UCSF Chimera
QUICK REFERENCE GUIDE
September 2005

Commands

*reverse function ~**command** available

2dlabels	create arbitrary text labels and place them in 2D
ac	enable accelerators (keyboard shortcuts)
addaa	add an amino acid to a peptide C-terminus
addh	add hydrogens
*alias**	create an alias or list aliases
align	align two atoms along the line of sight
angle	measure a bond angle or torsion angle
*bond**	add/delete bonds
*bondcolor**	color bonds independently from atoms
bonddisplay	control how bond display depends on atom display
bondrepr	control the representation of bonds (wire, stick)
brotation	make a bond rotatable
cd	change the working directory
center	center the view on specified atoms
chain	chain specified atoms, undisplay the others
chirality	report the R/S configuration of a chiral center
*clip**	move clipping planes
close	close a model
*cofr**	report or change the center of rotation
*color**	color atoms/bonds, ribbons, 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
defattr	assign attribute values to atoms, residues, or models
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
*hbonds**	(*findhbond*) identify possible hydrogen bonds
help	display the manual page for a command
ksdssp	determine secondary structure from protein coordinates
*label**	display atom labels
labelopt	control the information in atom 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
matrixget	write the current transformation matrices to a file
matrixset	read and apply transformation matrices from a file
mmaker	(*matchmaker*) align models in sequence and then superimpose them accordingly
modelcolor	set color at the model level
*modeldisplay**	set display at the model level
move	translate along the X, Y, or Z axis
movie	capture image frames and assemble them into a movie
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 residues, chains, models over a range (default blue to red)
rangecolor	color over a range according to attribute values
read	execute a command file, updating the display 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, edged, round)
*rlabel**	display residue labels
rmsd	evaluate the RMSD between specified sets of atoms
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 display continually
stereo	switch amongst stereo options and mono viewing
stop	exit from Chimera
*surface**	calculate and display molecular surface
surfcat	(*msms cat*) group atoms for subsequent surface calculations
surfcolor	set whether surface color is determined at the atom or model level
surfrepr	(*msms repr*) control surface representation (solid, mesh, dot)
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
writesel	write a parsable text file containing specifications of the currently selected (or unselected) items
x3dsave	save the graphical scene as an X3D file

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
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 Controls...Side View
Command Line	Tools...General Controls...Command Line
Reply Log	Tools...Utilities...Reply Log
Preferences	Favorites...Preferences
listing of tools/extensions	Tools category of Preferences (above); also specify which tools start when Chimera starts, which appear in the Favorites menu, and which icons appear in the tool bar

Atom Specification Symbols

Symbol	Function	Usage
#	model number	# *model* (integer)
#.	submodel number	**#.** *submodel* (integer)
:	residue	**:** *residue* (name or number)
::	residue name	**::** *residue*
:.	chain ID	**:.** *chain*
@	atom name	**@***atom*
@.	alternate location ID	**@.** *alt_loc*
–	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	matches whole atom or residue names, *e.g.*,**:*@CA** specifies the alpha carbons of all residues
=	partial wildcard	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
;	command separator	separates multiple commands on a single line
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 < gives the complement.
&	intersection	intersection of specified sets
|	union	union of specified sets
~	negation	negation of specified set (when space-delimited)

Atom Attributes

Usage	Description
@/altLoc=*altloc*	*altloc* is the alternate location ID
@/bfactor=*bfactor*	*bfactor* is the B-factor
@/color=*color*	*color* is the color assigned on a per-atom basis
@/drawMode=*mode*	*mode* can be 0 (dot, as in wireframe), 1 (sphere, as in CPK), 2 (endcap, as in stick), or 3 (ball, as in ball-and-stick)
@/defaultRadius=*rad*	*rad* is the default VDW radius
@/display	whether display is enabled at the atom level
@/element=*atno*	*atno* is the atomic number
@/idatmType=*type*	*type* is the atom type
@/label	whether the atom is labeled
@/label=*label*	*label* is the text of the atom label
@/labelColor=*labcolor*	*labcolor* is the color of the atom label
@/name=*name*	*name* is the atom name
@/occupancy=*occupancy*	*occupancy* is the occupancy
@/radius=*radius*	*radius* is the current radius (may have been changed 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 molecular surface
@/surfaceDisplay	whether molecular surface display is turned on for the atom
@/vdw	whether VDW surface display is turned on for the atom

Residue Attributes

Usage	Description
:/isHelix	whether the residue is in an alpha helix
:/isHet	whether the residue is in HETATM records in the input PDB file
:/isStrand *or* **:/isSheet**	whether the residue is in a beta strand
:/isTurn	whether the residue is in a turn according to PDB TURN records
:/kdHydrophobicity=*value*	*value* is the Kyte-Doolittle hydrophobicity
:/ribbonColor=*ribcolor*	*ribcolor* is the color of the residue's ribbon segment
:/ribbonDisplay	whether ribbon display is turned on for the residue (can be true for residues such as water that cannot be shown with ribbon)
:/type=*resname*	*resname* is the residue name

Molecule Model Attributes

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 wireframe linewidth
#/pointSize=*size*	*size* is the font size of labels
#/vdwDensity=*density*	*density* is the dot density used for VDW surfaces

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/isHelix
- asparagine residues in alpha helices

#1:asp,glu & #0 z<10
- aspartate and glutamate residues in model 1 within 10 angstroms of model 0

solvent & Ng+ z<3 | solvent & N3+ z<3
- solvent residues within 3 angstroms of guanidinium nitrogens or *sp*3-hybridized, formally positive nitrogens

@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions