

#<sup>1</sup>\$<sup>2</sup>+<sup>3</sup>

# RasMol V2.3

## Molecular Visualisation Program

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1rasmol  
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## +<sup>5</sup>#<sup>6</sup>\$<sup>7</sup> **Introduction**

RasMol2 is an X11 windows system tool intended for the visualisation of proteins and nucleic acids. RasMol requires either an 8bit pseudo colour or a 24bit (32bit) true colour display. The program reads in a specified Brookhaven protein databank (PDB) file and determines the connectivity from the residue information provided. This may then rendered on the screen in a variety of formats and colour schemes. Currently available molecule representations include depth-cued wireframes, sticks, space filling 'union of spheres', ball and stick models and protein ribbon diagrams.

5doc  
6chintro  
7Introduction

## +<sup>8</sup><sub>μ</sub><sup>9</sup>\$<sup>10</sup> **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.

<u>backbone</u>	<u>colour</u>	<u>exit</u>	<u>hbond</u>
<u>help</u>	<u>load</u>	<u>quit</u>	<u>reset</u>
<u>restrict</u>	<u>ribbon</u>	<u>rotate</u>	<u>save</u>
<u>script</u>	<u>select</u>	<u>set</u>	<u>show</u>
<u>slab</u>	<u>spacefill</u>	<u>structure</u>	<u>ssbond</u>
<u>translate</u>	<u>wireframe</u>	<u>write</u>	<u>zap</u>

8doc

9chcomref

10Command Reference

+<sup>11</sup>#<sup>12</sup>\$<sup>13</sup>^<sup>14</sup>**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 parameter 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.

11doc  
12backbone  
13Backbone  
14backbone

+<sup>15</sup>#<sup>16</sup>\$<sup>17</sup>K<sup>18</sup>**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.

15doc

16background

17Background

18background

+<sup>19</sup>#<sup>20</sup>#<sup>21</sup>\$<sup>22</sup>K<sup>23</sup>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.

19doc  
20center  
21centre  
22Centre  
23centre

+<sup>24</sup>#<sup>25</sup>#<sup>26</sup>\$<sup>27</sup>K<sup>28</sup> 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, 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, 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>.

24doc  
25color  
26colour  
27Colour  
28colour



+<sup>29</sup><sub>4</sub>#<sup>30</sup><sub>4</sub>#<sup>31</sup><sub>4</sub>\$<sup>32</sup><sub>4</sub>K<sup>33</sup><sub>4</sub>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.

29doc  
30hbond  
31hbonds  
32HBonds  
33hbonds

+<sup>34</sup> <sup>35</sup># <sup>36</sup>\$ <sup>37</sup>K **Help**

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

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

34doc  
35help  
36Help  
37help

+<sup>38</sup><sub>44</sub>#<sup>39</sup><sub>5</sub>\$<sup>40</sup><sub>1</sub><sup>41</sup><sub>1</sub> **Load**

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

Load either a Brookhaven Protein Databank (PDB) file or Alchemy(tm) format file into RasMol2. Only a single PDB file may be loaded at a time. This command selects all the atoms in the molecule, and sets the default representation to be a cpk coloured wireframe model.

38doc  
39load  
40Load  
41load

+<sup>42</sup>#<sup>43</sup>#<sup>44</sup>\$<sup>45</sup>K<sup>46</sup>Quit

**Syntax:**    quit  
              exit

Exit from the RasMol program.

42doc  
43exit  
44quit  
45Quit  
46quit

+<sup>47</sup><sub>48</sub><sup>49</sup><sub>50</sub><sup>51</sup> # # \$ K **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.

47doc  
48renum  
49renumber  
50Renumber  
51renumber

+<sup>52</sup>/<sub>53</sub>g<sup>54</sup>r<sup>55</sup>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, 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.

52doc  
53reset  
54Reset  
55reset

+<sup>56</sup>#<sup>57</sup>\$<sup>58</sup>K<sup>59</sup>**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.

56doc

57restrict

58Restrict

59restrict

+6061626364Ribbons

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

The RasMol **ribbons** command displays the currently loaded protein 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 width of the ribbon at each position is determined by the optional parameter in the usual RasMol units. By default this value is 380, which produces a ribbon 1.52 Angstroms wide. The number of strands in the ribbon may be altered using the RasMol set strands command. The rendering of the ribbon may also be changed using the set ribbons command.

60doc  
61ribbon  
62ribbons  
63Ribbons  
64ribbons



+<sup>65</sup> #<sup>66</sup> \$<sup>67</sup> K<sup>68</sup> **Rotate**

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

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.

65doc  
66rotate  
67Rotate  
68rotate

+<sup>69</sup><sub>44</sub><sup>70</sup><sub>6</sub><sup>71</sup><sub>1</sub><sup>72</sup><sub>7</sub> 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.

