



RasMol v2.6

Quick Reference Card

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v2.6 features added May, 1997.

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 Script

quit Terminate pgn 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

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

set monitor on (off) Show distance monitor labels

set backfade on (off) Shade to any background color

set display selected Currently selected portion

set picking Series of eight commands:
off | ident | distance
angle | torsion | label
monitor | center

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 molecule

zoom [boolean] Scale molecule

zoom <value> Specify magnification

slab [boolean] Enable/disable slabbin

slab <value> Move Z-clipping plane

set slabmode <slabmode> Control slabbing methn

centre [expression] Set centre of rotation

reset Initial transformation

set stereo [boolean] Control L & R images

Scripted Commands

pause Suspend script execution

echo Display text on command line

refresh Redraw local 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(8,0,ligand)

Predefined Sets

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

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 bonds [boolean]	Double and triple bonds
cartoons [boolean]	MolScript-style display
set cartoons [number]	Depth of display
trace [boolean]	Draw a smooth CA spline
trace [value]	Specify trace width

Export Commands

write [format] <filename>	Output image file
gif	CompuServe GIF format
ps, epsf	Encapsulated PostScript
monops	Monochrome PostScript
vecpts	'Cartoon' PostScript
bmp	Microsoft Bitmap format
pict	Apple 'PICT' file
ppm	Portable Pixmap
sun, sunrle	Sun Rasterfile
set vecpts <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
clipboard	Copy image to clipboard
print	Image to local printer
save <filename>	Save selected atoms
set transparent <filename>	Output transparent gif

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
hetero <boolean>	Excludes HETATMs if false
hydrogen <boolean>	Excludes hydrogens if false
hourglass <boolean>	Enables "hour glass" cursor
set menus <boolean>	Enables menu buttons/bar

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	Movebackward/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]
Sodium	blue*	[0,0,255]
Iron	orange*	[255,165,0]
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]

*Same as the Predefined Colours on the first page.