**Command Reference**

RasMol allows the execution of interactive commands typed at the '**RasMol>**' prompt in the terminal window. Each command must be given on a separate line. Keywords are case insensitive and may be entered in either upper or lower case letters. All whitespace characters are ignored except to separate keywords and their arguments.

The commands/keywords currently recognised by RasMol are given below.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| [Backbone](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22backbone)  | [Background](http://www.openrasmol.org/doc/rasmol.html#background)  | [Bond](http://www.openrasmol.org/doc/rasmol.html#bond)  | [Cartoon](http://www.openrasmol.org/doc/rasmol.html#cartoon)  | [Centre](http://www.openrasmol.org/doc/rasmol.html#centre)  | [Clipboard](http://www.openrasmol.org/doc/rasmol.html#clipboard)  | [Colour](http://www.openrasmol.org/doc/rasmol.html#colour)  | [Connect](http://www.openrasmol.org/doc/rasmol.html#connect)  |
| [CPK](http://www.openrasmol.org/doc/rasmol.html#spacefill)  | [CPKnew](http://www.openrasmol.org/doc/rasmol.html#cpknew)  | [Define](http://www.openrasmol.org/doc/rasmol.html#define)  | [Depth](http://www.openrasmol.org/doc/rasmol.html#depth)  | [Dots](http://www.openrasmol.org/doc/rasmol.html#dots)  | [Echo](http://www.openrasmol.org/doc/rasmol.html#echo)  | [English](http://www.openrasmol.org/doc/rasmol.html#english)  | [Exit](http://www.openrasmol.org/doc/rasmol.html#quit)  |
| [French](http://www.openrasmol.org/doc/rasmol.html#french)  | [HBonds](http://www.openrasmol.org/doc/rasmol.html#hbonds)  | [Help](http://www.openrasmol.org/doc/rasmol.html#help)  | [Italian](http://www.openrasmol.org/doc/rasmol.html#italian)  | [Label](http://www.openrasmol.org/doc/rasmol.html#label)  | [Load](http://www.openrasmol.org/doc/rasmol.html#load)  | [Molecule](http://www.openrasmol.org/doc/rasmol.html#molecule)  | [Monitor](http://www.openrasmol.org/doc/rasmol.html#monitor)  |
| [Pause](http://www.openrasmol.org/doc/rasmol.html#pause)  | [Print](http://www.openrasmol.org/doc/rasmol.html#print)  | [Quit](http://www.openrasmol.org/doc/rasmol.html#quit)  | [Refresh](http://www.openrasmol.org/doc/rasmol.html#refresh)  | [Renumber](http://www.openrasmol.org/doc/rasmol.html#renumber)  | [Reset](http://www.openrasmol.org/doc/rasmol.html#reset)  | [Restrict](http://www.openrasmol.org/doc/rasmol.html#restrict)  | [Ribbons](http://www.openrasmol.org/doc/rasmol.html#ribbons)  |
| [Rotate](http://www.openrasmol.org/doc/rasmol.html#rotate)  | [Save](http://www.openrasmol.org/doc/rasmol.html#save)  | [Script](http://www.openrasmol.org/doc/rasmol.html#script)  | [Select](http://www.openrasmol.org/doc/rasmol.html#select)  | [Set](http://www.openrasmol.org/doc/rasmol.html#set)  | [Show](http://www.openrasmol.org/doc/rasmol.html#show)  | [Slab](http://www.openrasmol.org/doc/rasmol.html#slab)  | [Source](http://www.openrasmol.org/doc/rasmol.html#script)  |
| [Spacefill](http://www.openrasmol.org/doc/rasmol.html#spacefill)  | [Spanish](http://www.openrasmol.org/doc/rasmol.html#spanish)  | [SSBonds](http://www.openrasmol.org/doc/rasmol.html#ssbonds)  | [Star](http://www.openrasmol.org/doc/rasmol.html#star)  | [Stereo](http://www.openrasmol.org/doc/rasmol.html#stereo)  | [Strands](http://www.openrasmol.org/doc/rasmol.html#strands)  | [Structure](http://www.openrasmol.org/doc/rasmol.html#structure)  | [Surface](http://www.openrasmol.org/doc/rasmol.html#surface)  |
| [Trace](http://www.openrasmol.org/doc/rasmol.html#trace)  | [Translate](http://www.openrasmol.org/doc/rasmol.html#translate)  | [UnBond](http://www.openrasmol.org/doc/rasmol.html#unbond)  | [Wireframe](http://www.openrasmol.org/doc/rasmol.html#wireframe)  | [Write](http://www.openrasmol.org/doc/rasmol.html#write)  | [Zap](http://www.openrasmol.org/doc/rasmol.html#zap)  | [Zoom](http://www.openrasmol.org/doc/rasmol.html#zoom)  |  |

**Backbone**

Syntax: backbone {<boolean>}

 backbone <value>

 backbone dash

The RasMol '**backbone**' command permits the representation of a polypeptide backbone as a series of bonds connecting the adjacent alpha carbons of each amino acid in a chain. The display of these backbone 'bonds' is turned on and off by the command parameter in the same way as with the '**[wireframe](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22wireframe)**' command. The command '**backbone off**' turns off the selected 'bonds', and '**backbone on**' or with a number turns them on. The number can be used to specify the cylinder radius of the representation in either Ångstrom or RasMol units. A parameter value of 500 (2.0 Ångstroms) or above results in a "Parameter value too large" error. Backbone objects may be coloured using the RasMol '**[colour backbone](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command.

The reserved word backbone is also used as a predefined set ("help sets") and as a parameter to the '**[set hbond](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22sethbonds)**' and '**[set ssbond](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22setssbonds)**' commands. The RasMol command '**trace**' renders a smoothed backbone, in contrast to '**backbone**' which connects alpha carbons with straight lines.

The backbone may be displayed with dashed lines by use of the '**backbone dash**' command.

**Background**

Syntax: background <colour>

The RasMol '**background**' command is used to set the colour of the "canvas" background. The colour may be given as either a colour name or a comma separated triple of Red, Green and Blue (RGB) components enclosed in square brackets. Typing the command '**[help colours](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22help)**' will give a list of the predefined colour names recognised by RasMol. When running under X Windows, RasMol also recognises colours in the X server's colour name database.