69doc  
70save  
71Save  
72save

## +<sup>73</sup>#<sup>74</sup>\$<sup>75</sup>K<sup>76</sup> 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 complicated sequences of actions to be executed.

73doc  
74script  
75Script  
76script

+<sup>77</sup><sub>44</sub><sup>78</sup><sub>79</sub><sup>80</sup><sub>80</sub> \$ K **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.

77doc  
78select  
79Select  
80select

+<sup>81</sup>#<sup>82</sup>\$<sup>83</sup>K<sup>84</sup>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 type [help set <parameter>](#).

<u><a href="#">ambient</a></u>	<u><a href="#">background</a></u>	<u><a href="#">bondmode</a></u>	<u><a href="#">hbonds</a></u>
<u><a href="#">hetero</a></u>	<u><a href="#">hourglass</a></u>	<u><a href="#">hydrogen</a></u>	<u><a href="#">mouse</a></u>
<u><a href="#">shadow</a></u>	<u><a href="#">slabmode</a></u>	<u><a href="#">specular</a></u>	<u><a href="#">specpower</a></u>
<u><a href="#">ssbonds</a></u>	<u><a href="#">strands</a></u>		

81doc  
82set  
83Set  
84set

+<sup>85</sup>#<sup>86</sup>\$<sup>87</sup>K<sup>88</sup> Show

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

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.

85doc  
86show  
87Show  
88show

+<sup>89</sup>#<sup>90</sup>\$<sup>91</sup>K<sup>92</sup>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.

89doc  
90slab  
91Slab  
92slab

+<sup>93</sup> #<sup>94</sup> \$<sup>95</sup> K<sup>96</sup> **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.

93doc  
94spacefill  
95Spacefill  
96spacefill



+<sup>97</sup>#<sup>98</sup>#<sup>99</sup>\$<sup>100</sup>K<sup>101</sup>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.

97doc  
98ssbond  
99ssbonds  
100SSBonds  
101ssbonds

+<sup>102</sup>#<sup>103</sup>\$<sup>104</sup>K<sup>105</sup>**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 determined using Kabsch and Sander's DSSP algorithm. Once finished the program reports the number of helices and ladders found.

102doc

103structure

104Structure

105structure

+<sup>106</sup>#<sup>107</sup>\$<sup>108</sup>K<sup>109</sup>**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.

106doc  
107translate  
108Translate  
109translate

+<sup>110</sup>#<sup>111</sup>\$<sup>112</sup>K<sup>113</sup>**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.

110doc  
111wireframe  
112Wireframe  
113wireframe

+<sup>114</sup>#<sup>115</sup>\$<sup>116</sup>K<sup>117</sup>**Write**

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

Write the current image to a file in a standard raster format. Currently supported 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). This command should not be confused with the RasMol save command which save the currently selected portion of the molecule.

114doc  
115write  
116Write  
117write

+<sup>118</sup>#<sup>119</sup>\$<sup>120</sup>K<sup>121</sup>**Zap**

**Syntax:**     **zap**

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

118doc  
119zap  
120Zap  
121zap

+<sup>122</sup>#<sup>123</sup>\$<sup>124</sup>K<sup>125</sup>**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.

122doc  
123zoom  
124Zoom  
125zoom

## +<sup>126</sup>μ<sup>127</sup>\$<sup>128</sup>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.

<u>ambient</u>	<u>background</u>	<u>bondmode</u>	<u>hbonds</u>
<u>hetero</u>	<u>hourglass</u>	<u>hydrogen</u>	<u>mouse</u>
<u>shadow</u>	<u>slabmode</u>	<u>specular</u>	<u>specpower</u>
<u>ssbonds</u>	<u>strands</u>		

126doc

127chsetopt

128Internal Parameters



+<sup>129</sup>#<sup>130</sup>\$<sup>131</sup>K<sup>132</sup> **Set Ambient**

K<sup>133</sup> **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 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.

129doc  
130setambient  
131Set Ambient  
132set ambient  
133ambient

+<sup>134</sup>#<sup>135</sup>\$<sup>136</sup>K<sup>137</sup> **Set Background**

K<sup>138</sup> **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.

