A Molecular Visualisation Program

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1 Introduction

RasMol is an menu- and command-driven interactive utility for the visualisation of molecular structures. The program will run on any BSD-like UNIX system, optionally displaying frames to either an 8 bit or 24 bit colour frame buffer available over the X Window System. Support is also provided for a dials box (via the XInput extensions) if one is connected to the system.

RasMol v2.1 accepts atomic co-ordinates in the standard Brookhaven Protein Data Bank (PDB) format, optionally supplemented David Baconjs Raster3D colour scheme specifications. The program interactively displays the molecule on the screen in a variety of representations, including wireframe, backbone, union-of-spheres, sticks and ball-and-stick. Different portions of the molecule may be rendered in any representation and colour independent of the rest of the model. The molecule may be rotated, translated, zoomed and z-clipped interactively, either from the keyboard, scroll bars or dials attached to the workstation. Finally, the rendered image may be written to a file in a variety of file formats.

2 General Operation

2.1 Running RasMol

To invoke the RasMol molecular visualisation tool, the user should type the command i`rasmol`j from the unix prompt. Immediately upon starting, the program displays the following message to identify the version number of the running program:

```
RasMol Molecular Renderer
Roger Sayle, June 1991
Version 2.1B
```

Immediately underneath this banner message, appears the programjs command line prompt i`RasMol>` j. If the program is being executed under the X Window System, the program determines the type of the display being used. If the screen has either an 8 bit or 24 bit colour frame buffer, RasMol creates another window, which is used to display menu options and the rendered images. If a suitable screen is not available, RasMol may only be used from the command line. Commands may be typed to manipulate the model, and to output the generated image to a raster file.

If an optional argument is given on the unix command line, this is taken to be a Brookhaven Protein Data Bank (PDB) file which is automatically loaded by the program (see the `load` command). If the file is found, the program displays the usual statistics after reading in the file, otherwise the error message i`Error: File not found!`j is displayed, before the user is presented the RasMol prompt.

In order to leave RasMol, the user can type the command `quit` or `exit` at the RasMol prompt, and the program will return the user to the familiar unix prompt. Alternatively, if a prompt other than the main RasMol prompt is being displayed, the user may hit control-C (`^C`) to leave the program. The message i`*** Quit ***`j will be output to the terminal, before the usual unix prompt is redisplayed. The program may also be terminated by selecting the **Quit** menu option, on the bottom of the main menu.

2.2 Display Window

If the program is run under the X Window System environment with a suitable colour screen, RasMol creates an additional window to display the rendered molecule interactively, as it is manipulated. This window is subdivided into three main regions. The left hand side of the window, called the icanvasj, is used to draw the images of the molecule. By default this area initially displays a black background. Both below and to the right of the canvas are two scroll bars used to rotate the molecule interactively. Finally, to the far right of the window are the buttons that form the menu.

While the mouse pointer is located within the canvas area of the display window, the mouse pointer is drawn as a cross-hair cursor, to enable the ipickingj of objects being displayed (see later); otherwise the mouse pointer is drawn as an arrowhead. Any characters that are typed at the keyboard while the display window is in ifocusj are redirected to the command line in the terminal window.

The display window may be resized at any point during the session. This has the effect of simply rescaling the image displayed on the canvas. RasMol imposes limits on the size of the display window such that the window must be large enough to display the menu and scroll bars and yet small enough to fit on a single screen. Attempts to enlarge the screen may fail owing to insufficient memory on the host machine, in which case RasMol reports the error message i`Renderer Error: Unable to allocate frame buffer!`j or some similar error.

On eight bit displays, when the number of colours required by the program exceeds the number of free colours on the screen, the program uses its own colourmap. This has the effect of temporarily displaying all windows other than the display window in false colours while the mouse pointer is within the display windows. If the mouse pointer is moved outside the display windows, the original colours of the other windows return, and the image on the canvas is shown in ifalse colourj. Once the number of colours required by the program drops again, the presentation of colours returns to normal.

