



RasMol v2.7.1

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.

Mac	Windows	Action
---	Left	Rotate X-Y
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
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

Display Commands

wireframe [boolean] Display wireframe
wireframe <value> 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

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 nine commands:
 off | ident | distance
 angle | torsion | label
 monitor | center | coord

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	YellowTont

Atom Colour Schemes:

cpk	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

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

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'

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]

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 Sheeet	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]

Rasmol commands that you will need for the homework assignment

Atom expressions (used with select or restrict commands below):

Amino acid number or DNA base number:

eg.: glu (selects all glu residues)
glu41 (selects only glu residue 41)
glu41:A (selects only glu residue 41 in chain A)
41 (selects amino acid or nucleotide residue 41)
41:A (selects amino acid or nucleotide residue 41 in chain A)
41-50 (selects residues 41-50)
* wild-card designator meaning "all"
*:A all residues in chain A
hetero a "hetero" atom is any non-protein or non-nucleotide residue. It includes water, miscellaneous inhibitor or extraneous atoms like metals, prosthetic groups, & salts.

Atom numbers in any residue:

eg.: atomno=469 (selects the single atom # 469 in the coordinate file)

Note: if you click on an atom in the coordinate file you will see something like this on the command line window:

CE 886 Group: LYS 70 Chain:A

This means that you have clicked on the □ carbon atom with an atom # designation 886 of a Lysine residue # 70 on chain A in the coordinate file. Use the "886" in the "atomno=" expressions (eg. atomno=886) and the 70 or the lys70 for the amino acid expressions above.

General commands:

Select <atom expression>

eg.: select protein (selects all protein residues)
select glu41 (selects protein glu residue 41)

Select commands will allow the program to "hold" those residues so that anything you subsequently do will be performed **ONLY** on those residues.

Restrict <atom expression>

eg.: restrict protein (selects all protein residues and eliminates the display of anything except the protein residues)
restrict glu41 (selects protein glu residue # 41 and eliminates the display of anything except the glu41 residue)

Note: after using the restrict command the visible residues are also now "selected" so that anything that you subsequently do will be executed only on those residues.

Note: unusual example of the select command: "select within" or "restrict within"

eg.: select within(3.5,DNA) (selects any atoms within 3.5Å of dna)
NOTE THE SYNTAX: the number must have a decimal, 3.5 means 3.5Å and 5 means 0.5Å.

You can add "Boolean operators" to select or restrict commands:

eg.: select within(3.5,dna) and not dna and not water (selects any atoms within 3.5Å of the dna, but not the dna itself or any water that is within 3.5Å of the dna)
select within(3.5,atomno=356) and not protein (selects any atom within 3.5Å of the atom with designation # 356, but excluding any protein atoms)

Other miscellaneous commands:

Center selected (use this command after using a select... command. It will center the rotation around the selected atom)

Zoom (some number between 100 and 1000)

eg.: zoom 400 (zooms in 4x, relative to the unzoomed structure at zoom 100)

Color (a color name)

eg.: color green (use after a select..... command. It will change the selected atom to the color that you chose)