134doc  
135setbackground  
136Set Background  
137set background  
138background

+<sup>139</sup>#<sup>140</sup>\$<sup>141</sup>K<sup>142</sup>Set BondMode

K<sup>143</sup>Syntax: set bondmode and  
set bondmode or

set bondmode

139doc

140setbondmode

141Set BondMode

142set bondmode

143bondmode

+<sup>144</sup><sub>#</sub><sup>145</sup><sub>\$</sub><sup>146</sup><sub>K</sub><sup>147</sup> **Set Display**

<sup>148</sup>**Syntax:**   **set display selected**  
                  **set display normal**

set display

144doc  
145setdisplay  
146Set Display  
147set display  
148display

+<sup>149</sup>#<sup>150</sup>\$<sup>151</sup>K<sup>152</sup>Set HBonds

K<sup>153</sup>K<sup>154</sup>K<sup>155</sup>**Syntax:**    **set hbonds backbone**  
                  **set hbonds sidechain**

set hbonds

149doc  
150sethbonds  
151Set HBonds  
152set hbonds  
153hbonds  
154sidechain  
155backbone

+<sup>156</sup>#<sup>157</sup>\$<sup>158</sup>K<sup>159</sup>**Set Hetero**

K<sup>160</sup>**Syntax:**    **set hetero** <boolean>

set hetero

156doc  
157sethetero  
158Set Hetero  
159set hetero  
160hetero

+<sup>161</sup>#<sup>162</sup>\$<sup>163</sup>K<sup>164</sup>**Set HourGlass**

K<sup>165</sup>**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.

161doc  
162sethourglass  
163Set HourGlass  
164set hourglass  
165hourglass

+<sup>166</sup>#<sup>167</sup>\$<sup>168</sup>K<sup>169</sup> **Set Hydrogen**

K<sup>170</sup> **Syntax:**    **set hydrogen** <boolean>

set hydrogen

166doc  
167sethydrogen  
168Set Hydrogen  
169set hydrogen  
170hydrogen



+<sup>171</sup>#<sup>172</sup>\$<sup>173</sup>K<sup>174</sup>**Set Mouse**

K<sup>175</sup>K<sup>176</sup>K<sup>177</sup>K<sup>178</sup>**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.

171doc  
172setmouse  
173Set Mouse  
174set mouse  
175mouse  
176rasmol  
177insight  
178quanta

+<sup>179</sup>#<sup>180</sup>\$<sup>181</sup>K<sup>182</sup> **Set Ribbons**

K<sup>183</sup>K<sup>184</sup>K<sup>185</sup> **Syntax:**    **set ribbons strands**  
                          **set ribbons solid**

The RasMol **set ribbons** command controls the way that macromolecular ribbons are displayed. The default value **strands** display macromolecular ribbons as parallel depth-cued strands that pass along the protein or nucleic acid backbone. The number of strands in the ribbon may be altered using the RasMol [set strands](#) command. The **set ribbons solid** command renders the macromolecular ribbon as a solid shaded ribbon.

179doc  
180setribbons  
181Set Ribbons  
182set ribbons  
183ribbons  
184strands  
185solid

+<sup>186</sup>#<sup>187</sup>\$<sup>188</sup>K<sup>189</sup> **Set Shadow**

K<sup>190</sup> **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 appropriate viewpoint is selected, to provide a greater impression of depth.

186doc  
187setshadow  
188Set Shadow  
189set shadow  
190shadow

+<sup>191</sup>#<sup>192</sup>\$<sup>193</sup>K<sup>194</sup>**Set SlabMode**

K<sup>195</sup>K<sup>196</sup>K<sup>197</sup>K<sup>198</sup>K<sup>199</sup>K<sup>200</sup>**Syntax: set slabmode <slabmode>**

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

191doc  
192setslabmode  
193Set SlabMode  
194set slabmode  
195slabmode  
196reject  
197half  
198hollow  
199solid  
200section

## <sup>+201</sup><sub>#</sub><sup>202</sup><sub>\$</sub><sup>203</sup><sub>K</sub><sup>204</sup> **Set Specular**

<sup>K</sup><sup>205</sup> **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.

201doc  
202setspecular  
203Set Specular  
204set specular  
205specular

+<sup>206</sup>#<sup>207</sup>\$<sup>208</sup>K<sup>209</sup> **Set SpecPower**

K<sup>210</sup> **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 coefficient 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.

206doc  
207setspecpower  
208Set SpecPower  
209set specpower  
210specpower

+<sup>211</sup>#<sup>212</sup>\$<sup>213</sup>K<sup>214</sup>Set SSBonds

K<sup>215</sup>K<sup>216</sup>K<sup>217</sup>**Syntax:**    **set ssbonds backbone**  
                  **set ssbonds sidechain**

set ssbonds

211doc  
212setssbonds  
213Set SSBonds  
214set ssbonds  
215ssbonds  
216backbone  
217sidechain

+<sup>218</sup>#<sup>219</sup>\$<sup>220</sup>K<sup>221</sup> **Set Strands**

K<sup>222</sup> **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 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.

