UCSF Chimera
QUICK REFERENCE GUIDE
October 2009

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
addcharge	assign partial charges to atoms
addh	add hydrogens
*alias**	create an alias or list the existing aliases
align	align two atoms or sets of atoms along the line of sight
angle	measure a bond angle or torsion angle
*aniso**	show thermal ellipsoids
*aromatic**	show ring aromaticity
*bond**	add/delete bonds
*bondcolor**	color bonds independently from atoms
bonddisplay	control how bond display depends on atom display
bondrepr	control bond style (wire, stick)
*bondzone**	make zoning tools use points along bonds
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, molecular surfaces
colordef	define a new color
combine	combine molecule models into a single model
conic	create a shadowed space-filling image
coordset	play through frames of a trajectory
copy	save an image (Chimera graphics or POV-Ray)
crystalcontacts	identify clashes between PDB symmetry copies
defattr	assign attribute values to atoms, residues, or models
*define**	calculate axes, planes for sets of atoms
delete	delete atoms and bonds
*display**	display specified atoms
*distance**	measure the distance between two atoms
echo	send text to the status line and Reply Log
export	save the scene (x3d, vrml, pov-ray, renderman, obj)
*fillring**	show rings as filled
*findclash**	identify clashes and/or contacts
fly	smoothly traverse a series of saved positions
*focus**	adjust the view and center of rotation
freeze	stop all motion
getcrd	report untransformed coordinates
*hbonds**	(*findhbond*) identify possible hydrogen bonds
help	display the manual page for a command
hkcage	create icosahedron as hexagon/pentagon mesh
intersurf	generate and display interface surfaces
ksdssp	determine secondary structure from protein coordinates
*label**	display atom labels
labelopt	control the information in atom labels
linewidth	control the width of wire bonds
*longbond**	show/hide pseudobonds representing missing segments
mask	extract volume data bounded by surfaces
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
*mclip**	control per-model clipping
mcopy	copy settings from one molecule model to another
measure	perform calculations on structures, surfaces, maps
meshmol	create a "molecule" from surface mesh for stick display
minimize	energy-minimize structures
mmaker	(*matchmaker*) align models in sequence, then in 3D
modelcolor	set color at the model level
*modeldisplay**	set display at the model level
molmap	create a density map from atomic coordinates
morph	create a morph trajectory from two or more structures
move	translate along the X, Y, or Z axis
movie	capture image frames and assemble them into a movie
*msc**	color multiscale surfaces to match atoms
namesel	name and save the current selection
neon	create a shadowed stick/tube image (not on Windows)
nucleotides	create special nucleotide representations
*objdisplay**	display graphical objects
*open**	read local files or fetch by ID
pause	pause script execution until the user presses a key
pdbrun	send an annotated PDB file to the system shell
*perframe**	specify an alias to be executed at each display frame
preset	apply a predefined combination of display settings
rainbow	color residues, chains, or models over a range
rangecolor	color over a range according to attribute values
read	execute a command file, updating display at the end
represent	control atom/bond style (wire, stick, bs, sphere)
reset	restore default or saved orientations
*ribbackbone**	allow display of both ribbon and backbone atoms
*ribbon**	display ribbon
*ribinsidecolor**	set a separate color for inside protein helix ribbons
ribrepr	control ribbon style (flat, edged, rounded)
ribscale	control ribbon scaling (Chimera default, licorice)
*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
runscript	run Python script with command-line arguments
save	save the current Chimera session
*savepos**	save the current orientations
*scale**	scale the view
scolor	color surfaces by volume data or geometry
section	move the clipping planes in parallel
*select**	activate models for motion or select atoms
*set**	set background color, visual effects, individual rotation
*setattr**	set an attribute to a specified value
shape	create a surface of a specified geometric shape
*show**	display specified atoms, undisplay the others
sleep	pause script execution for a specified time
solvate	add solvent using AmberTools
sop	edit a surface model
split	make chains of a molecule model separate submodels
start	start Chimera tools by name
stereo	switch amongst stereo options and mono viewing
stop	exit from Chimera
*surface**	calculate and display molecular surfaces
surfcat	(*msms cat*) group atoms for surface calculations
surfcolor	set molecular surface color source
surfrepr	(*msms repr*) control surface style (solid, mesh, dot)
*surftransparency**	adjust surface transparency
swapaa	mutate amino acids or swap rotamers
swapna	mutate nucleic acid residues
*sym**	generate symmetry-related copies of a structure
system	send a command to the system shell
thickness	move the clipping planes in opposite directions
*tile**	arrange models in a plane
topography	plot values in a volume data plane as surface heights
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 Chimera version
viewdock	start ViewDock and load docking results
volume	visualize volume data such as electron density
vop	edit volume data to create a new volume data set
wait	suspend command processing until motion has stopped
window	adjust the view to contain the specified atoms
windoworigin	set graphics window location
*windowsize**	adjust the dimensions of the graphics window
write	save atomic coordinates (pdb, mol2)
writesel	write a list of the currently selected (or unselected) items