The '**background**' command is synonymous with the RasMol '**[set background](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22setbackground)**' command.

**Bond**

Syntax: bond <number> <number> +

 bond <number> <number> pick

 bond rotate {<boolean>}

The RasMol command '**bond <number> <number> +**' adds the designated bond to the drawing, increasing the bond order if the bond already exists. The command '**bond <number> <number> pick**' selects the two atoms specified by the atom serial numbers as the two ends of a bond around which the '**[rotate bond <angle>](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22rotate)**' command will be applied. If no bond exists, it is created.

Rotation around a previously picked bond may be specified by the '[**rotate bond <angle>**](http://www.openrasmol.org/doc/rasmol.html#rotate)' command, or may also be controlled with the mouse, using the '**bond rotate on/off**' or the equivalent '[**rotate bond on/off**](http://www.openrasmol.org/doc/rasmol.html#rotate)' commands.

**Cartoon**

Syntax: cartoon {<number>}

The RasMol '**cartoon**' command does a display of a molecule '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)' as Richardson (MolScript) style protein '**cartoons**', implemented as thick (deep) ribbons. The easiest way to obtain a cartoon representation of a protein is to use the '**Cartoons**' option on the '**Display**' menu. The '**cartoon**' command represents the currently selected residues as a deep ribbon with width specified by the command's argument. Using the command without a parameter results in the ribbon's width being taken from the protein's secondary structure, as described in the '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)' command. By default, the C-termini of beta-sheets are displayed as arrow heads. This may be enabled and disabled using the '[**set cartoons**](http://www.openrasmol.org/doc/rasmol.html#setcartoon)' command. The depth of the cartoon may be adjusted using the '[**set cartoons <number>**](http://www.openrasmol.org/doc/rasmol.html#setcartoon)' command. The '[**set cartoons**](http://www.openrasmol.org/doc/rasmol.html#setcartoon)' command without any parameters returns these two options to their default values.

**Centre**

Syntax: centre {<expression>} {translate|center}

 center {<expression>} {translate|center}

The RasMol '**centre**' command defines the point about which the '[**rotate**](http://www.openrasmol.org/doc/rasmol.html#rotate)' command and the scroll bars rotate the current molecule. Without a parameter the centre command resets the centre of rotation to be the centre of gravity of the molecule. If an atom expression is specified, RasMol rotates the molecule about the centre of gravity of the set of atoms specified by the expression. Hence, if a single atom is specified by the expression, that atom will remain 'stationary' during rotations.

Type '**[help expression](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22help)**' for more information on RasMol atom expressions.

Alternatively the centring may be given as a comma separated triple of [CenX, CenY, CenZ] offsets in RasMol units (1/250 of an Ångstrom) from the centre of gravity. The triple must be enclosed in square brackets.

The optional forms '**centre ... translate**' and '**centre ... center**' may be used to specify use of a translated centre of rotation (not necessarily in the centre of the canvas) or a centre of rotation which is placed at the centre of the canvas. Starting with RasMol 2.7.2, the default is to center the new axis on the canvas.

**Clipboard**

Syntax: clipboard

The RasMol '**clipboard**' command places a copy of the currently displayed image on the local graphics 'clipboard'. Note: this command is not yet supported on UNIX or VMS machines. It is intended to make transfering images between applications easier under Microsoft Windows or on an Apple Macintosh.

When using RasMol on a UNIX or VMS system this functionality may be achieved by generating a raster image in a format that can be read by the receiving program using the RasMol '[**write**](http://www.openrasmol.org/doc/rasmol.html#write)' command.

**Colour**

Syntax: colour {<object>} <colour>

 color {<object>} <colour>

Colour the atoms (or other objects) of the selected region. The colour may be given as either a colour name or a comma separated triple of Red, Green and Blue (RGB) components enclosed in square brackets. Typing the command '[**help colours**](http://www.openrasmol.org/doc/rasmol.html#help)' will give a list of all the predefined colour names recognised by RasMol.

Allowed objects are '**atoms**', '**bonds**', '[**backbone**](http://www.openrasmol.org/doc/rasmol.html#backbone)', '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)', '[**labels**](http://www.openrasmol.org/doc/rasmol.html#label)', '[**dots**](http://www.openrasmol.org/doc/rasmol.html#dots)', '**[hbonds](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22hbonds)**' and '**[ssbonds](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22ssbonds)**'. If no object is specified, the default keyword '**atom**' is assumed. Some colour schemes are defined for certain object types. The colour scheme '**none**' can be applied to all objects except atoms and dots, stating that the selected objects have no colour of their own, but use the colour of their associated atoms (*i.e.* the atoms they connect). '**Atom**' objects can also be coloured by '**[alt](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22altcolours)**', '[**amino**](http://www.openrasmol.org/doc/rasmol.html#aminocolours)', '[**chain**](http://www.openrasmol.org/doc/rasmol.html#chaincolours)', '[**charge**](http://www.openrasmol.org/doc/rasmol.html#chargecolours)', '**[cpk](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22cpkcolours)**', '[**group**](http://www.openrasmol.org/doc/rasmol.html#groupcolours)', '[**model**](http://www.openrasmol.org/doc/rasmol.html#nmrmodelcolours)', '[**shapely**](http://www.openrasmol.org/doc/rasmol.html#shapelycolours)', '[**structure**](http://www.openrasmol.org/doc/rasmol.html#structurecolours)', '[**temperature**](http://www.openrasmol.org/doc/rasmol.html#temperaturecolours)' or '[**user**](http://www.openrasmol.org/doc/rasmol.html#usercolours)'. Hydrogen bonds can also be coloured by '[**type**](http://www.openrasmol.org/doc/rasmol.html#hbondtypecolours)' and dot surfaces can also be coloured by '[**electrostatic potential**](http://www.openrasmol.org/doc/rasmol.html#potentialcolours)'. For more information type '**[help colour <colour>](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22chcolours)**'.

**Connect**

Syntax: connect {<boolean>}

The RasMol '**connect**' command is used to force RasMol to (re)calculate the connectivity of the current molecule. If the original input file contained connectivity information, this is discarded. The command '**connect false**' uses a fast heuristic algorithm that is suitable for determining bonding in large bio-molecules such as proteins and nucleic acids. The command "**connect true**" uses a slower more accurate algorithm based upon covalent radii that is more suitable to small molecules containing inorganic elements or strained rings. If no parameters are given, RasMol determines which algorithm to use based on the number of atoms in the input file. Greater than 255 atoms causes RasMol to use the faster implementation. This is the method used to determine bonding, if necessary, when a molecule is first read in using the '[**load**](http://www.openrasmol.org/doc/rasmol.html#load)' command.

