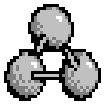

RasMol Quick Reference

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Mouse Buttons (PC)

Clicking on an atom identifies that atom in the command window.

Left Button	Rotate X-Y
Right Button	Translate X-Y
Shift Left Button	Zoom
Shift Right Button	Rotate Z
Control Left Button	Z-Clipping (Slab)

General Commands

load [format] <filename> Load a molecule
- **pdb** Brookhaven Protein Databank
- **others** see documentation

zap Delete molecule
exit Exit from RasMol

help [topic [subtopic]] Display on-line help topic

Selection

select <expression> Update part of molecule
restrict <expression> Display only part of mol.

*	All atoms
cys	Atoms in cysteines
hoh	Atoms in water molecules
as?	Atoms in 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 of chain P
.;A	Atoms in alternate conformation A
*/4	All atoms in model 4

Atom Expressions

Predefined Sets:	alpha hydrophobic
Residue Ranges:	3,16,12 9-20
Boolean Operators:	backbone and not alpha ligand or 196-199 not (hydrogen or hetero) not *.FE and hetero
Primitive Expressions:	cys, glu, arg, as? ser70a, **p, glu24:1 hem*p.fe, *.sg
Comparison Operators:	atomno=4,atomno=6 temperature>=900
Within Expressions:	within(8.0,ligand)

Predefined Sets

at	**acidic**	**acyclic**	**aliphatic**
alpha	**amino**	**aromatic**	**backbone**
basic	**bonded**	**buried**	**cg**
charged	**cyclic**	**cystine**	**helix**
hetero	**hydrogen**	**hydrophobic**	**ions**
large	**ligand**	**medium**	**neutral**
nucleic	**polar**	**protein**	**purine**
pyrimidine	**selected**	**sheet**	**sidechain**
small	**solvent**	**surface**	**turn**
water			

define <identifier> <expression> User-defined sets

Rendering Commands

background <colour> Set background colour
set ambient [value] Depth-cueing/lighting
set shadows [boolean] Enable/disable shadows
set specular [boolean] Enable atom highlights
set specpower [value] Control atom 'shininess'

Display Commands

thickness values are in 1/250 Å units

wireframe [boolean] Display wireframe
wireframe <value> Display stick bonds

spacefill [boolean] Display spacefill spheres
spacefill <value> Specify atom sphere radius
spacefill temperature

backbone [boolean] Display alpha backbone
backbone <value> Specify backbone radius

ribbons [boolean] Display solid ribbons
ribbons <value> Specify ribbon width

cartoon [boolean] Display ribbon & direction
cartoon <value> Specify width

label [boolean] Draw default atom labels
label <string> Label with arbitrary text
set fontsize <value> Set label font height

ssbonds [boolean] Display disulphide bonds
ssbonds <value> Specify ssbond radius

set ssbonds backbone SSBonds between alphas
set ssbonds sidechain SSBonds between sulphurs

hbonds [boolean] Display hydrogen bonds
hbonds <value> Specify hbond radius

set hbonds backbone HBonds between alphas
set hbonds sidechain HBonds donor/acceptor

monitor <#>, <#> Draw bond and distance between arbitrary atoms
monitor [boolean] Turn monitor on and off
set monitor [boolean] Turn monitor label on/off

dots [boolean] Display dot surface
dots <value> Specify dot density

set solvent [boolean] VDW or solvent surface
set radius <value> Specify probe sphere rad.

Colour Commands

colour [object] <colour> Colour representation

Objects:

atoms	**bonds**	**backbone**
ribbons	**labels**	**hbonds**
ssbonds	**dots**	**axes**
ribbons1	**ribbons2**	

Predefined Colours:

blue	**black**	**cyan**	**green**
greenblue	**magenta**	**orange**	**purple**
red	**redorange**	**violet**	**white**
yellow			

Atom Colour Schemes:

cpk	**amino**	**shapely**
group	**chain**	**structure**
temperature	**charge**	**user**

colour hbonds type Colour hbonds by offset
colour dots potential Display potential surface

Colour Schemes

CPK Atom Colours

Carbon	**light grey**	**[200,200,200]**
Oxygen	**red**	**[240,0,0]**
Nitrogen	**light blue**	**[143,143,255]**
Hydrogen	**white**	**[255,255,255]**
Sulphur	**yellow**	**[255,200,50]**
Phosphorous	**orange**	**[255,165,0]**
Chlorine	**green**	**[0,255,0]**
Ca, Metals	**dark grey**	**[128,128,144]**
Unknown	**deep pink**	**[255,20,147]**

Amino Acid Colours

ASP, GLU	**bright red**	**[230,10,10]**
CYS, MET	**yellow**	**[230,230,0]**
LYS, ARG	**blue**	**[20,90,255]**
SER, THR	**orange**	**[250,150,0]**
PHE, TYR	**mid blue**	**[50,50,170]**
ASN, GLN	**cyan**	**[0,220,220]**
GLY	**light grey**	**[235,235,235]**
LEU, VAL, ILE	**green**	**[15,130,15]**
ALA	**dark grey**	**[200,200,200]**
TRP	**pink**	**[180,90,180]**
HIS	**pale blue**	**[130,130,210]**
PRO	**flesh**	**[220,150,130]**

Secondary Structure Colours

Alpha Helix	**magenta**	**[240,0,128]**
Beta Sheet	**yellow**	**[255,255,0]**
Turns	**pale blue**	**[96,128,255]**
Other	**white**	**[255,255,255]**

Hydrogen Bond Type Colours

Offset +2	**white**	**[255,255,255]**
Offset +3	**magenta**	**[255,0,255]**
Offset +4	**red**	**[255,0,0]**
Offset +5	**orange**	**[255,165,0]**
Offset -3	**cyan**	**[0,255,255]**
Offset -4	**green**	**[0,255,0]**
default	**yellow**	**[255,255,0]**

Manipulation Commands

rotate <axis> [-] <value> Rotate molecule

translate <axis> [-] <value> Translate molecule

zoom [boolean] Scale molecule
zoom <value> Specify magnification

slab [boolean] Enable/disable slabbing
slab <value> Move Z-clipping plane

centre [expression] Set centre of rotation

reset Initial transformation

Export Commands

write [format] <filename> Output image file

gif	CompuServe GIF format
ps, epsf	Encapsulated PostScript
monops	Monochrome PostScript
vectps	'Cartoon' PostScript
bmp	Microsoft Bitmap format
pict	Apple 'PICT' file
ppm	Portable Pixmap
sun, sunrle	Sun Rasterfile

set vectps <boolean> Enable cartoon outlines

write script <filename> Generate RasMol script
write molscript <filename> Output MolScript script
write kinemage <filename> Output Kinemage file
set kinemage <boolean> Set Mage file detail

Misc. Commands

structure	DSSP secondary structure
connect [boolean]	Recalculate connectivity
renumber	Sequentially number chains
show information	Display molecule statistics
show sequence	Display molecule sequence
show symmetry	Display crystal space group

Command Line Editing

In addition to the cursor keys, the following 'emacs' control keys may be used to edit the command line.

Ctrl-H / Ctrl-DDelete previous/next character
Ctrl-B / Ctrl-F Move backward/forward a character
Ctrl-A / Ctrl-E Move to beginning/end of line
Ctrl-P / Ctrl-N Display previous/next history