RasMol v2.7.3 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.

Mac	Windows	Action
---	Left	Rotate X-Y (or Z)
Command	Right	Translate X-Y
Shift	Shift Left	Zoom
Shift-Cmnd	Shift Right	Rotate Z
Control	Control Left	Z-Clipping (Slab)

General Commands

load [format] <filename> Load a molecule (up to 5)

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
mopac	J.P. Stewart's MOPAC file format
cif	IUCr CIF or mmCIF file format

exit Exit from RasMol Script
quit Terminate pgm execution

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

Bond Commands

bond <src> <dst> + Add a bond
bond <src> <dst> pick Pick bond for rotation
unbond <src> <dst> Remove a bond

Display Commands

wireframe [boolean] Display wireframe
wireframe <rad> Display stick bonds
set bondmode all Mark all atoms
set bondmode none Mark no atoms
set bondmode not bonded Mark non-bonded atoms
spacefill [boolean] Display spacefill spheres
spacefill <value> Specify atom sphere radius
spacefill temperature
spacefill user
star ... Display stars for spheres
surface molecule <value>
surface solvent <value> Display molecule surface
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> [FS|PS] Set label font height
set fontstroke<value> Set label stroke width

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

set monitor [boolean] Show distance monitor labels
set backfade [boolean] Shade to any background color
set display selected Currently selected portion
set picking Series of 13 commands:
off | ident | distance| angle
| torsion | label | monitor | center
coord | bond | atom | group | chain

Colour Commands

colour [object] <colour> Colour representation

Objects:

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

Predefined Colours:

Black	**Blue**	**BlueTint**	**Brown**
Cyan	**Gold**	**Grey**	**Green**
GreenBlue	**GreenTint**	**HotPink**	**Magenta**
Orange	**Pink**	**PinkTint**	**Purple**
Red	**RedOrange**	**SeaGreen**	**SkyBlue**
Violet	**White**	**Yellow**	**YellowTon t**

Atom Colour Schemes:

cpk, cpknew	**amino**	**shapely**
group	**chain**	**structure**
temperature	**charge**	**user**
alt	**model**	

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

Manipulation Commands

depth[boolean] Enable/disable back-clipping
depth <value> Move back-clipping plane

molecule <number> Specify molecule to manipulate

rotate <axis> [-] <value> Rotate molecule
rotate bond Rotate bond
rotate molecule Rotate selected molecule
rotate all Rotate all molecules

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] {centre|translate} Set centre of rotation

reset Initial transformation

set stereo [boolean] Control L&R images

Scripted Commands

load [format] inline	Load molecule from script
pause	Suspend script execution
echo	Display text on command line
refresh	Redraw image
set write [boolean]	Save & write in scripts

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'
set shadepower [value]	Control atom 'contrast'

Language Commands

English	English menus and messages
French	French menus and messages
Italian	Italian menus and messages
Spanish	Spanish menus and messages

Export Commands

write [format] <filename>	Output image file
gif	CompuServe GIF format
iris	IRIS RGB
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 povray <filename>	Generate POVray data
write vrml<filename>	Generate VRMLdata
write molscript <filename>	Output MolScript script
write kinemage <filename>	Output Kinemage file
save <filename>	Save selected atoms
set kinemage <boolean>	Set Mage file detail
set transparent<boolean>	Allow transparent GIFs
write phipsi<filename>	Generate phi-psi data
write RDF<filename>	Ramachandran plot data
write RPP<filename>	Ramachandran printer plot

Misc. Commands

structure	DSSP secondry structure
connect [boolean]	Recalculate connectivity
renumber	Sequentially number chains
show information	Display molecule statistics
show phipsi	Display trosion angles
show RPP	Ramachandran printer plot
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
set cisangle	CIS angle cutoff

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	**sky blue**	**[143,143,255]**
Hydrogen	**white**	**[255,255,255]**
Sulphur	**yellow**	**[255,200,50]**
Phosphorous	**orange**	**[255,165,0]**
Chlorine	**green**	**[0,255,0]**
Bromine, Zinc	**brown**	**[165,42,42]**
Calcium	**dark grey**	**[128,128,144]**
Unknown	**deep pink**	**[255,20,147]**

CPKnew Atom Colours

Carbon	**light grey**	**[211,211,211]**
Oxygen	**red**	**[255,0,0]**
Nitrogen	**sky blue**	**[135,206,235]**
Hydrogen	**white**	**[255,255,255]**
Sulphur	**yellow**	**[255,255,0]**
Phosphorous	**orange**	**[255,170,0]**
Chlorine	**green**	**[0,255,0]**
Bromine, Zinc	**brown**	**[128,40,40]**
Calcium	**dark grey**	**[105,105,105]**
Unknown	**deep pink**	**[250,22,145]**

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]**
others	**tan**	**[190,160,110]**

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]**