**Define**

Syntax: define <identifier> <expression>

The RasMol '**define**' command allows the user to associate an arbitrary set of atoms with a unique identifier. This allows the definition of user-defined sets. These sets are declared statically, *i.e.* once defined the contents of the set do not change, even if the expression defining them depends on the current transformation and representation of the molecule.

**Depth**

Syntax: depth {<boolean>}

 depth <value>

The RasMol '**depth**' command enables, disables or positions the back-clipping plane of the molecule. The program only draws those portions of the molecule that are closer to the viewer than the clipping plane. Integer values range from zero at the very back of the molecule to 100 which is completely in front of the molecule. Intermediate values determine the percentage of the molecule to be drawn.

This command interacts with the '[**slab <value>**](http://www.openrasmol.org/doc/rasmol.html#slab)' command, which clips to the front of a given z-clipping plane.

**Dots**

Syntax: dots {<boolean>}

 dots <value>

The RasMol '**dots**' command is used to generate a van der Waals' dot surface around the currently selected atoms. Dot surfaces display regularly spaced points on a sphere of van der Waals' radius about each selected atom. Dots that would are 'buried' within the van der Waals' radius of any other atom (selected or not) are not displayed. The command '**dots on**' deletes any existing dot surface and generates a dots surface around the currently selected atom set with a default dot density of 100. The command '**dots off**' deletes any existing dot surface. The dot density may be specified by providing a numeric parameter between 1 and 1000. This value approximately corresponds to the number of dots on the surface of a medium sized atom.

By default, the colour of each point on a dot surface is the colour of its closest atom at the time the surface is generated. The colour of the whole dot surface may be changed using the '**[colour dots](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command.

**Echo**

Syntax: echo {<string>}

The RasMol '**echo**' command is used to display a message in the RasMol command/terminal window. The string parameter may optionally be delimited in double quote characters. If no parameter is specified, the '**echo**' command displays a blank line. This command is particularly useful for displaying text from within a RasMol '[**script**](http://www.openrasmol.org/doc/rasmol.html#script)' file.

**English**

Syntax: English

The RasMol '**English**' command sets the menus and messages to the English versions. The commands '**[French](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22french)**', '**[Italian](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22italian)**' and '**[Spanish](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22spanish)**' may be used to select French, Italian and Spanish menus and messages.

**French**

Syntax: French

The RasMol '**French**' command sets the menus and messages to the French versions. The commands '[**English**](http://www.openrasmol.org/doc/rasmol.html#english)', '[**Italian**](http://www.openrasmol.org/doc/rasmol.html#italian)' and '[**Spanish**](http://www.openrasmol.org/doc/rasmol.html#spanish)' may be used to select English, Italian and Spanish menus and messages.

**HBonds**

Syntax: hbonds {<boolean>}

 hbonds <value>

The RasMol '**hbond**' command is used to represent the hydrogen bonding of the protein molecule's backbone. This information is useful in assessing the protein's secondary structure. Hydrogen bonds are represented as either dotted lines or cylinders between the donor and acceptor residues. The first time the '**hbond**' command is used, the program searches the structure of the molecule to find hydrogen bonded residues and reports the number of bonds to the user. The command '**hbonds on**' displays the selected 'bonds' as dotted lines, and the '**hbonds off**' turns off their display. The colour of hbond objects may be changed by the '**[colour hbond](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. Initially, each hydrogen bond has the colours of its connected atoms.

By default the dotted lines are drawn between the accepting oxygen and the donating nitrogen. By using the '[**set hbonds**](http://www.openrasmol.org/doc/rasmol.html#sethbonds)' command the alpha carbon positions of the appropriate residues may be used instead. This is especially useful when examining proteins in backbone representation.

**Help**

Syntax: help {<topic> {<subtopic>}}

 ? {<topic> {<subtopic>}}

The RasMol '**help**' command provides on-line help on the given topic.

**Italian**

Syntax: Italian

The RasMol '**Italian**' command sets the menus and messages to the Italian versions. The commands '[**English**](http://www.openrasmol.org/doc/rasmol.html#english)', '[**French**](http://www.openrasmol.org/doc/rasmol.html#french)' and '[**Spanish**](http://www.openrasmol.org/doc/rasmol.html#spanish)' may be used to select English, French and Spanish menus and messages.

**Label**

Syntax: label {<string>}

 label <boolean>

The RasMol '**label**' command allows an arbitrary formatted text string to be associated with each currently selected atom. This string may contain embedded 'expansion specifiers' which display properties of the atom being labelled. An expansion specifier consists of a '%' character followed by a single alphabetic character specifying the property to be displayed (similar to C's printf syntax). An actual '%' character may be displayed by using the expansion specifier '%%'.

Atom labelling for the currently selected atoms may be turned off with the command '**label off**'. By default, if no string is given as a parameter, RasMol uses labels appropriate for the current molecule. RasMol uses the label '%n%r:%c.%a' if the molecule contains more than one chain, '%e%i' if the molecule has only a single residue (a small molecule) and '%n%r.%a' otherwise.

The colour of each label may be changed using the '**[colour label](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. By default, each label is drawn in the same colour as the atom to which it is attached. The size and spacing of the displayed text may be changed using the '[**set fontsize**](http://www.openrasmol.org/doc/rasmol.html#setfontsize)' command. The width of the strokes in the displayed text may be changed using the '[**set fontstroke**](http://www.openrasmol.org/doc/rasmol.html#setfontstroke)' command.