2.3 Scroll Bars

The scroll bar across the bottom of the canvas area is used to rotate the molecule about the y-axis, i.e. to spin the nearest point on the molecule left or right; and the scroll bar to the right of the canvas rotates the molecule about the x-axis, i.e. the nearest point up or down. Each scroll bar has a iindicatorj to denote the relative orientation of the molecule, which is initially positioned in the centre of the scroll bar. These scroll bars may be operated in either of two ways. The first is by clicking any mouse button on the dotted scroll bar background to indicate a direct rotation relative to the current indictor position; the second is by clicking one of the arrows at either end of the scroll bar to rotate the molecule in fixed sized increments. Rotating the molecule by the second method may cause the indicators on the scroll bars to wrap around from one end of the bar to the other. A complete revolution is indicated by the indicator travelling the length of the scroll bar. The angle rotated by using the arrows depends upon the current size of the display window. No facility is provided for depressing the mouse button and idraggingj the indicator along the scroll bar.

2.4 Menu Buttons

The menu consists of a vertical column of large buttons that are selected by depressing and releasing any of the mouse buttons while the mouse pointer is over a menu button. Each menu option either directly changes the system options, or displays a submenu from which the user can select a further option. The number of menu buttons displayed on the screen varies from menu to menu. Most menus have the option Cancel to allow the user to return to the menu without affecting any of the current options. When selection of a menu option causes the program to prompt the user for additional information in the terminal window, the current command line being edited is erased (see later). When RasMol first starts executing, the menu area of the display window presents the main menu. The bottom option from this menu, Quit, allows the user to terminate the program directly, and return to the UNIX prompt.

2.5 Picking

In order to identify a particular atom or bond being displayed, RasMol allows the users to ipickj objects on the screen. The mouse is used to position the cross-hair cursor over the appropriate item, and then any of of the mouse button is depressed. Provided that the pointer is located close enough to a visible object, the program determines the identity of the nearest atom to the point identified.

The program will display, in the terminal window, the atomjs type, serial number, residue name and residue number. If the atom is a member of a named chain, the chain identifier is also displayed. Two examples of the output generated by selecting an atom are displayed below:

```
Atom: CA 349  Group: SER 70
Atom: O  526  Hetero: HOH 205  Chain: P
```

The first line describes the alpha carbon of the serine-70 amino acid in a protein. The unique Brookhaven serial number for this atom is 349. The following line describes the oxygen atom in a water molecule attached to the P chain of the main molecule. The word iHeteroj distinguishes heterogenous molecules (such as cofactors) from the residues in the main molecule, noted by iGroupj. [These two atoms are referred to by the two atom expressions k`SER70.CA`l and k`HOH205P.O`l, respectively, when using the RasMol commands `select` and `restrict`.]

2.6 Dials Box

If RasMol detects a idials boxj attached to the userjs workstation, it also allows the molecule to be manipulated interactively by the dials. Once RasMol starts up, it labels the LED displays above each dial, kROTATE Xl, kROTATE Yl, kROTATE Zl and kZOOMl across the top row from left to right, and kTRANS Xl, kTRANS Yl, kTRANS Zl and kSLABl from left to right across the bottom row. Rotating any of the knobs will automatically transform and redisplay the molecule interactively. The dials only have effect while the mouse pointer is within the display window. If more than one application is using the dials box at a time, care must be taken to remember the dial labels assigned by each program, as each application may overwrite the dial-label LEDs.

The rotation about the X and Y axes automatically updates the indicators on the appropriate scroll bars. All the rotation dials rotate the molecule for a complete revolution of the dial. All the remaining dials clamp their values to permissible ranges; turning these dials past their limits has no effect.
The kZOOMl dial allows the interactive zooming of the molecule between 10% and 200% of the original default magnification. Rotating the dial clockwise magnifies the molecule and anticlockwise shrinks it. A complete revolution of the dial corresponds to a 100% change in scale.
The kSLABl dial, which is only effective when slabbing is enabled, allows the user to move the front z-clipping plane from the nearest point on the molecule to the furthest. A complete rotation of the SLAB dial corresponds to moving the clipping plane half the distance between the front and back of the molecule. Turning the SLAB knob clockwise moves the clipping plane closer to the viewer (increasing the number of objects displayed), and turning it anticlockwise moves it further away (preventing more objects from being displayed). Slabbing mode is enabled by selecting the **Slab** menu button on the **Options** menu, or by using the `slab` command on the command line.
The translation along the X and Y axis allows the centre of the molecule to be moved within the canvas area of the screen. Rotation and zooming are still performed relative to the centre of the molecule, which may often not be at the centre of the canvas. The TRANS Z dial currently has no effect.

