RasWin 2.4 Help

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RasMol V2.4

Molecular Visualisation Program

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Introduction

RasMol2 is a molecular graphics program intended for the visualisation of proteins, nucleic acids and small molecules. The program is aimed at teaching, display and generation of publication quality images. RasMol runs under Microsoft Windows and also UNIX and VMS systems with an 8bit or 24bit (32bit) colour X Windows display (X11R4 or later). The program reads in a molecule co-ordinate file and interactively displays the molecule on the screen in a variety of representations and colour schemes. Currently available molecule representations include depth-cued wireframes, 'drieding' sticks, spacefilling (CPK) spheres, ball and stick, biomolecular ribbon (either solid or strands) and dots.

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	background	centre	colour
dots	define	exit	hbond
help	load	quit	renumber
reset	restrict	ribbon	rotate
save	script	select	set
show	slab	spacefill	strands
structure	ssbond	translate	wireframe
write	zap	zoom	

Backbone

Syntax: **backbone {<boolean>}**
backbone <value>

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 paramater the same as the wireframe 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 determine the cylinder radius of the representation in 0.004 angstrom units. Backbone objects may be coloured using the RasMol colour backbone command. A parameter value of 500 (2 angstroms) or above results in an "Integer argument too large" error.

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 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.

Centre

Syntax: **center {<expression>}**

centre {<expression>}

The RasMol **centre** command defines the point about which the 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 for more information on RasMol atom expressions.

Colour

Syntax: **colour {<object>} <colour>**
color {<object>} <colour>

Colour the atoms (or other objects) of the selected zone. 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 will give a list of all the predefined colour names recognised by RasMol.

Allowed objects are **atoms, bonds,** backbone, dots, hbonds, ribbons and ssbonds. 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 all objects accept 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 amino, cpk, chain, group, shapely, structure, temperature and user and hydrogen bond objects can also be coloured by type. For more information type help colour <colour>.

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.

Dots

Syntax: **dots {<boolean>}**
dots {<value>}

The RasMol **dots** command is used to generate a Van der Waal's 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 Waal's 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 it's closest atom at the time the surface is generated. The colour of the whole dot surface may be changed using the colour dots 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 file.

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 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 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.

Load

Syntax: **load {<format>} <filename>**

Load a molecule co-ordinate file into RasMol2. Valid molecule file formats are **pdb** (Brookhaven Protein Databank), **mdl** (Molecular Design Limited's MOL file format), **alchemy** (Tripos' Alchemy file format), **mol2** (Tripos' Sybyl Mol2 file format), **charmm** (CHARMm file format) or **xyz** (MSC's XMol XYZ file format). If no file format is specified, **pdb** is assumed by default. Only a single molecule may be loaded at a time. To delete a molecule prior to loading another use the RasMol zap 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.

Quit

Syntax: **quit**
exit

Exit from the RasMol program.

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 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 it default value, zoom 100, the centre of rotation is set to the geometric centre of the currently loaded molecule, centre all, 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 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 active zone 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 effect only the currently selected zone. 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 command, except restrict disables the wireframe, spacefill and backbone representations in the non-active zone.

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 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 for nucleic acids (which produces a ribbon 2.88 Angstroms wide). The default width of protein alpha helices and beta sheets is 380 (1.52 Angstroms) and 100 (0.4 Angstroms) 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 command. This command is similar to the RasMol command strands which renders the biomolecular ribbon as parallel depth-cued curves.

Rotate

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

Rotate the molecule about the specified axis. Permited 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.

Save

Syntax: **save {pdb} <filename>**
save alchemy <filename>

Save the currently selected set of atoms in either a Brookhaven Protein Database (PDB) or Alchemy(tm) format file. This command should not be confused with the RasMol write command which generates either image or script files.

Script

Syntax: **script <filename>**

The RasMol **script** command reads a set of commands sequentially from a text file and executes them. This allows sequences of commonly used commands to be stored and performed by a single command. A RasMol script file may contain a further script command up to a maximum "depth" of 10, allowing compilicated sequences of actions to be executed.