218doc  
219setstrands  
220Set Strands  
221set strands  
222strands



## <sup>+223</sup><sub>#</sub><sup>224</sup><sub>\$</sub> 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 backbone atoms, not the protein and [nucleic] acid backbone atoms!

- Primitive Expressions
- Predefined Sets
- Comparison Operators
- Within Expressions
- Example Expressions

## +<sup>226</sup>#<sup>227</sup>\$<sup>228</sup>K<sup>229</sup>Example Expressions

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

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

226doc

227exampleexpressions

228Example Expressions

229example expressions

RasMol primitive expressions are the fundamental building blocks of atom expressions. There are two basic 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 permitted. For example, **SER70**. Care must be taken when specifying both residue name and number, if 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.

## +<sup>234</sup><sub>#</sub><sup>235</sup><sub>\$</sub><sup>236</sup><sub>K</sub><sup>237</sup> 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**

234doc  
235comparisonoperators  
236Comparison Operators  
237comparison operators

## +<sup>238</sup>#<sup>239</sup>\$<sup>240</sup>K<sup>241</sup> Within Expressions

K<sup>242</sup> 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 usefull for selecting the atoms around an active site.

238doc  
239withinexpressions  
240Within Expressions  
241within expressions  
242within

+<sup>243</sup><sub>#</sub><sup>244</sup><sub>\$</sub><sup>245</sup><sub>K</sub><sup>246</sup>**Predefined Sets**

K<sup>247</sup> RasMol atom expressions may contain predefined sets. These 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.

<u>at</u>	<u>acidic</u>	<u>acyclic</u>	<u>aliphatic</u>
<u>alpha</u>	<u>amino</u>	<u>aromatic</u>	<u>backbone</u>
<u>basic</u>	<u>buried</u>	<u>cg</u>	<u>charged</u>
<u>cyclic</u>	<u>cystine</u>	<u>helix</u>	<u>hetero</u>
<u>hydrogen</u>	<u>hydrophobic</u>	<u>large</u>	<u>medium</u>
<u>neutral</u>	<u>nucleic</u>	<u>polar</u>	<u>protein</u>
<u>purine</u>	<u>pyrimidine</u>	<u>selected</u>	<u>sheet</u>
<u>sidechain</u>	<u>small</u>	<u>surface</u>	<u>turn</u>
<u>water</u>			

243doc  
244predefinedsets  
245Predefined Sets  
246predefined sets  
247sets

+<sup>248</sup>#<sup>249</sup>\$<sup>250</sup>K<sup>251</sup>AT Set

K<sup>252</sup>This set contains the atoms in the complementary nucleotides adenosine and thymidine (A and T respectively). All nucleotides are classified as either the set **at** or the set cg This set is equivalent to the RasMol atom expressions "a,t" and "nucleic and not cg"

248doc  
249atset  
250AT Set  
251at set  
252at

+<sup>253</sup>#<sup>254</sup>\$<sup>255</sup>K<sup>256</sup> **Acidic Set**

K<sup>257</sup>The set of acidic amino acids. These are the residue types Asp, Glu and Tyr. All amino acids are classified as either **acidic**, basic or neutral. This set is equivalent to the RasMol atom expressions "**asp, glu, tyr**" and "**amino and not (basic or neutral)**"

253doc  
254acidicset  
255Acidic Set  
256acidic set  
257acidic



+<sup>258</sup>#<sup>259</sup>\$<sup>260</sup>K<sup>261</sup> **Acyclic Set**

K<sup>262</sup>The set of atoms in amino acids not containing a cycle or ring. All amino acids are classified as either cyclic or **acyclic**. This set is equivalent to the RasMol atom expression "**amino and not cyclic**"

258doc

259acyclicset

260Acyclic Set

261acyclic set

262acyclic

+<sup>263</sup>#<sup>264</sup>\$<sup>265</sup>K<sup>266</sup> **Aliphatic Set**

K<sup>267</sup>This set contains the aliphatic amino acids. These are the amino acids Ala, Gly, Ile, Leu and Val. This set is equivalent to the RasMol atom expression "**ala, gly, ile, leu, val**"

263doc  
264aliphaticset  
265Aliphatic Set  
266aliphatic set  
267aliphatic

+<sup>268</sup>#<sup>269</sup>\$<sup>270</sup>K<sup>271</sup> **Alpha Set**

K<sup>272</sup>The set of alpha carbons in the protein molecule. This set is approximately equivalent to the RasMol atom expression "**\*.CA**" This command should not be confused with the predefined set helix which contains the atoms in the amino acids of the protein's alpha helices.

268doc  
269alphaset  
270Alpha Set  
271alpha set  
272alpha

<sup>273</sup>+<sup>274</sup>#<sup>275</sup>\$<sup>276</sup>K **Amino Set**

<sup>277</sup>K This set contains all the atoms contained in amino acid residues. This is useful for distinguishing the protein from the nucleic acid and heterogenous atoms in the current molecule database.

