL2 file as a ligand source (menu `Docking/Ligand Setup/From Database`). As in docking, rundock UNIX shell script can be used to start simulations.

Score Threshold

An important parameter of the VLS run is the score threshold. Docked conformation for a particular ligand will only be stored by ICM VLS procedure if its binding−score is below the threshold. Edit the project .tab file to adjust this value:

```
#>r DOCK1.r_ScoreThreshold
  −35.
```

The choice of the threshold can be done in two ways:

1. based on the scores calculated by docking known ligands. Generally, a value somewhat above typical score observed for known ligands is a good guess.
2. if no ligands are known, a pre−simulation can be run using ~1000 compounds from the target database. Using the resulting statistics for the scores, the threshold should be set to retain ~1% of the ligands.

Potential of mean force score

Potential of mean force calculation (`pmf`) provides an independent score of the strength of ligand−receptor interaction. The pmf−parameters are stored in the `icm.pmf` file. To enable calculation of the pmf−score, define the `PROJECTNAME.r_mfScoreThreshold` threshold paramter to the table:

```
#>r PROJECTNAME.r_mfScoreThreshold
  999.
```

Other selection criteria

ICM VLS uses a number of criteria to pre−select compounds before docking. Edit the project .tab file to change their defaults:

```
#>i DOCK1.i_maxHdonors
 5
#>i DOCK1.i_maxLigSize
 500
#>i DOCK1.i_maxNO
 10
#>i DOCK1.i_maxTorsion
 10
#>i DOCK1.i_minLigSize
 100
```

Parallelization

If the database size exceeds several thousand compounds, it is desirable to run a number of VLS jobs in parallel to speed up calculations. Use −f and −t options of rundock to start multiple jobs on different parts of the database, e.g.

```
rundock −f 1     −t 10000 −o
rundock −f 10001 −t 20000 −o
rundock −f 20001 −t 30000 −o
..
```

Running VLS jobs in PBS UNIX cluster environment

Jobs on the Linux cluster are run through PBS queuing system. Several scripts are provided to facilitate submission of vls jobs. To submit a single job, use pbs script 'pbsrun', which is a pbs wrapper for rundock

qsub $ICMHOME/pbsrun −v"JOBARGS=−f 1 −t 1000 −o MYPROJECT"

Note that the rundock arguments go in the quotes after JOBARGS= . The qsub command is a part of PBS.

To submit multiple jobs, there is a simple shell script 'pbsscan' which executes multiple qsub's for database stripes:

$ICMHOME/pbsscan MYPROJECT 1 6000 1000

−submits 6 jobs, 1 to 1000; 1001 to 2000 ... 5001 to 6000. Currently this script only supports default rundock arguments, copy/edit to change.

The command qstat is a part of PBS and can be used to check the status of the jobs. In addition, $ICMHOME/scanstat script can be used to monitor the progress of the VLS jobs. It analyses the *.ou rundock output files.

$ICMHOME/scanstat *.ou

To delete the jobs, use PBS command qdel:

qdel 1234 # delets job number 1234

Where to find the scores of the compounds

Once the compounds are docked, if VLS option is installed, the procedure evaluates the score and stores it in the 'comment' of the ligand object. When browsing scan answers, the SCORE>... line appears for each object viewed, containing the value of the score and it's component terms. It can also be extracted from the icm object in shell using Namex(a_1.) function, and Field() can be used to get particular component or the total: Field(Namex(a_1.) "Score=" 1). The SCORE lines also appear in the output file and can be extracted by simple unix grep command grep SCORE *.ou

The MFScore was recently added, it's calculated if `r_mfScoreThreshold` variable is defined in the project .tab file. It can be added manually:

```
#>r PROJECTNAME.r_mfScoreThreshold
  999.
```

Analysis of the results

The hits found by the screening procedure and stored in *answers*.ob files can be visualized in ICM (menu `Docking/Browse Scan Solutions`). If necessary, they can also be exported as SD file using (menu `Docking/Tools/Export scan answers as mol`). The score and its components are stored in the resulting SD file as well. Simple analysis of the score distribution can be performed by making a histogram (menu `Docking/Tools/Scan results histogram`).

3.12. Example scripts

3.12.1. How to predict 3D structure of a peptide from its sequence

In the following script you are going to search for the lowest energy conformation using the Biased Probability Monte Carlo procedure to generate new conformations and full−atom energy plus solvation electrostatics, surface and entropy contributions. Start 3 or more independent simulations and let them run to convergence. Two features are indicative of convergence: the plot of the best energy achieved should be flat for sufficiently long (store the output in f1.ou and run the following macro:

```
 plotBestEnergy "f1" 100. "append display"
```

); and the lowest energy conformation in different simulations are close, e.g.:

```
# peptide "pep.se" ; runs: "f1" and "f2"
  build "pep"
  display
  read conf "f1" 0
```

```
 show stack
 read conf "f2" 0
 show stack
```

Watching movies f1.mov and f2.mov may also be useful. (See also How to evaluate helicity of a peptide from the BPMC simulation and How to calculate an ensemble average). Now, the script:

```
                    # Example folding script. Use as directed.
read libraries
build "pep16"       # your peptide sequence is in pep16.se file.
rename a_*. "f2"    # specifies current name.
                    # Several runs (f2,f3, etc.) are recommended
nvar = Nof( v_//* ) # number of variables

nProc=4             # if you are using parallel version.

mncallsMC    = nvar*50000  # maximal number of energy evaluations
mncalls      = 170+nvar*3  # maximal n_of minimization calls after
                           # each random change
temperature  = 600   # optimal temperature for the simulation
tolGrad      = 0.01  # exit minimization when gradient is < 0.01
mcBell       = 1.0   # the default width of the MC probability distributions
mnconf       = 40    # maximal n_of low-energy conformations saved
                     # in the stack (f2.cnf file)
mnvisits     = 25    # if stuck for >= 25 times, push it out
mnreject     = 10
mnhighEnergy = 30
l_bpmc       = yes   # use biased probability
electroMethod = "MIMEL"
surfaceMethod = "constant tension"
set terms "vw,14,hb,el,to,sf,en"
                     # ECEPP/2 energy + solvation + entropy (see icm.hdt file)

fix v_//?vt*         # exclude irrelevant virtual variables specifying
                     # absolute molecular position
set vrestraint a_/*  # load preferred backbone and side-chain angle zones
                     # for the  biased probability MC
randomize v_//!omg 180.0  # create random starting conformation
vicinity = 15.0
compare v_//phi,psi  # use these variables to compare structure
montecarlo movie     # run it and record a movie.
                     # watch the movie later by:
                     # read movie "f2"; display ribbon
                     # display movie "f2" 4. 8.
                     # analyze the best conf. in the stack by:
                     # build "pep16"; read stack; show stack all
                     # load conf 1
quit
```

3.12.2. How to perform local flexible docking of two protein molecules

using the grid potentials

This is a so called "local docking procedure" which docks all orientations of the protein ligand to a certain orientation of the protein receptor. The "global docking procedure" is somewhat different.

You may follow the menu items in Docking.Protein−protein or run the docking scripts directly. To illustrate the principal commands and functions we will also consider a series of shell commands to perform a docking procedure. We will use the following steps from the shell to dock the proteins chymotrypsin (5cha) and APPI (1aap). The real structure of the complex is known (1ca0), which can help us to test the validity of the method. This procedure has been recently tested in a dataset of 24 known protein−protein complexes (`Fernández−Recio,Totrov,Abagyan, 2002`)

The procedure includes the following steps:

1. Creating two ICM objects for both proteins with the `convertObject` macro
2. Specify project parameters in a special table
3. Orient molecules, choose the docking box and make potentials.
4. Dock the protein ligand into the potentials.
5. Refine the solutions.

3.12.3. How to perform an explicit flexible docking of two simplified protein molecules

This procedure is relatively old and was used previously to explicitly dock two proteins starting from simplified objects. The best solutions are refined in all−atom representation. Currently we prefer docking into grid (see above).

1. Create ICM−objects of the two proteins you want to dock.
2. Use macro `makeSimpleDockObj` to create two simplified objects.
3. Combine two simplified objects into one and prepare it for docking simulation using _makeComplex script. During the execution you will be prompted for orientation of the first molecule, which should face the second one with the expected epitope.
4. Run the docking simulation using _dock2mol script. To insure the completeness of the search, run 3−4 simulations in parallel and compare the resulting stacks, the top 5−7 conformations should be the same except for 1−2. Combine the stacks using "read stack append" command with subsequent filtering by

```
vicinity = 4.
compare static a_2//ca
compress stack
```

5. Prepare .var files with optimized surface sidechain conformations for individual proteins by running _surfSideChainOpt script.
6. Run _makeFullAtom script to create full atom models from the simplified conformations accumulated in the stack.
7. Run _refineComplex script on each of the full atom models
8. Complex with the best energy after the optimization is (hopefully) the answer.

3.12.4. How to build a model by homology

Have an alignment and a pdb file with the template handy, say "sx.ali" "x.brk". If you have a *homology* module key you can use the `build model` command and refine the model with the `refineModel` macro. The `build model` command builds a complete model and searches for matching loops in all pdb files. You can run the build model command from the GUI interface (menu `Homology`)

`alignSS` is a good macro to make a sequence−structure alignment. It incorporates solvent accessibility and secondary structure into the alignment procedure. Alternatively, allow the `build model` command to perform the alignment on the fly.

In the absence of the `Homology` module, use the following macros/scripts:

- homodel macro: fast interactive model building.
- _homFast for fast model building (substitute nonidentical side−chains, assign the most likely rotamer).
- _hom for more rigorous model building for one polypeptide chain: side−chains are optimally placed loops are automatically recognized and simulated.
- _homMult the same as the above script, but for a multichain protein molecule, e.g. an immunoglobulin molecule. Requires a set of separate files for each alignment.