Select

Syntax: **select {<expression>}**

Define the currently active zone of the molecule. All subsequent RasMol commands that manipulate a molecule or modify its colour or representation, only effects the currently selected zone. The parameter of a **select** command is a RasMol expression that is evaluated for every atom of the current molecule. The currently selected (active) zone of the molecule are those atoms that cause the expression to evaluate true. To select the whole molecule use the RasMol command **select all.**

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, ommiting the paramter option resets that parameter to its default value. A list of valid parameter names is given below. For more information on each internal parameter typehelp set parameter.

ambient	axes	background	bondmode
boundbox	display	hbonds	hetero

hourglass	hydrogen	menus	mouse
shadow	slabmode	specular	specpower
ssbonds	strands	unitcell	vectps

Show

Syntax: **show information**
show sequence
show symmetry

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 sequence** lists the residues that compose each chain of the molecule.

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.

Spacefill

Syntax: **spacefill {<boolean>}**
spacefill temperature
spacefill user
spacefill <value>

Represent the currently selected zone as a spacefilling union of spheres model. An integer parameter may be used to specify the radius of each atom given in 4nm units. If no parameter is given, each atom is drawn as a sphere of its Van der Waals radius.

The **temperature** option is used to set the radius of each selected sphere to the value in the temperature field of the molecule file. A zero or negative value causes no change in the selected atom. Temperature values greater than 2.00 are truncated to 2.00 Angstrom radius.

The **user** option allows the radius of the selected spheres to be determined by matching each atom against optional lines in the input data file. Details of the wildcard pattern matching used by Raster3D's COLOR

records is given in the manual.

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 angstroms 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 command. The colour of disulphide bonds may be changed using the colour ssbonds 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 command the position of the cysteine's alpha carbons may be used instead.

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 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 colour of the central and outermost strands may be coloured independently using the colour ribbon1 and colour ribbon2 commands respectively. The number of strands in the ribbon may be altered using the RasMol set strands 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 Angstroms wide). The default width of protein alpha helices and beta sheets is 380 (1.52 Angstroms) and 100 (0.4 Angstroms) 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 command. This command is similar to the RasMol command 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 and SHEET) these are discarded. Initially, the hydrogen bonds of the current molecule are found, if this hasn't been done already. The secondary structure is the determined using Kabsch and Sander's DSSP algorithm. Once finished the program reports the number of helices and ladders found.

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. Permited 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.

Wireframe

Syntax: **wireframe {<boolean>}**
wireframe <value>

Represent each bond within the selected zone of the molecule as either a cylinder or depth-cued vector. If no parameter is given, RasMol draws each bond as a hither-and-yon shaded narrow vector. An integer parameter specifies the radius of a cylinder, given in 4nm units, to be used as a stick bond.

Write

Syntax: **write {<format>} <filename>**

Write the current image to a file in a standard raster format. Currently supported image file formats include "**gif**" (Compuserve GIF), "**ppm**" (Portable Pixmap), "**ras**" (Sun rasterfile), "**ps**" and "**epsf**" (Encapsulated PostScript), "**monops**" (Monochrome Encapsulated PostScript) and "**bmp**" (Microsoft bitmap). 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 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.

This command should not be confused with the RasMol save command which save the currently selected portion of the molecule.

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 between 10 and 200 specifies the desired magnification as a percentage of the default scale.

Internal Parameters

RasMol has a number of internal parameters that may be modified using the set command. These parameters control a number of program options such as rendering options and mouse button mappings.

A complete list of internal parameter names is given below.

ambient	axes	background	bondmode
boundbox	display	hbonds	hetero
hourglass	hydrogen	menus	mouse
shadow	slabmode	specular	specpower
ssbonds	strands	unitcell	vectps

Set Ambient

K**Syntax:** **set ambient {<value>}**

The RasMol **ambient** parameter is used to control the amount of ambient (or surrounding) light in the scene. The **ambient** value must be between 0 and 100 that controls the percentage intensity of the darkest shade of an object. For a solid object, this is the intensity of surfaces facing away from the light source or in

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K ambient

shadow. For depth-cued objects this is the intensity of objects furthest from the viewer.

This parameter is commonly used to correct for monitors with different "gamma values" (brightness), to change how light or dark a hardcopy image appears when printed or to alter the feeling of depth for wireframe or ribbon representations.

Set Axes

K**Syntax: set axes <boolean>**

The RasMol **axes** parameter controls the display of orthogonal co-ordinate axes on the current display. The co-ordinate axes are those used in the molecule data file, and the origin is the centre of the molecule's bounding box. The **set axes** command is similar the the commands set boundbox and set unitcell that display the bounding box and the crystallographic unit cell respectively.

Set Background

K**Syntax: set background <colour>**

The RasMol **background** parameter 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, Blue (RGB) components enclosed in square brackets. Typing the command help colours 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.

Set BondMode

K**Syntax: set bondmode and**
set bondmode or

The RasMol **set bondmode** command controls the mechanism used to select individual bonds. When using the select and restrict commands, a given bond will be selected if i) the bondmode is **or** and either of the connected atoms is selected, or ii) the bondmode is **and** and both atoms connected by the bond are selected. Hence an individual bond may be uniquely identified by using the command "**set bondmode and**" and then uniquely selecting the atoms at both ends.

K axes
K background
K bondmode

Set BoundBox

K **Syntax: set boundbox <boolean>**

The RasMol **boundbox** parameter controls the display of the current molecules bounding box on the display. The bounding box is orthogonal to the data file's original co-ordinate axes. The **set boundbox** command is similar the the commands set_axes and set_unitcell that display orthogonal co-ordinate axes and the bounding box respectively.

Set Display

K **Syntax: set display selected**
set display normal

This command controls the display mode within RasMol. By default, **set display normal,** RasMol displays the molecule in the representation specified by the user. The command **set display selected** changes the display mode such that the molecule is temporarily drawn so as to indicate currently selected portion of the molecule. The user specified colour scheme and representation remains unchanged. In this representation all selected atoms are shown in yellow and all non selected atoms are shown in blue. The colour of the background is also changed to a dark grey to indicate the change of display mode. This command is typically only used by external Graphical User Interfaces (GUIs).

Set HBonds

K **Syntax: set hbonds backbone**
set hbonds sidechain

The RasMol **hbonds** parameter determines whether hydrogen bonds are drawn between the donor and acceptor atoms of the hydrogen bond, **set hbonds sidechain** or between the alpha carbon atoms of the protein backbone and between the phosphorous atoms of the nucleic acid backbone, **set hbonds backbone.** The actual display of hydrogen bonds is controlled by the hbonds command. Drawing hydrogen bonds between protein alpha carbons or nucleic acid phosphorous atoms is useful when the rest of the molecule is shown in only a schematic representation such as backbone, ribbons or strands. his parameter is similar to the RasMol ssbonds parameter.

K boundbox
K display
K backbone;hbonds;sidechain

Set Hetero

K **Syntax:** **set hetero <boolean>**

set hetero

Set HourGlass

K **Syntax:** **set hourglass {<boolean>}**

The RasMol **hourglass** parameter allows the user to enable and disable the use of the `hour glass' cursor used by RasMol to indicate that the program is currently busy drawing the next frame. The command **set hourglass on** enable the indicator, whilst **set hourglass off** prevents RasMol from changing the cursor. This is useful when spinning the molecule, running a sequence of commands from a script file or using interprocess communication to execute complex sequences of commands. In these cases a `flashing' cursor may be distracting.

Set Hydrogen

K **Syntax:** **set hydrogen <boolean>**

set hydrogen

Set Menus

K **Syntax:** **set menus <boolean>**

The RasMol **set menus** command enables the canvas window's menu buttons or menu bar. This command is typically only used by graphical user interfaces or to create as large as image as possible.

K hetero
K hourglass
K hydrogen
K menus

Set Mouse

K **Syntax:** **set mouse rasmol**
set mouse insight
set mouse quanta

The RasMol **set mouse** command sets the rotation, translation, scaling and zooming mouse bindings. The default value is **rasmol** which is suitable for two button mice (for three button mice the second and third buttons are synonymous); X-Y rotation is controlled by the first button, and X-Y translation by the second. Additional functions are controlled by holding a modifier key on the keyboard. [Shift] and the first button performs scaling, [shift] and the second button performs Z-rotation, and [control] and the first mouse button controls the clipping plane. The **insight** and **quanta** provide the same mouse bindings as other packages for experienced users.