273doc  
274aminoset  
275Amino Set  
276amino set  
277amino

<sup>278</sup>+<sup>279</sup>#<sup>280</sup>\$<sup>281</sup>K **Aromatic Set**

<sup>282</sup>K The set of atoms in amino acids containing aromatic rings. These are the amino acids His, Phe, Trp and Tyr. Because they contain aromatic rings all members of this set are member of the predefined set cyclic. This set is equivalent to the RasMol atom expressions "**his, phe, trp, tyr**" and "**cyclic and not pro**"

278doc

279aromaticset

280Aromatic Set

281aromatic set

282aromatic

+<sup>283</sup><sub>#</sub><sup>284</sup><sub>\$</sub><sup>285</sup><sub>K</sub><sup>286</sup>**Backbone Set**

<sup>287</sup>This set contains the four atoms of each amino acid that form the polypeptide N-C-C-O backbone of proteins, and the atoms the sugar phosphate backbone of nucleic acids. Use the RasMol predefined sets **protein** and **nucleic** to distinguish between the two forms of backbone. Atoms in nucleic acids and proteins are either **backbone** or sidechain. This set is equivalent to the RasMol expression "(protein or nucleic) and not sidechain

283doc  
284backboneset  
285Backbone Set  
286backbone set  
287backbone

<sup>+288</sup><sub>#</sub><sup>289</sup><sub>\$</sub><sup>290</sup><sub>K</sub><sup>291</sup>**Basic Set**

<sup>292</sup><sub>K</sub>The set of basic amino acids. These are the residue types Asp, Glu and Tyr. All amino acids are classified as either acidic, **basic** or neutral. This set is equivalent to the RasMol atom expressions "**asp, glu, tyr**" and "**amino and not (acidic or neutral)**"

288doc  
289basicset  
290Basic Set  
291basic set  
292basic

+<sup>293</sup>#<sup>294</sup>\$<sup>295</sup>K<sup>296</sup>**Buried Set**

K<sup>297</sup>This set contains the atoms in those amino acids that tend (prefer) to buried inside protein, away from contact with solvent molecules. This set refers to the amino acids preference and not the actual solvent accessability for the current protein. All amino acids are classified as either surface or **buried**. This set is equivalent to the RasMol atom expression "**amino and not surface**"

293doc  
294buriedset  
295Buried Set  
296buried set  
297buried



<sup>+298</sup><sub>#</sub><sup>299</sup><sub>\$</sub><sup>300</sup><sub>K</sub><sup>301</sup>**CG Set**

<sup>302</sup><sub>K</sub> This set contains the atoms in the complementary nucleotides cytidine and guanine (C and G respectively). All nucleotides are classified as either the set at or the set **cg** This set is equivalent to the RasMol atom expressions "**c,g**" and "**nucleic and not at**"

298doc  
299cgset  
300CG Set  
301cg set  
302cg

+<sup>303</sup>#<sup>304</sup>\$<sup>305</sup>K<sup>306</sup> **Charged Set**

K<sup>307</sup>This set contains the charged amino acids. These are the amino acids that are either acidic or basic. Amino acids are classified as being either **charged** or neutral. This set is equivalent to the RasMol atom expressions "**acidic or basic**" and "**amino and not neutral**"

303doc  
304chargedset  
305Charged Set  
306charged set  
307charged

+<sup>308</sup>#<sup>309</sup>\$<sup>310</sup>K<sup>311</sup>**Cyclic Set**

K<sup>312</sup>The set of atoms in amino acids containing a cycle or rings. All amino acids are classified as either **cyclic** or **acyclic**. This set consists of the amino acids His, Phe, Pro, Trp and Tyr. The members of the predefined set aromatic are members of this set. The only cyclic but non-aromatic amino acid is proline. This set is equivalent to the RasMol atom expressions "**his, phe, pro, trp, tyr**" and "**aromatic or pro**" and "**amino and not acyclic**"

308doc

309cyclicset

310Cyclic Set

311cyclic set

312cyclic

+<sup>313</sup><sub>#</sub><sup>314</sup><sub>\$</sub><sup>315</sup><sub>K</sub><sup>316</sup> **Cystine Set**

<sup>317</sup>K This set contains the atoms of cysteine residues that form part of a disulphide bridge, i.e. half cystines. RasMol automatically determines disulphide bridges, if neither the predefined set **cystine** nor the RasMol ssbonds command have been used since the molecule was loaded. The set of free cysteines may be determined using the RasMol atom expression "**cys and not cystine**"

313doc  
314cystineset  
315Cystine Set  
316cystine set  
317cystine

+<sup>318</sup>#<sup>319</sup>\$<sup>320</sup>K<sup>321</sup>**Helix Set**

K<sup>322</sup>This set contains all atoms that form part of a protein alpha helix as determined by either the PDB file author or Kabsch and Sander's DSSP algorithm. By default, RasMol uses the secondary structure determination given in the PDB file if it exists. Otherwise, it uses the DSSP algorithm as used by the RasMol structure command.