Miscellaneous Operations (Default Settings)

selection from screen	Ctrl-left mouse button
add/toggle selection	Shift-Ctrl-left mouse button
XY-rotation	left mouse button inside "spaceball"
Z-rotation	left mouse button outside "spaceball"
XY-translation	middle mouse button
Z-translation	Ctrl-middle mouse button
scaling	right mouse button or Side View
preferences	Favorites... Preferences...
searching help	Help... Search Documentation...

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, **za<***zone* specifies all atoms (rather than entire residues) within that distance. Using > instead of < gives the complement.
&	intersection	intersection of specified sets
|	union	union of specified sets
~	negation	negation of specified set (when space-delimited)

Selected Atom Attributes

Usage	Description
@/altLoc=*altloc*	alternate location ID
@/areaSAS=*sasa*	solvent-accessible surface area
@/areaSES=*sesa*	solvent-excluded surface area
@/bfactor=*bfactor*	B-factor
@/color=*color*	atom-level color assignment
@/defaultRadius=*rad*	default VDW radius
@/display	whether the atomic display bit is "on"
@/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)
@/element=*atno*	atomic number
@/idatmType=*type*	Chimera atom type
@/label	whether the atom is labeled
@/label=*label*	text of the atom label
@/labelColor=*labcolor*	color of the atom label
@/name=*name*	atom name
@/occupancy=*occupancy*	crystallographic occupancy
@/radius=*radius*	current VDW radius
@/serialNumber=*n*	serial number in the input file
@/surfaceCategory=*category*	surface calculation category (main, ligand, *etc.*)
@/surfaceDisplay	per-atom surface display bit (can be true for buried atoms with no surface)

Selected Residue Attributes

Usage	Description
:/areaSAS=*sasa*	solvent-accessible surface area
:/areaSES=*sesa*	solvent-excluded surface area
:/isHet	whether the residue is in PDB HETATM records (or the mmCIF equivalent)
:/isHelix	whether the residue is in an alpha helix
:/isStrand *or* **:/isSheet**	whether the residue is in a beta strand
:/kdHydrophobicity=*value*	Kyte-Doolittle amino acid hydrophobicity
:/phi=*angle*	protein/peptide backbone phi angle
:/psi=*angle*	protein/peptide backbone psi angle
:/ribbonColor=*ribcolor*	color of the residue's ribbon segment
:/ribbonDisplay	per-residue ribbon display bit (can be true for residues such as water that cannot be shown with ribbon)

Selected Molecule Model Attributes

Usage	Description
#/ballScale=*factor*	ball radius relative to VDW radius
#/color=*color*	model-level color assignment
#/display	model display bit
#/lineWidth=*width*	linewidth of wire representation
#/stickScale=*factor*	stick radius relative to bond radius

Specification Examples

#
- all models

#0
- model 0

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

:lys,arg
- lysine and arginine residues

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

:12-15,26-28.a,45.b
- residues 12-15 in all chains (except het/water), 26-28 in chain A, and 45 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