2.7 Command Line Interface

RasMol allows the execution of interactive commands typed at the RasMol prompt in the terminal window. Characters typed into either the terminal or the display window are processed on the command line. Each command must be given on a separate line terminated by a newline or carriage return character. Keywords are case insensitive and may be entered in both lower and upper case letters. All whitespace (space, tab and formfeed) characters are ignored, except to separate the keyword and the arguments of a command. Blank lines (those containing only whitespace) are ignored. There is an internal restriction that command lines are limited to a maximum of 256 characters. Strings may be delimited by matching single or double quotation marks. Placing a hash i#j character anywhere outside quotes terminates the line. RasMol will ignore the rest of the line, which may be used to comment on the command.

If a syntax error is detected on entering an interactive command, RasMol indicates the location of the error on the command line by placing the i^j character under the offending word or character, and writing an error message on the following line. If a command is not recognised by RasMol, the program will generate an i`Unrecognised command!`j error and redisplay the main prompt. If surplus information is given at the end of a command line, RasMol will execute the recognised command, but issue the warning message i`Warning: Ignoring rest of command!`j. Some commands may prompt the user for more information. These commands display a different prompt and are discussed in the command reference.
Whenever RasMol outputs diagnostic or error messages to the screen owing to selecting options from the menu or picking objects on the screen, the current command line is cleared. And the prompt redisplayed after any text has been displayed.

2.8 Command Line Editing

RasMol allows basic editing of the command line. Pressing either backspace, delete or `^H` will delete the previous character, and the key `^D` may be used to delete the character under the cursor. Several characters may be used to move the cursor along the command line. The characters `^B`, `^F`, `^A` and `^E` move the cursor back a single character, forward a single character, to the beginning of the line and to the end of the line, respectively. When the cursor is not at the end of the command line, typed characters are inserted into the line and do not overwrite existing characters. After a command line has been edited, a newline or carriage return will enter the entire line, regardless of where the cursor is positioned. Because RasMol is unable to move the cursor up to the previous line, care must be taken when editing commands that wrap over several lines. In the event that another process overwrites or corrupts the command line, the character `^L` may be used to redisplay the line on the screen.

RasMol maintains a history of recently used commands, so the that the user never needs to type the same commands repeatedly. Typing `^P` on the command line will display the previous command in the history and `^N` will display the following command. These commands may be edited using the features described above. Moving forward or backward through the command history undoes the modifications made to the current line. The number of commands retained in the history depends upon their length. RasMol can retain more short command lines and fewer long ones.
For users of kvt100l and compatible terminals (such as an kxterml), RasMol also understands the cursor control characters on the keyboard. The right and left cursor keys have the same affect as `^F` and `^B`, moving the cursor forward and back a single character respectively. Similarly, the up and down cursor keys have the same function as `^P` and `^N`, producing the previous and next entries in the command history respectively.

2.9 Start-up File

When RasMol is first run, it searches for an initialisation file of commands to run before the command prompt is presented to the user. The file is called **.rasmolrc** on UNIX systems, and **RASMOL.INI** on MS-DOS and Microsoft Windows Systems. The format and execution of the this file is identical to that of the `script` command described in section ? of this manual.
RasMol first looks for the initialisation file in the current directory, and if it is not found will look for it in the userjs home directory. On MSDOS systems the environment variable i`HOME`j may be used name the appropriate directory. Unlike the command i`script ".rasmolrc"`j, the program will not generate an error message if the file is not found.

3 Menu Options

3.1 Main Menu

When RasMol is started up at the beginning of a session, the menu area on the right hand side of the display window presents the main menu. This is the root menu for the RasMol menu system, and this menu is redisplayed after each operation selected from a menu is performed.