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4.5. Credits

5. Glossary

5.1. A

add

a family of commands adding things. It is also used as an option equivalent to `append` in `write` command.

alignment

or *sequence group*. Individual sequences in the group may be just combined and left−justified (no insertions/deletions, e.g. as an output of `group` command) or actually aligned (or realigned) with either pairwise function `Align` (*seq1, seq2*) or multiple alignment command `align` *sequence_group*

Pairwise sequence alignment is performed with the `ZEGA` (Zero End−Gap Alignment) algorithm. You can `read`, `write`, `list`, `show`, `delete` or `edit` an *alignment*. Flag `l_showSstructure` allows you to show the secondary structure string which belong to a participating `sequence` to be displayed. When you `show` the alignment, the consensus string appears on top. The meaning of consensus characters is explained `below` and the string can be extracted with the `Consensus`( ) function.

A table with relative amino acid numbers for all sequences in the alignment is returned by the `Table`(*ali_*) function. An array of mean scores for each column of a multiple sequence alignments is returned by the `Rarray`(ali [`exact`]) function.

Coloring 3D models by local alignment strength. Space averaging

See: `selectSphereRadius` and `ribbonColorStyle` = "reliability"

Arithmetics:

- extracting a domain (i.e. a certain position range) from an alignment `alignment[i1:i2]` or `alignment[i]`
- extracting an alignment of a group of sequences from a larget alignment `Align(aliLarge,` *I_seqNumbers*)
- projected alignment: concatenation of two alignments sharing the same sequence. The shared sequence serves as a ruler for merging the two alignments. The alignments can be of arbitrary size and number of sequences. In the simplest case of three sequences a, b, c and alignments ab and bc, the operation ab//bc will create an alignment of three sequences a b c. The function Align(ab//bc,{1,3}) will extract the, so called, projected alignment of **a** and **c** through **b.** Example:

```
  ali1    //    ali2  returns   Projected ali.
a VYRWA−W     b FK−WG−−KW     a  VYR−WA−−−W
b −FKWGKW     c AKGWAPGKW     b  −FK−WG−−KW
                              c  −AKGWAPGKW
```

- projecting a numerical property from a sequence to alignment: `Rarray`(*R_property,seq_,ali_,r_gapDefault*).

- projecting a numerical property from alignment to a sequence : `Rarray( ~R_ali,ali_from,seq_|i_seqNumber )`

Deleting some sequences from an alignment To delete a list of sequences from an alignment use the following command: `delete` *alignmentName* `only` *seq1 seq2 ...*

To delete sequences *selected* via the graphics user interface from an alignment use the `delete` *alignmentName* `only selection` command.

Example

```
delete sh3 only Fyn
delete sh3 only selection
```

Functions:

function name	description
`Align`	pairwise alignment from 2 sequence, or subalignment extracted from another alignment, or alignment extracted from tethers in an ICM−molecular object.
`Consensus( )`	the consensus string
`Deletion( )`	residue selection of deleted residues
`Distance( )`	pairwise distance matrix between sequences.
`Insertion( )`	residue selection of inserted residues
`Matrix( )`	distance matrix
`Name( )`	string array of names of sequences
`Nof( )`	number of sequences
`Profile( )`	a profile derived from the alignment
`Res( )`	residue selection corresponding to the aligned sequence
`Score( )`	sequence identity, similarity or alignment score for a pairwise alignment
`String( )`	a multiline string of the alignment (contains '−')
`Table( )`	a table with relative sequence numbers (0 for gaps)

Examples:

```
read alignment "globins.msf"
list alignments
glob_fragment = globins[10:36]
show glob_fragment
delete alignments
```

all

an option used in several commands where whole list of items involved should be invoked (e.g. `show terms`).

alpha helix

alpha−helical conformation. Average angles (phi=−63.2,psi=−38.5). Referred to as 'a' in `variable restraint` names: e.g. alpha−zone for histidine is called "ha".

See also commands `assign sstructure` , `set vrestraint` and file `icm.rst` .

amber

a force field for simulations of proteins and DNA in the Cartesian coordinate space.

See the reference.

append

used as option mostly in `read` and `write` commands, for example:

```
write matrix "fil.mat" append
read stack "mc12" append
```

arrays. ICM−shell allows 3 types of arrays:

- iarray − integer array,
- rarray − real array,
- sarray − string array

These arrays are legal elements of the ICM−shell.

iarray−constant looks like this: `{2, 4, 67, −4}.`

rarray−constant looks like this: `{2.0, −4., .67, −4.3433}.`

sarray−constant looks like this: `{"a−word","b−word","c−word","..."}` .

Commas are optional unless you have negative elements in integer or real arrays. Array ICM−shell variables can be created by direct assignment: (e.g. `a={2, 4, 67, −4}` or `b={"wow","oops","ouch"}`), `read` (e.g. `read iarray "numb.iar"`), and `written` to a file (e.g. `write numb "numb"`). You can specify a `subset` of an integer array (e.g. a[2:15]). Besides, there all kinds of `operations` and `functions` on the ICM arrays. There are many ways to create an array:

- read an array from a file: read rarray "a.dat"
- create by direct assignment: a={1, −2, 3, 14}
- use arithmetic expressions: a=Sin(Cos(a))*b
- use functions `Iarray`, `Rarray`, or `Sarray`, e.g.: a=Rarray(15, 2.)
- concatenate two elements, e.g.: a=2//3

atom

(Greek): indivisible; the smallest particle of a chemical element that can exist alone or in combination (cool, isn't it?).

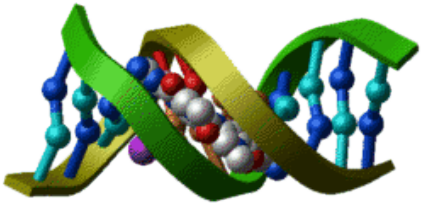
axis

an imaginary straight line passing through a point or a body.

5.2. B

base

Use option `base` to display cartoon representations of the bases on the DNA/RNA ribbons. In DNA and RNA ribbons, bases can be displayed/colored separately from the ribbon itself (e.g. `color ribbon base a_1/* white`), the default coloring being A−red, C−cyan, G−blue, T or U−gold.



ball

a solid sphere representing an atom in the graphics window. Its size is defined by the `GRAPHICS.ballRadius` ICM−shell variable.

Examples:

```
display ball a_//ca         # does not make much sense
```

See also: `xstick`

beta

an extended conformation ("E" in one−character notation). Referred to as 'b' in `variable restraint` names: e.g. beta−zone for alanine is called "ab".

See also: `assign sstructure` , `set vrestraint` and file `icm.rst` .

boundary element

See REBEL . See also: `electroMethod`, `delete boundary`, `show energy"`, `term "el"`, `Potential( )`.

BPMC

is an acronym for the Biased Probability Monte Carlo method (Abagyan and Totrov, 1994). The method is based on a theorem establishing that if the Monte Carlo procedure is used for global optimization, rather than generation of a Boltzmann ensemble, random moves based on known local probability distributions (e.g. alpha and beta regions for peptide backbone conformations) maximize the optimization efficiency. Practically, the procedure randomly choose a group of coupled angles and changes them according to probabilities defined in the `icm.rst` file. Do not forget to use the `set vrestraint a_/*` command before the `montecarlo` command to activate the biasing.

5.3. C

cavity

is the free space inside a molecule. Here we use a limited definition of a cavity as a fully *enclosed* space inside a molecule. See the `icmCavityFinder` macro which identifies and characterizes cavities.

To generate a cavity an `skin` is generated and converted into `grob.` We then `split` this grob into individual connected entities.

charge

is an electric charge in electron units. You may redefine charges with the `set charge` command.

clipping plane

An invisible graphical plane which truncates the view. There two clippings planes: the front one and the back one. The front clipping plane determines the beginning of the visible part of your object, while the back clipping plane is where the visible parts ends. The planes can be moved independently, or in concert (so called "slicing"). In the `"FOG"` mode the image gradually disappears between the front and the back planes.

coil

is an irregular conformation ("_" in one−character notation). It is displayed as spaghetti when the `ribbon` type of representation is used. To assign a residue fragment to coil, do something like this: `assign sstructure` a_/13:40 "_".

column

indicates a layout format of several arrays (`iarray`s, `rarray`s, `sarray`s) with the same number of elements as side−by−side columns. The column format look like this:

```
#>  a   b   c
   1.  15  "alpha"
   2.  18  "beta"
   5.  10  "gamma"
```

It is also useful to show arrays of a `table` (see also `database`).

current map

usually is the last map loaded by the `read map` command or created by the `make map` command. The current map may be changed by the `set map` command. To find out which one is the current, use `list` *maps.*

current object

usually is the last object loaded by the `read object` command or created by the `build` command. The current object may be changed by the `set object` [*os_object*] command. To find out which is the current one, use `list object` or `show object` [*os_object].*

You may refer to the current object as **a_**

current table

usually is the last table loaded by the `read table` command or created by the `group table` command. The current table may be changed by the `set table` command. To find out which one is the current, use `list` *tables.*

command

an instruction one can execute in the ICM−shell interactively or from an ICM script file. Typically a command consists of a verb (like `read` or `delete`) and a bunch of arguments. The word order in the argument list is not important, if arguments have different types. For example:

```
display a_//ca,c,n yellow # is as good as ...
display yellow a_//ca,c,n # ... inverse
```

There are exceptions,

- if two or more arguments are of the same type, e.g.

  `write "This line" "filename"`

  or `superimpose` *as_select1 as_select2* ,

- a complex argument consists of two parts: e.g. `delete label` *i_number* or `grid["x"]` in the `plot` command. In the latter case if the "x" string is not preceded by `grid` word, it will not be considered.

comp_matrix

a residue comparison matrix used by the `align`ment algorithms. The matrix is loaded automatically together with other library files from the icm.cmp file and can be reloaded later (if you need another matrix) using the `read comp_matrix` command.

