NAME

AddAco – add angle constraints

SYNOPSIS

AddAco expr expr

DESCRIPTION

Add an angle constraint for all selected angles. The first argument gives the minimal value, the second the maximal value in degrees.

EXAMPLE

```
AddAco -20 130
```

SEE ALSO

ReadAco, SelectAngle, RemoveAco, AddUpl, AddLol

DATE

950302

NAME
AddAngle - add dihedral angle

SYNOPSIS
AddAngle name

DESCRIPTION
Add a dihedral angle with the given name, defined by the four selected atoms. Exactly four atoms must be selected before this command is executed, an error message will be issued otherwise.

Two of the atoms must be from the same residue, one also from the same residue or the previous residue, one from the same residue or the next residue.

The name must be unique within the residue.

The new angle cannot be used immediately for commands like RotateAngle, only angles that were in the residue library can be used for that purpose. The command is intended to be used in conjunction with WriteRes to generate library entries for non-standard residues.

EXAMPLE
AddAngle "RHO"

SEE ALSO
AddAtom, AddBond, CalcBond, WriteLib

DATE
961219

NAME

AddAtom - add new atom

SYNOPSIS

```
AddAtom name name1 name2 name3 expr expr expr
```

DESCRIPTION

Add an atom with the name given as first argument to all selected residues.

name1 is the name of the atom where the new atom is attached. name2 is the name of the atom that is used to define the axis of the dihedral angle together with the atom name1. name3 is the name of the atom relative to which the dihedral angle is given.

The first numeric argument gives the dihedral angle, the next one the angle between the axis of the dihedral angle and the bond between atom name1 and the new atom. The last argument gives the bond distance.

If name1, name2 and name3 do not exist in a selected residue, or if name already exists, then no new atom is added for this residue, without an error message.

A bond between the new atom and atom name1 is automatically added.

EXAMPLE

```
AddAtom "HB2" "CB" "CA" "HB1" 120 120 1.5
```

SEE ALSO

SelectRes, AddPseudo, RemoveAtom, WriteLib

DATE

961206

NAME

AddBond - add bond between two atoms

SYNOPSIS

AddBond

DESCRIPTION

Add a bond between the two selected atoms. Exactly two atoms must be selected before this command is executed, an error message will be issued otherwise.

EXAMPLE

AddBond

SEE ALSO

RemoveBond, CalcBond, AddAtom

DATE

931126

NAME

AddCircles - add circles around atoms

SYNOPSIS

AddCircles expr

DESCRIPTION

Add circles around atoms. This is typically used to indicate mobility or exactness. A circle will be drawn around every selected atom. The selected bonds are used to determine the direction of the circles. The user will normally select atoms of the backbone (e. g. all CA) and all bonds of the backbone before executing this command.

The created primitives have the property "circle".

EXAMPLES

```
AddCircles 0.5
AddCircles bfactor
```

SEE ALSO

SelectAtom, SelectBond,
ColorPrim, LinePrim, RemovePrim

DATE

970723

NAME

AddCylinder - add cylinder for schematic drawing

SYNOPSIS

AddCylinder (least_square | spacing)

DESCRIPTION

Add a cylinder that approximates the selected atoms. The argument selects between two fit criteria. 'least_square' does a least square fit of the cylinder surface to the atoms, 'spacing' takes the axis direction that gives the most regular spacing of atoms. The results are normally very similar, but 'spacing' works better than 'least_square' if very few atoms are given.

A cylinder is added for each molecule that has selected atoms. A minimum number of atoms (5 for least_square, 4 for spacing) must be selected, otherwise the cylinder cannot be determined and an error message is issued.

Cylinders can be used for showing alpha helices in schematic drawings. For good results, it is recommended to either select the CA or all backbone atoms within a helix region.

The created primitives have the property "cylinder".

EXAMPLE

```
AddCylinder spacing
```

SEE ALSO

SelectAtom, StyleCylinder, ColorPrim, LengthPrim, RemovePrim, AddRibbon, AddSolid, AddDipole

DATE

970930

NAME

AddDipole - add arrow showing dipolar moment

SYNOPSIS

AddDipole

DESCRIPTION

Add an arrow that shows the dipolar moment of the selected atoms. A separate arrow is created for each molecule that has selected atoms.

The arrow is in fact a cylinder, like it is created with AddCylinder, and can be manipulated with the corresponding commands, like StyleCylinder or LengthPrim.

The created primitives have the properties "dipole" and "cylinder".

EXAMPLE

```
AddDipole
```

SEE ALSO

SelectAtom, StyleCylinder, ColorPrim, LengthPrim, RemovePrim, AddCylinder

DATE

970723

NAME
AddDist - add distance between two atoms

SYNOPSIS
AddDist

DESCRIPTION
Add a distance between the two selected atoms. Exactly two atoms must be selected before this command is executed, an error message will be issued otherwise.

EXAMPLE
AddDist

SEE ALSO
RemoveDist, CalcDist, AddUpl, AddLol

DATE
961219

NAME
    AddDrawobj - add line, rectangle or circle

SYNOPSIS
    AddDrawobj (line | rect | circle) (2D | 3D)

DESCRIPTION
    Add a line, rectangle or circle for annotation.
    The first argument selects the type of drawing object.

    If the second argument is 2D, the object is placed at a default location and can be moved to the desired place. It will always keep its screen position and is not related to any atoms.

    If the second argument is 3D, a label is added for each molecule that has selected atoms. The initial position in space is calculated as the average of the coordinates of all selected atoms of the molecule. The positon relative to these atoms can be changed with the mouse or with the MoveDrawobj command.

    The created primitives have the property "drawobj".

EXAMPLES
    AddDrawobj line 3D

SEE ALSO
    SelectAtom, ColorPrim, LinePrim, StyleDrawobj, MoveDrawobj, RemovePrim, AddTitle, AddText

DATE
    970930

NAME

AddHbond - add H-bond between two atoms

SYNOPSIS

AddHbond

DESCRIPTION

Add an H-bond between the two selected atoms. Exactly two atoms must be selected before this command is executed, an error message will be issued otherwise.

An H-bond is a special kind of distance and the corresponding commands are used for manipulating it.

EXAMPLE

AddHbond

SEE ALSO

CalcHbond, RemoveDist

DATE

950221

NAME

AddIsosurface - add isosurface of potential

SYNOPSIS

AddIsosurface fileName expr

DESCRIPTION

Add an isosurface of the electrostatic potential of the selected molecule. Exactly one molecule must be selected. The file given as first argument must contain the electrostatic potential in the format generated by CalcPot, see the help page of ReadPot for a description.

The second argument gives the level for the isosurface.

The created primitives have the properties "surface" and "isosurface".

EXAMPLE

```
AddIsosurface tt.pot -0.01
```

SEE ALSO

SelectMol, CalcPot, AddSurface, ReadPot, ColorPrim, RemovePrim

DATE

970723

NAME

AddLol - add lower limit between two atoms

SYNOPSIS

AddLol expr

DESCRIPTION

Add a lower limit between the two selected atoms. Exactly two atoms must be selected before this command is executed, an error message will be issued otherwise.

EXAMPLE

```
AddLol 2.3
```

SEE ALSO

SelectAtom, CheckLol, RemoveDist, AddUpl

DATE

950221

NAME
    AddPlates - add plates for rings

SYNOPSIS
    AddPlates

DESCRIPTION
    Add plates for all rings consisting entirely of selected atoms. Rings are only detected if all atoms belong to the same residue.

    The created primitives have the property "plate".

EXAMPLES
    AddPlates

SEE ALSO
    SelectAtom, ColorPrim, SizePlate, RemovePrim

DATE
    970723

NAME

AddPseudo - add new pseudo atom

SYNOPSIS

AddPseudo name

DESCRIPTION

Add a pseudo atom with the name given as first argument to all selected residues.

The new pseudo atom will correspond to all selected atoms of the corresponding residue. If less than two atoms are selected in a residue, no pseudo atom is added.

EXAMPLE

AddPseudo "QD"

SEE ALSO

SelectRes, SelectAtom, AddAtom, RemoveAtom, WriteLib

DATE

961206

NAME

    AddRes - add residue to molecule

SYNOPSIS

    AddRes (first | last) name

DESCRIPTION

    Add a residue as first or last residue of all selected molecules.

    The new residue can only be docked properly if the coordinates of the 3 atoms that overlap for subsequent residues are known for the last residue. If this is not the case, which happens frequently if a coordinate file was read, the missing atom coordinates (mostly the 'N' for proteints) should be calculated with the CalcAtom command first.

EXAMPLE

    AddRes last "ALA"

SEE ALSO

    NewMol, SelectMol, CalcAtom, ChangeRes, RemoveRes

DATE

    970401

NAME

AddRibbon - add ribbons (schematic drawing)

SYNOPSIS

AddRibbon

DESCRIPTION

Create a schematic drawing with ribbons. The ribbons will go through the currently selected atoms, this will normally be all CA atoms in a protein.

If ribbons for helices and sheets are desired, certain properties of the residues must be set to give the necessary secondary structure information. The following properties are used:

```
helix
helix1, helix2,...
sheet
sheet1, sheet2,...
strand1_1, strand1_2,...
```

These properties are set when a PDB file containing secondary structure information (HELIX and SHEET records) is read, or they can be calculated with the CalcSecondary command. They can also be set/modified using the DefPropRes command, a more convenient way for modifying the result of CalcSecondary is often to use the WriteSecondary command.

For sheets, the neighbour of the residues should be set with the SetNeigh command if the secondary structure was not read from a PDB file or calculated with CalcSecondary.

The created primitives will have exactly one of the following properties set:

```
helix
sheet
coil
```

and for helix and sheet the numbered one from the residue (helix1,...) is also copied.

In addition, all created primitives have the property "ribbon".

EXAMPLE

AddRibbon

SEE ALSO

ReadPdb, CalcSecondary, SelectAtom, WriteSecondary, DefPropRes, SetNeigh, LengthPrim, ColorPrim, TintPrim, ShadePrim, TypeRibbon, StyleRibbon, SizeRibbon, PaintRibbon

```
     LengthBond, RemovePrim

DATE
     970723
```

NAME

AddSheet - add sheet for schematic drawing

SYNOPSIS

AddSheet

DESCRIPTION

Create a surface that serves as schematic drawing of a beta sheet. The surface will approximate all selected atoms that belong to the same sheet. An atom is considered belonging to a sheet if the residue it belongs to has the 'sheet' property set. Even if multiple atoms of one residue are selected, only one of them is taken for determining the surface, it is recommended to select just the CA atoms.

The surface will not exactly pass through the atoms, but a smoothing algorithm is applied. To get nice smoothing at the borders, it is good to select not just the sheet atoms, but also atoms that are adjacent to the sheet.

The command is very easy to use for structures that have just one beta sheet. Then the user can just select all CA atoms and execute the command, provided that the secondary structure is known from the PDB file or calculated using the CalcSecondary command.

If a structure has multiple beta sheets, they have to be created one after the other. It is best to start with all CA selected, create one sheet, deselect the atoms belonging to that sheet, creating the second sheet, etc.

The created primitives have the property "sheet".

EXAMPLE

AddSheet

SEE ALSO

ReadPdb, CalcSecondary, SelectAtom, DefPropRes, AddRibbon, ColorPrim, TintPrim, ShadePrim, RemovePrim

DATE

970723

NAME

AddSolid - add solid for schematic drawing

SYNOPSIS

```
AddSolid ( sphere | ellipsoid | cylinder |
    cone | box ) expr
```

DESCRIPTION

Add a solid that (partly) covers the selected atoms for each selected molecule. The first parameter selects the desired shape. The second parameter gives the fraction of atoms that must be inside the solid.

The program tries to determine the solid with the smallest volume that covers the desired number of atoms. This is done by a randomized algorithm, so it is possible that the same input parameters do not always lead to exactly the same solid.

The calculation can take up to a few minutes, depending on the shape, the number of atoms, and the coverage.

The created primitives have the property "solid".

EXAMPLE

```
AddSolid ellipsoid 0.8
```

SEE ALSO

SelectAtom, ColorPrim, RemovePrim

DATE

970723

NAME

AddSurface - add surface

SYNOPSIS

AddSurface expr (vdw | solvent | contact) expr
(dots | shaded) (0 | 1)

DESCRIPTION

Add a surface for the selected atoms. The precision (density of the dots) depends on DrawPrec.

The first argument is the radius of the atoms, you will normally not change the default value ’vdw’.

The second argument gives the type of surface:

vdw: van der Waals surface

solvent: surface given by the center of spheres (solvent) touching the atoms

contact: contact surface (Richards)

The third argument gives the solvent radius for solvent and contact surfaces.

The fourth argument gives the type of surface, dots or a solid, shaded surface can be selected.

The final option selects whether a report with the approximate areas and volumes of all surface parts is desired. The volumes are mainly interesting for cavities. Note that the numbers are not highly precise.

Depending on the precision, shaded surfaces can use a lot of memory. If the machine runs out of memory, the program may crash occasionally.

This command supports groups for shaded surfaces, the resulting surface will belong to the first group member.

EXAMPLE

```
AddSurface vdw contact 1.4 dots 0
```

SEE ALSO

SelectAtom, RadiusAtom, DrawPrec, Group, ColorPrim, RemovePrim, CalcSurface

DATE

970723

NAME

AddText - add 3D text annotation

SYNOPSIS

AddText expr string

DESCRIPTION

Add a 3D text annotation. The first argument gives the initial size, the second argument the text.

A label is added for each molecule that has selected atoms. The initial position in space is calculated as the average of the coordinates of all selected atoms of the molecule. It can be moved with the mouse or with the MovePrim command.

For an explanation on how to enter greek letters, sub- and superscript, see the manual page of the EditText command.

The created primitives have the property "text".

EXAMPLES

```
AddText 0.15 "Label"
```

SEE ALSO

SelectAtom, EditText, ColorPrim, LinePrim, MovePrim, SizeText, AddTitle, RemovePrim

DATE

970930

NAME

AddTitle - add 2D text annotation

SYNOPSIS

AddTitle <coord> expr string

DESCRIPTION

Add a text annotation at a given screen position. The screen position must be entered by a mouse click or on the command line. The second argument is the size, the third the string to be displayed.

The origin of the screen coordinates is at the center of the window. The x-axis runs from left to right, the y-axis from bottom to top. The range for y is -1.0 to 1.0, the one for x depends on the aspect ratio, e. g. it would be -1.5 to 1.5 if the window width is 50% larger than the window height.

For an explanation on how to enter greek letters, sub- and superscript, see the manual page of the EditText command.

The created primitives have the properties "text" and "title".

EXAMPLES

```
AddTitle 0.5 0.3 0.15 "Label"
```

SEE ALSO

EditText, ColorPrim, LinePrim, MovePrim, SizeText, AddText, RemovePrim

DATE

970723

NAME

AddTrajec - add trajectories

SYNOPSIS

AddTrajec

DESCRIPTION

Add trajectories for all selected atoms. The same number of atoms has to be selected in all selected molecules, the corresponding atoms of all selected molecules will be connected with a polyline. This is mainly used for displaying results of MD runs.

The created primitives have the property "trajec".

EXAMPLES

AddTrajec

SEE ALSO

SelectAtom, ColorPrim, StyleTrajec, RemovePrim

DATE

970723

NAME
    AddUpl - add upper limit between two atoms

SYNOPSIS
    AddUpl expr

DESCRIPTION
    Add an upper limit between the two selected atoms.
    Exactly two atoms must be selected before this command
    is executed, an error message will be issued otherwise.

EXAMPLE
    AddUpl 3.7

SEE ALSO
    RemoveDist, CheckUpl, RemoveDist, AddLol

DATE
    950302

NAME

AttrAtom - list attributes of atoms
AttrBond - list attributes of bonds
AttrDist - list attributes of distances
AttrPrim - list attributes of primitives

SYNOPSIS

AttrAtom
AttrBond
AttrDist
AttrPrim

DESCRIPTION

Lists the values of the attributes of all selected atoms, bonds, distances or primitives. All items have to share the same set of attributes, an error message is issued otherwise.

Also creates a macro that can be used to set all the attributes to these values.

EXAMPLES

AttrAtom

SEE ALSO

Select*, Color*, Material*, Texture*, Style*, Line*

DATE

960213

NAME
```
     BackColor - change background color
```

SYNOPSIS
```
     BackColor expr expr expr
```

DESCRIPTION

Set the background color. The color is given by its Red, Green and Blue component, all in the range between 0.0 and 1.0.

EXAMPLE
```
     BackColor 1.0 0.2 0.7
```

DATE

931126

NAME

BondMode - choose bond display mode

SYNOPSIS

BondMode (normal | pseudo)

DESCRIPTION

Choose whether the regular bonds or bonds to pseudo atoms are displayed. This is a global switch, it is currently not possible to change this for individual bonds.

EXAMPLE

```
BondMode pseudo
```

WARNING

Rings look somewhat weird in 'pseudo' mode.

DATE

950606

NAME

CalcAngle - calculate angular order parameters

SYNOPSIS

CalcAngle

DESCRIPTION

Generate a report with angular order parameters for all selected angles in all selected molecules. The same number of angles must be selected in all selected molecules.

The first column of the report will show an average angle. This is not an arithmetic average, but the angle of the resulting vector sum used for the calculation of the angular order parameters.

The second number is the standard deviation from this average.

The third number is the angular order parameter.

EXAMPLE

CalcAngle

REFERENCE

Hyberts, SG, Goldberg, MS, Havel, TF, Wagner, G.
The solution structure of eglin c based on measurements of many NOEs and coupling constants and its comparison with X-ray structures.
Protein Science, 1 (1992) 736-751.

SEE ALSO

SelectAngle, CheckAco, FigAngles

DATE

960621

NAME

CalcAtom - calculate missing atom coordinates

SYNOPSIS

CalcAtom name

DESCRIPTION

Calculate coordinates of atoms that were missing in the input file (e. g. protons in PDB files of crystal structures).

The command uses the standard geometry from the residue library to calculate the coordinates of the atoms with the given name in all selected residues. If there are not enough known atoms to determine the orientation (e. g. if only the O of a water is given), the program will choose a random orientation. Atom oordinates that are known already will not be changed.

The name can contain wildcards (?, *).

EXAMPLE

CalcAtom "H*"

SEE ALSO

SelectRes, AddAtom

DATE

951110

NAME

CalcAxis - calculate lengths of principal axes

SYNOPSIS

CalcAxis (0 | 1)

DESCRIPTION

Generate a report with the relative lengths of the principal axes of all selected molecules. Only the selected atoms of each molecule are used, the same mass is used for all atoms.

The lengths are listed relatively to the shortest axis, the average for all structures is given at the end.

The option selects whether a list with the angles of all selected bonds relative to the principal axes should be printed.

This command supports groups.

EXAMPLE

```
CalcAxis
```

SEE ALSO

SelectAtom, Group, Fit

DATE

960317

NAME

CalcBond - calculate bonds between close atoms

SYNOPSIS

CalcBond expr (0 | 1) (0 | 1)

DESCRIPTION

Find pairs of selected atoms that have a small distance, but are not connected by a bond. An atom pair is a candiate if the distance is less than the sum of the bond radii stored in the file:

$MOLMOLHOME/setup/AtomRadius

Depending on the options, the command will create a report with the missing bonds, will add them to the structure, or both. Only bonds that appear in a minimal number of structures given as first argument appear in the report.

This command is useful after reading a PDB file that contains unknown residues, or a DG file with unknown residues and missing connection informations.

This command supports groups.

EXAMPLE

CalcBond 5 1 0

SEE ALSO

PathNames, ReadPdb, ReadDg, Group, AddBond

DATE

960317

NAME

CalcCluster - reduce number of structures

SYNOPSIS

CalcCluster expr expr expr

DESCRIPTION

Takes a bundle of superimposed structures and determines a smaller number of structures that represent the same bundle as well as possible. This is done by clustering similar structures into groups, and taking the "central" structure of each group.

The command acts on all selected molecules and only considers the selected atoms of these molecules for the calculation.

The first argument gives the desired number of structures. The second argument gives the minimal RMSD between two resulting groups, where the RMSD between two groups is defined as the maximal RMSD between a member of one group and a member of the other group. The third argument gives the maximal RMSD of two members of a group. Due to these restrictions, the number of calculated clusters can be different from the one given as first argument.

The property "cluster" is set on all molecules that represent a group. From each group, the one with the smallest sum of RMSDs to all other members is chosen.

This command supports groups.

EXAMPLE

CalcCluster 5 0.02 1

SEE ALSO

SelectMol, SelectAtom, Group, Fit, MeanMol

DATE

960317

NAME

CalcDist - find short distances between atoms

SYNOPSIS

```
CalcDist expr expr expr
    ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
    [ name ] [ name ]
```

DESCRIPTION

Find pairs of selected atoms that have a distance smaller than the one given as first argument, but are not connected over one or two bonds.

Distances between residues that are closer in sequence than given by the second arument are not considered.

The first option determines whether distances within structures or distances between atoms of different structures are desired.

The second option determines whether a report with short distances is created.

The third option determines whether a peak list (XEASY format) containing expected NOESY peaks is created. Only distances between atoms where the chemical shift is known (see ReadShift) lead to an entry in the peak list.

The fourth option determines whether the found distances are added to the display as upper distance limits.

Only distances that appear in a minimal number of structures given as third argument appear in the report and peak list.

The optional last two arguments give the names of two properties, only pairs where the first atom has the first of these properties and the second atom has the second one are considered. The default corresponds to pairs where both atoms are selected.

This command supports groups.

EXAMPLE

```
CalcDist 3.5 4 5 0 1 0 0
```

SEE ALSO

SelectAtom, Group, ReadShift, RemoveDist

DATE

960317

NAME

CalcHbond - find H-bonds

SYNOPSIS

CalcHbond expr expr expr
(0 | 1) (0 | 1) (0 | 1) (0 | 1)

DESCRIPTION

Find pairs of selected atoms where the first one is a donor and the second one an acceptor for an H-bond, the distance between the two atoms is smaller than the first argument, and the angle between the line from the atom connected to the donor and the donor and the line from the atom connected to the donor and the acceptor is smaller than the second argument.

The first option determines whether H-bonds within structures or H-bonds between atoms of different structures are desired.

Depending on the other three options, the command will create a report with the H-bonds, a macro to add the H-bonds to all selected structures (can e. g. be used to add them to a mean structure later) and will add them to the display. Only H-bonds that appear in a minimal number of structures given as third argument appear in the report and the macro.

This command supports groups.

EXAMPLE

CalcHbond 2.4 35 10 0 1 0 1

SEE ALSO

SelectAtom, Group, AddHbond, RemoveDist

DATE

960317

NAME

CalcHelix - calculate angles between helix axes

SYNOPSIS

CalcHelix

DESCRIPTION

Generate a report with angles between helix axes. Cylinders have to be added for all helices to be considered by this command, and at least two such cylinders have to be selected. The command will create a two-dimensional table with angles for all pairs, indexed with the primitive numbers of the cylinders.

EXAMPLE

CalcHelix

SEE ALSO

AddCylinder, SelectPrim

DATE

961126

NAME

CalcMatch - calculate best matching structure parts

SYNOPSIS

CalcMatch expr expr

DESCRIPTION

Determines which parts of all selected molecules can be superimposed with the smallest RMSD, taking into account all selected atoms of all selected residues. The structures do not need to be identical, but the same number of residues with the same number of atoms each must be selected. The structures do not need to be superimposed before executing the command.

The first argument gives the minimal number of residues that must be superimposed, the second argument the maximal RMSD (to the mean) desired.

The algorithm is relatively simple, it superimposes the structures with the current set of atoms (starting with all selected ones), and in each step it leaves away the atoms from the residue that has the largest global displacement. This is repeated until one of the conditions given by the arguments is met.

A protocol of the progress, giving RMSD and largest displacement, is printed. All values are to the mean. At the end, an expression for selecting the superimposed residues for each molecule is printed. The property "match" is set on all these residues.

This command supports groups.

EXAMPLE

CalcMatch 50 0.7

SEE ALSO

SelectMol, SelectAtom, Group, Fit, CalcRmsd

DATE

960323

NAME

CalcPot - calculate electrostatic potential

SYNOPSIS

```
CalcPot expr expr expr expr expr expr
    expr ( zero | debye ) fileName
```

DESCRIPTION

Calculate the electrostatic potential of all selected molecules, and write the result to a file with the given name. The resolution (grid density) depends on DrawPrec.

The first argument is the radius of the atoms, you will normally not change the default value 'vdw'.

The second argument determines the charge of the atoms, typical values are:

charge: partial charges on all atoms

heavycharge: partial charges of protons transferred to heavy atoms

avgcharge: partial charges on heavy atoms, averaged over neighbours

simplecharge: charges only on one or two atoms of charged residues, as specified in the setup file AtomCharges

The third argument gives the dielectricity constant for the molecule, typically in the range 2 to 4, the fourth for the solvent, normally 80.

The fifth argument gives the solvent radius, normally 1.4 for water.

The sixth argument gives the salt concentration as ionic strength. For simple salts, this is twice the concentration, so the default value of 0.3 corresponds to a salt concentration of 150 mMol.

The seventh argument gives the salt radius.

The eighth argument gives the size in Angstroms that (on each side) the box that the potential is calculated in is larger than the extent of the molecule. Values of 10 to 15 are recommended. Smaller values reduce the calculation time, but may introduce artifacts from the boundary conditions.

The ninth argument selects the kind of boundary condition, either values fixed at zero, or Debye-Hueckel. Using zero is faster, and there does not seem to be a noticable difference between the two.

For correct results, special care should be taken that the residue definitions with the correct charges are used. This is expecially important when using PDB files, because the residue names in there normally do not contain the charges. There is a standard macro called pdb_charge.mac that can be run after reading PDB files, it should normally do the necessary corrections. For the N and C termini, the molecules should have charged end groups, or special forms of the residues that contain the necessary charges.

Depending on the precision, this function can use a lot of memory, an error message will be given if the memory runs out.

This command supports groups.

EXAMPLE

```
CalcPot vdw charge 2.0 80.0 1.4 0.3 2.0
    10.0 zero foo.pot
```

REFERENCE

Nicholls, A, Honig, B.
A rapid finite difference algorithm, utilizing successive over-relaxation to solve the Poisson-Bolzmann equation.
Journal of Computational Chemistry, 12 (1990) 435-445

SEE ALSO

SelectMol, SelectAtom, DrawPrec, Group, PathNames, AddSurface, ReadPot, PaintSurface

DATE

960621

NAME

CalcRmsd - calculate RMSDs and displacements

SYNOPSIS

```
CalcRmsd ( fit_pairs | as_is ) region
    name name nameList name nameList nameList
```

DESCRIPTION

Calculate RMSDs and displacements of all selected molecules. The first argument selects whether each pair of molecules is superimposed before calculating the RMSD, or whether the current orientation is used. This can be useful to calculate RMSDs of structures already overlaid with the Fit command.

The second arguments selects the residue range used for superposition when calculating global RMSDs and global displacements.

The third argument selects the name of the first property that is used for superposition. The user can either give a property defined with DefProp or one of the predefined properties. The RMSD values will be printed in the upper right part of the matrix. This property is also used for the superpositions when calculating displacements.

The forth argument selects the name of the second property that is used for superposition. The RMSD values will be printed in the lower left part of the matrix.

The fifth argument is a space separated list of property names. It defines the groups of molecules that are compared. All the molecules of a group must be given a common property with DefPropMol (e. g. g1 and g2), and the list of these properties must be given here.

The sixth argument is the name of a property of the molecule that is used as reference for displacements and local RMSDs, typically the mean structure. If no name is given, average pairwise values will be calculated.

The seventh argument is a space separated list of property names. The global displacements will be calculated for all the given properties. The property used for the superposition is always the one given as third argument.

The eighth argument is a space separated list of property names. The local RMSDs will be calculated for all the given properties. The local RMSD of a residue is calculated by superimposing 3 residues centered at the given residue, using the property given as third argument, and calculating the RMSD of all 3 residue.

The ninth argument is a space separated list of property names. The local displacements will be calculated for all the given properties. The local displacement of a residue is calculated by superimposing 3 residues centered at the given residue, using the property given as third argument, and calculating the RMSD of the middle residue.

This command supports groups.

EXAMPLE

```
CalcRmsd fit_pairs '5..32,37..55' 'bb' 'heavy' ''
    'bb heavy heavysc' '' 'bb heavy'
```

SEE ALSO

SelectMol, DefPropMol, DefPropAtom, Group, Fit

DATE

960317

NAME

CalcSecondary - calculate secondary structure

SYNOPSIS

CalcSecondary

DESCRIPTION

Calculate the secondary structure of a protein using the algorithm published by Kabsch/Sander. The command operates on all selected residues of all selected molecules. It will set various properties on these residues, depending on the secondary structure. These properties are listed in a text window. They are used by the AddRibbon command to produce schematic drawings.

Note that editing the text has no effect on the definitons used. For changing the definitons it is most convenient to use the WriteSecondary command.

Since the calculation is based on hydrogen bonding patterns, the coordinates of HN atoms are required. So before using the command for a structure without coordinates for hydrogen atoms (X-ray), use the CalcAtom command for adding them.

EXAMPLE

CalcSecondary

SEE ALSO

SelectMol, SelectRes, CalcAtom, DefPropRes, WriteSecondary, AddRibbon

DATE

960815

NAME
     CalcShift - calculate ring current shifts

SYNOPSIS
     CalcShift (1 | 0) (1 | 0) string expr expr

DESCRIPTION
     Calculate ring current and bond polarization shifts of all selected atoms, taking into account all rings/atoms of the same molecule.

     The first argument selects whether ring current shifts should be calculated, the second one whether bond polarization shifts should be calculated. At least one of the two should be selected, a warning is issued otherwise.

     The third argument gives the name of the model for the calculation. The description of the models is read from the file:

```
$MOLMOLHOME/setup/RingShift
```

     The fourth argument selects a cutoff, contributions to the ring current shifts above this value are listed individually *before* the sum.

     The fifth argument gives a maximal distance for the atoms considered for the calculation of bond polarization shifts. Larger values will lead to longer calculation times.

     The results are listed for each molecule separately, a summary with average, minimal and maximal values is given at the end.

     For all protons but HN, a ring belonging to the same residue as the proton is not considered for the calculation of the ring current shift.

     The same is the case for the bond polarization: atoms of the same residue are not considred for the field calculation, except for HN atoms. A more elaborate strategy would have to be used to make the calculated numbers more useful as expected difference to random coil shift, especially for HN atoms.

EXAMPLE
```
CalcShift 1 0 Heigh-Mallion 0.5 5.0
```

REFERENCE
     Case, DA.
     Calibration of ring-current effects in proteins and nucleic acids.
     Journal of Biomolecular NMR, 6 (1995) 341-346

WARNING

The results for bond polarization shifts were not compared to the results of other programs, so there is no guarantee given on their correctness and usefulness.

SEE ALSO

SelectAtom, PathNames

DATE

960621

NAME

CalcSurface - calculate solvent accessible surface

SYNOPSIS

CalcSurface expr expr

DESCRIPTION

Generate a report with solvent accessible surfaces of each residue. The first argument gives the radius of the solvent, the second the desired precision. A reasonably good approximation will be obtained with precisions of 2 or 3, higher values will lead to even better results.

Only selected atoms are used for the calculation. The first surface given for each residue is the accessible surface in the context of the molecule, the second one is the surface of the isolated residue.

The results are listed for each molecule separately, a summary with average, minimal and maximal values is given at the end. If not all molecules have the same structure, or if not the same atoms are selected in all molecules, these values will not make much sense.

The calculation will take some time, especially if a high precision is desired. The time grows exponentially with the precision, so values of more than 4 or 5 are not recommended.

This command supports groups.

EXAMPLE

```
CalcSurface 1.4 2
```

SEE ALSO

SelectAtom, Group, AddSurface

DATE

960317

NAME
    CalcVdw - find Van der Waals violations

SYNOPSIS
    CalcVdw expr expr (0 | 1) (0 | 1) (0 | 1)

DESCRIPTION
    Find pairs of selected atoms with Van der Waals violations larger than the cutoff given as first argument.

    The first option determines whether violations within structures or violations between atoms of different structures are desired.

    Depending on the other two options, the command will create a report with the violations, will add them to the display as lower distance limits, or both. Only violations that occur in a minimal number of structures given as third argument appear in the report.

    This command supports groups.

EXAMPLE
    CalcVdw 0.3 1 0 1 0

SEE ALSO
    SelectAtom, Group, RemoveDist

DATE
    960317

NAME

Center - change rotation center

SYNOPSIS

Center

DESCRIPTION

Change the center for future rotations to the center of gravity of all selected atoms.

At least one atom must be selected before this command is executed, an error message will be issued otherwise.

EXAMPLE

```
Center
```

DATE

970417

NAME

ChangeRes - change residue type

SYNOPSIS

ChangeRes (angles | atoms) name

DESCRIPTION

Exchange all selected residues with a different residue type given as second argument. If the first argument is 'angles', the old conformation is maintained by copying the values of the common dihedral angles from the old residue to the new residue. If it is 'atoms', the old conformation is maintained by copying the coordinates of the common atoms from the old residue to the new residue.

EXAMPLE

```
ChangeRes angles "ARG"
```

SEE ALSO

NewMol, AddRes

DATE

960411

NAME

CheckAco - check angle constraints

SYNOPSIS

CheckAco expr expr

DESCRIPTION

Check all selected angles for violations of angle constraints. The command will generate a report with all violations greater than the cutoff given as first argument if it occurs in at least the number of structures given as second argument.

EXAMPLE

```
CheckAco 5.0 1
```

SEE ALSO

ReadAco, AddAco, RemoveAco, SelectAngle

DATE

950302

NAME

CheckBond - check number of bonds

SYNOPSIS

CheckBond

DESCRIPTION

Check all selected atoms for a correct number of bonds. The minimal and maximal number of bonds for each atom type is stored in the third and fourth column of the file:

```
$MOLMOLHOME/setup/AtomRadius
```

This is useful after adding bonds with the command CalcBond.

EXAMPLE

```
CheckBond
```

SEE ALSO

PathNames, CalcBond, AddBond, RemoveBond

DATE

950704

NAME

CheckLol - check lower limits

SYNOPSIS

CheckLol expr expr

DESCRIPTION

Check all selected lower limits for violation in any of the selected molecules. The command will generate a report with all violations greater than the cutoff given as first argument if it occurs in at least the number of structures given as second argument.

The lower limits do not have to be read/added for all structures, it is enough if they are defined for one structure. If different lower limits are present in different structures, the largest one is considered for the report.

This command supports groups.

EXAMPLE

CheckLol 0.3 1

SEE ALSO

ReadLol, AddLol, Group, RemoveDist, SelectDist, CheckUpl, CheckAco

DATE

960317

NAME

CheckUpl - check upper limits

SYNOPSIS

CheckUpl expr expr

DESCRIPTION

Check all selected upper limits for violation in any of the selected molecules. The command will generate a report with all violations greater than the cutoff given as first argument if it occurs in at least the number of structures given as second argument.

The upper limits do not have to be read/added for all structures, it is enough if they are defined for one structure. If different upper limits are present in different structures, the smallest is considered for the report.

This command supports groups.

EXAMPLE

CheckUpl 0.3 1

SEE ALSO

ReadUpl, AddUpl, Group, RemoveDist, SelectDist, CheckLol, CheckAco

DATE

960317

NAME

    ClipPos - set position of clipping planes
    ClipSize - set distance of clipping planes

SYNOPSIS

    ClipPos expr
    ClipSize expr

DESCRIPTION

Set new values for the distance of the near and far clipping planes. By ClipPos, the user sets the position of the middle between the two planes, by ClipSize the distance:

```
near = pos - size / 2
far  = pos + size / 2
```

EXAMPLES

```
ClipPos 8.0
ClipSize 5.0
```

DATE

950124

NAME

    ColorAtom - set color of atoms

SYNOPSIS

    ColorAtom expr expr expr

DESCRIPTION

    Set the color of all selected atoms. The color is given by its Red, Green and Blue component, all in the range between 0.0 and 1.0. By using expressions, it is possible to give each atom a different color, depending e. g. on the B factor.

EXAMPLES

```
ColorAtom 1.0 0.0 0.0
ColorAtom 0.5*bfactor 1.0-0.5*bfactor 0.0
```

SEE ALSO

    SelectAtom, DialColor

DATE

    940119

NAME

ColorBond - set color of bonds

SYNOPSIS

ColorBond expr expr expr

DESCRIPTION

Set the color of all selected bonds. The color is given by its Red, Green and Blue component, all in the range between 0.0 and 1.0. By using expressions, it is possible to give each bond a different color, depending e. g. on the B factor of the first atom.

EXAMPLES

```
ColorBond 1.0 0.0 0.0
ColorBond atom1.bfactor 1.0-atom1.bfactor 0.0
```

SEE ALSO

SelectBond, DialColor

DATE

940119

NAME

ColorDist - set color of distances

SYNOPSIS

ColorDist expr expr expr

DESCRIPTION

Set the color of all selected distances. The color is given by its Red, Green and Blue component, all in the range between 0.0 and 1.0. By using expressions, it is possible to give each distance a different color, depending e. g. on the value of the distance.

EXAMPLES

```
ColorDist 0.0 0.0 1.0
ColorDist val/5 1.0-val/5 0.0
```

SEE ALSO

SelectDist, DialColor

DATE

940119

NAME

    ColorPrim - change color of primitives

SYNOPSIS

    ColorPrim expr expr expr

DESCRIPTION

    Set the color of the selected circles, cylinders, texts, ribbons, etc. The color is given by its Red, Green and Blue components, all in the range between 0.0 and 1.0.

EXAMPLE

```
ColorPrim 1.0 0.0 0.0
```

SEE ALSO

    SelectPrim, TintPrim, DialColor

DATE

    950407

NAME

```
DefPropMol   - define molecule property
DefPropRes   - define residue property
DefPropAtom  - define atom property
DefPropBond  - define bond property
DefPropAngle - define angle property
DefPropDist  - define distance property
DefPropPrim  - define primitive property
```

SYNOPSIS

```
DefPropMol propertyName expr
DefPropRes propertyName expr
DefPropAtom propertyName expr
DefPropBond propertyName expr
DefPropAngle propertyName expr
DefPropDist propertyName expr
DefPropPrim propertyName expr
```

DESCRIPTION

Define a property with the given name by the given expression. See SelectMol for a description of the expression syntax. Properties can be used in other property definitions or selections. The Select commands are actually just special cases of the DefProp commands, they defines the property with the name "selected". The following properties are used internally by the program and should not be defined by this command:

```
all
visible
```

The value of the "visible" property is maintained by the program, it is set for all atoms, bonds, distances and primitives that have their attributes (Style*) set in a way to make them visible. This is very convenient for selecting only visible items.

The "displayed" property is used by the program to decide which items should be displayed. It is not recommended to modify it, it is normally better to use the Style* commands for changing the visibility. It is very useful for molecules, however, but the molecule dialog (DialMol command) is more convenient for modifying it in this case.

The "movable" property is used by the program to decide which items are moved by rotations etc. It only has an influence for molecules, and the molecule dialog (DialMol command) command is more convenient for modifying it.

Some properties are predefined, they can be seen in the file:

```
$MOLMOLHOME/setup/PropDef
```

or with the HelpProp command.

EXAMPLES

```
DefPropRes 'helix' 'num >= 47 & num <= 56'
DefPropAtom 'helixCA' 'name = "CA" & res.helix'
```

SEE ALSO

DialSelect, Select*, DialMol, HelpProp, ListProp*

DATE

950704

NAME

DialColor - switch color dialog on and off

SYNOPSIS

DialColor (off | on)

DESCRIPTION

Switch color dialog on and off. The color dialog is a convenient interface to the commands BackColor, ColorAtom, ColorBond, ColorDist, TintDist, ColorPrim and TintPrim.

The central part of the dialog shows the currently chosen color. A selection of commonly used colors is available from the list on the right side of the dialog. These colors can also be selected by typing their name in the top text field on the left side. Arbitrary colors can be chosen by typing their RGB (Red-Green-Blue) components in the range 0.0 to 1.0 in the corresponding text fields on the left side of the dialog.

When an interactive selection is made in the drawing area, the dialog reflects the color of the selected item.

The currently chosen color can be applied to selected items by activating the corresponding button from the bottom of the dialog.

The OK button closes the dialog, the Help button shows this help page.

The list of colors displayed in the dialog is taken from the file:

    $MOLMOLHOME/setup/ColorList

An alternate file can be chosen with the PathNames command. An extensive list of colors is supplied in the file:

    $MOLMOLHOME/auxil/ColorList

EXAMPLE

DialColor on

SEE ALSO

BackColor, ColorAtom, ColorBond, ColorDist, TintDist, ColorPrim, TintPrim, PathNames

DATE

980409

NAME

DialMeasure - switch measurement dialog on and off

SYNOPSIS

DialMeasure (off | on)

DESCRIPTION

Switch measurement dialog on and off.

The measurement dialog displays bond lengths, bond angles, atom distances and dihedral angles of interactively selected atoms, bonds and angles.

The top line of the dialogs reflects the bond and atom selections that are used for the measurements. All other lines correspond to one measurement, where the left text field shows the bond(s)/atoms involved, and the result of the measurement (distance or angle) is displayed in the right text field.

The "Bond Length" line displays the length of the most recently selected bond.

The "Bond Angle" line displays the angle between the two most recently selected bonds.

The "Bond Dih." line displays the dihedral angle between the three most recently selected bonds.

The "Atom Dist." line displays the distance between the two most recently selected atoms.

The "Atom Angle" line displays the angle defined by the three most recently selected atoms.

The "Atom Dih." line displays the angle defined by the four most recently selected atoms.

The OK button closes the dialog, the Help button shows this help page.

EXAMPLE

DialMeasure on

SEE ALSO

AddDist, WriteAng

DATE

980409

NAME

DialMol - switch molecule dialog on and off

SYNOPSIS

DialMol (off | on)

DESCRIPTION

Switch molecule dialog on and off. The molecule dialog can be used to select molecules and for toggling their displayed and movable states. It is a convenient interface to the commands SelectMol and DefPropMol.

The radio buttons at the top of the dialog allow the selection of the property that is displayed/modified.

The list contains all currently loaded molecules, where the ones with the corresponding property are highlighted. The property can be modified by selecting and unselecting entries in the list. Note that you can make multiple/extended selections by holding down the Shift or Ctrl key while clicking on entries in the list.

The OK button closes the dialog, the Help button shows this help page.

EXAMPLE

DialMol on

SEE ALSO

SelectMol, DefPropMol

DATE

980409

NAME

DialRmsd - switch RMSD dialog on and off

SYNOPSIS

DialRmsd (off | on) [expr]

DESCRIPTION

Switch RMSD dialog on and off. The RMSD dialog is a convenient interface to the commands Fit and CalcRmsd, especially for comparisons of different molecules.

The optional second argument gives the number of groups of molecules for which residue ranges can be selected in the dialog. The default is the number of different molecules loaded.

The top two parts of the dialog allow selection of the two properties for which the global RMSDs are calculated. The common choices 'bb' (backbone) and 'heavy' (all heavy atoms) can be selected directly. A different property can be selected by chosing the 'other' button, and entering the name of the property in the corresponding text field on the right hand side. If 'other' is selected, and the text field is left empty, no global RMSDs will be calculated.

The third part of the dialog is for entering residue ranges used for superposition. Different ranges can be used for different sets of molecules given by the range in the left side text field, this is useful for comparing different molecules. Both molecule ranges and residue ranges are given in the short selection syntax, e. g. 3-10,15,18-23. The number of lines for molecule ranges is chosen when opening the dialog, and can only be changed by closing the dialog and opening it again.

The check boxes in the fourth part of the dialog select the properties that global displacements, local RMSDs, and local displacements are calculated for.

The check boxes at the bottom of the dialog select some options. The first one has to be activated when a fit with segments in a different order than their residue numbering is desired, see the Fit help page for more details. The remaining options are used for RMSD calculation. They select whether each pair of molecules is fitted before calculating the RMSDs, whether local RMSDs and displacements should be reported relative to the mean structure or as average pairwise values, and whether RMSDs between groups of molecules (as defined by the molecule ranges in the third part of the dialog) should be calculated.

The buttons at the bottom right activate the Fit or CalcRmsd command with the selected options.

The OK button closes the dialog, the Help button shows this help page.

EXAMPLE

DialRmsd on

SEE ALSO

Fit, CalcRmsd

DATE

980409

NAME

DialSelect - switch selection dialog on and off

SYNOPSIS

DialSelect (off | on)

DESCRIPTION

Switch selection dialog on and off. The selection dialog is a convenient interface to the commands SelectMol, SelectRes, SelectAtom, SelectBond, SelectAngle and SelectDist.

For making a selection, enter an expression (see the Select* help page) in one of the text fields, and either click the corresponding button on the left side, or hit the Return key). When the Return key is used, the expression is stored in a history which can be recalled by the cursor keys or the small arrows on the right side of the text fields.

The button/field "R+A+B+A" makes a selection with the same expression for residues, atoms, bonds and angles. This can be convenient in some cases, also if the user is unsure what kind of selection a command requires.

The OK button closes the dialog, the Help button shows this help page.

EXAMPLE

DialSelect on

SEE ALSO

Select*, DefProp*

DATE

980409

NAME

DialStyle - switch style dialog on and off

SYNOPSIS

DialStyle (off | on)

DESCRIPTION

Switch style dialog on and off. The style dialog is a convenient interface to the commands StyleAtom, StyleBond and StyleDist.

The style for the selected atoms, bonds or distances is changed by clicking on the corresponding button.

The OK button closes the dialog, the Help button shows this help page.

EXAMPLE

```
DialStyle on
```

SEE ALSO

SelectAtom, SelectBond, SelectDist, DialSelect, StyleAtom, StyleBond, StyleDist

DATE

980409

NAME

DrawDelay – set drawing delay

SYNOPSIS

DrawDelay expr

DESCRIPTION

Set a delay for drawing. The program will pause for the given time (in milliseconds) after each redraw. This can be useful on machines without double buffering, to avoid too much flickering.

EXAMPLE

```
DrawDelay 100
```

DATE

940325

NAME

DrawPrec - set drawing precision

SYNOPSIS

DrawPrec expr

DESCRIPTION

Set the precision for certain drawing operations, e. g. for the approximation of spheres. Making this value larger improves the drawing quality, but makes the drawing slower. Reasonable values are in the range between 2 (moderate quality) and 4 (good quality).

The value used for plotting can be set seperately with the PlotPar command.

EXAMPLE

DrawPrec 3

SEE ALSO

PlotPar

DATE

950613

NAME

DrawSize - set size of drawing area

SYNOPSIS

DrawSize (set | restore) [expr expr]

DESCRIPTION

If the fist argument is 'set', set the size of the drawing are to the given width and height (in pixels). This can be useful in connection with plotting, so that the user can enforce a certain aspect ratio for the resulting plot.

With the first argument 'restore', the command restores the drawing area to the last size given with the 'set' option. The saved size is also stored in parameter and dump files, so this command is mainly used for saving a desired window (and plot) size in a dump file, and restoring it after reading it back.

EXAMPLE

```
DrawSize set 1000 750
DrawSize restore
```

SEE ALSO

PlotPar

DATE

961213

NAME

EditText - edit text annotation

SYNOPSIS

EditText string

DESCRIPTION

Change the text of all selected text annotations.

Besides the normal characters, greek letters can be used by entering a \ (backslash)followed by the corresponding latin character (e. g. \a for alpha).

Subscript is started with an _. If more than one character should be displayed in subscript, they have to be enclosed in braces.

Superscript is analogous to subscript, only that the ^ character is used instead of _.

EXAMPLES

```
EditText "New Text"
EditText "C_\a"
EditText "a^{2 * x}"
```

SEE ALSO

AddTitle, AddText, ColorPrim, LinePrim, MovePrim, SizeText, RemovePrim

DATE

950407

NAME

FigAngles – show angle distribution bars

SYNOPSIS

FigAngles nameList expr

DESCRIPTION

Create a figure showing the angle distributions as points inside bars. Only selected angles are shown. The first argument is a space separated list of all angle names shown in the plot. If there is a gap greater than the value given as second argument, the bar indicating the angle range will be split.

The user can select angles by clicking on symbols in the plot.

This command supports groups.

EXAMPLE

```
FigAngles 'PHI PSI' 45
```

SEE ALSO

SelectAngle, Group, FigOff, FigCircles

DATE

960317

NAME

FigCircles - show angle distribution circles

SYNOPSIS

FigCircles expr expr

DESCRIPTION

Create a figure showing the angle distributions as polylines inside circles. The first argument gives the number of rows over which the circles are distributed, the second argument is the font size relative to the radius of the circles.

The same number of angles has to be selected in all selected molecules, the corresponding angles from all molecules will be drawn in one circle, from the inside to the outside. 0 is at the top, 90 degrees at the right side of the circle.

This kind of figure is mainly used for analyzing results of MD runs.

This command supports groups.

EXAMPLE

FigCircles 4 0.3

SEE ALSO

SelectMol, SelectAngle, Group, FigOff, FigAngles

DATE

960317

NAME

FigContact - show contact map

SYNOPSIS

FigContact name name name name expr expr

DESCRIPTION

Create a figure showing a contact map of residues. The first argument gives a property name, the residues with this property set will be shown on the horizontal axis. The residues with the property given as second argument will be shown on the vertical axis.

For each of these residues, only the atoms with the property given as third argument will be considered for the contacts shown on the top-left side of the diagonal, the ones with the property given as fourth argument will be considered for the bottom-right side of the diagonal.

Two distances are given as fifth and sixth argument. Nothing will be drawn if the smallest distance between two atoms of the corresponding residues is larger than the maximal distance. A black square will be drawn if it is smaller than the minimal distance. Values in between are shown with increasing levels of grey.

If more than one molecule is selected, they all need to have the same structure. The distance of each atom pair is calculated as average over the distances in each individual molecule. So what is used for the plot is the minimal average distance of atom pairs between the corresponding residues.

This command supports groups.

EXAMPLE

```
FigContact 'selected' 'selected' 'bb' 'all' 3.0 5.0
```

SEE ALSO

DefPropRes, DefPropAtom, Group, FigOff, FigLimit, CalcDist

DATE

961126

NAME

FigDist - show distance vs. structure number

SYNOPSIS

FigDist expr expr expr (0 | 1) (0 | 1)

DESCRIPTION

Create a figure showing distances on the vertical axis vs. structure numbers on the horizontal axis. The first argument gives the number of rows over which the plots are distributed.

The second and third argument give the distance range on the vertical axis.

A plot will be made for all selected distances of the first selected molecule, the corresponding distances from all selected molecules will be shown.

The first option selects whether residue numbers are written as subscripts. The second option selects whether the values of constraints are shown as horizontal lines.

This kind of figure is mainly used for analyzing results of MD runs.

This command supports groups.

EXAMPLE

```
FigDist 4 3.0 7.0 0 1
```

SEE ALSO

SelectMol, SelectDist, Group, FigOff, FigAngles, FigCircles

DATE

960317

NAME

FigLimit - show map of distance constraints

SYNOPSIS

FigLimit name name expr expr expr

DESCRIPTION

Create a figure showing a map with the number of distance constraints between residue pairs. The first argument gives a property name, the residues with this property set will be shown on the horizontal axis. The residues with the property given as second argument will be shown on the vertical axis.

All selected distances are considered. If the two properties given as first and second argument are the same, upper limits are shown on the top-left side of the diagonal, lower limits on the bottom-right side. If the properties are different, the number of upper and lower limit constraints is shown together.

The third argument gives the number of constraints required for a fully black square, the fourth argument the minimum number of constraints required for a square to be shown at all. The grey value of these squares is given as fifth argument (0.0 is black, 1.0 is white).

This command supports groups.

EXAMPLE

```
FigLimit 'selected' 'selected' 5 1 0.7
```

SEE ALSO

ReadUpl, ReadLol, DefPropRes, Group, FigOff, FigContact

DATE

961127

NAME

FigOff - switch from figure to normal display

SYNOPSIS

FigOff

DESCRIPTION

When a figure (e. g. Ramachandran plot) is displayed, this command will switch back to the normal molecule display.

EXAMPLE

```
FigOff
```

SEE ALSO

FigRamach, FigAngles, FigCircles, FigDist, FigContact, FigLimit

DATE

950123

NAME

FigRamach - Ramachandran plot

SYNOPSIS

```
FigRamach name name nameList
    ( none | normal | VAL-ILE-THR | GLY )
    ( dot | plus | cross | res | res_box |
    mol | mol_box )
    ( dot | plus | cross | res | res_box |
    mol | mol_box )
    ( 0 | 1) ( 0 | 1 )
```

DESCRIPTION

Create a Ramachandran plot with the first angle name on the x-axis and the second angle name on the y-axis. Only residues where both angles are selected are shown.

The third argument is a space separated list of alternative residues (typically GLY).

The fourth argument selects the background (allowed regions). The allowed regions were determined from 378 different crystal structures with a resolution of 2.5 A or better. The regions where the density of points (PHI/PSI) from this statistic is highest are marked with color. The green regions contain 80% of all points, the green and yellow regions together 95%, all colored regions together 98%. There is a background for all non-GLY/PRO residues, one for VAL/ILE/THR and one for GLY.

The fifth argument selects the display style of residues not listed as alternative, the sixth argument the one for alternative residues.

If the color option is selected, he colors of the markers is taken from the bond corresponding to the angle, otherwise they are all black.

If the last option is selected and all angles shown in the plot have the same angle constraints, the allowed region is indicated in light grey.

The user can select residues by clicking on symbols in the plot.

EXAMPLE

```
FigRamach 'PHI' 'PSI' 'GLY' normal dot plus 1 0
```

SEE ALSO

ReadAco, SelectAngle, FigOff

DATE

960519

NAME

FirstMol - move molecules to front of molecule list

SYNOPSIS

FirstMol

DESCRIPTION

Move all selected molecules to the front of the molecule list. This can be useful for commands that are sensitive to the order of molecules, most notably Fit.

EXAMPLE

FirstMol

SEE ALSO

SelectMol, DialMol, Fit

DATE

970722

NAME

Fit - calculate structure superpositions

SYNOPSIS

```
Fit ( to_axes | to_first | circular | to_mean )
    nameList
```

DESCRIPTION

Calculate a superposition of all selected molecules, using the selected atoms (or the atoms with properties given by the second argument, see below). The number of selected atoms of all selected molecules must be the same, otherwise an error message is issued.

If the option 'to_axes' is selected, the principal axes of the structures are aligned to the axes of the coordinate system. This is useful for obtaining a standard orientation.

If the option 'to_first' is selected, the RMSD of each structure to the first structure is minimized separately.

If the option 'circular' is selected, the sum of the RMSDs from the first to the second, from the second to the third, ... and from the last to the first structure is minimized.

If the option 'to_mean' is selected, the sum of all RMSDs to the resulting mean structure is minimized.

The options 'circular' and 'to_mean' use a less efficient algorithm than 'to_first', they can take very long to calculate. Their use is therefore generally not recommended. They can help in rare cases where the algorithm used in 'to_first' is numerically unstable.

At least one molecule has to be selected for 'to_axes', at least two for all other options.

For only two selected molecules, all algorithms give the same result.

The RMSD to the mean averaged over all molecules for the selected atoms after the fit is printed on the status line.

The optional second argument gives a list of properties of atoms to be fitted, where the default is just all selected atoms. If several properties are given, the corresponding atoms are fitted in this order. This is useful when superimposing different molecules, and the fragments to be superimposed are not in the same order in all molecules. E. g. for superimposing fragments of two molecules like this:

```
mol 1      mol 2
10-20 <--> 15-25
30-40 <--> 55-65
50-60 <--> 35-45
```

Just selecting all these atoms would take all fragments in ascending order, making the following superposition:

```
mol 1      mol 2
10-20 <--> 15-25
30-40 <--> 35-45
50-60 <--> 55-65
```

For getting the desired result:

```
DefPropAtom 'fragm1' '(#1:10-20 #2:15-25) & bb'
DefPropAtom 'fragm2' '(#1:30-40 #2:55-65) & bb'
DefPropAtom 'fragm3' '(#1:50-60 #2:35-45) & bb'
Fit to_first 'fragm1 fragm2 fragm3'
```

This command supports groups.

EXAMPLE

```
Fit to_first 'selected'
```

SEE ALSO

SelectAtom, Group, DialMol

DATE

961217

NAME

FlipAtom - flip atoms for better superposition

SYNOPSIS

FlipAtom nameList

DESCRIPTION

Exchanges sets of atom names in all selected residues if that leads to a better superposition to the first structure. The sets of atoms that can be exchanged is listed in the file:

$MOLMOLHOME/setup/FlipAtoms

The specifications in this file list atoms that are part of one potential exchange operation on one line. Each set of (typically 2 or 3) atoms that will be permuted by this operation is inside a pair of parentheses.

The atoms that can be exchanged are normally the atoms of rings that do not have a fixed orientation in an NMR structure (PHE, TYR), and the protons of methyl groups.

This command is typcially used before calculating mean structures, or RMSDs that involve side chains.

The command will make a report listing the atoms that were exchanged.

EXAMPLE

FlipAtom "PHE TYR"

SEE ALSO

PathNames, MeanMol, CalcRmsd

DATE

950922

NAME

Fog - setup of fog (depth cueing)

SYNOPSIS

Fog (off | exp | exp2 | linear) expr expr expr

DESCRIPTION

Set fog mode and parameters. The first argument selects the mode (off, exponential, squared exponential, linear). The second argument selects the density for both kinds of exponential fog. The third and fourth argument give the start and end distance for linear fog.

Negative values for any of the numerical arguments will leave the value unchanged, this is useful for changing only one value if the command is put on a slider.

Not all fog modes are supported on all hardware.

EXAMPLE

```
Fog linear 0.1 7.0 13.0
```

DATE

960305

NAME

Fullscreen - switch fullscreen display on and off

SYNOPSIS

Fullscreen (off | on)

DESCRIPTION

Switch fullscreen display on and off. Fullscreen mode is usefull for making screen photos and it is required for stereo display on some machines. Note that the menu and the command line are not visible in fullscreen mode. If the Fullscreen command is in the popup menu (right mouse button), this is the easiest way to switch back to normal mode. You can also type commands in fullscreen mode, but it is not very convenient because there is no feedback.

EXAMPLE

Fullscreen on

SEE ALSO

Stereo

DATE

931129

NAME

Group - define molecule groups

SYNOPSIS

Group expr

DESCRIPTION

Define groups with the currently selected molecules. The argument gives the number of members of each group. The default value is all selected molecules. If a smaller number is given, multiple groups with the desired number of molecules each are defined. E. g. the value 2 will make a group with the first and second selected molecule, another one with the third and fourth, etc.

Defining groups changes the behaviour of a number of commands, mostly the ones for calculation. They will treat the molecules in a group as if they were only one molecule. This is commonly used when dealing with complexes, so that e. g. CalcSurface will calculate the surface of the whole complex, and not of each molecule individually.

The help page of every command that deals with groups has the remark "this command supports groups" at the bottom.

EXAMPLE

Group 2

SEE ALSO

SelectMol

DATE

960317

NAME

    HelpAbout - show program version and copyright

SYNOPSIS

    HelpAbout

DESCRIPTION

    Show a message box with program name, version and
    copyright.

EXAMPLE

    HelpAbout

DATE

    970224

NAME
    HelpApropos - locate commands by keyword

SYNOPSIS
    HelpApropos string

DESCRIPTION
    Show a list of all commands that have the given keyword in their one-line description. The menu that the command can be found in is given in parentheses. The keyword may contain wildcard characters (?, *), the search is case insensitive.

EXAMPLE
    HelpApropos "plot"

SEE ALSO
    HelpCmd

DATE
    950727

NAME

HelpButton – show definition of buttons

SYNOPSIS

HelpButton

DESCRIPTION

Show the file that contains the definition of the buttons.

EXAMPLE

HelpButton

SEE ALSO

PathNames

DATE

950411

NAME
    HelpCmd - get help on command

SYNOPSIS
    HelpCmd

DESCRIPTION
    Switch to help mode. The next command that is entered on the command line or selected in the menu will not be executed, but the according help text will be displayed instead.

    Instead of displaying help texts in a simple text window, it is possible to use a web browser to see the hypertext versions of the help pages. This can be selected with the HelpViewer command.

EXAMPLE
    HelpCmd

SEE ALSO
    HelpViewer, HelpApropos

DATE
    971002

NAME

HelpMouse - show help text about using the mouse

SYNOPSIS

HelpMouse

DESCRIPTION

Show a text that explains how to use the mouse.

EXAMPLE

HelpMouse

DATE

950411

NAME

HelpProp - show definition of standard properties

SYNOPSIS

HelpProp

DESCRIPTION

Show the file that contains the definition of the standard properties.

EXAMPLE

HelpProp

SEE ALSO

PathNames, DefProp*, Select*

DATE

950302

NAME

HelpViewer - set viewer for help files

SYNOPSIS

```
HelpViewer ( UNIX-Netscape | Windows-Explorer |
    builtin | custom ) string
```

DESCRIPTION

Choose a viewer for displaying help files. The first two options set commonly used web browsers on the corresponding platform. With 'builtin', a simple text window is used. When 'custom' is selected, the command given as second argument is used for starting a web browser. For UNIX, this has to be a complete command string, where %f will be replaced by the name of the HTML file. For Windows, it is only the name of a web browser, this must be capable of DDE with the same protocol as Explorer.

Once a help file has been displayed, choosing a different option with this command may only take effect after restarting the program.

EXAMPLE

```
HelpViewer UNIX-Netscape ''
```

SEE ALSO

HelpCmd

DATE

971002

NAME

InitAll - delete and initialize everything

SYNOPSIS

InitAll (yes | no)

DESCRIPTION

Delete all data and initialize the program. This can be used before starting with something new. It is also needed after changing certain parameters (e. g. ResLib) to make sure that they take effect.

The command asks for a confirmation.

EXAMPLE

InitAll yes

SEE ALSO

PathNames, RemoveMol

DATE

940411

NAME

LabelAtom – set format of atom label

SYNOPSIS

LabelAtom string

DESCRIPTION

Set the format of the label of all selected atoms. If the character 'R' appears in the string, it is replaced by the residue name. 'N' is replace by the residue number, 'A' by the atom name. All other characters are displayed in the label unchanged.

EXAMPLE

```
LabelAtom "R N"
```

SEE ALSO

SelectAtom

DATE

940119

NAME

LabelDist - choose label of distances

SYNOPSIS

```
LabelDist ( invisible | val | limit | viol )
```

DESCRIPTION

Choose the label of all selected distances.
The following possibilities are supported:

```
invisible: no label
val:       current value of the distance
limit:     limit of distance constraints
viol:      violation of distance constraints
```

EXAMPLE

```
LabelDist val
```

SEE ALSO

SelectDist

DATE

941122

NAME

LengthBond - set length of bonds for display

SYNOPSIS

LengthBond expr expr

DESCRIPTION

Set the displayed length of all selected bonds. The first argument gives the start parameter, the second argument the end parameter, the parameter range 0 to 1 refers to the original size of the bond.

Note that this command does not actually modify coordinates that would e. g. be written to a coordinate file, it only changes the way bonds are displayed. The command is especially useful when drawing side chains in ribbon diagrams, where the bonds from CA to CB would otherwise not match with beta strands.

EXAMPLES

```
LengthBond -0.5 1
```

SEE ALSO

SelectBond, AddRibbon

DATE

970219

NAME

LengthPrim - set length of primitives

SYNOPSIS

LengthPrim expr expr

DESCRIPTION

Set the length of all selected ribbons. The first argument gives the start parameter, the second argument the end parameter. The parameter value is 1 for the first atom used for AddRibbon, 2 for the second atom, etc.

The command can also be used for changing the length of a cylinder. In this case, the parameter range 0 to 1 refers to the current size of the cylinder, and the new parameter values are interpreted relative to these values.

Entering 0 for any of the parameters will leave this value unchanged.

EXAMPLES

```
LengthPrim 12.5 20.5
LengthPrim 0.1 1.1
```

SEE ALSO

AddRibbon, SelectPrim, MovePrim,
TypeRibbon, StyleRibbon, SizeRibbon, PaintRibbon

DATE

951123

NAME

Light - setup of light source

SYNOPSIS

Light (off | point | infinite) expr expr expr

DESCRIPTION

The first argument selects between no light source, a point light source or a light source at infinity. The coordinates are used as position if a point light source was chosen as point, or only as direction for an infinite light source. Point light sources might not be supported on all hardware, or they may be slower than infinite light sources.

Coordinates are so that the origin is at the center of the screen, the x-axis points to the right, the y-axis to the top, and the z-axis out of the screen. The viewpoint (eye, camera) is at (0, 0, 10).

EXAMPLE

```
Light point 0 5 5
```

DATE

950824

NAME

LineAtom - set style and width of atom lines

SYNOPSIS

LineAtom (solid | dashed) expr

DESCRIPTION

Set the style and width of the lines used for drawing all selected atoms. Lines are used for atoms if the style is 'tetrahedron', or if it is 'sphere' and the shading is set to 'lines'.

EXAMPLE

LineAtom solid 3

SEE ALSO

SelectAtom, StyleAtom, ColorAtom, ShadeAtom

DATE

950324

NAME

LineBond - set style and width of bond lines

SYNOPSIS

LineBond (solid | dashed) expr

DESCRIPTION

Set the style and width of the lines used for drawing all selected bonds. The default width of 0 is the minimal width that can be drawn, it is also the one that can be drawn fastest.

EXAMPLE

```
LineBond solid 3
```

SEE ALSO

SelectBond, StyleBond, ColorBond

DATE

940119

NAME

LineDist - set style and width of distance lines

SYNOPSIS

LineDist (solid | dashed) expr

DESCRIPTION

Set the style and width of the lines used for drawing all selected distances. The default width of 0 is the minimal width that can be drawn, it is also the one that can be drawn fastest.

EXAMPLE

```
LineDist solid 3
```

SEE ALSO

SelectDist, StyleDist, ColorDist

DATE

940119

NAME

LinePrim - set style and width of primitive lines

SYNOPSIS

LinePrim (solid | dashed) expr

DESCRIPTION

Set the style and width of the lines used for drawing all selected primitives. The default width of 0 is the minimal width that can be drawn, it is also the one that can be drawn fastest.

EXAMPLE

```
LinePrim solid 3
```

SEE ALSO

SelectPrim, ColorPrim

DATE

951013

NAME

```
ListPropMol   - list all molecule properties
ListPropRes   - list all residue properties
ListPropAtom  - list all atom properties
ListPropBond  - list all bond properties
ListPropAngle - list all angle properties
ListPropDist  - list all distance properties
ListPropPrim  - list all primitive properties
```

SYNOPSIS

```
ListPropMol
ListPropRes
ListPropAtom
ListPropBond
ListPropAngle
ListPropDist
ListPropPrim
```

DESCRIPTION

Lists the set properties of all selected molecules, residues, atoms, bonds, angles, distances or primitives. All items have to share the same set of properties, an error message is issued otherwise.

EXAMPLES

```
ListPropRes
```

SEE ALSO

DefProp*, Select*

DATE

960213

NAME

MaterialAtom - set material properties of atoms
MaterialBond - set material properties of bonds
MaterialDist - set material properties of distances
MaterialPrim - set material properties of primitives

SYNOPSIS

MaterialAtom expr expr expr expr expr expr expr
MaterialBond expr expr expr expr expr expr expr
MaterialDist expr expr expr expr expr expr expr
MaterialPrim expr expr expr expr expr expr expr

DESCRIPTION

Set the material properties of all selected atoms, bonds, distances or primitives. The first three paramters give the coefficients for ambient, diffuse and specular reflection. These values should all be between 0 and 1, for good results the ambient and diffuse terms should sum up to around 1.

The fourth parameter gives the shininess, it only has an effect if the specular coefficient is not zero. Higher values for the shininess result in smaller specular highlights. Values can be from 1.0 (very dull) to 200 and more (highly polished metal).

The fifth parameter gives the reflection. 1.0 results in a complete reflection of other objects in the scene (mirror), 0.0 in no reflection.

The sixth parameter gives the opacity. 1.0 results in a completely opaque material, 0.0 in complete transparency.

The seventh parameter gives the index of refraction, it only has an influence for (partly) transparent materials. 1.0 gives no refraction, 1.5 is the value for glass, 2.4 for diamond.

Transparency is not supported on most hardware, and only to a limited amount on machines with high-end graphics. It is mainly useful for preparing files for ray tracing (PlotPov). Reflection is not supported on screen, it is only used for ray tracing.

Giving a value less than 0.0 for any value will not change it, this is useful for changing only part of the parameters.

EXAMPLES

MaterialAtom 0.3 0.7 0.4 30 0.0 1.0 1.0

SEE ALSO

Select*, Texture*, PlotPov

DATE

950824

NAME

MeanMol - create mean molecule

SYNOPSIS

```
MeanMol name
    ( avg_bfactor | max_disp | rms_disp | x_ray )
    ( mean_only | set_all )
```

DESCRIPTION

Create a new molecule with the given name. The new molecule will be the mean structure of all selected molecules. At least one molecule must be selected, and all selected molecules must have the same structure.

The second argument determines how the B-factors of the new molecule are set:

avg_bfactor: average value of all B-factors

max_disp: maximal displacement from mean structure

rms_disp: root mean square of all displacements

x_ray: values corresponding to B-factors used for X-ray structures (mean square displacement multiplied by 8/3 * pi * pi)

If the third argument is mean_only, this B-factors are only set in the new mean structure, if it is set_all, the B-factors of all selected structures are set to this value.

The newly created molecule will have the property "mean".

EXAMPLE

```
MeanMol "mean" rms_disp mean_only
```

SEE ALSO

SelectMol, RemoveMol

DATE

960314

Definiton of Actions

click: press one (or multiple) mouse button(s) and release them without moving the mouse

click+mod: hold down a modifier key (Shift or Ctrl) and click.

drag: press one (or multiple) mouse button(s), move the mouse, and release the button(s)

Table of Actions

	click	click+mod	drag
left	select	select add.	rotate
middle (in text)	toggle text select		move/resize text
middle (elsewhere)	select	select add.	move molecules
left+middle			zoom
right	popup		

NAME

MoveDrawobj - move draw object

SYNOPSIS

MoveDrawobj expr expr expr expr

DESCRIPTION

Move all selected draw objects (like lines or rectangles) by the given amount. The first argument gives the index of the control point (starting at 0) to be moved, the rest of the arguments give the amount of movement in each direction.

Moving the control points of drawing objects is normally done interactively by using the middle mouse button.

EXAMPLE

```
MoveDrawObj 0 0.3 0.1 0.2
```

SEE ALSO

AddDrawobj, SelectPrim

DATE

950618

NAME

MovePrim - move primitive

SYNOPSIS

MovePrim expr expr expr

DESCRIPTION

Move all selected primitives by the given amount. Only circles, cylinders and texts can currently be moved. Moving texts is normally done interactively by using the middle mouse button.

EXAMPLE

```
MovePrim 0.3 0.1 0.2
```

SEE ALSO

SizeText, RadiusPrim, LengthPrim

DATE

950407

NAME
MoveX - move molecule in X direction

SYNOPSIS
MoveX expr

DESCRIPTION
Move all movable (set with DialMol) molecules by the given amount in X direction. Moving is normally done interactively by pressing the middle mouse button. This command is useful for being used in macros or for setting up the slider box.

EXAMPLE
MoveX 10

SEE ALSO
DialMol, DefPropMol, MoveY, MoveZ

DATE
931129

NAME

MoveY - move molecule in Y direction

SYNOPSIS

MoveY expr

DESCRIPTION

Move all movable (set with DialMol) molecules by the given amount in Y direction. Moving is normally done interactively by pressing the middle mouse button. This command is useful for being used in macros or for setting up the slider box.

EXAMPLE

```
MoveY 10
```

SEE ALSO

DialMol, DefPropMol, MoveX, MoveZ

DATE

931129

NAME
     MoveZ - move molecule in Z direction

SYNOPSIS
     MoveZ expr

DESCRIPTION
     Move all movable (set with DialMol) molecules by the given amount in Z direction. Moving in Z direction is very similar to zooming, which is normally done interactively by pressing the left and the middle mouse buttons simultanously. The effect is somewhat different if a perspective projection is chosen, and also the clipping planes work differently.

EXAMPLE
     MoveZ 10

SEE ALSO
     DialMol, DefPropMol, MoveX, MoveY, Zoom*,
     ClipPos, ClipSize, Projection

DATE
     950124

NAME

NameMol - change molecule name

SYNOPSIS

NameMol name expr expr

DESCRIPTION

Change the name of all selected molecules. When multiple molecules are renamed, they can be given unique names by appending a number to the name.

The first argument gives the (base) name, the second one the starting number for numbering molecules, the third one the number of digits for numbering.

When changing the name of only one molecule, the number of digits (third argument) should be 0, so that the name given as first argument is directly used as name.

EXAMPLES

```
NameMol bpti 1 0
NameMol bpti 21 3
```

SEE ALSO

NewMol, DialMol

DATE

980319

NAME

NearPrim - set near clipping plane of primitives

SYNOPSIS

NearPrim expr

DESCRIPTION

Set the position of the near clipping plane of all selected primitives. The position is given as distance from the viewing point, the center of the display has distance 10.0 from the viewing point. When a negative value is given, the current value will be unchanged. When 0.0 is given, no separate clipping will be done, the global clipping planes set by ClipPos and ClipSize are then used.

This command is mainly useful for surfaces, by clipping away the front part it is possible to see the inside.

EXAMPLE

```
NearPrim 8.0
```

SEE ALSO

SelectPrim, AddSurface, ClipPos, ClipSize, TrimSurface

DATE

970718

NAME
    NewMol - create new molecule

SYNOPSIS
    NewMol name

DESCRIPTION
    Create a new molecule with the given name. The new molecule will contain no residues, they must be added by using the command AddRes.

EXAMPLE
```
NewMol "My Molecule"
```

SEE ALSO
    AddRes, ChangeRes

DATE
    931129

NAME

PaintRibbon - set coloring style of ribbons

SYNOPSIS

PaintRibbon (one_color | two_color |
atom | atom_smooth | as_is)

DESCRIPTION

Set the coloring style of all selected ribbons. With the value one_color, the ribbon will be drawn entirely in the color set with ColorPrim. With two_color, one side will be drawn with the color set by TintPrim. With the value atom, the color for each section is taken from the color of the atom that was used to define the ribbon, normally the CA atom for proteins. atom_smooth will do the same, only that the color change between the sections is smooth. The value as_is will leave the value unchanged.

EXAMPLE

```
PaintRibbon one_color
```

SEE ALSO

AddRibbon, SelectPrim, ColorPrim, TintPrim

DATE

951210

NAME

PaintSurface - set coloring style of surfaces

SYNOPSIS

PaintSurface (one_color | atom | dist | center | access | pot) expr expr expr expr string

DESCRIPTION

Set the coloring style of all selected surfaces. With the value one_color, the surface will be drawn entirely in the color set with ColorPrim.

With the value atom, the color for each point is taken from the color of the closest selected atom. For this case, the third argument gives the maximum distance from the atom surface, the user will normally give the solvent radius used for calculating the surface for this argument.

With the value dist, the color for each point is calculated from the distance to the reference atom(s) defined with SetRef, using the mapping of values to colors described below.

With the value center, the color for each point is calculated from the distance to the center of gravity of all selected atoms, using the mapping of values to colors described below.

With the value access, the color for each point is calculated from the accessibility of the point, using the mapping of values to colors described below. The accessibility is calculated by an experimental (and relatively slow) algorithm that casts a number (4**p, where p is the precision given as fifth argument) of rays from each surface point, and counts how many of them intersect a selected atom within the distance range given by the second and third argument. A small offset given as fourth argument is normally applied to each surface point to avoid artefacts.

With the value pot, the color is calculated from a potential field read with ReadPot, using the mapping of values to colors described below.

For the options that require a mapping of values to colors, this mapping is given by the last argument. It consists of space separated tuples of the form:

```
v r g b
```

where v is the potential and r, g, b give the color as RGB (red, green, blue) components. Colors are interpolated between the values in the table.

Potentials have to be calculated with the CalcPot command, and then read with ReadPot, before using this command with the corresponding option.

EXAMPLE

```
PaintSurface atom 0.0 1.4 0.0 0 ''
PaintSurface dist 0.0 0.0 0.0 0
    '5.0 1 0 0 10.0 1 0 1 20.0 0 0 1'
PaintSurface access 3.0 8.0 0.2 2
    '0.4 1 0 0 0.5 1 1 0 0.8 0 1 0'
PaintSurface pot 0.0 0.0 0.0 0.0 '0.0 0 0 1 4.0 1 0 0'
```

SEE ALSO

AddSurface, SelectPrim, SetRef, CalcPot, ReadPot, ColorPrim, ColorAtom

DATE

980319

NAME
    PathNames - set path names

SYNOPSIS
    PathNames string string string string string
        string string string string

DESCRIPTION
    Set path names for some configuration files.
    Normally the program reads these file from the
    directory $MOLMOLHOME/setup.

    The following is a list of all configuration files:

        AtomRadius: Contains radii for atoms. Used for
            the commands CalcBond and CheckBond.

        AtomCharge: Contains charges for atoms. These
            are used when 'simplecharge' is referenced
            in an expression for an atom.

        FlipAtoms: Contains sets of atoms that can be
            exchanged by the FlipAtom command.

        RingShift: Contains definitions of models for
            the CalcShift command.

        PdbAtoms: Contains a table that is used to
            translate atom names from PDB files to
            atom names from the residue library.

        PropDef: Contains definitons of standard
            properties.

        ResLib: Residue library.

        MenuDir: Directory that contains menu definition
            files (MenuBar, *.menu, Popup, Valuator).

        ColorList: List of colors used for DialColor.

    Generally the configuration files are read when
    they are used the first time, and the contents is
    kept in memory. This means that changing the path
    only has an effect after leaving the program and
    starting it again. This is always true for MenuDir.
    It is also necessary for AtomRadius if the CalcBond
    or CheckBond command was used, for RingShift if the
    CalcShift command was used, for PdbAtoms if a PDB
    file was read or written, and for ColorList if the
    color dialog (DialColor) was opened.

    ResLib, together with AtomCharge, is read as soon as
    a molecule is read from a file. To use the new
    definitions after ResLib has been changed, the program
    has to be reinitialized by using the InitAll command,

and the molecules have to be read again. Just leaving the program and starting it again does not help, since the contents is stored in the molmol/dump file in the home directory. PropDef is handled in the same way.

If the file with the given path name cannot be openend, the program will silently fall back to the default file.

The special name "0" can be given for path names, in this case an empty file will be taken for the corresponding configuration file. This can be handy e. g. for PdbAtoms when you want to read a PDB file without using the normal translation for atom names.

EXAMPLE

```
PathNames "" "" "" "" "" "" "/home/joe/molmol/my.lib" "" ""
```

SEE ALSO

CalcBond, FlipAtom, CalcShift, ReadPdb, DialColor, InitAll, DefProp*

DATE

960416

NAME

PlotBmp - make a BMP (Windows bitmap) plot

SYNOPSIS

PlotBmp fileName

DESCRIPTION

Save the current screen contents as BMP file, the standard image file format used on Windows. The horizontal resolution can be set with the PlotPar command, the vertical resolution is calculated to maintain the aspect ratio of the screen.

This command is not supported on all machines and with all graphics systems. It will give an appropriate error message if it is not supported.

EXAMPLE

```
PlotBmp /home/joe/MyPlot.bmp
```

SEE ALSO

PlotPar, PlotTiff, PlotJpeg, PlotPng
PlotFm3, PlotFm4, PlotPs

DATE

970225

NAME

PlotFm3 - make a FrameMaker 3 plot
PlotFm4 - make a FrameMaker 4 plot

SYNOPSIS

PlotFm3 fileName
PlotFm4 fileName

DESCRIPTION

Make a plot of the current screen contents in MIF format. This can be imported into FrameMaker.

PlotFm3 produces a file that can be read by FrameMaker 3 or later. This only supports 8 different colors, and is therefore not suited for displays with shading. Its main use is for the output of figures from commands like FigAngles.

PlotFm4 makes use of color possibilities introduced in FrameMaker 4, these files cannot be read by earlier versions. They are also larger.

FrameMaker can currently not handle the files created with PlotFm4 well, they make it very slow. Unless this improves with future versions, PlotFm4 is only of limited usefulness.

EXAMPLE

PlotFm4 /home/joe/MyPlot.fm

SEE ALSO

PlotPar, PlotPs

DATE

950704

NAME

PlotJpeg - make a JPEG plot

SYNOPSIS

PlotJpeg fileName

DESCRIPTION

Save the current screen contents as JPEG File. The horizontal resolution can be set with the PlotPar command, the vertical resolution is calculated to maintain the aspect ratio of the screen.

Note that that JPEG uses a lossy compression scheme, the quality factor can be adjusted with the PlotPar command.

This command is not supported on all machines and with all graphics systems. It will give an appropriate error message if it is not supported.

The freely available JPEG library written by the Independent JPEG Group is used for writing the JPEG file.

EXAMPLE

```
PlotJpeg /home/joe/MyPlot.jpg
```

SEE ALSO

PlotPar, PlotTiff, PlotPng,
PlotFm3, PlotFm4, PlotPs

DATE

960625

NAME
    PlotMeta - make a Windows enhanced metafile plot

SYNOPSIS
    PlotMeta fileName

DESCRIPTION
    Make a plot of the current screen contents in the Windows enhanced metafile format.

    This command is not supported on all machines and with all graphics systems. It will give an appropriate error message if it is not supported.

EXAMPLE
    PlotMeta /home/joe/MyPlot.emf

SEE ALSO
    PlotPar, PlotFm*, PlotPs, PlotPov, PlotVrml

DATE
    970225

NAME

PlotPar - set plot parameters

SYNOPSIS

```
PlotPar expr expr expr expr expr
    ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
    expr expr expr
```

DESCRIPTION

Set size and options for plots. The first argument gives the width of the paper, the second one the height. The third argument gives the width of the plot, the fourth one the height. If one of the plot sizes is 0, it is calculated to correspond to the dimensions (aspect ratio) of the window. The plot is centered on the paper.

The current unit for these sizes is shown in the prompt, it can be changed with the PlotUnit command. The default paper size also depends on the current unit.

The fifth argument selects the horizontal resolution used for saving image (TIFF, JPEG, PNG) files.

The first option switches stereo plotting on or off.

The second option switches shading and hidden surface elimination for the plot. The third only has an influence if shading is switched on. If it is selected, a full hidden surface elimination is done. This can take a few minutes for complex plots, but it is necessary to produce perfect results as soon as the scene contains spheres, cylinders or primitives. If it is not selected, a simple depth sorting is used, which is much faster, but the result can contain slight errors. For important plots (publications), this option must always be switched on.

The fourth option selects whether the plot is rotated by 90 degrees to produce a landscape plot. Note that the size of the plot (arguments 3 and 4) is still given in the original orientation of the plot, before rotation. The size of the paper is given in the orientation used by the printer, which is normally portrait. So e. g. good size for a landscape plot on A3 format are 29.7 42 0 26.

The third but last parameter select the precision (resolution) of the plot. See DrawPrec for an explanation of this parameter.

The second but last parameter selects a gamma correction parameter. 1.0 will leave the colors unchanged, values less than 1.0 will make the colors brighter, values greater than 1.0 will make the colors darker. Note that the "correct" gamma value depends on the output device used, so using gamma correction when producing the file is in principal not the right thing to do. We offer this possibilty for convenience sake, it is often difficult to do decent gamma correction on the output file (e. g. for PostScript) with other possibilities.

The last parameter selects the quality for JPEG plots. Recommended values are between 50 (strong compression with reasonable quality) and 95 (excellent quality).

EXAMPLES

```
PlotPar 21 29.7 18 0 1000 0 0 1 0 3 1.0 75
PlotPar 21 29.7 0 18 2000 0 1 1 1 3 0.7 60
PlotPar 29.7 42 0 26 1500 0 1 1 1 4 0.5 90
```

SEE ALSO

PlotUnit, PlotPs, PlotFm*,
PlotTiff, PlotJpeg, PlotPng, DrawPrec

DATE

960321

NAME

PlotPng - make a PNG plot

SYNOPSIS

PlotPng fileName

DESCRIPTION

Save the current screen contents as PNG File. The horizontal resolution can be set with the PlotPar command, the vertical resolution is calculated to maintain the aspect ratio of the screen.

This command is not supported on all machines and with all graphics systems. It will give an appropriate error message if it is not supported.

The freely available PNG library written by Guy Eric Schalnat, Group 42, Inc., is used for writing the PNG file.

EXAMPLE

PlotPng /home/joe/MyPlot.png

SEE ALSO

PlotPar, PlotTiff, PlotJpeg,
PlotFm3, PlotFm4, PlotPs

DATE

960625

NAME

PlotPov - make a POV-Ray plot

SYNOPSIS

PlotPov fileName

DESCRIPTION

Make a plot of the current screen contents in POV-Ray format. This can be used as input file for the ray tracing package POV-Ray (Persistence of Vision Ray Tracer) to produce high quality pictures.

The POV-Ray software is available free of charge by anonymous ftp from ftp.povray.org, directory /pub/povray/Official. See the accompanying files for copyright conditions and instructions on installation and use of the program. The output files generally have to be rendered with version 3.0 (or higher) of POV-Ray. If certain features, like text, are not used, they may also work with POV-Ray 2.2, but this is not supported.

EXAMPLE

PlotPov /home/joe/MyPlot.pov

SEE ALSO

PlotFm*, PlotPs, PlotTiff, PlotJpeg, PlotPng

DATE

961204

NAME

PlotPs - make a PostScript plot

SYNOPSIS

PlotPs fileName

DESCRIPTION

Make a PostScript plot of the current screen contents. Selection of the desired parameters with the PlotPar command is essential for obtaining good results. Hidden surface elimination of complex scenes can take some time (up to a few minutes typically).

EXAMPLE

```
PlotPs /home/joe/MyPlot.ps
```

SEE ALSO

PlotUnit, PlotPar, Rendering, Stereo

DATE

961128

NAME

PlotTiff - make a TIFF plot

SYNOPSIS

PlotTiff fileName

DESCRIPTION

Save the current screen contents as TIFF File. The horizontal resolution can be set with the PlotPar command, the vertical resolution is calculated to maintain the aspect ratio of the screen.

This command is not supported on all machines and with all graphics systems. It will give an appropriate error message if it is not supported.

The freely available TIFF library written by Sam Leffler, Copyright (c) 1988-1995 Sam Leffler and Silicon Graphics, is used for writing the TIFF file.

EXAMPLE

```
PlotTiff /home/joe/MyPlot.tif
```

SEE ALSO

PlotPar, PlotJpeg, PlotPng,
PlotFm3, PlotFm4, PlotPs

DATE

960625

NAME

PlotUnit - set unit of plot parameters

SYNOPSIS

PlotUnit (cm | mm | inch)

DESCRIPTION

Set the unit used for paper and plot sizes in the PlotPar command. Changing the unit will also reset the paper size to the default associated with the unit, which is A4 for cm and mm and US Letter for inch.

EXAMPLE

```
PlotUnit cm
```

SEE ALSO

PlotPar

DATE

950727

NAME

PlotVrml - make a VRML plot

SYNOPSIS

PlotVrml fileName

DESCRIPTION

Make a plot of the current screen contents in VRML (Virtual Reality Modeling Language) format. VRML is the standard format for transferring and displaying three-dimensional geometry on the World Wide Web. The created files follow version 1.0 of the VRML specifications and can be displayed by any VRML browser.

EXAMPLE

PlotVrml /home/joe/MyPlot.wrl

WARNING

This command was not tested thoroughly. Not all display possibilities of MOLMOL are supported.

SEE ALSO

PlotFm*, PlotPs, PlotPov

DATE

960723

NAME

Projection - choose projection

SYNOPSIS

Projection (orthogonal | perspective)

DESCRIPTION

Choose between orthogonal and perspective projection.

EXAMPLE

Projection orthogonal

SEE ALSO

ClipPos, ClipSize, ViewAngle

DATE

950124

NAME

Quit - quit the program

SYNOPSIS

Quit (yes | no)

DESCRIPTION

Quit the program. If the argument is 'yes', it will save the program state ("dump") to the file molmol/dump in the users home directory. This file is read whenever the program is started again.

The program state can also be saved and recovered to an arbitrary file by using the commands WriteDump and ReadDump.

EXAMPLE

```
Quit yes
```

SEE ALSO

ReadDump, WriteDump

DATE

951013

NAME

RadiusAtom - set radius of atoms

SYNOPSIS

RadiusAtom expr

DESCRIPTION

Set the radius of all selected atoms. The radius is only visible if an atom is displayed as sphere or as tetrahedron.

EXAMPLES

```
RadiusAtom 1.0
RadiusAtom 0.5+bfactor
```

SEE ALSO

SelectAtom, StyleAtom

DATE

940119

NAME
    RadiusBond - set radius of bonds

SYNOPSIS
    RadiusBond expr

DESCRIPTION
    Set the radius of all selected bonds. The radius
    is only visible if an bond is displayed as cylinder.

EXAMPLES
    RadiusBond 0.5

SEE ALSO
    SelectBond, StyleBond

DATE
    940119

NAME

    RadiusDist - set radius of distances

SYNOPSIS

    RadiusDist expr

DESCRIPTION

    Set the radius of all selected distances. The radius is only important if an distance is displayed as cylinder.

EXAMPLES

    RadiusDist 0.5

SEE ALSO

    SelectDist, StyleDist

DATE

    950223

NAME

RadiusPrim - set radius of primitives

SYNOPSIS

RadiusPrim expr

DESCRIPTION

Set the radius used for drawing all selected primitives. If the radius of a spline is set to 0, the spline is drawn as line, otherwise it is drawn as tube with the given radius.

EXAMPLE

```
RadiusPrim 0.7
```

SEE ALSO

AddRibbon, AddTrajec, AddDrawobj, ColorPrim

DATE

931130

NAME
    ReadAco - read file with angle constraints

SYNOPSIS
    ReadAco fileName

DESCRIPTION
    Read a file with angle constraints. The format is the one that DIANA uses. The angle constraints are added to all selected molecules.

EXAMPLE
    ReadAco /home/joe/struct/my_prot.aco

SEE ALSO
    SelectMol, DialMol,
    ReadUpl, ReadLol, AddAco, RemoveAco, CheckAco

DATE
    950302

NAME

ReadAng - read DIANA dihedral angle file
ReadListAng - read list of DIANA dihedral angle files

SYNOPSIS

ReadAng fileName
ReadListAng fileName

DESCRIPTION

Read a dihedral angle file like it is generated by DIANA or DYANA. The file can contain more than one structure. If only one structure is stored in the file, the file name is taken as name of the molecule. If there are multiple structures, numbers are appended to the file name for generating the molecule names.

ReadListAng expects a file with one file name per line (empty lines allowed), and reads all these files.

All residues must appear in the residue library:

$MOLMOLHOME/setup/amber94.lib

Angle files can only represent structures if the only conformational changes from the standard geometry in the residue library are rotations about dihedral angles. This is the case for structures calculated in dihedral angle space (DIANA), but not e. g. for energy minimized structures. It is also essential to use the same library that was used for the calculations, otherwise structures can be distorted due to slight differences in the standard geometry in the different libraries. It is generally safer to use coordinate files to avoid these problems.

EXAMPLE

ReadAng /home/joe/struct/my_prot.ang
ReadListAng /home/joe/struct/my_prot.nam

SEE ALSO

PathNames, ReadDg, ReadPdb, WriteAng

DATE

950704

NAME

ReadDg - read DG file
ReadListDg - read list of DG files

SYNOPSIS

```
ReadDg fileName
ReadListDg fileName
```

DESCRIPTION

ReadDg reads a file in DG format. Since no clear separation of molecules is supported by the DG format, it is assumed that a new molecule starts whenever the residue number decreases.

ReadListDg expects a file with one file name per line (empty lines allowed), and reads all these files.

If residues appear in the residue library ($MOLMOLHOME/setup/amber94.lib by default), the covalent structure is taken from there. The optional connection information of the DG format is also read, bonds not already known from the residue library are inserted. If there is no connection information at all, the user can add bonds with the command CalcBond later.

EXAMPLE

```
ReadDg /home/joe/struct/my_prot.cor
ReadListDg /home/joe/struct/my_prot.nam
```

SEE ALSO

PathNames, ReadAng, ReadPdb, WriteDg, CalcBond

DATE

951116

NAME

ReadDump - read dump file

SYNOPSIS

ReadDump fileName

DESCRIPTION

Read a dump file. A dump file is a binary file that contains the complete program state. A dump file with the name molmol/dump in the users home directory is created whenever the user leaves the program. A dump file with an arbitrary name can be created anytime by using the command WriteDump.

EXAMPLE

ReadDump /home/joe/struct/my_prot.mol

SEE ALSO

WriteDump

DATE

950704

NAME

ReadLib - read and error check residue library

SYNOPSIS

ReadLib

DESCRIPTION

Read the residue library. This command is not normally used, the residue library is read automatically when needed. This command gives diagnostic output, however, where normally errors in the residue library are not reported. So this command is helpful for checking the library after modifications, or whenever problems are suspected.

EXAMPLE

ReadLib

SEE ALSO

PathNames, InitAll, WriteLib

DATE

961206

NAME

ReadLol - read file with lower limits

SYNOPSIS

ReadLol fileName

DESCRIPTION

Read a file with lower distance limits. The format is the one that DIANA/DYANA uses. The distance constraints are added to all selected molecules.

This command supports groups.

EXAMPLE

```
ReadLol /home/joe/struct/my_prot.lol
```

SEE ALSO

SelectMol, Group, ReadUpl, AddLol, CheckLol

DATE

960317

NAME

ReadPdb - read PDB file
ReadListPdb - read list of PDB files

SYNOPSIS

ReadPdb fileName
ReadListPdb fileName

DESCRIPTION

Read a PDB file. The file can contain more than one structure. If only one structure is stored in the file, the file name is taken as name of the molecule. If there are multiple structures, numbers are appended to the file name for generating the molecule names.

ReadListPdb expects a file with one file name per line (empty lines allowed), and reads all these files.

If residues appear in the residue library ($MOLMOLHOME/setup/amber94.lib by default, can be changed with the PathNames command), the covalent structure is taken from there. If a residue is not present in the library, just the atom coordianates are read from the PDB file. The user can add bonds with the command CalcBond later.

Because the PDB naming conventions do not fully correspond with the names in the residue library of MOLMOL, a translation table for atom names is used. This is $MOLMOLHOME/setup/PdbAtoms by default, and can be changed with the PathNames command.

The command also reads secondary structure information (HELIX and SHEET records) and sets the corresponding properties on the residues. They are used by the AddRibbon command to create schematic drawings.

EXAMPLE

```
ReadPdb /home/joe/struct/my_prot.pdb
ReadListPdb /home/joe/struct/my_prot.nam
```

SEE ALSO

PathNames, ReadAng, ReadDg, WritePdb,
CalcBond, AddRibbon

DATE

950704

NAME

ReadPot - read potentials for surface coloring

SYNOPSIS

ReadPot fileName

DESCRIPTION

Read a file with potentials, these are used for coloring surfaces. The file must contain values on a grid, the format is:

```
x0 xSize xInc
y0 ySize yInc
z0 zSize zInc
val val val ....
```

where x0, y0, z0 (float) are the coordinates of the grid origin, xSize, ySize and zSize (int) are the sizes of the grid in each dimension, and xInc, yInc and zInc (float) the spacing between two grid points in each dimention. This must be followed by xSize * ySize * zSize values (float), where the x-coordinate is the one that is running the fastest.

The potentials will be set for all selected surfaces, but the PaintSurface command has to be given to update the colors.

EXAMPLE

ReadPot /home/joe/struct/my_pot.dat

SEE ALSO

CalcPot, AddSurface, SelectPrim, PaintSurface

DATE

960509

NAME
    ReadSeq - read sequence

SYNOPSIS
    ReadSeq fileName

DESCRIPTION
    Read a sequence. The file must contain the name of
    a residue on each line. All residues must appear in
    the residue library:

        $MOLMOLHOME/setup/amber94.lib

    The molecule will be in an extended conformation,
    with the standard geometry used for all residues.

EXAMPLE
    ReadSeq /home/joe/struct/my_prot.seq

SEE ALSO
    PathNames, ReadAng, ReadDg, ReadPdb, WriteSeq

DATE
    950704

NAME
ReadShift - read file with chemical shifts

SYNOPSIS
ReadShift fileName

DESCRIPTION
Read a file with chemical shifts. Both the old and new formats used by EASY/XEASY can be read.

The old format is:

```
columns  1- 4: proton number
columns  6-12: shift
columns 33-37: atom name
columns 38-42: residue number
```

The new format is:

```
columns  1- 4: proton number
columns  6-12: shift
columns 20-24: atom name
columns 25-28: residue number
```

The chemical shifts are added to all selected molecules.

The chemical shifts can be used in expressions, e. g. for selection. The program can also generate an expected NOESY peak list with the command CalcDist.

EXAMPLE
ReadShift /home/joe/struct/my_prot.prot

SEE ALSO
DialMol, SelectMol, CalcDist

DATE
950810

NAME

ReadSybyl - read SYBYL Mol2 file

SYNOPSIS

ReadSybyl fileName

DESCRIPTION

ReadSybyl reads a file in the Mol2 file format used by the program SYBYL by Tripos. The entries MOLECULE, ATOM, BOND, SUBSTRUCTURE and SET (STATIC) are interpreted, everything else is ignored. Special characters (like $) in set (i. e. property) names are not allowed by MOLMOL, they are replaced with underscores while reading.

When necessary, numbers are added to residue and atom names to make them unique.

EXAMPLE

ReadSybyl /home/sybyl/demo/vit_c.mol2

SEE ALSO

PathNames, ReadDg, ReadAng, ReadPdb

DATE

960312

NAME

ReadUpl - read file with upper limits

SYNOPSIS

ReadUpl fileName

DESCRIPTION

Read a file with upper distance limits. The format is the same that DIANA/DYANA uses. The distance constraints are added to all selected molecules.

This command supports groups.

EXAMPLE

```
ReadUpl /home/joe/struct/my_prot.upl
```

SEE ALSO

SelectMol, Group, ReadLol, AddUpl, CheckUpl

DATE

960317

NAME
    ReadXyz - read XYZ file

SYNOPSIS
    ReadXyz fileName

DESCRIPTION
    Read a file in XYZ format. Bonds are automatically
    added based on the atom radii in:

        $MOLMOLHOME/setup/AtomRadius

EXAMPLE
    ReadXyz /home/joe/struct/my_mol.xyz

SEE ALSO
    PathNames, ReadAng, ReadDg, ReadPdb, ReadSybyl
    CalcBond

DATE
    970314

NAME

RecordMac – open macro recorder

SYNOPSIS

RecordMac

DESCRIPTION

Open a macro recorder. The text area shows the macro recorded so far, it can also be edited manually. The ’Add’ button adds the most recently executed commands, the number of commands is given in the text field. If ’automatic’ is switched on, each executed command is recorded automatically.

The ’Test’ button executes the recorded macro, the ’Save’ button stores it with the given file name.

EXAMPLE

RecordMac

SEE ALSO

XMacUser

DATE

950626

NAME
     Register - register as MOLMOL user

SYNOPSIS
     Register string string string string [string]

DESCRIPTION
     Send an E-mail to register as MOLMOL user. The first argument gives your name, the second argument the name of the organisation (university/company) where you work, the third argument the S-mail address, the fourth argument the E-mail address. The fifth argument is the program name and release, just leave the value that is automatically filled in.

     Getting registered is strongly recommended, so that we can inform you of new releases and send you other useful information.

EXAMPLE
```
Register "Joe User" "Useless Univ."
    "Street 42, Nowhere, USA" "joe@useless.edu"
```

DATE
     960111

NAME
RemoveAco - remove angle constraints

SYNOPSIS
RemoveAco

DESCRIPTION
Remove angle constraint for all selected angles.

EXAMPLE
RemoveAco

SEE ALSO
ReadAco, AddAco, SelectAngle

DATE
950302

NAME

    RemoveAngle - remove angles

SYNOPSIS

    RemoveAngle

DESCRIPTION

    Remove all selected angles.

EXAMPLE

    RemoveAngle

SEE ALSO

    SelectAngle, AddAngle

DATE

    950131

NAME

    RemoveAtom - remove atoms

SYNOPSIS

    RemoveAtom

DESCRIPTION

    Remove all selected atoms.

EXAMPLE

    RemoveAtom

SEE ALSO

    SelectAtom, AddAtom, WriteLib

DATE

    950131

NAME

RemoveBond – remove bonds

SYNOPSIS

RemoveBond

DESCRIPTION

Remove all selected bonds.

EXAMPLE

RemoveBond

SEE ALSO

SelectBond, AddBond

DATE

940119

NAME
     RemoveDist – remove distances

SYNOPSIS
     RemoveDist

DESCRIPTION
     Remove all selected distances.

EXAMPLE
     RemoveDist

SEE ALSO
     SelectDist, AddDist, AddHbond, AddLol, AddUpl

DATE
     950221

NAME

RemoveMol - remove molecules

SYNOPSIS

RemoveMol

DESCRIPTION

Remove all selected molecules.

EXAMPLE

```
RemoveMol
```

SEE ALSO

SelectMol, DialMol, InitAll

DATE

931201

NAME
    RemovePrim - remove primitive

SYNOPSIS
    RemovePrim

DESCRIPTION
    Remove all selected primitives (circles, cylinders, texts, ribbons, etc.).

EXAMPLE
    RemovePrim

SEE ALSO
    AddCircles, AddCylinder, AddTitle, AddText, AddRibbon, SelectPrim

DATE
    950407

NAME

RemoveRes - remove residues

SYNOPSIS

RemoveRes

DESCRIPTION

Remove all selected residues. Only residues at start and end of a molecule can be deleted. A warning is issued if not all selected residues could be deleted due to this restriction.

EXAMPLE

RemoveRes

SEE ALSO

SelectRes, AddRes, ChangeRes

DATE

960616

NAME

Rendering - set rendering options

SYNOPSIS

```
Rendering ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
    ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
```

DESCRIPTION

Set some rendering options. Depending on the output device, some options may always be enabled, no matter whether they are switched on or off by this command. Some of these options (like two-sided lighting) are also used to generate plots, so the appropriate options have to be set before giving the plotting command.

The following options are supported:

Anti Aliasing: Draw smooth lines. This may not be supported on all hardware.

Transparency: Use transparent drawing for objects that are not completely opaque. This may not be supported on all hardware.

Fast Spheres Drawing: Instead of approximating spheres with many polygons, they are drawn as circles. This makes shading impossible, but can make the display much faster.

Backface Elimination: Eliminate polygons that face away from the viewpoint at an early display step. This has normally no visual effect on the display, but can make it faster.

Shading: Color polygons depending on the angle from the light source and the view point. This is also necessary for the support of depth cueing on most devices, e. g. for plotting.

Two-sided Lighting: Normally lighting calculations are only done for the "outside" of an object. This triggers lighting calculation to be done for both sides. The effect is visible if objects are cut, mostly by the front clipping plane. It is not switched on by default on most devices because it can make all rendering slower.

Depth Sorting: Sort all display elements by depth before drawing. This gives a quick, but sometimes unexact, method for hidden surface elimination.

Hidden Surface Elimination: Eliminate display elements that are hidden by other elements closer to the viewpoint. If the hardware supports this feature, it is enabled by default. If it has to be emulated by the program, the display can get very slow.

EXAMPLE

```
Rendering 0 0 0 1 1 0 1 0
```

SEE ALSO

PlotPar, PlotPs, PlotFm*, Fog

DATE

960305

NAME

ReplaceDg - replace with DG file
ReplaceListDg - replace with list of DG files

SYNOPSIS

ReplaceDg fileName
ReplaceListDg fileName

DESCRIPTION

ReplaceDg reads coordinates from a file in DG format, replacing the coordinates of the currently selected molecule. If no molecule is selected, a new molecule will be created. The structure in the file should be identical to the structure of the selected molecule, otherwise the result will not be very useful.

ReplaceListDg expects a file with one file name per line (empty lines allowed), and reads coordinates from all these files, replacing the coordinates of the selected molecules.

See ReadDg for more information about the DG format.

EXAMPLE

```
ReplaceDg /home/joe/struct/my_prot.cor
ReplaceListDg /home/joe/struct/my_prot.nam
```

SEE ALSO

ReadDg, ReadListDg

DATE

950626

NAME

ReplacePdb - replace with PDB file
ReplaceListPdb - replace with list of PDB files

SYNOPSIS

ReplacePdb fileName
ReplaceListPdb fileName

DESCRIPTION

ReplacePdb reads coordinates from a file in PDB format, replacing the coordinates of the currently selected molecules. If not enough molecules are selected, new molecules will be created. The structures in the file should be identical to the structures of the selected molecules, otherwise the result will not be very useful.

ReplaceListPdb expects a file with one file name per line (empty lines allowed), and reads coordinates from all these files, replacing the coordinates of the selected molecules.

See ReadPdb for more information about the PDB format.

EXAMPLE

```
ReplacePdb /home/joe/struct/my_prot.pdb
ReplaceListPdb /home/joe/struct/my_prot.nam
```

SEE ALSO

ReadPdb, ReadListPdb

DATE

950626

NAME

RotateAngle - rotate dihedral angles

SYNOPSIS

RotateAngle expr { expr }

DESCRIPTION

Rotate all selected dihedral angles. The first argument gives the number of angles that should rotate the chain backwards (i. e. towards the N-terminus in a protein). The user will normally not enter the value of the angles on the command line, but use the dialog box to interactively vary the angles.

If backwards rotation is desired, the first argument should be adjusted *before* any of the angles are modified, otherwise it will not have the desired effect.

EXAMPLE

```
RotateAngle 1 -57.0 -47.0
```

SEE ALSO

SelectAngle, SetAngle

DATE

951208

NAME
RotateInit - undo all rotations

SYNOPSIS
RotateInit

DESCRIPTION
Bring all movable (set with DialMol) molecules back to their original orientation.

EXAMPLE
RotateInit

SEE ALSO
DialMol, RotateX, RotateY, RotateZ

DATE
941206

NAME

RotateX - rotate molecule around X axis

SYNOPSIS

RotateX expr

DESCRIPTION

Rotate all movable (set with DialMol) molecules by the given angle around the X axis. The X axis runs from left to right of the screen. Rotation is normally done interactively by pressing the left mouse button. This command is useful for being used in macros or for setting up the slider box.

EXAMPLE

```
RotateX 90
```

SEE ALSO

DialMol, RotateY, RotateZ

DATE

931201

NAME

RotateY – rotate molecule around Y axis

SYNOPSIS

RotateY expr

DESCRIPTION

Rotate all movable (set with DialMol) molecules by the given angle around the Y axis. The Y axis runs from bottom to top of the screen. Rotation is normally done interactively by pressing the left mouse button. This command is useful for being used in macros or for setting up the slider box.

EXAMPLE

```
RotateY 90
```

SEE ALSO

DialMol, RotateX, RotateZ

DATE

931201

NAME

RotateZ - rotate molecule around Z axis

SYNOPSIS

RotateZ expr

DESCRIPTION

Rotate all movable (set with DialMol) molecules by the given angle around the Z axis. The Z axis points out of the screen. Rotation is normally done interactively by pressing the left mouse button. This command is useful for being used in macros or for setting up the slider box.

EXAMPLE

```
RotateZ 90
```

SEE ALSO

DialMol, RotateX, RotateY

DATE

931201

NAME

```
SelectMol   - select molecules
SelectRes   - select residues
SelectAtom  - select atoms
SelectBond  - select bonds
SelectAngle - select angles
SelectDist  - select distances
SelectPrim  - select primitives
```

SYNOPSIS

```
SelectMol expr
SelectRes expr
SelectAtom expr
SelectBond expr
SelectAngle expr
SelectDist expr
SelectPrim expr
```

DESCRIPTION

Select molecules, residues, atoms, bonds, angles, distances or primitives that satisfy a conditions specified by an expression. The expression must give a result of type boolean (truth value).

There are two special values not covered by the expression syntax below. If an empty string is given as expression, everything is selected. If the value "0" is given, nothing is selected (i. e. everything deselected).

The following is a formal sytax description of expressions in EBNF notation. Typical examples are shown in the next section.

```
expr       = andExpr { "|" andExpr } .
andExpr    = relExpr { "&" relExpr } .
relExpr    = simpleExpr [ relOp setExpr ] .
relOp      = "=" | "!=" | "<=" |
             "<" | ">=" | ">" .
setExpr    = rangeExpr { "," rangeExpr } .
rangeExpr  = simpeExpr [ ".." simpleExpr ] .
simpleExpr = term { addOp term } .
addOp      = "+" | "-" .
term       = factor { mulOp factor } .
mulOp      = "*" | "/" | "%" .
factor     = [ "-" | "sqrt" | "log" | "!" ] primary .
primary    = constant | designator | "(" expr ")" .
constant   = string | int | float .
designator = [ qual "." ] field [ "[" int "]" ] .
qual       = "mol" | "mol1" | "mol2" |
             "res" | "res1" | "res2" | "atom" |
             "atom1" | "atom2" | "atom3" | "atom4" |
             "bond" | "angle" | "dist" | "prim" .
field      = "num" | "number" | "name" | "attr" |
             "shift" | "bfactor" | "vdw" | "d" |
             "charge" | "heavycharge" |
```

```
                 "avgcharge" | "simplecharge" |
                 "val" | "limit" | "viol" |
                 "upl" | "lol" | "hbond" |
                 propertyName .
```

For simple selections, there is a shorter notation of the form:

```
  expr       = exprPart { exprPart } .
  exprPart   = [ "#" molSet ] [ ":" resSet ]
               [ "@" atomSet ] .
  molSet     = molSel { "," molSel } .
  molSel     = string | range .
  resSet     = resSel { "," resSel } .
  resSel     = string | range .
  atomSet    = string { "," string ) .
  range      = int ".." int | int "-" int .
```

Strings are not quoted in this notation.

The full and the short notation can be mixed, in this case a part written in the short notation behaves like a primary with a boolean value.

EXAMPLES

```
SelectAtom 'name = "C*"'
    # C atoms
SelectAtom 'name = "CA" & res.num < 10 &
    bfactor > 2.0'
    # CA atoms in residues with number less than 10
    # and with B factor larger than 2
SelectAtom 'res.num = 10 & name = "CA"'
SetRef
SelectAtom 'd < 5.0'
    # atoms with distance less than 5.0 from CA
    # of residue 10
SelectBond 'atom1.name = "CA" & atom2.name = "CB"'
    # bonds from CA to CB
SelectAngle 'name = "OMEGA" & (val < 170 | val > 190)'
    # omega angles outside the range from 170 to 190
SelectDist 'res1.num = 7 | res2.num = 7'
    # distances involving residue 7
DefPropDist 'hnd' 'atom1.name = "HN" |
    atom2.name = "HN"'
    # define property 'hnd' as all distances that
    # have a HN atom on one side
SelectDist 'hnd & viol > 1.5'
    # constraints from HN atoms that have a violation
    # of more than 1.5
SelectDist '! hnd & viol > 2.0'
    # constraints that do not have a HN atom on either
    # side and that have a violation of more than 2.0
SelectPrim 'mol.num = 2'
    # primitives belonging to molecule number 2
DefPropRes 'helix' 'mol.name = "bpti*" &
    res.num = 47..56'
    # define helix region of all molecules that have a
```

```
        # name starting with "bpti"
    SelectAtom 'name = "CA" & res.helixres'
        # CA atoms in helix region

    SelectAtom '#1-5:10-20,25-30@N,CA,C'
        # N, CA and C atoms of residues 10 to 20 and 25 to 30
        # in molecules 1 to 5
    SelectAtom ':7@HN :12@HA'
        # HN of residue 7 and HA of residue 12
```

SEE ALSO

DialSelect, DefProp*, DialMol, SetRef

DATE

950525

NAME
    SetAngle - rotate dihedral angles

SYNOPSIS
    SetAngle expr

DESCRIPTION
    Set all selected dihedral angles to the given value.
    This command can be used to construct regular
    secondary structures.

EXAMPLE
    SetAngle -57.0

SEE ALSO
    SelectAngle, RotateAngle

DATE
    940119

NAME

SetNeigh - set sheet neighbours of residues

SYNOPSIS

SetNeigh expr expr expr expr

DESCRIPTION

Set the information about neighbouring residues used for schematic display of beta sheets. The arguments are applied to all selected molecules.

The first and second argument give the numbers of the start and end residues in the first strand, where the start number must be smaller than the end number. The third and fourth argument give the start and end numbers of residues in the second strand. For a parallel pair of strands, the start number must be smaller than the end number, for an antiparallel pair it must be larger. Both strands must have the same number of residues and must not overlap.

This command is only used if the secondary structure information was not read from a PDB file or calculated with CalcSecondary, or if the user wants to modify this information.

EXAMPLE

```
SetNeigh 18 24 35 29
```

SEE ALSO

ReadPdb, CalcSecondary, WriteSecondary, AddRibbon, TypeRibbon

DATE

950523

NAME
SetRef - set reference atoms

SYNOPSIS
SetRef

DESCRIPTION
Use the currently selected atoms as reference atoms. The reference atoms are used for selecting atoms by distance.

EXAMPLE
```
SetRef
```

SEE ALSO
SelectAtom

DATE
950525

NAME

SetUndo - set the number of possible undos

SYNOPSIS

SetUndo expr

DESCRIPTION

Set the number of possible undos. Each level can use a significant amount of memory, so setting the number too high is not recommended if the available memory is tight. There is also a certain overhead for each command as soon as the level is greater than zero, especially if many structures are loaded. So if the program seems to get too slow, try setting the value to zero.

EXAMPLE

```
SetUndo 3
```

SEE ALSO

Undo

DATE

950624

NAME

ShadeAtom - set shading of atoms

SYNOPSIS

```
ShadeAtom ( none | flat | gouraud | phong |
    dots | lines )
```

DESCRIPTION

Set the shading method for atoms if they are displayed as spheres.

```
none:    no shading
flat:    polygons shaded in uniform color
gouraud: color interpolated between vertices
phong:   normals interpolated, highest quality
dots:    draw surface using dots
lines:   draw surface using lines
```

Not all graphics devices support all shading methods.

EXAMPLE

```
ShadeAtom phong
```

SEE ALSO

SelectAtom, StyleAtom, ColorAtom

DATE

950309

NAME

ShadeBond - set shading of bonds

SYNOPSIS

```
ShadeBond ( none | flat | gouraud | phong |
    dots | lines )
```

DESCRIPTION

Set the shading method for bonds if they are displayed as cylinders.

```
none:    no shading
flat:    polygons shaded in uniform color
gouraud: color interpolated between vertices
phong:   normals interpolated, highest quality
dots:    draw surface using dots
lines:   draw surface using lines
```

Not all graphics devices support all shading methods.

EXAMPLE

```
ShadeBond phong
```

SEE ALSO

SelectBond, StyleBond, ColorBond

DATE

950309

NAME

ShadeDist - set shading of distances

SYNOPSIS

```
ShadeDist ( none | flat | gouraud | phong |
    dots | lines )
```

DESCRIPTION

Set the shading method for distances if they are displayed as cylinders.

```
none:    no shading
flat:    polygons shaded in uniform color
gouraud: color interpolated between vertices
phong:   normals interpolated, highest quality
dots:    draw surface using dots
lines:   draw surface using lines
```

Not all graphics devices support all shading methods.

EXAMPLE

```
ShadeDist phong
```

SEE ALSO

SelectDist, StyleDist, ColorDist

DATE

950309

NAME

ShadePrim - set shading of primitives

SYNOPSIS

```
ShadePrim ( none | flat | gouraud | phong |
    dots | lines )
```

DESCRIPTION

Set the shading method for primitives.

```
none:    no shading
flat:    polygons shaded in uniform color
gouraud: color interpolated between vertices
phong:   normals interpolated, highest quality
dots:    draw surface using dots
lines:   draw surface using lines
```

Not all graphics devices support all shading methods.

EXAMPLE

```
ShadePrim phong
```

SEE ALSO

SelectPrim, StyleDrawobj, StyleTrajec, ColorPrim

DATE

950309

NAME

SizePlate - set sizes of plates

SYNOPSIS

SizePlate expr

DESCRIPTION

Set the thickness of all selected plates to the given value. Entering 0 or a negative value will leave the size unchanged.

EXAMPLES

SizePlate 0.6

SEE ALSO

AddPlates, SelectPrim, ColorPrim

DATE

950426

NAME

SizeRibbon - set sizes of ribbons

SYNOPSIS

SizeRibbon expr [expr [expr [expr [expr]]]]

DESCRIPTION

Set the size of all selected ribbons. The first argument gives the width, the second argument the thickness, the third the length of the start part, the fourth the length of the end part and the fifth the width of the arrow as multiple of the ribbon width. Start/end length and arrow width only have an effect if the style is set accordingly (soft, arrow).

Entering 0 for any of the sizes will leave this value unchanged. This is useful when one wants to change part of the values for multiple ribbons at once.

EXAMPLES

```
SizeRibbon 3.0 0.5
SizeRibbon 2.5 0.4 2.0 2.0 1.4
```

SEE ALSO

AddRibbon, SelectPrim, LengthPrim,
TypeRibbon, StyleRibbon, PaintRibbon

DATE

950407

NAME
    SizeText - resize text

SYNOPSIS
    SizeText (abs | rel) expr

DESCRIPTION
    Resize all selected text primitives. If the first argument is 'abs', all sizes are set to the given value. If it is 'rel', the given value is added to the current size.

    Resizing texts is normally done interactively by using the middle mouse button.

EXAMPLE
```
SizeText abs 0.15
```

SEE ALSO
    MovePrim

DATE
    950407

NAME

SplitRibbon - split ribbons

SYNOPSIS

SplitRibbon

DESCRIPTION

Split all selected ribbons into two pieces of equal length. The length of the pieces can later be adjusted with LengthPrim.

To get rid of a ribbon, use the RemovePrim command.

EXAMPLE

SplitRibbon

SEE ALSO

SelectPrim, LengthPrim, RemovePrim

DATE

950523

NAME

StartAnim - start animation

SYNOPSIS

StartAnim (once | cycle) expr

DESCRIPTION

Start an animation. This can be used for displaying MD runs. If the first argument is 'once', every selected structure will be displayed once.

If it is 'cycle', the program will loop through all selected structures until the StopAnim command is executed.

The second argument is the minimal delay in milliseconds between displaying structures.

It is possible to execute the command while an animation is running, e. g. for changing the delay.

EXAMPLE

StartAnim cycle 50

SEE ALSO

SelectMol, DialMol, StopAnim

DATE

940216

NAME

StartRock - start rock

SYNOPSIS

```
StartRock ( once | cycle ) expr
    expr expr expr expr expr expr expr expr
```

DESCRIPTION

Start to rotate all movable (set with DialMol) molecules automatically. There are parameters for two phases, so that it is possible to rotate back and forth.

If the first argument is 'once', the movement will only happen once. If it is 'cycle', the program will repeat it until the StopRock command is executed.

The second argument is the minimal delay in milliseconds between rotations. The rest of the arguments are rotation angles for all three axis and number of steps.

It is possible to execute the command while rocking is running, e. g. for changing the delay.

EXAMPLE

```
StartRock cycle 50 0 10 0 18 0 -10 0 18
```

SEE ALSO

DialMol, StopRock

DATE

940331

NAME

Stereo - set stereo mode

SYNOPSIS

```
Stereo ( off | left | right | side_by_side |
    cross_eye | hardware )
```

DESCRIPTION

Set stereo mode. Hardware stereo is not supported by all hardware. If it is supported, it normally works only in fullscreen mode (see command Fullscreen).

Hardware stereo is also supported for certain plot devices. E. g. generating a PostScript plot in hardware stereo mode will produce a side by side stereo image with the correct eye distance, while the distance between the images will very likely be wrong when plotting in side_by_side mode.

EXAMPLE

```
Stereo side_by_side
```

SEE ALSO

Fullscreen

DATE

941205

NAME
    StopAnim - stop animation

SYNOPSIS
    StopAnim

DESCRIPTION
    Stop an animation started with StartAnim.

EXAMPLE
    StopAnim

SEE ALSO
    StartAnim

DATE
    940216

NAME

StopRock - stop rock

SYNOPSIS

StopRock

DESCRIPTION

Stop automatic rotation started with StartRock.

EXAMPLE

StopRock

SEE ALSO

StartRock

DATE

940331

NAME

StyleAtom – set display style of atoms

SYNOPSIS

StyleAtom (invisible | sphere | tetrahedron)

DESCRIPTION

Set the display style of all selected atoms.