The following table lists the current expansion specifiers:

 %a Atom Name

 %b %t B-factor/Temperature

 %c %s Chain Identifier

 %e Element Atomic Symbol

 %i Atom Serial Number

 %n Residue Name

 %r Residue Number

 %M NMR Model Number (with leading "/")

 %A Alternate Conformation Identifier (with leading ";")

**Load**

Syntax: load {<format>} <filename>

Load a molecule coordinate file into RasMol. Valid molecule file formats are '**pdb**' (Protein Data Bank format), '**mdl**' (Molecular Design Limited's MOL file format), '**alchemy**' (Tripos' Alchemy file format), '**mol2**' (Tripos' Sybyl Mol2 file format), '**charmm**' (CHARMm file format), '**xyz**' (MSC's XMol XYZ file format), '**mopac**' (J. P. Stewart's MOPAC file format) or '**cif**' (IUCr CIF or mmCIF file format). If no file format is specified, '**PDB**', '**CIF**', or '**mmCIF**' is assumed by default. Up to 5 molecules may be loaded at a time. To delete a molecule prior to loading another use the RasMol '[**zap**](http://www.openrasmol.org/doc/rasmol.html#zap)' command. To select a molecule for manipulation use the RasMol '[**molecule <n>**](http://www.openrasmol.org/doc/rasmol.html#molecule)' command.

The '**load**' command selects all the atoms in the molecule, centres it on the screen and renders it as a CPK coloured wireframe model. If the molecule contains no bonds (*i.e.* contains only alpha carbons), it is drawn as an alpha carbon backbone. If the file specifies fewer bonds than atoms, RasMol determines connectivity using the '[**connect**](http://www.openrasmol.org/doc/rasmol.html#connect)' command.

The '**load inline**' command also allows the storing of atom coordinates in scripts to allow better integration with WWW browsers. A load command executed inside a script file may specify the keyword '**inline**' instead of a conventional filename. This option specifies that the coordinates of the molecule to load are stored in the same file as the currently executing commands.

Typically this is used in the command '**load pdb inline**', which is followed by a number of RasMol commands terminated by the command '[**exit**](http://www.openrasmol.org/doc/rasmol.html#quit)'. The '**exit**' command terminates execution of the current script and returns control to the command line (or the calling script). This means any lines following '**exit**' are never interpreted by RasMol. These may be used to store atomic coordinates in PDB, CIF or mmCIF file format. One possible use is a standard RasMol script prefix that may be concatenated with an appropriate PDB file on-the-fly.

**Molecule**

Syntax: molecule <number>

The RasMol '**molecule**' command selects one of up to 5 previously loaded molecules for active manipulation. While all the molcules are displayed and may be rotated collectively (see the '[**rotate all**](http://www.openrasmol.org/doc/rasmol.html#rotate)' command), only one molecule at a time time is active for manipulation by the commands which control the details of rendering.

**Monitor**

Syntax: monitor <number> <number>

 monitor {<boolean>}

The RasMol '**monitor**' command allows the display of distance monitors. A distance monitor is a dashed (dotted) line between an arbitrary pair of atoms, optionally labelled by the distance between them. The RasMol command '**monitor <number> <number>**' adds such a distance monitor between the two atoms specified by the atom serial numbers given as parameters

Distance monitors are turned off with the command '**monitors off**'. By default, monitors display the distance between its two end points as a label at the centre of the monitor. These distance labels may be turned off with the command '[**set monitors off**](http://www.openrasmol.org/doc/rasmol.html#setmonitor)', and re-enabled with the command '[**set monitors on**](http://www.openrasmol.org/doc/rasmol.html#setmonitor)'. Like most other representations, the colour of a monitor is taken from the colour of its end points unless specified by the '**[colour monitors](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command.

Distance monitors may also be added to a molecule interactively with the mouse, using the '[**set picking monitor**](http://www.openrasmol.org/doc/rasmol.html#setpicking)' command. Clicking on an atom results in its being identified on the rasmol command line. In addition every atom picked increments a modulo counter such that, in monitor mode, every second atom displays the distance between this atom and the previous one. The shift key may be used to form distance monitors between a fixed atom and several consecutive positions. A distance monitor may also be removed (toggled) by selecting the appropriate pair of atom end points a second time.

**Pause**

Syntax: pause

 wait

The RasMol '**pause**' command is used in script files to stop the script file for local manipulation by a mouse, until any key is pushed to restart the script file. '**Wait**' is synonymous with '**pause**'. This command may be executed in RasMol script files to suspend the sequential execution of commands and allow the user to examine the current image. When RasMol executes a '**pause**' command in a script file, it suspends execution of the rest of the file, refreshes the image on the screen and allows the manipulation of the image using the mouse and scroll bars, or resizing of the graphics window. Once a key is pressed, control returns to the script file at the line following the '**pause**' command. While a script is suspended the molecule may be rotated, translated, scaled, slabbed and picked as usual, but all menu commands are disabled. The '**pause**' can probably be used most effectively with '[**echo**](http://www.openrasmol.org/doc/rasmol.html#echo)' commands in education pre-scripted demonstrations, where a description of the current image is presented to the user/student. Typically the command before a '**pause**' should be '**echo Press any key to continue**'.

Execution of a script can be cancelled by pressing Control-D or Control-Z (on VAX/VMS, Control-C) while standing at a pause. The command '[**set picking none**](http://www.openrasmol.org/doc/rasmol.html#setpicking)' disables picking, which avoids the display of spurious messages whilst a script is suspended at a pause.

**Print**

Syntax: print

The RasMol '**print**' command sends the currently displayed image to the local default printer using the operating system's native printer driver. Note: this command is not yet supported under UNIX or VMS. It is intended to take advantage of Microsoft Windows and Apple Macintosh printer drivers. For example, this allows images to be printed directly on a dot matrix printer.

When using RasMol on a UNIX or VMS system this functionality may be achieved by either generating a PostScript file using the RasMol '[**write ps**](http://www.openrasmol.org/doc/rasmol.html#write)' or '[**write vectps**](http://www.openrasmol.org/doc/rasmol.html#write)' commands and printing that or generating a raster image file and using a utility to dump that to the local printer.

**Quit**

Syntax: quit

 exit

Exit from the RasMol program. The RasMol commands '**exit**' and '**quit**' are synonymous, except within nested scripts. In that case, '**exit**' terminates only the current level, while '**quit**' terminates all nested levels of scripts.

**Refresh**

Syntax: refresh

The RasMol '**refresh**' command redraws the current image. This is useful in scripts to ensure application of a complex list of parameter changes.