The current matrix can be shown. All elements are properly reordered and multiplied by a factor such that the sum of occurrence−weighted diagonal elements (identities) of the matrix is 1.0 and stored in this form.

You can increase all the values in the matrix (a useful operation for low sequence identities) with the `set comp_matrix` command which has similar effect to reduction of the `gapOpen` parameter.

The `set comp_matrix` command also allows to modify weight for specific residue pairs (e.g. set comp_matrix 4. "CC"). Two matrices are recommended: the blosum50 with penalties 2.0/0.15 and the Gonnet matrix (the default) with penalties 2.4/0.15. A number of matrices are provided. You can use your own data file too.

Normalized matrices with diagonal elements equal to 1. Most of the matrices efficient for sequence alignment have different Cii weights. For example, two aligned tryptophanes will get better score than two aligned alanines. The Cij values can also be normalized as follows:

```
Cij_norm = Cij/Sqrt(Cii*Cjj)
```

This normalization is used in the `Score` () and `Rarray` () functions calculating conservation values for each position in an alignment.

conf

a conformation (actually a set of variables determining the conformation) stored in an ICM `stack` . You can add a conformation to the conformational stack or `load` a conformation from the stack.

Example:

```
% icm
 buildpep "ala his trp"
 montecarlo
 show stack
 iconf>       1       2       3       4       5       6       7
 ener>    -15.1   -14.6   -14.6   -14.2   -13.9   -11.4    -1.7
 rmsd>      0.3    39.2    48.0    44.1    27.4    56.6    39.3
 naft>        1       0       0       1       1       1       0
 nvis>        4       1       1       4       4       4       1
 print Nof(conf)
 7
 print Iarray(stack)  # returns {4 1 1 4 4 4 1}
 t = Table(stack)     # more conf parameters
 for i=1,Nof(conf)
   load conf i
   center
   pause  # hit return
 endfor
```

cpk

abbreviation of "Corey−Pauling−Koltun" who introduced space−filling solid models of atoms. In ICM graphics it means solid representation of van der Waals spheres. Spheres are drawn at van der Waals radii. See also: `display`

5.4. D

database

a format for storing entries containing several different types of information. The `column` format (multicolumn representation) is the alternative. The database should have the following format:

```
FieldName1 Number|String
FieldName2 Number|String
FieldName3 Number|String

FieldName1 Number|String
FieldName2 Number|String
FieldName3 Number|String
...
```

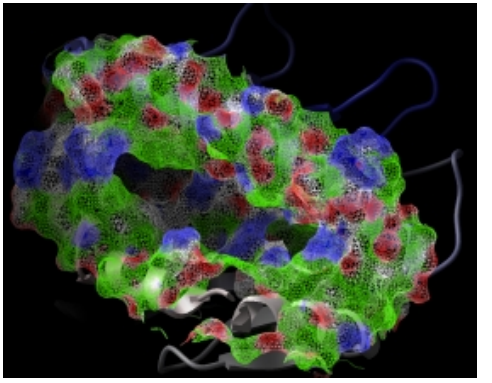
Fields can contain integers, reals and multiline strings.

Example:

```
id   jur1
iq   24
addr  LA
addr  California

id   jur2
iq   17
addr LA
```

Depth−cueing, or fog



a visual effect which makes objects disappear in a fog according to the screen Z−coordinate. Press

`Ctrl−D`

to invoke the effect and move the back clipping closer with MidMB to make the effect more dramatic. Also more the front clipping plane with `Ctrl−MidMB` to make the front brighter.

If you use `gui` adjust the front and back clipping planes using the buttons in the graphics tool bar and vertical movements with the left−mouse−button

Two parameters influence the **fog** effect:

- `fogStart` determines the relative Z−position at which the linear fog effect starts (the distance between the front and the back planes is 1.)
- `color volume` *color* command allows to color fog differently from the `background` (by default they are the same).

distance

a measure of proximity in three−dimensional or multidimensional space for all kinds of objects, including sequences and real arrays. See function `Distance` ().

distance geometry

is often used to calculate a set of Cartesian coordinates of a series of objects given all (or even a subset of) the inter−object distances (Crippen and Havel, 1988). ICM function `Disgeo`() allows to solve this sort of problems. See also `Distance`().

disulfide bond

(or SS−bond) a covalent bond between sulfur atoms of two cystein residues. In the PDB objects loaded by the `read pdb` command these bonds are automatically imposed on the basis of `SSBOND` records. Upon conversion of a PDB structure into the ICM−object with the `convert` command, the disulfide bonds are inherited. **Important:** commands `make disulfide bond` and `delete disulfide bond` are valid for ICM−type molecular objects only (and have no effect on, say, PDB structures). Both commands change the covalent structure of the modeled molecular object and expel/add hydrogens. In addition, SS−bonded **cys** residues are renamed to **cyss.** Therefore, to count the number of disulfide bonds you may simply count the **cyss** residues: `show Nof(a_/cyss)/2` . Distance restraints imposed to form such a bond are defined in the file `icm.cnt` .

drestraint

a distance restraint (sometimes abbreviated as **cn**) which imposes a penalty function on the distance between two atoms of the *same* object (in contrast, `tether` imposes a restraint to an atom in *another* object) . Distance restraints may have different characteristics and types. A drestraint is a basin with flat bottom between the upper and lower bounds (D_u and D_L) and bi−quadratic walls:

$P(d) = 0.25*(d^2 - D_u^2)^2 / D_u^2$ if $d > D_u$ (upper wall)
$P(d) = 0$ if $D_{L<d<D,,u}$ (flat bottom)
$P(d) = 0.25*(d^2 - D_L^2)^2 / D_L^2$ if $d < D_L$ (lower wall)

`drestraints` are mostly used in structure determination using the NMR NOE data.

Drestraints may be read, written, made, setn, shown, and displayed. The parameters of drestraints are written in `*.cn` files. See also: `icm.cnt` file description.

To activate the drestaint penalty term, use the `set terms "cn"` command.

drestraint type

a type of `distance restraint`(s). It describes well depth, lower and upper boundaries and has two forms: *global* and *local*. Local restraints become weaker and vanish as the distance between the corresponding atoms grows (similar to the van der Waals forces), while global restraints become stronger as you deviate further from the required distance range. Local type has an additional characteristic: sharpness. The types are given in `*.cnt` files.

The main list of types consists of general user−defined global and local types as well as a number of fixed named types used to impose `disulfide bond`s or `peptide bond`s. Drestraint types may be `read`, `written`, `set`, and `shown`.

See also: `*.cn` file description.

5.5. E−H

ecepp

a force field used in the ICM program. The latest version is called ECEPP/3 reported in Nemethy et al. (1992). See also the following references: Momany et al. (1975), Nemethy et al. (1983)

fasta

program **FASTA** (Pearson and Lipman, 1988) is used for search sequence databases, evaluate similarity scores and identify sequence similarities on the basis of local sequence similarity. The program is well suited for rapid database searches, because it does not handle insertions/deletions. In ICM, **fasta** also specifies one of the several allowed formats of sequence data storage and representation.

5.6. S

site

ICM sequences and objects may contain specific information about local sequence features, such as location of binding sites, disulfide bonds etc. These information is stored in the feature table (FT) section of the Swissprot protein sequence entries or after the SITE fields of `pdb` files. The sites in the feature table may look like this:

```
FT   ACT_SITE     15     15       ACTIVE SiTE HIS
FT   TRANSMEM    309    332       PROBABLE
FT   DOMAIN      333    362       CYTOPLASMIC TAIL.
FT   DISULFID    125    188       BY SIMILARITY.
```

We use one letter code (the second column) to specify the site type. The first column shows the priority value which is used by the `set site` command.

Priority	Char	SWISSPROT def.	Description
4	A	ACT_SITE	Amino acid(s) involved in the **A**ctivity of an enzyme.
2	B	BINDING	**B**inding site for any chem.group(co−enzyme,prosthetic group...)

5	C	CA_BIND	Extent of a **C**alcium−binding region.
5	D	DNA_BIND	Extent of a **D**NA−binding region.
4	F	SITE	Any other **Feature** on the sequence (i.e. SITE records in PDB).
2	G	CARBOHYD	**G**lycosylation site.
7	I	INIT_MET	The sequence is known to start with an **i**nitiator methionine.
2	L	LIPID	Covalent binding of a **L**ipidic moiety
2	M	METAL	Binding site for a **M**etal ion.
5	N	NP_BIND	Extent of a **N**ucleotide phosphate binding region.
6	O	PROPEP	Extent of a pr**O**peptide.
6	P	PEPTIDE	Extent of a released active **P**eptide.
5	R	REPEAT	Extent of an internal sequence **R**epetition.
6	S	SIGNAL	Extent of a **S**ignal sequence (prepeptide).
5	T	TRANSMEM	Extent of a **T**ransmembrane region.
1	V	VARIANT	Authors report that sequence **V**ariants exist.
1	X	CONFLICT	Different papers report differing sequences.
5	Z	ZN_FING	Extent of a **Z**inc finger region.
6	c	CHAIN	Extent of a polypeptide **C**hain in the mature protein.
5	d	DOMAIN	Extent of a **D**omain of interest on the sequence.
3	e	THIOLEST	Thiol**E**ster bond.
1	m	**M**UTAGEN	Site which has been experimentally altered.
2	p	MOD_RES	**P**ost−translational modification of a residue.
3	s	DISULFID	Di**S**ulfide bond.
3	t	THIOETH	**T**hioether bond.
1	v	VARSPLIC	Sequence **V**ariants produced by alternative splicing.
6	z	TRANSIT	Transit peptide(mitochondrial,chloroplastic,cyanelle,microbody)
5	~	SIMILAR	Extent of a similarity with another protein sequence.
4	−	NON_CONS	Non consecutive residues.
7	+	NON_TER	The residue at an extremity of seq.is not the terminal res.
4	?	UNSURE	Uncertainties in the sequence

The sites can be

- read from a swissprot entry with the `read sequence swiss` command
- set to a `sequence` or a molecular object with the

  `set site` [seq_from [ali_] {seq_|ms_} [only]

  command

- a new site can be set with the

  `set site` s_siteString {seq_|ms_} [only]

command (e.g. set site a_1.1 "FT SITE 15 15 important residue") .

