



RasMol v2.5

Quick Reference Card

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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.

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
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 boundingbox [boolean]	Display bounding box
set unitcell [boolean]	Display crystal unit cell

Colour Commands

colour [object] <colour>	Colour representation
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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
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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 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

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 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	
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]