The main menu of RasMol Version 2.1 contains six options.

3.1.1 Load

This option allows the user to specify the Brookhaven Protein Data Bank (PDB) file to be read in. The function of this button is identical to the interactive command i`load`j typed from the RasMol command line. The PDB file contains the Cartesian co-ordinates of each atom in the molecule to be displayed. A complete description of the PDB file format and records understood by the program (including the Raster3D colour scheme records) are given in section ? of this document. If a molecule has already been loaded from a PDB file, clicking the Load option has no effect.

On pressing **Load** the user is prompted by the message i`PDB file name:`j in the terminal window. The filename must be a valid UNIX filename without wildcard characters, and must be entered without string delimiters. Entering an empty filename will abort the operation and return the user to the main menu and RasMol command

line prompt. If the file exists it is loaded by the program, otherwise RasMol outputs the error message i`Error: File not found!`j, before returning the user to the main menu and the RasMol command line prompt.

Once the PDB file is loaded, the RasMol program determines the connectivity of the molecule by proximity of atoms: Two atoms within an appropriate interval of one another are considered to be bonded. Once these calculations have been performed, the program outputs statistics on the molecule together with any appropriate information found in the PDB file. Once all the required preprocessing has been performed, RasMol iselectsj all the atoms in the molecule and displays a monochrome depth-cued wireframe representation on the display window canvas. The exact details of the molecule preprocessing steps are discussed under the i`load`j command, section ? in the command reference section of this document.

3.1.2 Display

Selecting the Display menu button from the RasMol main menu presents the user with the RasMol display options submenu. This submenu allows the current representation of the molecule to be changed. The operation of the options on this submenu is described in detail in section ?, kDisplay Menul. These options allow the molecule to be represented as wireframe, alpha carbon backbone, stick bonds, space filling union-of-spheres or ball-and-stick models.

3.1.3 Colours

Clicking the Colours option on the RasMol main menu displays the colour submenu in the display window. These submenu options allow the user to modify the colour scheme of the atoms and bonds in the currently displayed molecule. The function of the buttons on the colour submenu are described in detail in section ?, kColours Menul. The options allow the molecule to be shown in monochrome or coloured according to atom type, amino acid type, residue number, polypeptide chain, temperature factor or a user-defined colouring scheme supplied in the moleculejs PDB file.

3.1.4 Options

The Options menu is used to access the RasMol miscellaneous options submenu. This submenu allows the user to modify the state of the regularly used RasMol variables. Details of each of the options available via the RasMol options menu are described in depth in section ?, kOptions Menul. These options are used to turn slabbing mode, shadowing and specular highlights on and off. In addition, the inclusion/exclusion of hydrogren atoms and heterogenous groups from the display may be altered by buttons on this submenu.

3.1.5 Save

The Save menu option on the RasMol main menu is for writing the currently displayed image to an output raster file. The functionality of this menu option is also available through the commands i`write gif`j, i`write epsf`j, i`write ppm`j and i`write sunrle`j. Selecting the Save button displays a submenu of raster file formats in which the current image may be stored. This menu has the five options GIF, EPSF, PPM, Rast and Cancel. The last option allows the user to abort writing the current image to a file, and return to the main menu. The first four options specify the file format to be used in writing the current frame, which correspond to compuserve GIF format, Encapsulated PostScript, raw portable pixmap format and run length encoded SUN rasterfile format.

Selecting any one of these three format options causes RasMol to prompt the user i`Output file name:`j. The filename must be a valid UNIX filename without wildcard characters and must be entered without string delimiters. Entering a empty filename causes the program to abort the save operation and redisplay the main menu and RasMol command prompt. Conventionally, GIF images have the filename extension i.gifj, PostScript files have the extension i.psj, raw PPM files have the extension i. ppmj and RLE SUN rasterfile images the extension i.rasj. If the program is unable to create the given filename for writing, RasMol aborts the command with the error message i`Output Error: Unable to create file i*j!`j. Once the file has been written (which may take a short time) the main menu and command line prompt are automatically redisplayed.