- and delete with the

  `delete site` {seq_|ms_} i_siteNumber

  command (e.g. delete site a_mol1 1) .

- To show sequence sites use the `show sequence swiss` command, and in objects: `show site` {seq_|ms_}

  command.

- Sites assigned to molecular objects can be selected (and thereby visualized) with the `a_/ F` *`SiteString`* selection
- Sites will be written to an object and restored upon reading under the `OBJECT.site` or `OBJECT.auto` preference.

The ICM−shell variable `l_showSites` toggles the appearance of the site information in the `show sequence` command.

The sites can be colored with the

```
color site rs_
```

command, e.g.

```
color site a_/FA red # features/sites from the active site
```

Example:

```
read pdb "1hla"  # this object Ca atoms of 2 molecules
make bond a_//ca # link them into a chain
rinx SWISS       #rinx is an alias to read index "...."
read seq swiss SWISS.ID=="1A02_HUMAN"
read seq swiss SWISS.ID=="B2MG_HUMAN"
read seq swiss SWISS.ID=="1A68_HUMAN"
set site a_1 1A02_HUMAN
set site a_1 1A68_HUMAN append
set site a_2 B2MG_HUMAN
show site B2MG_HUMAN
cool a_
ds cpk magenta a_/FV # display variants
ds cpk yellow a_/Fs  # display disulfides
```

grob

an abbreviation for a general GRaphics OBject, which contains dots, and/or lines and/or solid surfaces; it can be a geometrical body, a contoured electron density, 3D plot, an arrow, etc. If the graphics object contains triangles, it can be represented by solid surfaces. The order of points in the triangles defines the direction of the normals which in turn defines which of the two sides are lit. Grob−file format is straightforward and editable.

To merge two or several grobs, use the double−slash operator (e.g. `g = g1//g2//g3`) or the `write grob append` command.

Example:

```
read grob "icos"             # several example graphics objects
read grob "cube"             # are read in ...
read grob "oblate"
read grob "prolate"
gAll = g_cube//g_icos

display g_cube red           # ... and displayed
display solid g_icos blue
display g_oblate green
display g_prolate magenta
center
```

hbond− hydrogen bonds

are calculated according to ECEPP/3 potential. One can also display hbonds with their distances, deviations from linearity, colored by the strength parameter which takes the angle into account.

Related commands are `show hbond`, `display hbond`, `color`, and `undisplay` .

See also: `GRAPHICS.hbondWidth` , `GRAPHICS.hbondStyle`

svariablei, or ICM−shell variable

a named object stored in the program memory of one of the following types: `integer` (i), `real` (r), `string` (s), `logical` (l), `preference` (p), `iarray` (I), `rarray` (R), `sarray` (S), `matrix` (M), `sequence` (seq), `profile` (prf). alignments (ali), `maps` (m), graphics objects (grob) (g) . They can be created by direct assignment to a constant (e.g. `a={1 4 3 8}` , to a function (e.g. `a=Iarray(4)`) or `read` from a disk file (e.g. `read iarray "a"`) Most of ICM−shell variables can also be `written` to a disk file, and `show`n. They can take part in the arithmetic and logical `expressions`. For some of the variable types, `subsets` are defined (e.g. a[2:4]).

integer

numbers may exist in the ICM−shell as a named `variable` or a `constant (e.g. 123,2,−45 )`. There are several dozen `predefined integer variables`. Integers may be mentioned in `arithmetic expressions`, `commands` and `functions`.

Examples:

```
born =  1957 + 5              # she is 5 years younger
now  =  1996                  # lets pretend we live in 1996
if (now − born > 28) print "no, you are not 28, you are 27!"
```

label

usually a string displayed in the ICM graphics window. Types of labels:

- atom label # toggled by LeftMB clicking
- residue label # toggled by LeftMB double clicking
- variable label
- free string label # drag it with the Middle mouse button.

To display the free text label, type:

```
display "Below lies a black abyss"
```

To delete it `delete label` *`i_labelNumber`* e.g. delete label 2

To show:

```
show labels
```

logical

may exist in ICM−shell as a named `variable` or a `constant` (only two possibilities: `yes` and `no`) You can use exclamation mark for negation (**!)** and two operations: *and* (**&**) and *or* (|) There is a number of `predefined logical variables`. Logicals can be used in `arithmetic expressions`, most frequently in `if` (*logical*) ... expressions.

Examples:

```
l_nowIamDoingAStupidThing = yes yes

l_Polite = no                     # another logical variable
if (Error !l_Polite) print "And what do you think you are doing?"
```

macro

a group of ICM commands in a separate named function. See description `macro` in the command section.

map

a real function defined on a three−dimensional grid. Usually it is an electron density map or grid potential. See also: `icm.map` This ICM−shell object contains a descriptor (or header) with the following information:

- cell type (space group number) and parameters {a, b, c, alpha, beta, gamma};
- lattice and sublattice specifications (sizes and offsets for columns, rows and sections);
- characteristics of the density values: the mean value, standard deviation, the minimum and the maximum values.
- correspondence between X,Y,Z and sections, rows and columns

The map itself contains a stream of real density values for each node of the sublattice.

Maps can be `read`, `calculated` from structure factors, and created as a result of `map arithmetics`. Maps of 5 types of grid potentials can also be calculated with the `make map potential` command. The last map loaded or created becomes **the current map**. The current map is a convenient default for commands requiring map as an argument.

The following arithmetic operations between maps of compatible sizes are allowed: *map+map, map+i, map+r, i+map, r+map map−map, map−i, map−r, i−map, r−map map*r, map*i, i*map, r*map, map*map map/r, map/i.*

Map functions:

`Box`(map)	returns R_6box defining the map boundary
`Bracket`	same as Trim
`Cell`(map)	returns R_6 crystallographic cell parameters of the map
`Map`(map I_3_or_6 [simple])	a submap
`Min`(map)	minimal value
`Max`(map)	maximal value
`Nof`(map)	total number of grid points
`Rarray`(map)	returns all values from 3D−grid points as a linear real array
`Smooth`(map [expand])	space−average the map values
`Symgroup`(map)	string with the symmetry group name
`Trim`(map,vMin vMax)	trim by values outside the range
`Trim`(map,R_6box)	set values **outside** the box to zero

Simple arithmetic operations are allowed with the maps (map1 and map2 must have the same dimensions):

- plus (map1 + map2, map + r),
- minus (map1 − map2, map − r),
- multiply (map1 * map2, map*r, r*map),
- divide (map1 / map2, map/r),

One can also use expressions, e.g.

```
m = Smooth(m_ge)*2. − 1. + m_gc  # does not make much sense
```

matrix

a set of real numbers organized in rows and columns. The ICM−shell allows arbitrary size matrices [n,m], access to its elements (M[i,j]), rows (M[i]), columns (M[1:i,j]) or any submatrix (M[i1:i2,j1:j2]). Basic matrix `operations` such as

- plus (M1 + M2),
- minus (M1 − M2),
- multiply (M1 * M2),
- concatenate rows (M1 // M2),
- equal (M1 == M2),
- not equal (M1 != M2),

- `Transpose`(M), and
- inverse (`Power`(M,−1))

allow powerful matrix arithmetics. You can **create** a new matrix in the ICM−shell by `read`ing (`read matrix "a"`), assignment (`M_new=Transpose(M_old)`) or function `Matrix` (e.g. `M=Matrix(4,8)`. Matrix−related functions are the following:

- determinant of square matrix (`Det`(M))
- principal components or `"distance geometry"` (`Disgeo` (M)) function, i.e. if a given square matrix M[1:n,1:n] contains distances between n points find coordinates in (n−1) dimensional space and sort the space dimensions according to their contribution to the variation. If distances are 3−dimensional Euclidean distances, the first three coordinates will give you x,y,z.
- `Eigen` (M) function returns a matrix of eigenvectors; eigenvalues are stored in `R_out`
- `Distance`(*alignment)* − returns matrix of pairwise distances between sequences in an alignment.
- `Max` , `Min` , `Mean` and `Sum` functions return a row (actually a `real array`) with maximal, minimal, mean, or total values in each column, respectively
- `Nof`(M) and `Length`(M) − return ***n*** and ***m,*** respectively for matrix ***M[1:n,1:m]*** .
- `Power`(M, *i_exponent)* calculates different integer powers of a matrix, including matrix **inverse** (`inmat=Power(M,−1)`,
- `Random`(d1,d2,n,m) creates a matrix and fills it with random numbers,
- `Rmsd`(M) returns root−mean−square deviation,
- `Trace`(M) returns the trace of a square matrix,
- `Xyz`(*as_select)* returns a matrix of xyz coordinates of selected atoms.
- `Distance`(*matrix)* returns a matrix of pairwise distances between the row−vectors of the matrix.

