UCSF Chimera
QUICK REFERENCE GUIDE
October 2002

Midas Emulator Commands

ac	enable accelerators (keyboard shortcuts)
alias	create an alias or list aliases
align	align two atoms along the z axis
angle	measure a bond angle or torsion angle
brotation	make a bond rotatable
cd	change the current working directory
center	center the view on specified atoms
chain	chain specified atoms, undisplay the others
clip	move clipping planes
close	close a model
cofr	report or change the center of rotation
color	color atoms, labels and surfaces
colordef	define a new color
conic	create a shadowed space-filling image (static; UNIX only)
copy	send the display image to a printer or file
display	display specified atoms
distance	monitor distances between atoms
echo	place text in the reply area
freeze	stop all motion
getcrd	return coordinates for an atom
help	show information about a command
ksdssp	determine secondary structure from protein coordinates
label	display atom labels
labelopt	control the information in labels
linewidth	control the width of lines in the wireframe representation
load	restore a saved Chimera session
longbond	remove excessively long bonds
match	superimpose two models
matrixcopy	apply the transformation matrix of one model to another
modelcolor	set color at the model level
modeldisplay	set display at the model level
move	translate selected models
msms	create and display a molecular surface, alter its type (solid or filled, mesh, dot)
neon	create a shadowed solid stick image (static; UNIX only)
objdisplay	display graphical objects
open	open a structure or object as a model for display, or execute a Python command file
pdbrun	send an annotated PDB file of the current display to the system shell (UNIX only)
push,pop	push or pop images on the picture stack
rainbow	color chains ranging from red to blue
represent	control the representation of atoms and bonds (wire, stick, bs or b+s, sphere or cpk)
rescolor	set color at the residue level
reset	reset models to their original (or saved) orientations
resrepr	display and undisplay a rotatable ribbon representation (ribbon or flat, sharp, smooth, none)
ribbonjr	create a ribbon image (static; UNIX only)
rock	rock a structure about the x, y or z axis
roll	roll a structure about the x, y, or z axis
rotation	make a bond rotatable
save	save the current Chimera session
savepos	save the current orientation(s)
scale	scale the view
section	change the cross-section of the display (move clipping planes in parallel)
select	activate models for motion or select atoms for further operations
set,unset	set or unset options (see **Set/Unset Toggle Options**)
show	display only the specified atoms in a model
sleep	suspend command processing for a specified length of time
source	read and execute a command file
stop	terminate the current Chimera session
surface	create and display a molecular surface
surfcat	equivalent to *msms cat*
surfrepr	alter surface type (solid or filled, mesh, dot); equivalent to *msms repr*
system	execute a system command
tcolor	color using texture map colors
texture	define texture maps and associated colors
thickness	change the cross-section thickness (move clipping planes in opposite directions)
turn	rotate a structure about the x, y, or z axis
vdw	display van der Waals (VDW) surface
vdwdefine	set VDW radii
vdwdensity	set VDW surface dot density
version	show program version information
wait	suspend command processing until motion has stopped
window	adjust the view to contain the specified atoms
write	save a molecule model as a PDB file

Reverse Command Functions

~alias	delete an alias
~chain	break chaining for the specified atoms
~clip	stop an ongoing *clip*
~cofr	return to the default center of rotation
~color	remove a color assignment
~display	undisplay specified atoms
~distance	turn off a distance calculation
~label	undisplay atom labels
~modeldisplay	efficiently undisplay entire models or submodels
~objdisplay	undisplay graphical objects
~open	close a model (equivalent to *close*)
~savepos	forget a saved orientation
~scale	stop an ongoing *scale*
~select	deactivate models for motion or deselect atoms
~set	unset options (see **Set/Unset Toggle Options**)
~show	undisplay specified atoms
~surface	undisplay molecular surface
~vdw	undisplay VDW surface

Set/Unset Toggle Options

autocolor	make each newly opened model a unique color
independent	make each model rotate about its own center of mass instead of the combined center of mass

Miscellaneous Operations (Default Settings)

Action	Procedure
picking	Ctrl-left mouse button (can sweep out an entire area)
adding to a selection	Shift-Ctrl-left mouse button
xy-rotation	left mouse button when inside the "spaceball"
z-rotation	left mouse button when outside the "spaceball"
xy-translation	middle mouse button
z-translation	Ctrl-middle mouse button
scaling	right mouse button or the Side View (below)
Side View	open by selecting **Controllers...Side View** from the menu
Midas command line	open by activating **Controllers...Midas Emulator** in the menu
Python command line	open by selecting **Extensions... Programming...IDLE** from the menu
color well activation	click on the well to open the Color Editor and change the color
listing of extensions	list extensions and short descriptions by opening the Extension Manager (**Extensions...Manager**) and clicking the box labeled "Show descriptions"