If the 8-bit version of RasMol version 2.1 is running, all four file formats may be output; however, the 24-bit versions of RasMol 2.1 may only output EPSF, PPM and SUN rasterfile formats. If the user attempts to write out a 24-bit GIF image, the program warns the user with the message i`Output Error: 24 bit GIF files unsupported!`j. Although the portable pixmap format represents raster images with three bytes per pixel, the eight bit version of RasMol produces a maximum of 250 unique RGB triples.

3.1.6 Quit

The bottom button on the RasMol main menu is Quit. The function of this button is identical to that of the commands i`quit`j and i`exit`j from the command line. Quit terminates the RasMol program and returns the user to the UNIX prompt. When exiting, RasMol closes the display window and the image currently being displayed is lost. If a dials box is attached to the workstation, all the LED labels above each knob are turned off.

3.2 Display Menu

The display submenu allows the current representation of the molecule to be changed. This submenu is displayed by selecting the option Display on the RasMol main menu. The display submenu contains seven menu options. The first six change the representation of the current active zone (see section ? on the `select` command) and the final option, Cancel, is used to return the user to the main menu without modifying the current display.

3.2.1 Wireframe

This menu option displays the current active zone of the molecule as a depth-cued wireframe model. Each bond is represented as a narrow line between bonded atoms. Bonds nearer the viewer are brighter than those towards the back of the molecule, providing an impression of depth. The colour of a bond, or `none`, may be set with the `colour bond` command (section ?). If the bond has no colour of its own, it is represented as two half bond segments, each of which is given the colour of the nearest bonded atom. This menu option is equivalent to the RasMol commands `spacefill off`, `backbone off` and `wireframe on`.

3.2.2 Backbone

The Backbone menu option displays the current active zone of the molecule as a set of cylinders connecting the alpha carbons along the polypeptide backbone of the protein. Each ibondj is drawn as a 0.48Å diameter cylinder. The colour of the backbone may be set using the RasMol `colour backbone` command (section ?). If the colour of the backbone segment is set to `none`, the two halves of the cylinder are drawn the colours of the alpha carbon atoms that they join. This representation is especially useful for revealing the secondary structure and folding of a protein. This menu option is equivalent to the RasMol command sequence `spacefill off`, `wireframe off` and `backbone 80`.

3.2.3 Sticks

The Sticks menu option displays the current active zone of the molecule as a set of sticks model. Each bond is represented as a cylinder of 0.48Å diameter. The colour of a bond, or `none`, may be altered with the `colour bond` command (section ?). If the bond has no colour of its own, it is represented as two half bond cylinders, each of which is given the colour of the nearest bonded atom. This menu option is equivalent to the two RasMol commands `spacefill off` and `backbone off`, followed by the command `wireframe 80`.

3.2.4 Spacefill

This command represents the current active zone of the molecule as a union-of-spheres surface. Each atom is represented as a sphere of the appropriate van der Waals radius centred at the atomjs position. The colours of the atoms may be changed by either the Colours submenu (section ?) or the RasMol `colour atom` command (section ?). This menu option is equivalent to the RasMol commands `spacefill` and `wireframe off`, `backbone off`.

3.2.5 Ball & Stick

The RasMol Ball & Stick menu option draws the current active zone of the molecule as a ball-and-stick model. Each atom is represented as a sphere of 0.48Å radius, and each bond is represented as a narrow cylinder of 0.16Å radius. This representation is combination of both a spacefilling and stick bond models. The colours of the atoms and bonds may be altered with the `colour atom` and `colour bond` commands respectively. This menu option is equivalent to the four RasMol commands `spacefill 120`, `wireframe 40`, `backbone off` and `ribbons off`.

3.2.6 Ribbons

The RasMol Ribbons menu option draws the current active zone of the molecule as a ribbon model. This menu option is equivalent to the four RasMol commands ribbons 380, `spacefill off`, `wireframe off` and backbone off.

3.3 Colours Menu

The colours submenu options allow the user to modify the colour scheme of the atoms and bonds in the currently displayed molecule. This submenu is displayed by selecting the option Colours on the RasMol main menu. The colours submenu contains eight menu options. The first seven select a colour scheme for the currently active zone (see section ? on the `select` command) and the final option, Cancel, is used to return the user to the main menu without modifying the current colouring.