EXAMPLE

StyleAtom sphere

SEE ALSO

SelectAtom

DATE

940119

NAME

StyleBond - set display style of bonds

SYNOPSIS

```
StyleBond ( invisible | line | half_line |
    cylinder | half_cylinder | neon | half_neon |
    cone | half_cone )
```

DESCRIPTION

Set the display style of all selected bonds. The style 'cylinder' draws the bond as an open cylinder, 'neon' draws it as cylinder with round ends, 'cone' as cone, taking the radii of the connected atoms.

The styles 'half_line', 'half_cylinder', 'half_neon' and 'half_cone' draw the bonds in two parts, taking the colors of the connected atoms.

EXAMPLE

```
StyleBond cylinder
```

SEE ALSO

SelectBond, DialStyle

DATE

960606

NAME

StyleCylinder - set display style of cylinders

SYNOPSIS

StyleCylinder (invisible | normal | arrow)

DESCRIPTION

Set the display style of all selected cylinders.

EXAMPLE

StyleCylinder arrow

SEE ALSO

SelectPrim, AddCylinder, AddDipole, ColorPrim

DATE

970722

NAME

StyleDist - set display style of distances

SYNOPSIS

StyleDist (invisible | line | viol | cylinder | neon | cone)

DESCRIPTION

Set the display style of all selected distances. 'viol' is only meaningful for distance constraints, it will display the constraint in two colors showing both limit and actual distance.

EXAMPLE

```
StyleDist invisible
```

SEE ALSO

SelectDist, DialStyle, ColorDist, TintDist

DATE

960606

NAME

StyleDrawobj – set display style of draw objects

SYNOPSIS

StyleDrawobj (invisible | line | cylinder | neon)

DESCRIPTION

Set the display style of all selected draw objects (lines etc.). The style 'cylinder' draws the object as a cylinder with flat ends, 'neon' draws it as cylinder with round ends. Not all display styles are supported for all draw objects types.

EXAMPLE

```
StyleDrawobj cylinder
```

SEE ALSO

SelectPrim, AddDrawobj, ColorPrim

DATE

950713

NAME

StyleRibbon - set display style of ribbons

SYNOPSIS

```
StyleRibbon ( invisible | rect | round |
    rounded | ellip | lense | as_is )
    [ ( open | sharp | soft | as_is )
    [ ( open | sharp | soft | arrow | as_is )
    [ ( const | atom | as_is ) ] ] ]
```

DESCRIPTION

Set the display style of all selected ribbons. The first argument gives the profile of the middle part, the optional second and third argument determine the style of the start and the end.

The fourth argument only has an effect when the profile is 'round'. With the value 'atom', the radius is interpolated between the radii of the atoms used to define the spline, normally the CA atom for proteins. This can e. g. be used to show mobility by varying radius of the spline if the radius of the atoms is set to (a function of) the B-factor. For bundles of NMR structures, the B-factors can be calculated by MeanMol.

For all arguments, the value 'as_is' will leave the style unchanged, this is useful when one wants to change part of the values for multiple ribbons at once.

EXAMPLES

```
StyleRibbon rect
StyleRibbon rounded sharp arrow
StyleRibbon round open open atom
```

SEE ALSO

AddRibbon, SelectPrim, LengthPrim,
TypeRibbon, SizeRibbon, PaintRibbon,
MeanMol, RadiusAtom

DATE

950509

NAME

StyleTrajec – set display style of trajectories

SYNOPSIS

StyleTrajec (invisible | line | neon | ellipsoid)

DESCRIPTION

Set the display style of all selected trajectories. The style 'neon' draws the trajectory using cylinders with round ends. The style 'ellipsoid' draws an ellipsoid for the principal axes of the atoms that define the trajectory.

EXAMPLE

```
StyleTrajec neon
```

SEE ALSO

SelectPrim, AddTrajec, ColorPrim

DATE

980324

NAME

System – execute operating system command

SYNOPSIS

System string

DESCRIPTION

Pass the command given as argument for execution by the operating system. Since MOLMOL is currently only running on UNIX, this will generally be a UNIX command.

EXAMPLE

```
System 'lp tt.ps'
```

DATE

960418

NAME

TextureAtom - set texture of atoms
TextureBond - set texture of bonds
TextureDist - set texture of distances
TexturePrim - set texture of primitives

SYNOPSIS

TextureAtom string expr expr expr
TextureBond string expr expr expr
TextureDist string expr expr expr
TexturePrim string expr expr expr

DESCRIPTION

Set the texture mapping parameters of all selected atoms, bonds, distances or primitives. The first parameter gives the name of a texture, the second paramter its scaling factor.

The third parameter determines the amount of bumpiness of the surface. 0.0 results in a smooth surface, 1.0 in a very bumpy surface. The fourth paramter is a scaling factor for the bump pattern, a larger scaling factor will result in wider bumps.

Texture mapping is not supported on screen, these parameters are used for preparing files for ray-tracing (PlotPOV).

The texture name must appear in the texture definition file of POV-Ray (textures.inc). If a texture is selected, the attributes of this texture will override the colors and material properties selected otherwise. If the name has the extension ".gif", it is assumed to be the name of a GIF file which is used as image map.

Giving a value of 'as is' for the texture name or less than 0.0 for any numerical argument will not change it, this is useful for changing only part of the parameters.

EXAMPLES

```
TextureAtom 'Blood_Marble' 0.5 0.0 1.0
TextureBond '' 1.0 0.5 1.0
```

SEE ALSO

Select*, Color*, Material*, PlotPov

DATE

950606

NAME

TintDist - set secondary color of distances

SYNOPSIS

TintDist expr expr expr

DESCRIPTION

Set the secondary color of all selected distances. The color is given by its Red, Green and Blue component, all in the range between 0.0 and 1.0.

The secondary color is used to show the size of the violation for distance constraints if this display style is selected with StyleDist.

EXAMPLE

```
TintDist 1.0 0.0 0.0
```

SEE ALSO

SelectDist, StyleDist, ColorDist, DialColor

DATE

950407

NAME

TintPrim - change secondary color of primitives

SYNOPSIS

TintPrim expr expr expr

DESCRIPTION

Set the secondary color of the selected primitives. The color is given by its Red, Green and Blue components, all in the range between 0.0 and 1.0.

The secondary color is used for drawing ribbons in two colors and for one side of sheets.

EXAMPLE

```
TintPrim 1.0 0.0 0.0
```

SEE ALSO

SelectPrim, ColorPrim, PaintRibbon, DialColor, AddRibbon, AddSheet

DATE

950411

NAME

TrimSurface - cut away part of a surface

SYNOPSIS

TrimSurface expr

DESCRIPTION

Cut away part of all selected surfaces. The part that is trimmed off is given by the selected atoms, all surface parts that have a distance smaller than the value given as argument from a selected atom are cut away. The distance from an atom takes the VdW radius into account, the argument is an additional offset.

EXAMPLE

```
TrimSurface 1.0
```

SEE ALSO

SelectPrim, AddSurface, NearPrim

DATE

970718

NAME

TypeRibbon - set type of ribbons

SYNOPSIS

```
TypeRibbon ( interpol | smooth | as_is )
    ( free | cylinder | spacing | neighbour | as_is )
```

DESCRIPTION

Set the type of all selected ribbons. The first argument determines whether the ribbon goes through the atoms used for AddRibbon, or whether it is smoothed. The second argument determines how the ribbon is oriented.

Typically interpol/cylinder or interpol/spacing is used for helices, smooth/neighbour for sheets and smooth/free for turns and random coil.

'cylinder' does a least square fit of a cylinder surface to the atoms, 'spacing' fits a cylinder so that the spacing of atoms along the axis is as regular as possible. The results are very similar in most cases, but 'spacing' often looks better for very short helices or DNA.

The information about which residue is the neighbour of which other residue is read from the secondary structure information in PDB files or calculated by the CalcSecondary command. It can also be set with the SetNeigh command.

For both arguments, the value 'as_is' will leave the value unchanged, this is useful when one wants to change one of the values for multiple ribbons at once.

EXAMPLE

```
TypeRibbon smooth neighbour
```

SEE ALSO

ReadPdb, CalcSecondary, SetNeigh,
AddRibbon, SelectPrim, LengthPrim,
StyleRibbon, SizeRibbon, PaintRibbon

DATE

950307

NAME

UndefProp - undefine property

SYNOPSIS

UndefProp propertyName

DESCRIPTION

Undefine the property with the given name everywhere. This command is rarely used. The program cannot detect if a property is not used anymore. Executing this command with unused properties can help to avoid problems (like unnecessarily large dump files or overflow of internal tables), especially when a lot of different properties are used.

The number of different properties supported by the program is currently set to 2048.

EXAMPLES

```
UndefProp bb
```

SEE ALSO

DefProp*

DATE

940408

NAME

Undo - undo effect of last command

SYNOPSIS

Undo

DESCRIPTION

Undo the effect of the last executed command. Multiple undo is possible by entering the Undo command multiple times. The number of possible undos is set with the SetUndo command.

EXAMPLE

Undo

SEE ALSO

SetUndo, WriteDump

DATE

950624

NAME

UserInterface - switch elements of user interface

SYNOPSIS

```
UserInterface ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
    ( 0 | 1 ) ( 0 | 1 ) ( 0 | 1 )
```

DESCRIPTION

Switch various parts of the user interface on or off. The following elements can be switched:

Valuator Box
Log Window
Buttons
Command Line
Status Line
Menubar

The program makes sure that Command Line and Menubar are not switched off at the same time, because this would make it impossible to enter any more commands.

EXAMPLE

```
UserInterface 0 0 1 1 1 1
```

DATE

940818

NAME

ViewAngle - set view angle

SYNOPSIS

ViewAngle expr

DESCRIPTION

Set the view angle. For orthogonal projection, this influences only the size (zooming factor) of the display, for perspective projection, a larger view angle leads to a stronger perspective. The value is given in radians.

EXAMPLE

```
ViewAngle 0.5
```

SEE ALSO

Projection, ClipPos, ClipSize

DATE

931201

NAME

WriteAng - write DIANA dihedral angle file

SYNOPSIS

WriteAng fileName

DESCRIPTION

Write a dihedral angle file like it is generated by DIANA or DYANA. All selected molecules are written to the file.

EXAMPLE

```
WriteAng /home/joe/struct/my_prot.ang
```

SEE ALSO

DialMol, WriteDg, WritePdb, ReadAng

DATE

931203

NAME

WriteDg – write DG file

SYNOPSIS

WriteDg fileName

DESCRIPTION

Write a file in DG format. All selected molecules are written to the file.

EXAMPLE

```
WriteDg /home/joe/struct/my_prot.cor
```

SEE ALSO

DialMol, WriteAng, WritePdb, ReadDg

DATE

951116

NAME

WriteDump - write dump file

SYNOPSIS

WriteDump fileName

DESCRIPTION

Write a dump file. A dump file is a binary file that contains the complete program state. A dump file with the name molmol/dump in the users home directory is created whenever the user leaves the program. A dump file with an arbitrary name can be created anytime by using this command.

EXAMPLE

```
WriteDump /home/joe/struct/my_prot.mol
```

SEE ALSO

ReadDump

DATE

950704

NAME

WriteLib - write entries for residue library

SYNOPSIS

WriteLib fileName

DESCRIPTION

For all selected residues that were not in the residue library or that were modified by commands like AddAtom and AddBond, write an entry for the residue library into the given file.

For working with non-standard residues, the best strategy is:

1. Read a structure that contains the residue.
2. Define bonds with the commands CalcBond, AddBond and RemoveBond, use AddAtom, RemoveAtom and AddPseudo if necessary.
3. Define angles with AddAngle.
4. WriteLib xxx.lib.
5. Edit xxx.lib if necessary (e. g. the atom types).
6. Make a copy of the standard library ($MOLMOLHOME/setup/amber94.lib) and append xxx.lib.
7. InitAll.
8. Use PathNames to set name of new library.
9. Check the library by executing the command ReadLib.
10. Read structure.

EXAMPLE

WriteLib /home/joe/my_res.lib

SEE ALSO

AddAtom, AddPseudo, RemoveAtom, CalcBond, CheckBond, AddBond, RemoveBond, AddAngle, RemoveAngle, InitAll, PathNames, ReadLib

DATE

980303

NAME

WriteLol - write file with lower limits

SYNOPSIS

WriteLol fileName

DESCRIPTION

Write a file with lower distance limits. The format is the same that DIANA/DYANA uses. All selected lower distance limits are written. When a constraint between two atoms appears in more than one molecule, the largest constraint value is written.

This command supports groups.

EXAMPLE

```
WriteLol /home/joe/struct/my_prot.lol
```

SEE ALSO

SelectMol, Group, ReadLol, AddLol, CheckLol, WriteUpl

DATE

980326

NAME

WritePdb - write PDB file

SYNOPSIS

WritePdb fileName

DESCRIPTION

Write a PDB file. All selected molecules are written to the file.

See the help page of ReadPdb for an explanation of the handling of atom names.

EXAMPLE

WritePdb /home/joe/struct/my_prot.pdb

SEE ALSO

DialMol, PathNames, WriteAng, WriteDg, ReadPdb

DATE

940408

NAME

WriteRotation – write current rotation

SYNOPSIS

WriteRotation fileName

DESCRIPTION

Write the current rotation of the first selected molecule to a macro file. Executing this macro with XMacUser will restore the orientation. At least one molecule must be selected.

EXAMPLE

```
WriteRotation /home/joe/macros/rotate.mac
```

SEE ALSO

XMacUser, RotateInit, RotateX, RotateY, RotateZ

DATE

941206

NAME

WriteSecondary - write macro with secondary structure

SYNOPSIS

WriteSecondary

DESCRIPTION

Show a macro that describes the current definiton of secondary structure for all selected residues. Exactly one molecule must be selected. This macro can be edited and saved to a given file name. The macro can be executed with XMacUser to set the same (modified) secondary structure again.

The secondary structure can be read from a PDB file, calculated with CalcSecondary, or set manually with a set of DefPropRes and SetNeigh commands. The most convenient way is often to use CalcSecondary to get an intial definition, then use WriteSecondary to create a macro, edit it to the "correct" definitions, and then use XMacUser to set these.

EXAMPLE

WriteSecondary

SEE ALSO

ReadPdb, CalcSecondary, XMacUser, AddRibbon

DATE

951010

NAME

WriteSeq - write sequence

SYNOPSIS

WriteSeq fileName

DESCRIPTION

Write the sequence of the selected molecule to a file, the name of each residue on a line. Exactly one molecule must be selected.

EXAMPLE

```
WriteSeq /home/joe/struct/my_prot.seq
```

SEE ALSO

WriteAng, WriteDg, WritePdb, ReadSeq

DATE

941206

NAME

WriteUpl - write file with upper limits

SYNOPSIS

WriteUpl fileName

DESCRIPTION

Write a file with upper distance limits. The format is the same that DIANA/DYANA uses. All selected upper distance limits are written. When a constraint between two atoms appears in more than one molecule, the smallest constraint value is written. All selected distances are also written, for these the actual distance is taken as constraint value.

This command supports groups.

EXAMPLE

```
WriteUpl /home/joe/struct/my_prot.upl
```

SEE ALSO

SelectMol, Group, ReadUpl, AddUpl, CheckUpl, WriteLol

DATE

980326

NAME
    XMacStand - execute standard macro
    XMacUser - execute user macro

SYNOPSIS
    XMacStand fileName
    XMacUser fileName

DESCRIPTION
    Execute a macro file. A macro file is a sequence of commands like they are entered on the command line. A history of all executed commands of each session is maintained in the file molmol/history in the users home directory. It can be used as macro.

    The two commands only differ in their search path. XMacStand by default searches in $MOLMOLHOME/macros, while XMacUser uses the current directory as default search path.

    Additonally to regular commands, macros can also contain command definitons. Once a macro with a command definiton is read in, this command can be used like a builtin MOLMOL command. A command definition has the syntax:

```
define CommandName
help one-line-help
$arg1 = default1 prompt1
..
$argN = defaultN promptN
Command1
..
CommandN
end
```

    The help line is optional. The command can have any number of arguments (including zero). If no default value is given, the empty string is assumed the first time the command is executed, the previous value from there on. If the prompt is missing, the name of the argument is taken. If default values or prompts contain blanks or other special characters, they have to be written in single or double quotes.

    At least one command must be present in the body. Empty lines and comments (staring with #) are allowed, the lines can be indented for better readability.

    In the body, the arguments can be referenced by $arg or ${arg}. Any command can be used.

    Example:

```
define ZoomRotate
  help zoom and rotate in one step
```

```
          $Zoom = 1.5
          $rotY = 90 "Rotate Y"

          ZoomRel $Zoom
          RotateY $rotY
        end
```

EXAMPLE

```
XMacUser /home/joe/macros/my_favorite.mac
```

DATE

960208

NAME

ZoomAbs – zoom absolute
ZoomRel – zoom relative

SYNOPSIS

ZoomAbs expr
ZoomRel expr

DESCRIPTION

Enlarge/reduce the size of the display. ZoomRel changes the size by a given factor, relative to the current size. Factors greater than 1 make the display larger, factors less than 1 make it smaller. ZoomAbs sets the zoom factor to an absolute value.

ZoomAbs, in conjunction with PlotPar, can be used to produce different plots with the same scale. If the zoom factor and the plot size are set to the same values, the scales will be identical.

Zooming is normally done interactively by pressing the left and the middle mouse button.

EXAMPLES

```
ZoomAbs 0.2
ZoomRel 1.4
```

SEE ALSO

PlotPar

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