Matrix assignments

Examples:

```
a=Matrix(4,5)           # create a matrix, simple assignment
a[1,1]=9.               # a single matrix element
a[2,?]={1. 2. 3. 4. 5.} # assign only the 2−nd row
a[?,3]={1. 2. 3. 4.}    # assign only the 3−nd column
a[2:3,1:2]=Random(−1.,1.,2,2) # assign only the 2x2 submatrix
```

By simple arithmetic operations with matrices you can

- solve a system of linear equations (x=Power(A,−1)*B),
- find best set of parameters x[1:m] which fits your model A[1:n,1:m] (n > m) to data vector B[1:n]. Minimum of (A*x−B) is found by 3 steps:

```
M1=Transpose(A)*A
M2=Power(M1,−1)
x =(M2*Transpose(A))*B
```

MIMEL

an abbreviation of Modified IMage ELectrostatics algorithm (Abagyan and Totrov, 1994) developed for fast evaluation of both internal Coulomb and electrostatic polarization free energy for large molecules. This term has no analytical derivatives and has no effect on local energy minimization. It can be a part of the

energy function in global optimization such as `montecarlo` or `ssearch` . Three components of MIMEL can be shown using the `show energy` command. They are:

- Coulomb interactions of explicit atomic charges (note that it is divided by the `dielConst` ICM−shell parameter)
- "Self energy" (or interaction of explicit charges with their own images)
- "Cross energy" (or interaction of explicit charges with other charges' images)

The last two components together represent the electrostatic polarization energy which is returned in the `r_out` variable. REBEL gives a more accurate evaluation of the electrostatic solvation. For small molecules use mimelDepth = 0.3. For proteins the error in the solvation energy evaluation (returned in the r_out variable) is estimated as 15 − 20%.

mmff .

This word refers to the Merck molecular force field described in a series of 1994 and 1999 publications by Thomas Halgren. ICM can assign MMFF atom types using local chemical environment, formal charges and 3D topology. ICM also allows to calculate the mmff94 energy and minimize it both in the `cartesian` space with free covalent geometry and in the `internal coordinate` space with fixed covalent geometry or user−defined geometrical constraints.

See also:

- `ffMethod` − defines which force field to use
- `read library mmff` − sets the parameters `set type mmff` − identifies the atom types from the covalent geometry, `formal charges`, and `bond types`
- `minimize`

mol

This word refers to the MDL Information Systems, Inc. SD−file format for small molecules (see trademarks). ICM can read and write molecules in this format. They may look like this:

```
name
jscorina  12209406473DS
LongName
  7  6
   -0.0187    1.5258    0.0104 C   0  0  0  0  0
    0.0021   -0.0041    0.0020 C   0  0  0  0  0
    1.6831    2.1537   -0.0024 S   0  0  0  0  0
   -1.4333   -0.5336    0.0129 C   0  0  0  0  0
    2.0692    1.9811   -1.7665 C   0  0  0  0  0
   -1.4126   -2.0635    0.0045 C   0  0  0  0  0
    1.4620    3.1542   -2.5386 C   0  0  0  0  0
  2  1  1  0  0  0
  3  1  1  0  0  0
  4  2  1  0  0  0
  5  3  1  0  0  0
  6  4  1  0  0  0
  7  5  1  0  0  0

> <NSC>
```

```
19

> <CAS_RN>
638-46-0

$$$$
```

mol2

This word refers to the Tripos file format for small molecules (see trademarks). ICM can read and write molecules in this format. The default extension for this type of file is .ml2. They may look like this:

```
@<TRIPOS> MOLECULE
a1
     3     2
SMALL
USER_CHARGES

@<TRIPOS>ATOM
     1  ho1    -2.0000    0.0000   -1.0000    H          1  hoh     0.3280
     2  o      -2.4944    0.0000   -1.8229    O          1  hoh    -0.6550
     3  ho2    -3.4149    0.0000   -1.5503    H          1  hoh     0.3280

@<TRIPOS>BOND
     1      1      2    1
     2      2      3    1
```

more

an internal ICM−viewer, a little brother of the UNIX browser with the same name. Displays ICM output one screenful at a time. Control:

- spacebar: next page
- Return: scroll by one line
- /string: find string
- n find next
- q: quit

movie

a series of molecular conformations representing a `Monte Carlo` trajectory and saved in an ICM−formatted `.mov` binary file can be simply `display`ed or used for `animated`.

The icm `.mov` files are *not* quicktime movies, or series of images. Instead, they contain a compressed series of geometrical parameters determining object geometry for each accepted `montecarlo` iteration.

The *frames* of the trajectory/movie file can be separately analyzed and further filtered with an ICM script. For example, one can generate a shorter movie by retaining only the frames with lower energies.

See also: `display movie`, `load frame`

mute

an option in a number of commands (e.g. `find pattern`, `find prosite`, `show tether`, `show energy`, `show area`, `show volume`, etc). It is usually used in scripts when one wants to suppresses unnecessary output. In `macro` declaration, this option suppresses prompting for missing macro arguments.

only

frequent option in commands which means disregard or delete the previous status. Without `only` commands usually add or append to the current settings.

Examples:

```
display only g_icos      # undisplay everything which is in the
                         # graphics window (if any)
                         # and display icosahedron
```

parray

pointer array, abbreviated as **P.** An array of pointers to objects. Currently there is only one type of parrays, namely arrays of chemical compounds created by reading a mol or sdf file. This compounds do not exist outside this array as independent molecular objects, but can be converted to molecular objects.

Mol−arrays.

creating mol−arrays To create a molarray use the `read table mol` command and first column of this table will be such an array. Example:

```
read table mol "Maybridge.sdf"
```

pattern

a sequence consensus pattern like this, "[AG]?[!P]W", or this "C?G?\{2,3\}C". A pattern can be extracted from an alignment and searched against a sequence database. See also:

- `find pattern` − find a pattern in a single sequence,
- `find database pattern` − efficient parallel pattern search in a BLAST−formatted sequence databank.
- `Pattern`(*s_consensus)* − create a regular pattern expression from a consensus,
- `Pattern`(*alignment)* − create a regular pattern expression from an alignment,
- `regular expressions and pattern matching`
- `prosite` − a collection of sequence patterns

png

graphics image format. Stands for Portable Network Graphics and was designed to replace the GIF format and, to some extent, the much more complex TIFF format. While GIF allows for only 256 palette colors, PNG can handle a variety of color schemes like TIF (1,3,8, 24, etc. bit colors). Furthermore, PNG is free, while GIF is subject to licensing fees. PNG also supports alpha−channel. Since 1998 most browsers

correctly display PNG images. See also: `rgb`, `tif` .

Pattern matching and regular expressions. Use the following metacharacters to construct regular expressions (try guess what string is used in the examples!)

- ***** matches any string including an empty string (e.g. "*see*")
- **?** matches any single character (e.g. "???ee M")
- **[string]** matches any one of the enclosed characters. Two characters separated by dash represent a range of characters.

  Examples: [A−Z], [a−Z], [a−z], [0−9] (e.g. "[A−Z] see [A−Z]"

- [**!string]** negation. matches any but the enclosed characters (e.g. "I see [!K]")
- single−character multiplication: *character\{m,n\}* (e.g. "I?\{3,6\}M" − repeat any character, ?, from 3 to 6 times)

The example string was "I see M". Regular expressions may be used in `selections` (`a_*.//c?,n,c`), and in `list`, `group`, `delete` commands. Note that for the latter three commands the pattern must be quoted.

pdb or Protein Data Bank

a repository of macromolecular structures solved by crystallography or NMR (occasional theoretical models are frowned upon). It used to be at the Brookhaven National Laboratory, Now it is shared between UCSD and Rutgers University. The old citations: Bernstein et al., 1977; Abola et al., 1987). The new citations can be found at `http://www.rcsb.org/pdb/` . On November 20th, 2001 it contained 16596 entries.

An example ATOM record:

```
ATOM     52  N   HIS D  18      53.555  24.250  49.573  1.00 32.59
```

peptide bond

a covalent bond between C=O and N−H groups, which is imposed in ICM−objects as an extra set of `distance restraints`. These groups may belong to the terminal groups as to the amino acid side chains. **Important**: commands `make peptide bond` and `delete peptide bond` are valid for ICM−type molecular objects only (and have no effect on, say, PDB structures). Both commands change the covalent structure of the modeled molecular object and expel/add hydrogens. `Distance restraints` imposed to form such a bond are defined in `icm.cnt` file.

profile

a table of residue preferences for each residue type at each position on a protein fold or a sequence. The preferences may be derived from a multiple sequence alignment of from a 3D structure. Profile also contains gap opening and gap extension values for each sequence position. Profile provides a good way of representing a consensus sequence pattern of a protein family. One can search a new sequence against a library of profiles, or search a profile against a data base of protein sequences (see Abagyan, Frishman, and Argos, 1994). One can add two profiles (prf1 + prf2), multiply them (prf1 * prf2), concatenate two

profiles (prf1//prf2), and extract a `part` of a profile (prf[15:67]). Profile can be read from a `.prf` file and calculated from an alignment with the `Profile`() function. See also: `Sequence`() `Consensus`() `Align`().

prosite

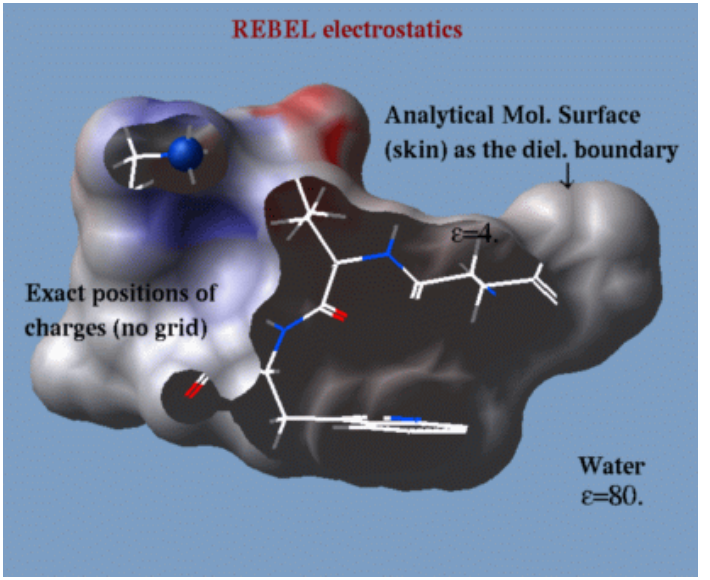
a dictionary of protein sites and patterns, (Copyright by Amos Bairoch, Medical Biochemistry Department, University of Geneva, Switzerland). ICM converts prosite patterns to standard string `patterns` containing regular expressions, like `"C?\{4,5\}CCS??G?CG????[FYW]C".`

The old releases of prosite can be found at
`ftp://ftp.expasy.org/databases/swiss-prot/sw_old_releases/`

See also:

- `read prosite`,
- `s_prositeDat`,
- `find prosite` − find all prosite patterns in a single sequence,
- find profile − find all prosite profiles in a single sequence

REBEL



a method to solve the Poisson equation for a molecule. REBEL is a new powerful implementation of the boundary element method with analytical molecular surface as dielectric boundary. This method is fast (takes seconds for a protein) and accurate. REBEL stands for Rapid Exact−Boundary ELectrostatics. The energy calculated by this method consists of the Coulomb energy and the solvation energy which is returned in the `r_out` system variable.