Set Shadow

K **Syntax:** **set shadow <boolean>**

The RasMol **set shadow** command enables and disables raytracing of the currently rendered image. Currently only the spacefilling representation is shadowed or can cast shadows. Enabling shadowing will automatically disable the Z-clipping (slabbing) plane using the command slab off. Raytracing typically takes about 10s for a moderately sized protein. It is recommended that shadowing is normally disabled whilst the molecule is being transformed or manipulated, and only enabled once an appropiate viewpoint is selected, to provide a greater impression of depth.

Set SlabMode

K **Syntax:** **set slabmode <slabmode>**

The RasMol **slabmode** parameter controls the rendering method of objects cut by the slabbing (z-clipping) plane. Valid slabmode parameters are "**reject**", "**half**", "**hollow**", "**solid**" and "**section**".

Set Specular

K insight;mouse;quanta;rasmol
K shadow
K half;hollow;reject;section;slabmode;solid

K**Syntax: set specular <boolean>**

The RasMol **set specular** command enables and disables the display of specular highlights on solid objects drawn by RasMol. Specular highlights appear as white reflections of the light source on the surface of the object. The current RasMol implementation uses an approximation function to generate this highlight.

The specular highlights on the surfaces of solid objects may be altered by using the specular reflection coefficient, which is altered using the RasMol set specpower command.

Set SpecPower

K**Syntax: set specpower {<value>}**

The **specpower** parameter determines the shininess of solid objects rendered by RasMol. This value between 0 and 100 adjusts the reflection coeffient used in specular highlight calculations. The specular highlights are enabled and disabled by the RasMol set specular command. Values around 20 or 30 produce plastic looking surfaces. High values represent more shiny surfaces such as metals, while lower values produce more diffuse/dull surfaces.

Set SSBonds

K**Syntax: set ssbonds backbone**
set ssbonds sidechain

The RasMol **ssbonds** parameter determines whether disulphide bridges are drawn between the sulphur atoms in the sidechain (the default) or between the alpha carbon atoms in the backbone of the cysteines residues. The actual display of disulphide bridges is controlled by the ssbonds command. Drawing disulphide bridges between alpha carbons is useful when the rest of the protein is shown in only a schematic representation such as backbone, ribbons or strands. his parameter is similar to the RasMol hbonds parameter.

Set Strands

K**Syntax: set strands {<value>}**

The RasMol **strands** parameter controls the number of parallel strands that are displayed in the ribbon representations of proteins. The permissible values for this parameter are 1, 2, 3, 4, 5 and 9. The default

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K specular
K specpower
K backbone;sidechain;ssbonds
K strands

value is 5. The number of strands is constant for all ribbons being displayed. However, the ribbon width (the separation between strands) may be controlled on a residue by residue basis using the RasMol ribbons command.

Set UnitCell

K**Syntax:** **set unitcell <boolean>**

The RasMol **unitcell** parameter controls the display of the crystallographic unit cell on the current display. The crystal cell is only enabled if the appropriate crystal symmetry information is contained in the PDB data file. The RasMol command show symmetry display details of the crystal's space group and unit cell axes. The **set unitcell** command is similar the the commands set axes and set boundbox that display orthogonal co-ordinate axes and the bounding box respectively.

Set VectPS

K**Syntax:** **set vectps <boolean>**

The RasMol **vectps** parameter is use to control the way in which the RasMol write command generates vector PostScript output files. The command **set vectps on** enables to use of black outlines around spheres and cylinder bonds producing `cartoon-like' high resolution output. However, the current implementation of RasMol incorrectly cartoons spheres that are intersected by more than one other sphere. Hence `ball and stick' models are rendered correctly by not large spacefilling spheres models. Cartoon outlines can be disabled, the default, by the command **set vectps off**

Atom Expressions

RasMol atom expressions uniquely identify an arbitrary group of atoms within a molecule. Atom expressions are composed of either primitive expressions, predefined sets, comparison operators, **within** expressions, or logical (boolean) combinations of the above expression types.

The logical operators allow complex queries to be constructed out of simpler ones using the standard boolean connectives **and, or** and **not.** These may be abbreviated by the symbols "**&**", "**|**" and "**!**" respectively. Parentheses (brackets) may be used to alter the precedence of the operators. For convenience, a comma may also be used for boolean disjunction.