3.3.1 Mono

The top menu button on the RasMol colours menu, Mono, is used to colour the current active zone of the molecule monochrome white. This is the default colour scheme on loading a PDB file using the `load` command. This menu option is equivalent to the command i`colour white`j.

3.3.2 CPK

The CPK option on the colours submenu is used to shade the current active zone of the molecule by atom type, using the Corey, Pauling and Kultun (CPK) colouring scheme. These are the colours commonly used by chemists to denote atom type. In this scheme, carbon appears light grey, hydrogen appears white, oxygen appears red, sulphur appears yellow, nitrogen appears light blue and phosphorous appears pink. Any unrecognised element is displayed in magenta. This menu option is equivalent to the command i`colour cpk`**j.**

3.3.3 Shapely

The Shapely menu button on the colours submenu, changes the colour of each atom in the current active zone to a shade determined by the atomjs residue type. For nucleic acids, each base is given a unique colour; for proteins, each amino acid sidechain is given a unique colour, and the the atoms of the polypeptide backbone are drawn in light grey. This is the colour scheme used by kShapely modelsl. This menu option is equivalent to the command i`colour shapely`**j.**

3.3.4 Group

The menu button Group on the RasMol colours submenu colours each atom of the current active zone in a colour based on its position along the macromolecule chain it belongs to. The actual colours use a irampedj colour map, beginning with dark blue at the start of each chain then slowly changing through cyan, green and yellow to red at the opposite end of the chain.

The matching of atom to colour is dependent upon the current status of the RasMol `hetero` variable (see the `set hetero` command). When the `hetero` variable is reset, and heterogenous groups are excluded from the default active zone, the colours are based directly on their position along the chain. Hence the N-terminal residue of proteins and the 5'-terminus of nucleic acids are coloured blue, and the C-terminal of proteins and 3'-terminus of nucleic acids are coloured red. If the `hetero` variable is set, and HETATM atoms are included in the default active zone, each heterogenous molecule associated with a chain is coloured as if it were appended to the end of the chain. Hence the last heterogenous molecule in the PDB file for each chain is drawn in red, and all atoms are coloured based on residue number.
Currently the functionality of this menu option is not replicated in the RasMol command line interface.

3.3.5 Chain

The Chain menu option on the colours submenu colours each atom in the current active zone using a colour based on the macromolecular chain to which it belongs, or with which it is assocaited. The chains are coloured arbitrarily by choosing the appropriate number of colours from a blue-to-red colour map as described in section ? above.

Currently the functionality of this menu option is not replicated in the RasMol command line interface.

3.3.6 Temperature

The colours menu option Temperature is used to colour the currently active atoms of a molecule in a colour based on their anisotropic temperature factors, as defined in the PDB file from which it was read. The actual colours use a irampedj colour map, beginning with the icoldestj atoms drawn in dark blue, then slowly changing through the colours cyan, green and yellow to red, as the atoms get warmer, with red representing the ihottestj atoms in the file.

The matching of atom to colour depends upon the current value of the RasMol `hetero` variable (see section ? and section ? on the `set hetero` command). If the heterogenous atoms are currently excluded from the default active zone, i.e. the `hetero` variable has the value `false`, the temperature of the red and blue atoms are determined by the maximum and minimum temperature factors of the atoms in the main molecule. Otherwise, if heterogenous groups are included in the default active zone because the `hetero` variable has the value `true`, then the colours are taken from the temperature range of all the atoms in the PDB file.
Currently the functionality of this menu option is not replicated in the RasMol command line interface.

3.3.7 User

The last colouring option on the RasMol colours submenu, User, allows the current active zone of the molecule to be coloured according to a user-defined colour scheme. This colour scheme is provided by including additional iCOLOj records in the PDB file containing the molecule. These colour records, which are not supported by Brookhaven National Laboratories, are based upon those used by David Baconjs Raster3D program [Bacon88b] and specify the colours of individual atoms by using a pattern matching algorithm. The exact format of these supplemental records is described in detail in section ? of this document.

