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

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]**

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]**