The atom expression is evaluated for each atom, hence **protein and backbone** selects protein bacbone atoms, not the protein and [nucleic] acid backbone atoms!

〈 Primitive Expressions

K unitcell
K vectps

〈 Predefined Sets
〈 Comparison Operators
〈 Within Expressions

〈 Example Expressions

Example Expressions

The following table gives some useful examples of RasMol atom expressions.

Expression	Interpretation
`*`	All atoms
`cys`	Atoms in cysteines
`hoh`	Atoms in heterogenous water molecules
`as?`	Atoms in either asparagine or aspartic acid
`*120`	Atoms at residue 120 of all chains
`*p`	Atoms in chain P
`*.n?`	Nitrogen atoms
`cys.sg`	Sulphur atoms in cysteine residues
`ser70.c?`	Carbon atoms in serine-70
`hem*p.fe`	Iron atoms in the Heme groups of chain P

Primitive Expressions

RasMol primitive expressions are the fundamental building blocks of atom expressions. There are two types of primitive expression. The first type is used to identify a given residue number or range of residue numbers. A single residue is identified by its number (position in the sequence), and a range is specified by lower and upper bounds separated by a hyphen character. For example **`select 5,6,7,8`** is also **`select 5-8.`** Note that this selects the given residue numbers in all macromolecule chains.

The second type of primitive expression specifies a sequence of fields that must match for a given atom. The first part specifies a residue (or group of residues) and an optional second part specifies the atoms within those residues. The first part consists of a residue name, optionally followed by a residue number and/or chain identifier.

A residue name typically consists of up to three alphabetic characters, which are case insensitive. Hence the primitive expressions **SER** and **`ser`** are equivalent, identifying all cysteine residues. Residue names that contain non-alphabetic characters, such as sulphate groups, may be delimited using square brackets, i.e. **`[SO4]`**

The residue number is the residue's position in the macromolecule sequence. Negative sequence numbers are permited. For example, **`SER70`** Care must be taken when specifying both residue name and number, it the group at the specified position isn't the specified residue no atoms are selected.

The chain identifier is typically a single case-insensitive alphabetic or numeric character. Numeric chain

identifiers must be distinguished or separated from residue numbers by a colon character. For example, **SER70A** or **SER70:1**

The second part consists of a period character followed by an atom name. An atom name may be up to four alphabetic or numeric characters.

An asterisk may be used as a wild card for a whole field and a question mark as a single character wildcard.

Comparison Operators

Parts of a molecule may also be distinguished using equality, inequality and ordering operators on their properties. The format of such comparison expression is a property name, followed by a comparison operator and then an integer value.

The atom properties that may be used in RasMol are **atomno** for the atom serial number, **resno** for the residue number, **radius** for the spacefill radius in RasMol units (or zero if not represented as a sphere) and **temperature** for the PDB anisotropic temperature value.

The equality operator is denoted either "**=**" or "**==**". The inequality operator as either "**<>**", "**!=**" or "**/=**". The ordering operators are "**<**" for less than, "**<=**" for less than or equal to, "**>**" for greater than, and "**>=**" for greater than or equal to.

```
Examples:    resno < 23
             temperature >= 900
             atomno == 487
```


Within Expressions

K A RasMol **within** expression allows atoms to be selected on their proximity to another set of atoms. A **within** expression takes two parameters separated by a comma and surrounded by parenthesis. The first argument is an integer value called the "cut-off" distance of the within expression and the second argument is any valid atom expression. The cut-off distance is expressed in RasMol 0.004 Angstrom units. An atom is selected if it is within the cut-off distance of any of the atoms defined by the second argument. This allows complex expressions to be constructed containing nested **within** expressions.

For example, the command **select within(800,backbone)** selects any atom within a 3.2 Angstrom radius of any atom in a protein or nucleic acid backbone. **Within** expressions are particularly useful for selecting the atoms around an active site.

K within

Predefined Sets

KRasMol atom expressions may contain predefined sets. Thsese sets are single keywords that represent portions of a molecule of interest. Predefined sets are often abbreviations primitive atom expressions, and in some cases of selecting areas of a molecule that could not otherwise be distinguished. A list of the currently predefined sets is given below.

K sets