**Renumber**

Syntax: renumber {{-} <value>}

The RasMol '**renumber**' command sequentially numbers the residues in a macromolecular chain. The optional parameter specifies the value of the first residue in the sequence. By default, this value is one. For proteins, each amino acid is numbered consecutively from the N terminus to the C terminus. For nucleic acids, each base is numbered from the 5' terminus to the 3' terminus. All chains in the current database are renumbered and gaps in the original sequence are ignored. The starting value for numbering may be negative.

**Reset**

Syntax: reset

The RasMol '**reset**' command restores the original viewing transformation and centre of rotation. The scale is set to its default value, '[**zoom 100**](http://www.openrasmol.org/doc/rasmol.html#zoom)', the centre of rotation is set to the geometric centre of the currently loaded molecule, '[**centre all**](http://www.openrasmol.org/doc/rasmol.html#centre)', this centre is translated to the middle of the screen and the viewpoint set to the default orientation.

This command should not be mistaken for the RasMol '[**zap**](http://www.openrasmol.org/doc/rasmol.html#zap)' command which deletes the currently stored molecule, returning the program to its initial state.

**Restrict**

Syntax: restrict {<expression>}

The RasMol '**restrict**' command both defines the currently selected region of the molecule and disables the representation of (most of) those parts of the molecule no longer selected. All subsequent RasMol commands that modify a molecule's colour or representation affect only the currently selected region. The parameter of a '**restrict**' command is a RasMol atom expression that is evaluated for every atom of the current molecule. This command is very similar to the RasMol '[**select**](http://www.openrasmol.org/doc/rasmol.html#select)' command, except '**restrict**' disables the '[**wireframe**](http://www.openrasmol.org/doc/rasmol.html#wireframe)', '**[spacefill](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22spacefill)**' and '[**backbone**](http://www.openrasmol.org/doc/rasmol.html#backbone)' representations in the non-selected region.

Type "help expression" for more information on RasMol atom expressions.

**Ribbons**

Syntax: ribbons {<boolean>}

 ribbons <value>

The RasMol '**ribbons**' command displays the currently loaded protein or nucleic acid as a smooth solid "ribbon" surface passing along the backbone of the protein. The ribbon is drawn between each amino acid whose alpha carbon is currently selected. The colour of the ribbon is changed by the RasMol '**[colour ribbon](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. If the current ribbon colour is '**none**' (the default), the colour is taken from the alpha carbon at each position along its length.

The width of the ribbon at each position is determined by the optional parameter in the usual RasMol units. By default the width of the ribbon is taken from the secondary structure of the protein or a constant value of 720 (2.88 Ångstroms) for nucleic acids. The default width of protein alpha helices and beta sheets is 380 (1.52 Ångstroms) and 100 (0.4 Ångstroms) for turns and random coil. The secondary structure assignment is either from the PDB file or calculated using the DSSP algorithm as used by the '[**structure**](http://www.openrasmol.org/doc/rasmol.html#structure)' command. This command is similar to the RasMol command '[**strands**](http://www.openrasmol.org/doc/rasmol.html#strands)' which renders the biomolecular ribbon as parallel depth-cued curves.

**Rotate**

Syntax: rotate <axis> {-} <value>

 rotate bond {<boolean>}

 rotate molecule {<boolean>}

 rotate all {<boolean>}

Rotate the molecule about the specified axis. Permitted values for the axis parameter are "**x**", "**y**" and "**z**". The integer parameter states the angle in degrees for the structure to be rotated. For the X and Y axes, positive values move the closest point up and right, and negative values move it down and left, respectively. For the Z axis, a positive rotation acts clockwise and a negative angle anti-clockwise.

Alternatively, this command may be used to specify which rotations the mouse or dials will control. If '**rotate bond true**' is selected, the horizontal scroll bar will control rotation around the axis selected by the '[**bond src dst pick**](http://www.openrasmol.org/doc/rasmol.html#bond)' command. If '**rotate all true**' is selected, and multiple molecules have been loaded, then all molecules will rotate together. In all other cases, the mouseand dials control the the rotation of the molecule selected by the '[**molecule n**](http://www.openrasmol.org/doc/rasmol.html#molecule)' command.

**Save**

Syntax: save {pdb} <filename>

 save mdl <filename>

 save alchemy <filename>

 save xyz <filename>

Save the currently selected set of atoms in a Protein Data Bank (PDB), MDL, Alchemy(tm) or XYZ format file. The distinction between this command and the RasMol '[**write**](http://www.openrasmol.org/doc/rasmol.html#write)' command has been dropped. The only difference is that without a format specifier the '**save**' command generates a '**PDB**' file and the '[**write**](http://www.openrasmol.org/doc/rasmol.html#write)' command generates a '**GIF**' image.

**Script**

Syntax: script <filename>

The RasMol '**script**' command reads a set of RasMol commands sequentially from a text file and executes them. This allows sequences of commonly used commands to be stored and performed by single command. A RasMol script file may contain a further script command up to a maximum "depth" of 10, allowing complicated sequences of actions to be executed. RasMol ignores all characters after the first '#' character on each line allowing the scripts to be annotated. Script files are often also annotated using the RasMol '[**echo**](http://www.openrasmol.org/doc/rasmol.html#echo)' command.

The most common way to generate a RasMol script file is to use the '[**write script**](http://www.openrasmol.org/doc/rasmol.html#write)' or '[**write rasmol**](http://www.openrasmol.org/doc/rasmol.html#write)' commands to output the sequence of commands that are needed to regenerate the current view, representation and colouring of the currently displayed molecule.

The RasMol command '**source**' is synonymous with the '**script**' command.

Scripts may also be created with a text editor.

**Select**

Syntax: select {<expression>}

Define the currently selected region of the molecule. All subsequent RasMol commands that manipulate a molecule or modify its colour or representation only affect the currently selected region. The parameter of a '**select**' command is a RasMol expression that is evaluated for every atom of the current molecule. The currently selected (active) region of the molecule are those atoms that cause the expression to evaluate true. To select the whole molecule use the RasMol command '**select all**'. The behaviour of the '**select**' command without any parameters is determined by the RasMol '[**hetero**](http://www.openrasmol.org/doc/rasmol.html#sethetero)' and '[**hydrogen**](http://www.openrasmol.org/doc/rasmol.html#set)' parameters.

Type "help expression" for more information on RasMol atom expressions.

