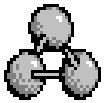

RasMol v2.5
Quick Reference Card

Mouse Buttons

Clicking on an atom identifies that atom in the command window. Moving the mouse whilst holding mouse buttons and/or control keys manipulates the molecule. The default bindings are described below.

RASWIN	*RASMAC*	*ACTION*
Left Button	SINGLE BUTTON	Rotate X-Y
Right Button	OPTION	Translate X-Y
Shift Left Button	SHIFT	Zoom
Shift Right Button	SHIFT + OPTION	Rotate Z
Control Left Button	CTRL	Z-Clipping (Slab)

General Commands

load [format] <filename> Load a molecule
- **pdb** Brookhaven Protein Databank
- **mdl** Molecular Design Limited's Mol file
- **mol2** Tripos' Sybyl Mol2 file format
- **alchemy** Tripos' Alchemy file format
- **charmm** CHARMm format card file
- **xyz** MSC's XMOL XYZ file format

exit Exit from RasMol
quit

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

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

set bondmode [mode] Change bond selection

script <filename> Execute file of commands

zap Delete molecule

Display Commands

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

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

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

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

strands [boolean] Draw ribbon as strands
strands <value> Specify ribbon width
set strands <value> Number of ribbon strands

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

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

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

set axes [boolean] Display co-ordinate axes
set boundbox [boolean] Display bounding box
set unitcell [boolean] Display crystal unit cell

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

Manipulation Commands

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

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

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

Atom Expressions

Predefined Sets:	alpha
	hydrophobic
Residue Ranges:	3,16,12
	9-20
Boolean Operators:	backbone and not alpha
	ligand or 196-199
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'

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 secondry 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
set mouse rasmol	Default mouse bindings
set mouse quanta	Polygen's Quanta bindings
set mouse insight	Biosym's Insight II bindings

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-D	Delete 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

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]**
Calcium, 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]**