# RasMol v2.7.4.1 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 (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
**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

## Language Commands

| | |
|---|---|
| **Bulgarian** | Bulgarian menus and messages |
| **Chinese** | Chinese menus and messages |
| **English** | English menus and messages |
| **French** | French menus and messages |
| **Italian** | Italian menus and messages |
| **Japanese** | Japanese menus and messages |
| **Spanish** | Spanish menus and messages |

## 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

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## Map Commands

**map {<map_selector>} {map_subcommand> <parameters>**
**<map_selector>: all, new, next or <number>**
manipulate maps for current molecule

**map {<map_selector>} generate {dots|mesh|surface}**
generate a map from the current atoms

**map {<map_selector>} level {MEAN} <number>**
select a coutour level

**map {<map_selector>} { load | save } <filename>**
load a CBF or CCP4 map, save a CBF map

**map {<map_selector>} mask { selected | <number> | none }**
generate a mask from selected atoms or an existing map by number

**map {<map_selector>} { resolution | spacing | spread } <number>**
set spacing and/or spread, spacing=resolution
spread = 2/3 resolution

**map {<map_selector>} {restrict | select}** select maps
if restrict disable display of the others

**map {<map_selector>} show**
show information about selected maps

**map {<map_selector>} zap**
erase selected maps

## Atom Expressions

| | |
|---|---|
| **Predefined Sets:** | alpha<br>hydrophobic |
| **Residue Ranges:** | 3,16,12<br>9-20 |
| **Boolean Operators:** | backbone and not alpha<br>ligand or 196-199 |
| **Primitive Expressions:** | cys, glu, arg, as?<br>ser70a, **p, glu24:1<br>hem*p.fe, *.sg |
| **Comparison Operators:** | atomno=4,atomno=6<br>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' |

## 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]** |