**Set**

Syntax: set <parameter> {<option>}

The RasMol '**set**' command allows the user to alter various internal program parameters such as those controlling rendering options. Each parameter has its own set or permissible parameter options. Typically, omitting the paramter option resets that parameter to its default value. A list of valid parameter names is given below.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| [Ambient](http://www.openrasmol.org/doc/rasmol.html#setambient)  | [Axes](http://www.openrasmol.org/doc/rasmol.html#setaxes)  | [Background](http://www.openrasmol.org/doc/rasmol.html#setbackground)  | [BackFade](http://www.openrasmol.org/doc/rasmol.html#setbackfade)  | [BondMode](http://www.openrasmol.org/doc/rasmol.html#setbondmode)  | [Bonds](http://www.openrasmol.org/doc/rasmol.html#setbonds)  | [BoundBox](http://www.openrasmol.org/doc/rasmol.html#setboundbox)  | [Cartoon](http://www.openrasmol.org/doc/rasmol.html#setcartoon)  |
| [CisAngle](http://www.openrasmol.org/doc/rasmol.html#setcisangle)  | [Display](http://www.openrasmol.org/doc/rasmol.html#setdisplay)  | [FontSize](http://www.openrasmol.org/doc/rasmol.html#setfontsize)  | [FontStroke](http://www.openrasmol.org/doc/rasmol.html#setfontstroke)  | [HBonds](http://www.openrasmol.org/doc/rasmol.html#sethbonds)  | [Hetero](http://www.openrasmol.org/doc/rasmol.html#sethetero)  | [HourGlass](http://www.openrasmol.org/doc/rasmol.html#sethourglass)  | [Hydrogen](http://www.openrasmol.org/doc/rasmol.html#sethydrogen)  |
| [Kinemage](http://www.openrasmol.org/doc/rasmol.html#setkinemage)  | [Menus](http://www.openrasmol.org/doc/rasmol.html#setmenus)  | [Monitor](http://www.openrasmol.org/doc/rasmol.html#setmonitor)  | [Mouse](http://www.openrasmol.org/doc/rasmol.html#setmouse)  | [Picking](http://www.openrasmol.org/doc/rasmol.html#setpicking)  | [Radius](http://www.openrasmol.org/doc/rasmol.html#setradius)  | [ShadePower](http://www.openrasmol.org/doc/rasmol.html#setshadepower)  | [Shadow](http://www.openrasmol.org/doc/rasmol.html#setshadow)  |
| [SlabMode](http://www.openrasmol.org/doc/rasmol.html#setslabmode)  | [Solvent](http://www.openrasmol.org/doc/rasmol.html#setsolvent)  | [Specular](http://www.openrasmol.org/doc/rasmol.html#setspecular)  | [SpecPower](http://www.openrasmol.org/doc/rasmol.html#setspecpower)  | [Stereo](http://www.openrasmol.org/doc/rasmol.html#setstereo)  | [SSBonds](http://www.openrasmol.org/doc/rasmol.html#setssbonds)  | [Strands](http://www.openrasmol.org/doc/rasmol.html#setstrands)  | [Transparent](http://www.openrasmol.org/doc/rasmol.html#settransparent)  |
| [UnitCell](http://www.openrasmol.org/doc/rasmol.html#setunitcell)  | [VectPS](http://www.openrasmol.org/doc/rasmol.html#setvectps)  | [Write](http://www.openrasmol.org/doc/rasmol.html#setwrite)  |  |  |  |  |  |

**Show**

Syntax: show information

 show centre

 show phipsi

 show RamPrint

 show rotation

 show selected { group | chain | atom }

 show sequence

 show symmetry

 show translation

 show zoom

The RasMol '**show**' command display details of the status of the currently loaded molecule. The command '**show information**' lists the molecule's name, classification, PDB code and the number of atoms, chains, groups it contains. If hydrogen bonding, disulphide bridges or secondary structure have been determined, the number of hbonds, ssbonds, helices, ladders and turns are also displayed, respectively. The command '**show centre**' shows any non-zero centering values selected by the '[**centre [CenX, CenY, CenZ]**](http://www.openrasmol.org/doc/rasmol.html#centre)' command. The command '**show phipsi**' shows the phi and psi angles of the currently selected residues and the omega angles of cis peptide bonds. The command '**show RamPrint**' (or 'show RPP' or 'show RamachandranPrinterPlot') shows a simple Ramachandran printer plot in the style of Frances Bernstein's fisipl program. The command '**show rotation**' (or 'show rot' or 'show 'rotate') shows the currently selected values of z, y, x and bond rotations, if any. The command '**show selected**' (or 'show selected group' or 'show selected chain' or 'show selected atom' ) shows the groups (default), chains or atoms of the current selection. The command '**show sequence**' lists the residues that comprise each chain of the molecule. The command '**show symmetry**' shows the space group and unit cell of the molecule. The command '**show translation**' shows any non-zero translation values selected by the '[**translate <axis> <value>**](http://www.openrasmol.org/doc/rasmol.html#translate)' command. The command '**show zoom**' shows any non-zero zoom value selected by the '[**zoom <value>**](http://www.openrasmol.org/doc/rasmol.html#zoom)' command.

**Slab**

Syntax: slab {<boolean>}

 slab <value>

The RasMol '**slab**' command enables, disables or positions the z-clipping plane of the molecule. The program only draws those portions of the molecule that are further from the viewer than the slabbing plane. Integer values range from zero at the very back of the molecule to 100 which is completely in front of the molecule. Intermediate values determine the percentage of the molecule to be drawn.

This command interacts with the '[**depth <value>**](http://www.openrasmol.org/doc/rasmol.html#depth)' command, which clips to the rear of a given z-clipping plane.

**Spacefill**

Syntax: spacefill {<boolean>}

 spacefill temperature

 spacefill user

 spacefill <value>

The RasMol '**spacefill**' command is used to represent all of the currently selected atoms as solid spheres. This command is used to produce both union-of-spheres and ball-and-stick models of a molecule. The command, '**spacefill true**', the default, represents each atom as a sphere of van der Waals radius. The command '**spacefill off**' turns off the representation of the selected atom as spheres. A sphere radius may be specified as an integer in RasMol units (1/250th Ångstrom) or a value containing a decimal point. A value of 500 (2.0 Ångstroms) or greater results in a "Parameter value too large" error.