Atom Specification Symbols

Symbol	Function	Usage
#	model number	**#** *model_number*, where *model_number* is an integer
#.	submodel	**#.** *submodel*, where *submodel* is an integer (specifies MODEL in a multi-MODEL file)
:	residue	**:** *residue*, where *residue* is a residue name or number
::	residue	**::** *residue*, where *residue* is a residue name
:.	chain	**:.** *chain*, where *chain* is a chain identifier such as HET, A or B
@	atom name	**@***atom_name*, where *atom_name* is an atom name
@.	alternate location	**@.** *alt_loc*, where *alt_loc* is an alternate location identifier
–	range	specifies a range of models, submodels, or residues
,	name separator	separates models or residues, ranges of models or residues, or names of atoms
*****	whole wildcard match	matches whole atom or residue names, *e.g.*,**:*@CA** specifies the alpha carbons of all residues
=	partial wildcard match	matches partial atom or residue names, *e.g.*, **@C=** specifies all atoms with names beginning with C
?	single char wildcard	used for atom and residue names only, *e.g.*, **:G??** selects all residues with three-letter names beginning with G
z<	zone specifier	**z<***zone* or **zr<***zone* specifies all residues within *zone* angstroms of the indicated atoms, and **za<***zone* specifies all atoms (rather than entire residues) within *zone* angstroms of the indicated atoms. Using > instead of < results in the complementary set of atoms.
&	intersection	specifies the atoms that meet both sets of criteria (on either side of the **&** symbol), *e.g.*, **#1 & #2:1 zr<10** specifies all residues in model 1 that are within 10 angstroms of residue 1 in model 2
;	command separator	separates multiple commands on a single line

Atom Descriptors

Usage	Description
@/altLoc=*altloc*	*altloc* is the alternate location identifier of the atom
@/color=*color*	*color* is the color of the atom (assigned on a per-atom basis)
@/drawMode=*mode*	*mode* can be 0 (dot, as in wireframe models), 1 (sphere, as in CPK models), 2 (endcap, as in stick models), or 3 (ball, as in ball-and-stick models)
@/display	whether the atom is displayed
@/element=*atno*	*atno* is the atomic number
@/label	whether the atom is labeled
@/label=*label*	*label* is the text of the atom's label
@/labelColor=*labcolor*	*labcolor* is the color of the atom's label
@/name=*name*	*name* is the atom name
@/surfaceCategory=*catname*	*catname* is the category the atom belongs to for surface calculation purposes
@/surfaceColor=*surfcolor*	*surfcolor* is the color of the atom's surface
@/surfaceDisplay	whether the atom's molecular surface is displayed
@/vdw	whether the atom's VDW surface is displayed
@/vdwRadius=*radius*	*radius* is the VDW radius of the atom in angstroms

Residue Descriptors

Usage	Description
:/color=*color*	*color* is the color assigned on a per-residue basis
:/isHelix	whether the residue is in an alpha helix
:/isSheet	whether the residue is in a beta strand
:/isStrand	whether the residue is in a beta strand
:/isTurn	whether the residue is in a turn according to PDB TURN records
:/type=*resname*	*resname* is the residue name

Chimera was developed by the Computer Graphics Laboratory at the University of California, San Francisco under support of the National Institutes of Health grant P41-RR01081. The software is copyrighted and licensed by the Regents of the University of California.

Model Descriptors

Usage	Description
#/color=*color*	*color* is the color assigned on a per-model basis
#/display	whether display is enabled at the model level
#/explicitHydrogens	whether the model has hydrogen atoms
#/lineWidth=*width*	*width* is the linewidth of the model in the wireframe representation
#/pointSize=*size*	*size* is the font size of labels on the model
#/vdwDensity=*density*	*density* is the dot density used for VDW surfaces on the model

Atom Specification Examples

#0
- all atoms in model 0

:lys,arg
- all lysine and arginine residues

#3:45-83,90-98
- residues 45 through 83 and 90 through 98 in model 3

:12,14@ca
- alpha carbons in residue 12 and residue 14

:12:14@ca
- all atoms in residue 12 and the alpha carbon in residue 14

ligand
- any/all residues automatically classified as ligand

:.A@ca,c,n,o
- peptide backbone atoms in chain A

#1:50.het
- HETATM residue 50 in model 1

:50.B,.D
- residue 50 in chain B and all residues in chain D

:522.water
- water residue 522 (HETATM residue 522 which is named HOH or WAT)

:12-15,16-18.a,15.b@ca
- CA atoms within the following residues: 12 through 15 (with no chain ID), 16 through 18 in chain A, and 15 in chain B

#0.1-3,5
- submodels 1-3 of model 0 and all of model 5

#0.1-3,.5
- submodels 1-3 of model 0 and submodel 5 of all models

@ca/!label and color!=green and color!=red
- atoms named CA which are not labeled, and are not green or red

@/color=yellow or color=blue and label
- atoms that are yellow and atoms that are both blue and labeled

:asn/isTurn
- asparagine residues in a turn according to PDB TURN records

#1:asp,glu & #0 z<10
- negatively charged amino acids in model 1 within 10 angstroms of model 0