This menu option is equivalent to the command i`colour user`j.

3.4 Options Menu

The options submenu allows user to alter commonly used display options and parameters used in rendering molecules. This menu option is presented by clicking the **Options** menu button on the RasMol main menu. The options submenu displays six menu options. The first five are used to toggle the values of parameters and the final option, **Cancel**, may be used to exit the options submenu without modifying the current state of the program.

3.4.1 Slab

The Slab menu option on the RasMol options submenu is used to toggle the front z-clipping function, slabbing. When slabbing is enabled, RasMol only renders those objects (atoms and bonds) that are greater than a given distance from the viewer. This allows the user to icut awayj the front part of the molecule to reveal internal or occluded detail. All wireframe bonds that intersect the clipping plane are subdivided, such that only the portion behind the z-clipping plane is drawn. The representation of spheres that intersect the clipping plane is governed by the `slabmode` variable (see section ? on the `set slabmode` command). By default, `slabmode` has the value `solid` which depicts clipped atoms as solid filled spheres.

When RasMol is first started, the position of the z-clipping mode is 50% of the way through the molecule (drawing only the furthest half of the structure), with slabbing switched off. The current position of the z-clipping plane may be altered by executing a `slab` command, or by using the kSLABl dial on the dials box (if attached). The position of the slabbing plane is moved by turning the kSLABl dial even when slabbing is disabled.
This menu button works as a toggle button, alternatively turning on and off slabbing depending on the current setting. The user should avoid setting the position of the slab plane to the value 100, as the operation of the **Slab** will appear ineffective, since the whole molecule remains displayed. Similarly, because there is a performance degradation associated with rendering z-clipped images, it is recommended that slabbing is switched off, rather than moving the slabbing plane in front of the molecule. Shadowing may not be performed while slabbing is enabled, so shadowing is automatically disabled when slabbing is switched on. This menu option performs the same task as the two RasMol commands `slab on` and `slab off`.

3.4.2 Hydrogen

The Hydrogen option on the options menu allows the user to enable and disable the display of hydrogen atoms from the menu interface. Normally hydrogen atoms are not resolved by X-ray crystallography and only appear in data files generated by energy minimization programs. In order to enable the underlying structure of the molecule to be visualised, it is often necessary to disable the large number of hydrogen atoms that obscure the molecule. This is done by changing the current value of the `hydrogen` variable and selecting or restricting the current active zone as required. By default, the `hydrogen` variable has the value `true` and all hydrogen atoms and bonds are displayed along with the rest of the model. The default active zone, as defined by the `select` and `restrict` commands without parameters, relies on the current setting of `hydrogen`.

If **Hydrogen** is clicked when RasMol is currently permitting the display of hydrogen atoms, then the `hydrogen` variable is assigned the value `false`, the `restrict` command is used to force only the default active zone to be rendered and the message i`Hydrogens removed!`j is output to the terminal window. The `restrict` command causes all objects (atoms and bonds) not in the default active zone to be removed from the display. In normal operation, this means that all the hydrogen atoms/ bonds disappear from the screen. If the `hetero` flag is currently `false`, any displayed heterogenous groups will also disappear from the display. This has the same effect as the command sequence `set hydrogen off` followed by the command `restrict`.
If the RasMol `hydrogen` variable is `false` when the **Hydrogen** menu option is clicked, then the `hydrogen` flag is set to `true`, the `select` command is used to set the current active zone to the new default active zone and the message i`Hydrogens selected!`j is written to the terminal window. The actual image drawn in the display window canvas does not change, but all subsequent representation and colouring commands will affect the moleculejs hydrogen atoms. If the `hetero` variable is currently true, all heterogenous atoms will also be iselectedj. This has the same effect as the command sequence `set hydrogen true` followed by the command `select`.