Related parameters and steps:

- `electroMethod` = "boundary element";

- `dielConst` (the default is usually OK);
- `dielConstExtern` (the default is usually OK);
- `set charge` *as_ r_Charge* (modify charges if you like);
- `make boundary` (if you want to make several evaluations of energy or `Potential`( ) with the same boundary. The "boundary" parameters depend only on conformation and do NOT depend on charges. You can redefine charges afterwards and get a corrects energy evaluation);
- `delete boundary` (if you do not need it);
- `show energy` (make sure the "el" term is on);
- `Potential`(*as_targets as_charges)* (if the boundary exists, returns potentials from charges at the target atoms);
- `color grob potential` (create graphics object, say, with `make grob skin` actually it can be any `grob` and `color it by the REBEL potential);`

The polarization charges can be returned by the `Rarray`(as_) function after the equation is solved, e.g.:

```
electroMethod = 4

show energy "el"

Rarray( a_//* )
```

real

number may exist in the ICM−shell as a named `variable` or a `constant` (e.g. `12.3, 2.0, −4.501`). There are a number of `predefined real variables`. Reals may be mentioned in `arithmetic expressions`, `commands` and `functions`.

Examples:

```
a = −1.2
b = Abs(Sin( 2.3 * a − 3.0 / a))
```

regularization

procedure for fitting a protein model with the ideal covalent geometry of residues (as represented in the `icm.res` residue library) to the atom positions of a target PDB structure (usually provided by X−ray crystallography or NMR). Regularization is required because the experimentally determined PDB−structures often lack hydrogen atoms and positional errors may result in the unrealistic van der Waals energy even if these structures were energetically refined (since the refinement of the crystallographic structures typically ignores hydrogen atoms and employs different force fields). The following steps are required to create the regularized and energy refined ICM−model of an experimental structure:

- an extended all−atom model of a particular protein is generated with regular geometry characteristics (see the `build` command and the `IcmSequence` function);
- the non−hydrogen atoms in the model are assigned to the equivalent atoms in the model (see `set tether`);
- the regularized structure is built starting from the N−terminus by adding atoms one−by−one (see `minimize tether`);
- methyl groups are rotated to reduce van−der−Waals clashes;

- combined geometry and energy function is optimized;
- polar hydrogen positions are adjusted;
- optionally the model may be additionally minimized, now without tethers to observe a "stability" of the model in the local energy minimum.

See macro `regul`.

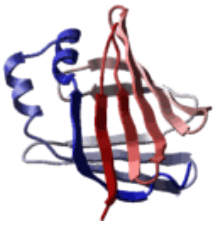
residue

a chemical building block or complete chemical compound, usually an amino−acid residue. The ICM hierarchy: atom −> residue −> molecule −> object. Individual small molecules may contain only one residue. Residues are described in the `icm.res` file. You may create your own residues with the `write library` command. Residues can be selected with the ICM−selection expression (e.g. `a_/ala, a_/15, a_/15:20, a_/"RDGE"` etc.), labeled with the `display residue label` *rs_* command, by double clicking with the right mouse button, via a pop−up menu, or from the GUI menu.

rgb

red−green−blue. It is of interest, that the combination of these three can produce any other color. In addition, this is the name of the SGI image format used in the ICM commands `write image` and `display movie`. ICM also generates the fourth channel on top of the RGB information. This fourth number is called alpha−channel and generates the opacity index for each pixel of the image. This information is interpreted by a number of applications, i.e. the IRIX showcase and dmconvert (the SGI moviemaker). See also `tif`, `targa`, `postscript`.

ribbon



a graphical representation of a polypeptide chain backbone by a smooth solid ribbon. DNA and RNA can be also displayed in a ribbon style.

There are three types of elements of the ribbon display depending on the `secondary structure` assigned to a given residue.

Residues marked as alpha−helices ('H') will be shown by a flat ribbon, those marked as beta−sheets ('E') will be flat ribbon with an arrow−head, and the rest will be shown by a cylindrical "worm". The ICM−shell parameter `GRAPHICS.wormRadius` defines its radius. Default ribbon colors are defined in the `icm.clr` file. Note that minor secondary structure elements like 3/10 helix ('G'), Pi−helix ('I') are colored by the corresponding colors (the `threetenRibbn` and `piRibbon` parameters in the `icm.clr` file), 'Y' type is colored by the `alphaRibbon` color, and 'L','P' and 'B' (isolated beta−residue) residues are colored by the `"betaRibbon"` color. DNA and RNA ribbons are colored according to the base type: A−red, C−cyan, G−blue, T or U − gold. Preference `ribbonStyle` allows to display a simplified `segment` representation of the secondary structure elements instead of (or together with) the ribbon.

The DNA/RNA ribbons consists of two parts the backbone ribbon and the bases shown with the sticks and balls. To selectively display and undisplay the bases, you can do the following:

Example:

```
read pdb "1dnk"         # contains 2 dna mol.
display ribbon a_1.2,3  # both bases and backbone
undisplay ribbon base a_1.2    # bases disappear
display ribbon base only a_1.2 # only bases
display ribbon a_1.2,3 yellow  # both bases and backbone
color ribbon a_1.3 magenta     # the second chain backbone
color ribbon a_1.2,3 bases     # default by base type
cool a_  # cool is a rich macro. View the whole thing
```

script

(or ICM script) means a collection of `ICM commands` stored in a file which can be `call`ed from `ICM-shell`.

Example:

```
call _demo_fold # find demo_fold file and start the script
```

sequence

an ICM-shell object containing an amino-acid or DNA sequence. The ICM-shell is tuned to work with very large sets sets of millions of genomic sequences at once. To work with the sets larger than 2 Gigabytes in size use the 64-bit binary executable (it is standard on Cray and Dec, unavailable on Windows and optional on SGI). One can `read a sequence` from a sequence file in different formats, create it with the `Sequence`() function, `make sequence` command, or by assignment (e.g., aseq = bseq [2:18], new sequence aseq is a 2:18 fragment of sequence bseq). A valid amino-acid sequence contains an uppercase string of one-characters amino-acid names. Please distinguish this ICM-shell object from the "sequence" in the ICM-sequence file which contains detailed 3 (or 4)-character notations of residues from the icm residue library. One can concatenate two sequences (seq1 // seq2) and extract a `part` of it (seq[15:67]). Sequence object may contain the secondary structure string (e.g. EEE___HHH_) of the same length as the sequence. It is automatically created by the `make sequence` command and the `Sequence`( ) function or can be directly set with the `set sstructure` command. If logical `l_showSstructure` is set to `yes`, the secondary structure string will be shown in `alignment`s.

Examples:

```
aseq=Sequence("ASSAARTYIP")
read sequences "aa.seq"
aseq[3:4]="WW"

read object "crn"
crn_seq = Sequence(a_/*)
```

Resetting sequence type

ICM is trying to guess sequence type. To set sequence type explicitly, use the set type [protein|nucleotide] command. E.g.

```
a=Sequence("AAAATAAAA")
set type a protein  # or if you change your mind
set type a nucleotide
```

Properties of a sequence can be projected to an alignment in which the sequence participates with the `Rarray`(*R_property,seq_,ali_,r_gapDefault*) function. The opposite action, i.e. projecting from alignment to a particular sequence can be achieved with another form of the Rarray function: `Rarray`(*R_ali,ali_from,seq_|i_seqNumber*)

segment

an element of the simplified representation of a protein topology in terms of its secondary structure elements (Abagyan and Maiorov, 1988). One element (referred to as a segment) is a vector of the best axis of the element. Loop segments are represented by a straight line between the end of the previous segment and the beginning of the next one. This representation can be used for a fold search through a library of precalculated segment descriptions of the protein topologies (foldbank.seg). See also `ribbonStyle.`

(ICM)−shell

user−friendly, high−level command interpreter combined with a collection of tools allowing you to interact conveniently with the kernel of the ICM software.

skin

a solid graphical representation of the molecular surface, also referred to as the Connolly surface. It is a smooth envelope touching the van der Waals surface of atoms as the solvent probe of the `waterRadius` size rolls over the molecule. "Skin" is important for analysis of recognition, electrostatics, energetics, ligand binding and protein `cavities`. The surface is calculated with a new fast analytical **contour−buildup** algorithm (Totrov and Abagyan, 1996) and can be generated as a general `graphics object` with the `make grob skin` command. 'Skin' consists of three types of elements: convex spherical elements, concave spherical elements, and torus−shaped elements. ICM allows the calculation of the `volume` confined by the 'skin' and its surface area. In a general case skin is defined by **two** atom−selections:

1. atoms the skin is calculated for
2. atoms surrounding the atoms from the previous selection

One can calculate/display only a patch within a context of the rest (as_part a_*), or skin around one molecule as the rest does not exist (as_part as_part):

```
read object "complex"
display a_//ca,c,n
pocket = a_1//!h* Sphere(a_2//!h*)
display skin pocket a_1//!h* # 5A sphere around the second subunit
set plane 2                  # or F2 : to avoid deletion of the previous patch
display skin a_2//!h* a_2//!h* green # ignore everything but the second molecule
```

Colored molecular surface can be saved as:

- bitmap image (tif, targa, gif, postscript bitmap) (`write image "file"`)

- vectorized postscript containing triangles, not pixels (`write postscript "file"`)
- the skin can be converted into a uniform color grob (`make grob skin`)
- the skin can be colored by potential and ((`color grob potential` try also: `show dsRebel`)
- Warning: `make grob image` does not generate correct normals because of a feature in OpenGL, however, this command works fine for molecular representations such as `cpk` , `ribbon` , `xstick` , etc.