The '**temperature**' option sets the radius of each sphere to the value stored in its temperature field. Zero or negative values have no effect and values greater than 2.0 are truncated to 2.0. The '**user**' option allows the radius of each sphere to be specified by additional lines in the molecule's PDB file using Raster 3D's COLOUR record extension.

The RasMol command '**cpk**' is synonymous with the '**spacefill**' command.

The RasMol command '**cpknew**' is synonymous with the '**spacefill**' command, except that a slightly different set of colours is used.

**Spanish**

Syntax: Spanish

The RasMol '**Spanish**' command sets the menus and messages to the Spanish versions. The commands '[**English**](http://www.openrasmol.org/doc/rasmol.html#english)', '[**French**](http://www.openrasmol.org/doc/rasmol.html#french)' and '[**Italian**](http://www.openrasmol.org/doc/rasmol.html#italian)' may be used to select English, French and Italian menus and messages.

**SSBonds**

Syntax: ssbonds {<boolean>}

 ssbonds <value>

The RasMol '**ssbonds**' command is used to represent the disulphide bridges of the protein molecule as either dotted lines or cylinders between the connected cysteines. The first time that the '**ssbonds**' command is used, the program searches the structure of the protein to find half-cysteine pairs (cysteines whose sulphurs are within 3 Ångstroms of each other) and reports the number of bridges to the user. The command '**ssbonds on**' displays the selected "bonds" as dotted lines, and the command '**ssbonds off**' disables the display of ssbonds in the currently selected area. Selection of disulphide bridges is identical to normal bonds, and may be adjusted using the RasMol '[**set bondmode**](http://www.openrasmol.org/doc/rasmol.html#setbondmode)' command. The colour of disulphide bonds may be changed using the '**[colour ssbonds](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. By default, each disulphide bond has the colours of its connected atoms.

By default disulphide bonds are drawn between the sulphur atoms within the cysteine groups. By using the '[**set ssbonds**](http://www.openrasmol.org/doc/rasmol.html#setssbonds)' command the position of the cysteine's alpha carbons may be used instead.

**Star**

Syntax: star {<boolean>}

 star temperature

 star user

 star <value>

The RasMol '**star**' command is used to represent all of the currently selected atoms as stars (six strokes, one each in the x, -x, y, -y, z and -z directions). The commands '**select not bonded**' followed by '**star 75**' are useful to mark unbonded atoms in a '[**wireframe**](http://www.openrasmol.org/doc/rasmol.html#wireframe)' display with less overhead than provided by '**[spacefill 75](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22spacefill)**'. This can be done automatically for all subsequent wireframe displays with the command '[**set bondmode not bonded**](http://www.openrasmol.org/doc/rasmol.html#setbondmode)'.

The command '**star true**', the default, represents each atom as a star with strokes length equal to van der Waals radius. The command '**star off**' turns off the representation of the selected atom as stars. A star stroke length may be specified as an integer in RasMol units (1/250th Ångstrom) or a value containing a decimal point. A value of 500 (2.0 Ångstroms) or greater results in a "Parameter value too large" error.

The '**temperature**' option sets the stroke length of each star to the value stored in its temperature field. Zero or negative values have no effect and values greater than 2.0 are truncated to 2.0. The '**user**' option allows the stroke length of each star to be specified by additional lines in the molecule's PDB file using Raster 3D's COLOUR record extension.

The RasMol '**[spacefill](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22spacefill)**' command can be used for more artistic rendering of atoms as spheres.

**Stereo**

Syntax: stereo on

 stereo <number>

 stereo off

The RasMol '**stereo**' command provides side-by-side stereo display of images. Stereo viewing of a molecule may be turned on (and off) either by selecting '**Stereo**' from the '**Options**' menu, or by typing the commands '**stereo on**' or '**stereo off**'.

Starting with RasMol version 2.7.2.1, the '**Stereo**' menu selection and the command '**stereo**' without arguments cycle from the initial state of '**stereo off**' to '**stereo on**' in cross-eyed mode to '**stereo on**' in wall-eyed mode and then back to '**stereo off**'.

The separation angle between the two views may be adjusted with the '[**set stereo [-] <number>**](http://www.openrasmol.org/doc/rasmol.html#setstereo)' command, where positive values result in crossed eye viewing and negative values in relaxed (wall-eyed) viewing. The inclusion of '**[-] <number>**' in the '**stereo**' command, as for example in '**stereo 3**' or '**stereo -5**', also controls angle and direction.

The stereo command is only partially implemented. When stereo is turned on, the image is not properly recentred. (This can be done with a '[**translate x -<number>**](http://www.openrasmol.org/doc/rasmol.html#translate)' command.) It is not supported in vector PostScript output files, is not saved by the '**write script**' command, and in general is not yet properly interfaced with several other features of the program.

**Strands**

Syntax: strands {<boolean>}

 strands <value>

The RasMol '**strands**' command displays the currently loaded protein or nucleic acid as a smooth "ribbon" of depth-cued curves passing along the backbone of the protein. The ribbon is composed of a number of strands that run parallel to one another along the peptide plane of each residue. The ribbon is drawn between each amino acid whose alpha carbon is currently selected. The colour of the ribbon is changed by the RasMol '**[colour ribbon](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. If the current ribbon colour is '**none**' (the default), the colour is taken from the alpha carbon at each position along its length. The central and outermost strands may be coloured independently using the '**[colour ribbon1](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' and '**[colour ribbon2](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' commands, respectively. The number of strands in the ribbon may be altered using the RasMol '[**set strands**](http://www.openrasmol.org/doc/rasmol.html#setstrands)' command.

The width of the ribbon at each position is determined by the optional parameter in the usual RasMol units. By default the width of the ribbon is taken from the secondary structure of the protein or a constant value of 720 for nucleic acids (which produces a ribbon 2.88 Ångstroms wide). The default width of protein alpha helices and beta sheets is 380 (1.52 Ångstroms) and 100 (0.4 Ångstroms) for turns and random coil. The secondary structure assignment is either from the PDB file or calculated using the DSSP algorithm as used by the '[**structure**](http://www.openrasmol.org/doc/rasmol.html#structure)' command. This command is similar to the RasMol command '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)' which renders the biomolecular ribbon as a smooth shaded surface.