This command should not be confused with the predefined set alpha which contains the alpha carbon atoms of a protein.

318doc  
319helixset  
320Helix Set  
321helix set  
322helix

+<sup>323</sup><sub>#</sub><sup>324</sup><sub>\$</sub><sup>325</sup><sub>K</sub><sup>326</sup>**Hetero Set**

K<sup>327</sup> This set contains all the heterogenous atoms in the molecule. These are the atoms described by HETATM entries in the PDB file. These typically contain water, cofactors and other solvents and ligands. The RasMol predefined set water is often used to partition this set.

323doc  
324heteroset  
325Hetero Set  
326hetero set  
327hetero

+<sup>328</sup>#<sup>329</sup>\$<sup>330</sup>K<sup>331</sup> **Hydrogen Set**

K<sup>332</sup> This predefined set contains all the hydrogen and deuterium atoms of the current molecule.

328doc  
329hydrogenset  
330Hydrogen Set  
331hydrogen set  
332hydrogen

+<sup>333</sup><sub>μ</sub><sup>334</sup>#<sup>335</sup>\$<sup>336</sup>K<sup>337</sup>Hydrophobic Set

K<sup>337</sup>This set contains all the hydrophobic amino acids. These are the amino acids Ala, Leu, Val, Ile, Pro, Phe, Met and Trp. All amino acids are classified as either **hydrophobic** or polar. This set is equivalent to the RasMol atom expressions "**ala, leu, val, ile, pro, phe, met, trp**" and "**amino and not polar**"

333doc  
334hydrophobicset  
335Hydrophobic Set  
336hydrophobic set  
337hydrophobic



+<sup>338</sup>#<sup>339</sup>\$<sup>340</sup>K<sup>341</sup>**Large Set**

K<sup>342</sup> All amino acids are classified as either small, medium or **large**. This set is equivalent to the RasMol atom expression "**amino and not (small or medium)**"

338doc  
339largeset  
340Large Set  
341large set  
342large

+<sup>343</sup><sub>#</sub><sup>344</sup><sub>\$</sub><sup>345</sup><sub>K</sub><sup>346</sup>**Medium Set**

K<sup>347</sup> All amino acids are classified as either small, **medium** or large. This set is equivalent to the RasMol atom expression "**amino and not (large or small)**"

343doc  
344mediumset  
345Medium Set  
346medium set  
347medium

+<sup>348</sup>#<sup>349</sup>\$<sup>350</sup>K<sup>351</sup>Neutral Set

K<sup>352</sup>The set of neutral amino acids. All amino acids are classified as either acidic, **basic** or neutral. This set is equivalent to the RasMol atom expression "**amino and not (acidic or basic)**"

348doc

349neutralset

350Neutral Set

351neutral set

352neutral

+<sup>353</sup>#<sup>354</sup>\$<sup>355</sup>K<sup>356</sup>**Nucleic Set**

K<sup>357</sup>The set of all atoms in nucleic acids.

353doc

354nucleicset

355Nucleic Set

356nucleic set

357nucleic

+<sup>358</sup>#<sup>359</sup>\$<sup>360</sup>K<sup>361</sup> **Polar Set**

K<sup>362</sup>This set contains the polar amino acids. All amino acids are classified as either hydrophobic or **polar**. This set is equivalent to the RasMol atom expression "**amino and not hydrophobic**"

358doc

359polarset

360Polar Set

361polar set

362polar

+<sup>363</sup><sub>#</sub><sup>364</sup><sub>\$</sub><sup>365</sup><sub>K</sub><sup>366</sup>**Protein Set**

<sup>367</sup>K The set of all atoms in proteins. This consists of the RasMol predefined set amino and common post-translation modifications.