ICM can also generate smooth `gaussian surfaces` with the following commands:

```
make map potential Box( a_ 3. )   # build gaussian map
make grob m_atoms solid exact 0.5 # contour it
display g_atoms                   # display the envelope grob
```

smiles

Simplified Molecular Input Line Entry Specification. The acronym introduced by David Weininger to represent chemical valence model by a string (e.g. CC=O). It can also be used as an exchange format for chemical data. The algorithm was published in 1988 and is described in detail at the WWW site of Daylight Chemical Information Systems, Inc.

See also the `Smiles` function and the `build smiles` command.

sln

Sybyl line notation, a string representation of molecular structure similar to Smiles. The sln string is returned by the `String`(*as_* `sln`) function.

stack

a set of `conf`ormations of a particular object. The stack can be just a place to store (with the `store conf` command) a number of complete descriptions of different conformations regardless of the way they have been created. The maximal number of stack conformations is determined by the `mnconf` parameter. The stack conformations can be created manually in the course of interactive procedure, or created automatically as a result of a `montecarlo` run. The energies of stack conformations can be shown with the `show stack [all]` command. The stack can be saved into a `.cnf` file, and you can also `read stack`. Stack in Biased Probability Monte Carlo procedure represents best energy representatives of different conformational families (see Abagyan and Argos, 1992). Measure of difference (or distance) is defined by the `compare` command and `vicinity` parameter. Stack can influence the search via the following variables: `mnvisits`, `mnhighEnergy`, `mnreject`, `visitsAction`, `highEnergyAction` and `rejectAction` .

See also:

- `conf` (has good examples),
- `Table(stack)` stack conformation parameters
- `Iarray(stack)` (the number of visits to each stack conformation).
- `Nof` (conf)
- `load conf i`

stick

graphical representation of a covalent bond as a solid cylinder. Its radius is defined by the `GRAPHICS.stickRadius` ICM−shell variable.

string

may exist in the ICM−shell as a named `variable` or a `constant` (e.g. `"1crn", "A b\n c"`). There is a number of `predefined string variables` in the ICM−shell. You can concatenate strings ("aaa" **+"bbb"** or "aaa" //**"bbb"** −> "aaabbb"), sum a string and a number ("aaa"+4.5 −> "aaa4.5"), compare them (if (s_pdbDir == "/data/pdb/", or if (s1 > s2)). Strings may be used in `arithmetic expressions`, `commands` and `functions`.

Examples:

```
s  = "1crn"
s1 = s1 + ".brk"
if (s != "2ins") print "wrong protein"
```

structure factor (factor)

a named ICM−shell `table` containing information about reflections. A structure factor table header may contain maximal absolute values of h k and l.

```
#>I igd.HKL
 31 36 37
```

It will be calculated on the fly if absent and is important for Fourier transformation. You may also have any number of additional members in the header section for your convenience. For example, real values for the minimal and maximal resolution, etc.

The "column" part of a table contains mandatory integer arrays of h,k and l. Some of the other arrays with fixed names may be necessary for specific operations. They are:

- **fo** : `real array` of observed amplitudes (used by the `"xr" term`)
- **fc** : `real array` of calculated amplitudes. They are added and updated automatically by the `"xr" term calculations`.
- **ac** and **bc** : `real array` of Real and Imaginary components of calculated structure factors. **ac** and **bc** may be read from a file, calculated in the ICM−session, and/or added and updated automatically by the `"xr" term calculations`. These two arrays are used as the input arrays for the `make map factor` command.
- **w** : `real array` of weights of individual reflections which are used if defined in the `"xr" term calculations`. Note, that multiplicity will be automatically taken into account, do not multiply your weights by it to avoid double counting.
- **free** : `integer array` of 0 and non−zeros to mark reflections for R−free calculations. Reflections marked with non−zeros will not be used in the `"xr" term calculations`. They

will be used instead by the `Rfree`(*T_factor)* function.

One can add any number of additional arrays to the factor−table. Of course, the table can be `read`, `written`, `sorted`, `shown`, etc. You may also use powerful table arithmetics and expressions to generate new columns and specify subsets.

Examples:

```
                                  # new columns
group table append F Sqrt(F.ac*F.ac+F.bc*F.bc) \
      "fc" Atan2(F.bc,F.ac) "ph_calc"

F.ac = (2*F.fo−F.fc)*Cos(F.ph_calc)
F.bc = (2*F.fo−F.fc)*Sin(F.ph_calc)
make map factor F    # 2Fo − Fc map is ready

F1= F.fc > 1. # another table of strong reflections
F2= F.h < 20 F.k < 30 F.l < 20 # another subset
```

See also: How to manipulate with structure factors

The command word "factor" serves to read/write the XPLOR formatted structure−factor−files.

surface area

in the ICM−shell means a solvent−accessible surface (center of water−sphere). **Important**: Do not confuse this surface with the molecular or Connolly surface which is referred to as `skin` . (see also `Acc` function, `Area` function, `display skin`,`display surface`, `show area surface`,`show area skin`, `show volume surface` `"sf" term`).

Important: There are two ways to calculate the surface area: via the `show area surface` or the `show energy "sf"` commands. In both cases individual atomic accessibilities are calculated and assigned to individual atoms. These accessibilities can be shown with the `show as_` command, or can be accessed with the `Area`(*as_)* function. However, the two commands use different atomic radii:

- show area surface
  - ♦ uses van der Waals radii as defined in the `icm.vwt` file
  - ♦ calculates areas for all atoms including hydrogens
- show energy "sf"
  - ♦ uses special radii designed for calculations of the solvation energy. The radii are defined in the `icm.hdt` file ;
  - ♦ employs a united atom model, in which hydrogens are ignored and radii increased accordingly;
  - ♦ calculates areas only for non−hydrogen atoms, ignores hydrogens.

Examples:

```
                  # dipeptide
build string "se nter ala his cooh"
                  # fill out individual accessibilities
                  # (incl. hydrogens)
show area surface  # takes all atoms w. vdWaals radii into account
```

```
 show a_//*         # look at the accessibilities
 show Area(a_//n*)  # extract atomic accessibilities for all nitrogens
#
 show energy "sf"   # only heavy atom accessibilities used in energy calc.
 show a_//*         # look at these new accessibilities
 show Area(a_//n*)  # "energy" accessibilities for nitrogens
```

5.7. T

table

an ICM object which unite several other `ICM-objects`. It consists of two parts:

- a header which is a set of any `ICM-objects` and
- a spreadsheet composed of `iarray`s, `rarray`s, `sarray`s, or `parray`s, of the same length. A `parray`, or pointer-array can contain chemical structures (see `read table mol` command).

Tables can be `read`, `written`, and `shown`. Tables can also be created by

`group table` *obj1 obj2* ...

command and returned by some functions such as:

- `Energy(stack)` returns a table with energy values for the stack conformations
- `Table(s_out)` interprets an output of an HTML form.
- `Find` performs search in all entries and returns the matching entries

One can inserted to empty rows, or duplicate rows or , insert rows from a different table with the add table command.

Tables can be merged with the `append column` command.

Pairwise table expressions:

- !(Table selection) negation
- T.I_ **?** i_ (**?** is one of: **==, !=,** <=, >=, <, >)
- T.R_ **?** r_ (**?** is one of: **==, !=,** <=, >=, <, >)
- T.S_ **?** s_ (**?** is one of: **==, !=, ~, !~,** i.e. exact of `fuzzy` comparisons)
- T.S_ **?** S_ (**?** is one of: **==, ~,** equivalent to `T.S_ ? S_[1] | T.S_ ? S_[2] | ...`)
- T.S_ **?** S_ (**?** is one of: **!=, !~,** a complement to what is returned by the T.S_ == S_ or T.S_ ~ S_ comparison, respectively, equivalent to `T.S_ ? S_[1] T.S_ S_[2] ...`)

The result of the pairwise expression is a subset of the table involved. The pairwise expressions can be further combined with the **&** (AND) or **|** (OR) operations. A full expression can be assigned to a new table or used on the fly in a number of commands and functions. String comparison can use patterns (e.g. t.NA=="*_MOUSE"). The pattern may contain more sophisticated `\{n,m\}` expressions, if the first symbol is '*' or '^'.

Example:

```
group table t {"a","b","c"} "s" {1 2 3} "i" # arrays t.s, t.i
show t
show t.s == {"c","a"} # shows the 1st and the 3rd lines
show t.s ~ "a*" | t.i < 3 # shows the 1st and the 2nd lines
```

Table operations

- split column values
- appending one table to another by a shared column
- grouping table rows by a column
- add/insert table rows

table subsets:

Table subsets can also be defined explicitly through the three types of index expressions:

- T[i_element], e.g. t[3]
- T[i_from:i_to], e.g. t[3:15]
- T[I_indexArray], e.g. t[{3,14,18}]

Index arrays are returned by some commands or the Iarray(T_) function.