3.4.3 Het Atoms

The option menu Het Atoms button allows the user to enable and disable the display of heterogenous groups from the menu interface. Typically water atoms and cofactors are also resolved by X-ray crystallography, along with the atoms of the protein or nucleic acid. Sometimes these heterogenous groups are important in the functioning of the macromolecule, but more generally they are solvent moieties that co-crystallize with the main molecule. The Het Atoms option allows the user to define whether these atoms, contained as HETATM records in the PDB file, should currently be displayed. This is done by changing the current value of the `hetero` variable and selecting or restricting the current active zone as required. By default, the `hetero` variable has the value `true`, and all heterogenous atoms and bonds are displayed along with the rest of the model. The default active zone, as defined by the `select` and `restrict` commands without parameters, relies on the current setting of `hetero`.

If **Het Atoms** is clicked when RasMol is currently permitting the display of heterogenous atoms, then the `hetero` variable is reset to the value `false`, the `restrict` command is used to limit the display of objects to the default active zone and the message i`HETA atoms selected!`j is printed below the RasMol prompt. The `restrict` command causes all objects (atoms and bonds) not in the default active zone to be removed from the display. In normal operation, this means all the heterogenous atoms/bonds disappear from the screen. If the `hydrogen` variable is currently `false`, any displayed hydrogen atoms will also disappear from the display. This has the same effect as the command sequence `set hetero off` followed by the command `restrict`.
If the RasMol `hetero` variable is `false` when the **Het Atoms** menu option is clicked, then the `hetero` flag is assigned `true`, the `select` command is used to set the current active zone to the new default active zone and the i`HETA atoms selected!`j diagnostic is displayed in the terminal window. The actual image drawn on the display window canvas does not change, but all subsequent representation and colouring commands will affect the molecule and the associated hetero groups. If the

RasMol `hydrogen` variable is set, all hydrogen atoms will also be iselectedj. This menu option is identical to the command sequence `set hetero true` followed by the command `select`.

3.4.4 Specular

This menu option performs the same task as the two RasMol commands `set specular on` **and** `set specular off`.

3.4.5 Shadow

The Shadow button on the RasMol options menu toggles the value of the `shadow` **variable. When this parameter has the value** `true`**, the macromolecular structure is rendered with cast shadows from a single light source, otherwise the shadowing is not calculated. Although by comparison RasMol is extremely fast at rendering shadowed images, testing which parts of a molecule are occluded from the light source is computationally expensive. It is recommended that, on slower machines, the correct orientation of the molecule is performed using the normal lighting model and then, once the desired position is determined, shadowing is enabled.**

Slabbing may not be performed while shadowing is enabled, and so slabbing is automatically disabled when shadowing is switched on.
This menu option performs the same task as the two RasMol commands `set shadow on` and `set shadow off`.

4 Atom Expressions

4.1 Primitive Expressions

The main constituent of an atom expression is the primitive expression. A primitive expression uniquely identifies a related group of atoms within a molecule. A primitive expression consists of four major fields, only the first of which is compulsory. The first field specifies the residue type, the second specifies the residue number, the third identifies the chain (if applicable) and the final field identifies the atoms within the residue. A primitive expression may not contain any whitespace. Each of the fields is described in detail below.

Syntax:`<residue-type><residue-number><chain>.<atom-type>`
The first field consists of one to three alphabetic or question mark (i?j) characters that identify the type of residue to be selected. The characters are matched against the residue name of each atom in the molecule, with the question mark acting as a wildcard character that matches any letter. For proteins, this means that the three letter codes for amino acids must be used. This field is case insensitive with all characters being converted to uppercase before the comparison is performed. A single asterisk (i*j) character may be used as a abbreviation for the field k???l. It is recommended that the asterisk is used whenever possible, for efficiency reasons. Unfortunately, residue names containing digits, such as kSO4l, cannot be specified.
The second field contains a number that identifies the residue number within the molecule. This field may be any number of numeric characters, or a single asterisk to match all residues. Normally, the first field contains an asterisk if this field is given. A numeric value in this field uniquely identifies a single residue (base or amino acid) in the macromolecule, and hence a residue type given in addition would be redundant.
The third field is a single alphabetic character used to identify a chain of the molecule (if appropriate), or either an asterisk or a question mark to indicate that all chains should be used in the match. If a character is specified, this is converted to uppercase before any comparison. If the residue number field is an asterisk, a digit may be used in this field if the chains are denoted by numerals.
The final field is a period or full-stop (i.j) character followed by