363doc  
364proteinset  
365Protein Set  
366protein set  
367protein

+<sup>368</sup>#<sup>369</sup>\$<sup>370</sup>K<sup>371</sup> **Purine Set**

K<sup>372</sup>The set of purine nucleotides. These are the bases adenosine and guanosine (A and G respectively). All nucleotides are either **purines** or pyrimidines. This set is equivalent to the RasMol atom expressions "**a,g**" and "**nucleic and not purine**"

368doc

369purineset

370Purine Set

371purine set

372purine

+<sup>373</sup><sub>μ</sub><sup>374</sup>#<sup>375</sup>\$<sup>376</sup>K<sup>377</sup>Pyrimidine Set

K<sup>377</sup>The set of pyrimidine nucleotides. These are the bases cytidine and thymidine (C and T respectively). All nucleotides are either **purineset purines** or **pyrimidines**. This set is equivalent to the RasMol atom expressions "**c,t**" and "**nucleic and not pyrimidine**"

373doc

374pyrimidineset

375Pyrimidine Set

376pyrimidine set

377pyrimidine



+<sup>378</sup>#<sup>379</sup>\$<sup>380</sup>K<sup>381</sup>**Selected Set**

K<sup>382</sup>This set contains the set of atoms in the currently active zone. The currently active zone is defined by the preceding select or restrict command and not the atom expression containing the **selected** keyword.

378doc  
379selectedset  
380Selected Set  
381selected set  
382selected

+<sup>383</sup><sub>μ</sub><sup>384</sup>#<sup>385</sup>\$<sup>386</sup>K<sup>387</sup>Sheet Set

K<sup>387</sup>This set contains all atoms that form part of a protein beta sheet as determined by either the PDB file author or Kabsch and Sander's DSSP algorithm. By default, RasMol uses the secondary structure determination given in the PDB file if it exists. Otherwise, it uses the DSSP algorithm as used by the RasMol structure command.

383doc  
384sheetset  
385Sheet Set  
386sheet set  
387sheet

+<sup>388</sup>#<sup>389</sup>\$<sup>390</sup>K<sup>391</sup> **Sidechain Set**

K<sup>392</sup>This set contains the functional sidechains of any amino acids and the base of each nucleotide. These are the atoms not part of the polypeptide N-C-C-O backbone of proteins or the sugar phosphate backbone of nucleic acids. Use the RasMol predefined sets **protein** and **nucleic** to distinguish between the two forms of sidechain. Atoms in nucleic acids and proteins are either backbone or **sidechain**. This set is equivalent to the RasMol expression "(protein or nucleic) and not backbone"

388doc  
389sidechainset  
390Sidechain Set  
391sidechain set  
392sidechain

+<sup>393</sup>#<sup>394</sup>\$<sup>395</sup>K<sup>396</sup> **Small Set**

K<sup>397</sup> All amino acids are classified as either **small**, medium or large. This set is equivalent to the RasMol atom expression "**amino and not (medium or large)**"

393doc  
394smallset  
395Small Set  
396small set  
397small

+<sup>398</sup>#<sup>399</sup>\$<sup>400</sup>K<sup>401</sup> **Surface Set**

K<sup>402</sup> This set contains the atoms in those amino acids that tend (prefer) to be on the surface of proteins, in contact with solvent molecules. This set refers to the amino acids preference and not the actual solvent accessibility for the current protein. All amino acids are classified as either **surface** or buried. This set is equivalent to the RasMol atom expression "**amino and not buried**"

398doc  
399surfaceset  
400Surface Set  
401surface set  
402surface

+<sup>403</sup><sub>#</sub><sup>404</sup><sub>\$</sub><sup>405</sup><sub>K</sub><sup>406</sup><sub>Turn Set</sub>

<sup>407</sup>This set contains all atoms that form part of a protein turns as determined by either the PDB file author or Kabsch and Sander's DSSP algorithm. By default, RasMol uses the secondary structure determination given in the PDB file if it exists. Otherwise, it uses the DSSP algorithm as used by the RasMol structure command.

403doc  
404turnset  
405Turn Set  
406turn set  
407turn

+<sup>408</sup>#<sup>409</sup>\$<sup>410</sup>K<sup>411</sup> **Water Set**

K<sup>412</sup> This set contains all the heterogenous water molecules in the current database. A large number of water molecules are sometimes associated with protein and nucleic acid structures determined by X-ray crystallography. These atoms tend to clutter an image.

408doc

409waterset

410Water Set

411water set

412water

## +<sup>413</sup>#<sup>414</sup>\$<sup>415</sup>Colour Schemes

The RasMol colour command allows different objects (such as atoms, bonds and ribbon segments) to be given a specified colour. Typically this colour is either a RasMol predefined colour name or an RGB triple. Additionally RasMol also supports amino, chain, group, shapely, structure, temperature, user and hbond type colour schemes. The currently predefined colour names are

413doc  
414chcolours  
415Colour Schemes



+<sup>416</sup>#<sup>417</sup>\$<sup>418</sup>K<sup>419</sup> **Amino Colours**

The RasMol **amino** colour scheme colours amino acids according to traditional amino acid properties. The purpose of colouring is to identify amino acids in an unusual or surprising environment. The outer parts of a protein are polar are visible (bright) colours and non-polar residues darker. Most colours are hallowed by tradition. This colour scheme is similar to the shapely scheme.