Look at this example of operations with tables. We read a database of secondary structures `foldbank.db` dump arrays into a table, add sequence length to a table, extract entries of interest, sort them and save the result.

```
read database "foldbank.db"          # load information into arrays
LE=Length(SS )                       # create iarray with sequence lengths
group table t $s_out LE              # create table t with all info + lengths
show t                               # press 'q' otherwise computer will explode
show t.NA == {"1gec.i","5pad*"}      # find these entries
a=t.RZ < 2.2 t.ER < 1. t.LE > 35 # select entries with resolution < 2.5,
                                     # converted with ER < 1. and longer
                                     # than 35 residues
sort a.LE a.RZ                       # resort entries according to
                                     # lengths/resolution
write database a "SUBSET"
```

Plotting table data

The ICM tables can have built−in plots. To add an automatically generated plot to a table, follow these steps:

- append the `plot` header field with a `sarray` of plots (e.g. `group table append t header {"x=A;y=B"} "plot"`).
- specify a subset of following options separated by semincolons and without space.

Syntax of a *plotString*, (*f* is the name of a column of the table, e.g. A)
x=f;y=f;[label=f;][color=f;][shape=SHAPE;][size=f;]:
[xbarFrom=f;xbarTo=f;|ybarFrom=f;ybarTo=f;]

[title=text;][xScale=from,to,nMajorTics,nMinorTics][yScale=from,to,nMajorTics,nMinorTics] : [regression={yes|no};][connect_dots;][rainbow=slash_separated_colors;] [element=element_specs]

The element section descrives additional sub−plots which can be added to the main plot. The element specifications are similar to the main plot specifications, but the fields for each element are separated by commas, rather than by semicolons.

```
element={rectangle|RECTANGLE},x=,y=,{x2=,y2=|w=,h=},color=,fillPattern=PATTERN,label=,labelPos
```

The following shape types are possible: None (i.e. dot), Ellipse , Rect , Diamond , Triangle , DTriangle , UTriangle , LTriangle , RTriangle

The following fillPattern styles are available:

Solid	solid color
Dense1	the most dense pattern
Dense2	
..	
Dense7	the lightest pattern
Hor	horizontal lines
Ver	vertical lines
Cross	cross pattern
BDiag	diagonal pattern
FDiag	another diagonal pattern
DiagCross	diagonal cross pattern
Custom	pixmap

Example:

```
S_plots = Sarray(1)
S_plots[1] = "x=i;y=MaxDev;color=Entropy;size=8;title=Quick plot"
# t has the following columns: i, MaxDev, Entropy,
group table append t header S_plots "plot"
```

tether

a harmonic restraint pulling an atom in the current object to a static point in space. This point is represented by an atom in another object. Typically, it is used to relate the geometry of an ICM molecular object with that of, say, an X−ray structure whose geometry is considered as a target (see also delete tether, minimize tether, show tether, set tether).

The restraint can also pull an atom to a z−plane (rather than to a point), if you specify tzMethod="z_only"

Atom specific weights can be imposed with tzMethod="weighted" via bfactors.

tzMethod="function" is the most flexible. It allows you to specify different strength, upper and lower boundaries for each tether, establish a flat area in which no penalty is imposed, and even exert

constant force. In this case one needs to set atom properties of the "dummy" object to which the "active" atoms are tethered.

Two other types of restraints are `drestraint` (distance restraints), and `vrestraint` (multidimensional variable restraints).

tif files

Tag(ged) Image File Format, used by default in the ICM commands `write image` and `display movie`. See also: `rgb`, `png`, `targa` .

transformation vector

an elementary space transformation is defined by a `rarray` where values {a1,a2,...,a12} define 3x3 rotation matrix and translation vector {a4,a8,a12}. The complete augmented affine 4x4 transformation matrix in direct space can be presented as:

```
a1  a2  a3  | a4
a5  a6  a7  | a8
a9  a10 a11 | a12
------------+----
0.  0.  0.  | 1.
```

The commands and functions related to transformation vector (referred to as *R_tv):*

- `transform` *ms_ R_tv* applies transformation to an object;
- `Symgroup`(*i_spaceGroupNumber)* returns a chain (R_[1:12*n]) of all n transformation vectors composing the specified space group;
- `Augment`(*R_tv)* converts 12−membered transformation vector into the augmented transformation matrix 4x4;
- `Vector`(*M_4x4)* converts a 4 by 4 transformation matrix into 12−membered transformation vector
- `superimpose` *as_1 as_2* ... returns *R_tv* in `R_out;`
- `Rmsd`(*as_1 as_2* [`exact`]) returns *R_tv* in `R_out;`
- `Axis`(*R_tv)* calculates the rotation axis *R_3* of the transformation. Rotation angle is returned in `r_out;`
- `Rot`(*R_tv)* extracts the 3x3 rotation matrix;
- `Trans`(*R_tv)* extracts the translation 3−vector which is applied after rotation.

5.8. U−Z

unique

an option of the `group sequence` command used to exclude from the group identical sequences (which may result from, e.g., from a set of PBD structures with the same sequence, but somewhat different conformation).

virtual atoms and variables

Additional immaterial geometrical points (referred to as "virtual atoms") attached to each molecule for technical reasons, and internal coordinates ("virtual bonds, angles, torsions and phases") associated with them. These points help to have a standard yet flexible treatment of parameters defining absolute position (translation and rotation) of each molecule with respect to the coordinate frame. Each molecule is connected to the origin via two virtual atoms attached to it. This part of the ICM−molecular tree is built in the following way:

- **o2, o1, o** three points with coordinates `{1,0,1}, {0,0,1}` and `{0,0,0},` respectively. They are the same for all molecules
- **vt1** the first virtual atom of a molecule. It is attached to the origin (**o**) via virtual bond length **bvt1,** planar angle **avt1** (**o1−o−vt1**) and a dihedral angle. The dihedral angle is a torsion angle **tvt1** (**o2−o1−o−vt1**) for the first molecule in the tree, but it is a phase angle **fvt1** (a difference between dihedrals **o2−o1−o−vt1**(*current−molecule)* and **o2−o1−o−vt1(** *1st−molecule))* for all molecules but the first one.
- **vt2** the second virtual atom attached to **vt1** via virtual bond length **bvt2** (usually fixed), planar angle **avt2** (**o−vt1−vt2**) and a a torsion angle **tvt2** (**o1−o−vt1−vt2**).
- **the first real atom of a molecule**. Torsion angle leading to it is called **tvt3**.

The absolute position of the first molecule as a rigid body is defined by six virtual variables:

```
   Name StdValue Type  Definition
1. tvt1 180. torsion   **o2−o1−o−vt1
2. avt1  90. angle     **o1−o−vt1
3. bvt1   1. bond      **o−vt1
4. tvt2 180. torsion   **o1−o−vt1−vt2
5. avt2  90. angle     **o−vt1−vt2
6. tvt3 180. torsion   **o−vt1−vt2−1stAtom
```

The

```
set a_1//vt1
```

command sets the first virtual atom to the center of mass of the corresponding molecule. After that you can control the distance to the origin by `vt1.` To understand it better, try the following short session (just paste it line by line):

```
build string "se ala\nml a\nse his" # two molecules
display virtual
varLabelStyle = "name"
display variable labels
display virtual atom labels a_//vt*
connect a_1   # move the 1st molecule with the mouse
connect a_2   # move the 2nd molecule with the mouse
set a_1//vt1
set a_2//vt1
set v_1//bvt1 2.
```

volume

measured in cubic Angstroms. One can calculate the van der Waals volume (see `Volume` function), the volume confined by solvent−accessible `surface` (see `show volume surface`) , or by molecular surface referred to as `skin` (see `show volume skin`) .

vrestraint

a multidimensional variable restraint (often abbreviated as **rs**) which restrains one or several geometrical variables (usually torsions) to certain ellipsoidal zones, described by Abagyan, Totrov and Kuznetsov (1994). Variable restraints may have different `characteristics and types`. The vrestraints are marked either for energy calculations or for description of probability distributions (fields 'rse' and 'rs', respectively). See also: `icm.rs` and `icm.rst` files.

vrestraint type

a type of multidimensional variable restraint. Each type specifies to which variables this type may be assigned, the average values and standard deviations (or well dimensions), and the well depth. The types are described in `*.rst` files. There are two kinds of vrestraint types depending on what they will be used for: energy kind marked with the 'rse' field and the probability type marked with the 'rs' field. The first kind will be used as an `"rs"` penalty term, while the second kind will be used for the BPMC random step.

wire

a default representation of a molecule, fast and simple. Bonds are shown by lines or arrows according to the `wireStyle` preference. Double bonds in the wireStyle "chemistry" mode are shown according to the `wireBondSeparation` parameter. Isolated atoms are shown according to the `atomSingleStyle` preference (usually by a small tetrahedron); line thinkness is controlled by the `lineWidth` parameter.

Examples:

```
display a__1crn./n,ca,c  # displays a wire model of crambin.
                         # (note, display command can also
                         # read in the 3D coordinates
                         # if double "_" used)
```

You would need to mention "wire" explicitly to undisplay it when other types of graphical representation are also present.

Examples:

```
display                 # wire is the default
display cpk a_/1:5      # adds CPK
undisplay wire          # remove wires, leave only CPK
```

xstick

a combination of `ball` and `stick` representations of atoms and bonds.

ZEGA

a pairwise `alignment` method based on the Needleman and Wunsch algorithm modified to use zero gap end penalties. This type of alignment was first described by Michael Waterman, who called it the "fit" alignment. The paper of Abagyan and Batalov, 1997 describes the statistics of the structural significance of the alignment score and optimization of the alignment parameters for the best recognition of structurally related proteins. This statistics is used in database search (see the `find database` command) to evaluate the significance of hits. This pairwise alignment algorithm is used in the `Align` function, `align` command, and database searching.

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