UCSF Chimera
QUICK REFERENCE GUIDE
December 2003

Commands

ac	enable accelerators (keyboard shortcuts)
alias	create an alias or list aliases
align	align two atoms along the line of sight
angle	measure a bond angle or torsion angle
brotation	make a bond rotatable
cd	change the 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/bonds, labels and surfaces
colordef	define a new color
conic	create a shadowed space-filling image (static; UNIX only)
copy	save or print the displayed image
delete	delete atoms and bonds
display	display specified atoms
distance	measure the distance between two atoms
echo	send text to the Reply Log
focus	adjust the view and center of rotation to the specified atoms
freeze	stop all motion
getcrd	report untransformed coordinates
help	display the manual page for 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	find and 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 along the X, Y, or Z axis
msms	(see *surfcat* and *surfrepr*)
neon	create a shadowed solid stick image (static; UNIX only)
objdisplay	display graphical objects
open	open structures or data for display or execute a 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 in gradations over a range (default blue to red)
read	execute a command file, only updating the view at the end
represent	control the representation of atoms and bonds (wire, stick, bs or b+s, sphere or cpk)
reset	restore default or saved orientations
ribbackbone	allow residue ribbon and backbone atoms to be displayed simultaneously
ribbon	display a secondary structure ribbon
ribbonjr	create a ribbon image (static; UNIX only)
ribcolor	set ribbon color
ribrepr	control the ribbon representation (flat, sharp, smooth)
rock	rock about the X, Y or Z axis
roll	roll about the X, Y, or Z axis
rotation	make a bond rotatable
save	save the current Chimera session
savepos	save the current orientations
scale	scale the view
section	move the clipping planes in parallel
select	activate models for motion or select atoms for further operations
set	set options (see **Set/Unset Options**)
show	display specified atoms, undisplay the others
sleep	suspend command processing for a specified length of time
source	execute a command file, updating the view continually
stereo	switch amongst stereo options and mono viewing
stop	exit from Chimera
surface	calculate and display molecular surface
surfcat	group atoms for subsequent surface calculations; equivalent to *msms cat*
surfcolor	set whether surface color is determined at the atom or model level
surfrepr	control surface representation (solid, mesh, dot); equivalent to *msms repr*
swapaa	mutate amino acid residues
swapna	mutate nucleic acid residues
system	send a command to the system shell
tcolor	color using texture map colors
texture	define texture maps and associated colors
thickness	move the clipping planes in opposite directions
turn	rotate 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 copyright information and which version of Chimera is being used
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
~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	turn off display at the model level
~objdisplay	undisplay graphical objects
~open	close a model (equivalent to *close*)
~ribbackbone	hide backbone atoms when ribbon is shown
~ribbon	undisplay ribbon
~ribcolor	deassign ribbon color
~savepos	forget saved orientations
~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

Set/Unset Value Options

bg_color	set background color; *value* can be any color name
dc_color	set depth cue color; *value* can be any color name

Miscellaneous Operations (Default Settings)

Action	Procedure
picking from the screen	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	**Tools...Viewing Parameters...Side View**
Command Line	**Tools...Keyboard...Command Line**
Model Panel	**Tools...Inspectors...Model Panel**
Python shell	**Tools...Programming...IDLE**
Reply Log	**Tools...Utilities...Reply Log**
color well activation	click on the well to open the Color Editor and change the color
listing of tools/extensions	also set which tools start at Chimera startup, which appear in the **Favorites** menu, and which icons appear in the tool bar using **Favorites...Preferences**, **Tools** category

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

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.

Atom Descriptors

Usage	Description
@/altLoc=*altloc*	*altloc* is the alternate location identifier of the atom
@/bfactor=*bfactor*	*bfactor* is the B-factor 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)
@/defaultRadius=*rad*	*rad* is the default VDW radius of the atom
@/display	whether the atom is displayed
@/element=*atno*	*atno* is the atomic number
@/idatmType=*type*	*type* is the IDATM atom type
@/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
@/occupancy=*occupancy*	*occupancy* is the occupancy value of the atom
@/radius=*radius*	*radius* is the radius of the atom (may have been changed by the user from the default VDW radius)
@/serialNumber=*n*	*n* is the atom serial number in the input file
@/surfaceCategory=*catname*	*catname* is the category the atom belongs to for surface calculation purposes (main, ligand, *etc.*)
@/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

Residue Descriptors

Usage	Description
:/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
:/ribbonColor=*ribcolor*	*ribcolor* is the color of the residue's ribbon segment
:/type=*resname*	*resname* is the residue name

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

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

:lys,arg
- lysine and arginine residues

: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

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

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

: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

ligand
- any/all residues automatically classified as ligand

element.S
- all sulfur atoms

@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
- aspartate and glutamate residues in model 1 within 10 angstroms of model 0