416doc  
417aminocolours  
418Amino Colours  
419amino colours

+<sup>420</sup>#<sup>421</sup>\$<sup>422</sup>K<sup>423</sup> **Chain Colours**

The RasMol **chain** colour scheme assigns each macromolecular chain a unique colour. This colour scheme is particularly usefull for distinguishing the parts of multimeric structure or the individual `strands' of a DNA chain.

420doc  
421chaincolours  
422Chain Colours  
423chain colours

## <sup>+424</sup><sub>#</sub><sup>425</sup><sub>\$</sub><sup>426</sup><sub>K</sub><sup>427</sup> CPK Colours

The RasMol **cpk** colour scheme is based upon the colours of the popular plastic spacefilling models which were developed by Corey, Pauling and later improved by Kultun. This colour scheme colour `atom' objects by the atom (element) type. This is the scheme conventionally used by chemists.

424doc  
425cpkcolours  
426CPK Colours  
427cpk colours

## <sup>+428</sup><sub>#</sub><sup>429</sup><sub>\$</sub><sup>430</sup><sub>K</sub><sup>431</sup> Group Colours

The RasMol **group** colour scheme colour codes residues by their position in a macromolecular chain. Each chain is drawn as a smooth spectrum from blue through green, yellow and orange to red. Hence the N terminus of proteins and 5' terminus of nucleic acids are coloured red and the C terminus of proteins and 3' terminus of nucleic acids are drawn in blue. If a chain has a large number of heterogenous molecules associated with it, the macromolecule may not be drawn in the full 'range' of the spectrum.

428doc  
429groupcolours  
430Group Colours  
431group colours

## <sup>+432</sup><sub>#</sub><sup>433</sup><sub>\$</sub><sup>434</sup><sub>K</sub><sup>435</sup> **Shapely Colours**

The RasMol **shapely** colour scheme colour codes residues by amino acid property. This scheme is based upon Bob Fletterick's "Shapely Models". Each amino acid and nucleic acid residue is given a unique colour. The **shapely** colour scheme is used by David Bacon's Raster3D program. This colour scheme is similar to the [amino](#) colour scheme.

432doc  
433shapelycolours  
434Shapely Colours  
435shapely colours

+<sup>436</sup><sub>#</sub><sup>437</sup><sub>\$</sub><sup>438</sup><sub>K</sub><sup>439</sup> **Structure Colours**

The RasMol **structure** colour scheme colours the molecule by protein secondary structure. Alpha helices are coloured magenta, beta sheets are coloured yellow, turns are coloured pale blue, [96,128,255] and all other residues are coloured white. The secondary structure is either read from the PDB file (HELIX and SHEET records), if available, or determined using Kabsch and Sander's DSSP algorithm. The RasMol structure command may be used to force DSSP's structure assignment to be used.

436doc  
437structurecolours  
438Structure Colours  
439structure colours

## <sup>+440</sup><sub>#</sub><sup>441</sup><sub>\$</sub><sup>442</sup><sub>K</sub><sup>443</sup><sub>T</sub>Temperature Colours

The RasMol **temperature** colour scheme colour codes each atom according to the anisotropic temperature (beta) value stored in the PDB file. Typically this gives a measure of the mobility/uncertainty of a given atom's position. High values are coloured in warmer (red) colours and lower values in colder (blue) colours. This feature is often used to associate a "scale" value [such as amino acid variability in viral mutants] with each atom in a PDB file, and colour the molecule appropriately.

440doc

441temperaturecolours

442Temperature Colours

443temperature colours

+<sup>444</sup><sub>#</sub><sup>445</sup><sub>\$</sub><sup>446</sup><sub>K</sub><sup>447</sup>**User Colours**

The RasMol **user** colour scheme allows RasMol to use the colour scheme stored in the PDB file. The colours for each atom are stored in COLO records placed in the PDB data file. This convention was introduced by David Bacon's Raster3D program.

444doc  
445usercolours  
446User Colours  
447user colours



#### <sup>+448</sup><sub>#</sub><sup>449</sup><sub>\$</sub><sup>450</sup><sub>K</sub><sup>451</sup> HBond Type Colours

The RasMol **type** colour scheme applies only to hydrogen bonds, hence is used in the command "**colour hbonds type**". This colour scheme colour codes each hydrogen bond according to the distance along a protein chain between hydrogen bond donor and acceptor. This schematic representation was introduced by Belhadj-Mostefa and Milner-White. This representation gives a good insight into protein secondary structure (hbonds forming alpha helices appear red, those forming sheets appear yellow and those forming turns appear magenta).

448doc  
449hbondtypecolours  
450HBond Type Colours  
451hbond type colours