**Structure**

Syntax: structure

The RasMol '**structure**' command calculates secondary structure assignments for the currently loaded protein. If the original PDB file contained structural assignment records (HELIX, SHEET and TURN) these are discarded. Initially, the hydrogen bonds of the current molecule are found, if this hasn't been done already. The secondary structure is then determined using Kabsch and Sander's DSSP algorithm. Once finished the program reports the number of helices, strands and turns found.

**Surface**

Syntax: surface molecule <value>

 surface solvent <value>

The RasMol '**surface**' command renders a Lee-Richards molecular surface resulting from rolling a probe atom on the selected atoms. The value given specifies the radius of the probe. If given in the first form, the evolute of the surface of the probe is shown (the solvent excluded surface). If given in the second form, the envelope of the positions of the center of the probe is shown (the solvent accessible surface).

**Trace**

Syntax: trace {<boolean>}

 trace <value>

 trace temperature

The RasMol '**trace**' command displays a smooth spline between consecutive alpha carbon positions. This spline does not pass exactly through the alpha carbon position of each residue, but follows the same path as '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)', '[**strands**](http://www.openrasmol.org/doc/rasmol.html#strands)' and '[**cartoons**](http://www.openrasmol.org/doc/rasmol.html#cartoon)'. Note that residues may be displayed as '[**ribbons**](http://www.openrasmol.org/doc/rasmol.html#ribbons)', '[**strands**](http://www.openrasmol.org/doc/rasmol.html#strands)', '[**cartoons**](http://www.openrasmol.org/doc/rasmol.html#cartoon)' or as a '**trace**'. Enabling one of these representations disables the others. However, a residue may be displayed simultaneously as backbone and as one of the above representations. This may change in future versions of RasMol. Prior to version 2.6, '**trace**' was synonymous with '**backbone**'.

'**Trace temperature**' displays the backbone as a wider cylinder at high temperature factors and thinner at lower. This representation is useful to X-ray crystallographers and NMR spectroscopists.

**Translate**

Syntax: translate <axis> {-} <value>

The RasMol '**translate**' command moves the position of the centre of the molecule on the screen. The axis parameter specifies along which axis the molecule is to be moved and the integer parameter specifies the absolute position of the molecule centre from the middle of the screen. Permitted values for the axis parameter are "**x**", "**y**" and "**z**". Displacement values must be between -100 and 100 which correspond to moving the current molecule just off the screen. A positive "**x**" displacement moves the molecule to the right, and a positive "**y**" displacement moves the molecule down the screen. The pair of commands '**translate x 0**' and '**translate y 0**' centres the molecule on the screen.

**UnBond**

Syntax: unbond <number> <number>

 unbond

The RasMol command '**unbond <number> <number>**' removes the designated bond from the drawing.

The command '**unbond**' without arguments removes a bond previously picked by the '[**bond <number> <number> pick**](http://www.openrasmol.org/doc/rasmol.html#bond)' command.

**Wireframe**

Syntax: wireframe {<boolean>}

 wireframe <value> {}

The RasMol '**wireframe**' command represents each bond within the selected region of the molecule as a cylinder, a line or a depth-cued vector. The display of bonds as depth-cued vectors (drawn darker the further away from the viewer) is turned on by the command '**wireframe**' or '**wireframe on**'. The selected bonds are displayed as cylinders by specifying a radius either as an integer in RasMol units or containing a decimal point as a value in Ångstroms. A parameter value of 500 (2.0 Ångstroms) or above results in an "Parameter value too large" error. Bonds may be coloured using the '**[colour bonds](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22colour)**' command. If the selected bonds involved atoms of alternate conformers then the bonds are narrowed in the middle to a radius of .8 of the specified radius (or to the radius specifed as the optional second parameter).

Non-bonded atoms, which could become invisible in an ordinary '**wireframe**' display can be marked by a preceding '[**set bondmode not bonded**](http://www.openrasmol.org/doc/rasmol.html#setbondmode)' command. If nearly co-linear bonds to atoms cause them to be difficult to see in a wireframe display, the '[**set bondmode all**](http://www.openrasmol.org/doc/rasmol.html#setbondmode)' command will add markers for '**all**' atoms in subsequent '**wireframe**' command executions.

**Write**

Syntax: write {<format>} <filename>

Write the current image to a file in a standard format. Currently supported image file formats include '**bmp**' (Microsoft bitmap) and '**gif**' (Compuserve GIF), '**iris**' (IRIS RGB), '**ppm**' (Portable Pixmap), '**ras**' (Sun rasterfile), '**ps**' and '**epsf**' (Encapsulated PostScript), '**monops**' (Monochrome Encapsulated PostScript), '**pict**' (Apple PICT), '**vectps**' (Vector Postscript). The '**write**' command may also be used to generate command scripts for other graphics programs. The format '**script**' writes out a file containing the RasMol '**[script](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22script)**' commands to reproduce the current image. The format '**molscript**' writes out the commands required to render the current view of the molecule as ribbons in Per Kraulis' Molscript program and the format '**kinemage**' the commands for David Richardson's program Mage. The following formats are useful for further processing: '**povray**' (POVRay 2), '**povray3**' (POVRay 3 -- under development), '**vrml**' (VRML file). Finally, several formats are provided to provide phi-psi data for listing or for '**phipsi**' (phi-psi data as an annotated list with cis omegas), '**ramachan**' and '**RDF**' and '**RamachandranDataFile**' (phi-psi data as columns of numbers for gnuplot), '**RPP**' and '**RamachandranPrinterPlot**' (phi-psi data as a printer plot).

The distinction between this command and the RasMol '**[save](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22save)**' command has been dropped. The only difference is that without a format specifier the '**[save](http://www.openrasmol.org/doc/rasmol.html%22%20%5Cl%20%22save)**' command generates a '**PDB**' file and the '**write**' command generates a '**GIF**' image.

**Zap**

Syntax: zap

Deletes the contents of the current database and resets parameter variables to their initial default state.

**Zoom**

Syntax: zoom {<boolean>}

 zoom <value>

Change the magnification of the currently displayed image. Boolean parameters either magnify or reset the scale of current molecule. An integer parameter specifies the desired magnification as a percentage of the default scale. The minimum parameter value is 10; the maximum parameter value is dependent upon the size of the molecule being displayed. For medium sized proteins this is about 500.