UCSF ChimeraX

QUICK REFERENCE GUIDE – BASICS

Essential command-line operations

SYNTAX command required-argument optional-keyword value. Atom specifications (**spec**) restrict the target; without one, many commands act on all applicable items.
Press Up and Down arrows to recall earlier or next commands.

`COLOR KEY command keyword / option atom specification (spec)`

FILES, MODELS & SESSIONS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`open 2wgj`	Fetch PDB entry; local paths and URLs also work.
`open ccd:VGH`	Fetch a Chemical Component Dictionary entry.
`open result.dock4 format swissdock`	Open SwissDock docking results.
`alphafold fetch P29474`	Fetch an AlphaFold Database model by UniProt ID.
`alphafold match #1/A`	Fetch the AlphaFold model matching a chain sequence.
`open file.cxs`	Restore a ChimeraX session.
`save work.cxs`	Save the current session.
`save figure.png width 2400`	Save an image at a specified pixel width.
`save figure.png transparentBackground true`	PNG with transparent background.
`save model.pdb models #1`	Write model #1 coordinates in file model.pdb.
`log clear`	Clear the Log.
`help color`	Open help for a command.
`close`	Close all models, keeping ChimeraX running.
`close #2`	Close model #2.
`exit`	Quit ChimeraX.

CONTROL & REUSE

COMMAND / PATTERN	PURPOSE / EXAMPLE
`undo / redo`	Undo or redo supported actions.
`alias name command`	Define a command-line shortcut.
`runscript file.py`	Run a Python script.
`command1 ; command2`	Run commands sequentially on one line.

SHOW, HIDE & REPRESENT

COMMAND / PATTERN	PURPOSE / EXAMPLE
`show spec atoms`	Show atoms/bonds for the atom specification (spec).
`hide spec atoms`	Hide specified atoms/bonds without deleting them.
`show spec cartoons`	Show cartoon representation.
`hide spec cartoons`	Hide cartoon representation.
`style spec stick`	Atom style. Available options: stick, ball, or sphere.
`cartoon style spec Xsection rectangle`	Use a rectangular cartoon cross-section.
`delete spec`	Delete atoms/bonds permanently.
`dssp spec`	Recalculate protein secondary structure.

COLOR & TRANSPARENCY

COMMAND / PATTERN	PURPOSE / EXAMPLE
`color spec cornflowerblue target acs`	Color atoms/bonds, cartoons, and surfaces.
`color spec byelement target a`	Color atoms/bonds by chemical element.
`color spec byhetero target a`	Keep carbon color; color heteroatoms by element.
`color spec red target c`	Color only cartoons.
`color spec blue target s`	Color only molecular surfaces.
`transparency spec 70 target s`	Make target surfaces 70% transparent.
`set bgColor white`	Set the graphics background.
`rainbow chains`	Apply a chain-based color gradient.
`rainbow residues`	Apply a residue-based color gradient.

MOLECULAR SURFACES

COMMAND / PATTERN	PURPOSE / EXAMPLE
`surface spec`	Calculate and display a molecular surface.
`surface hide spec`	Hide, but retain, an existing surface.
`surface show spec`	Show an existing surface.
`surface close spec`	Delete the corresponding surface model.
`surface style surface-spec mesh`	Set surface model style to solid, mesh, or dot (for example, #1.1).

! CAUTION - HIDE vs DELETE hide preserves items so they can be shown again. delete and surface close remove data or derived models; save a session before destructive edits.

VIEW, MOTION & CLIPPING

COMMAND / PATTERN	PURPOSE / EXAMPLE
`view`	Fit all displayed items in the window.
`view sel`	Center and fit the current selection.
`view orient`	Return to the standard scene orientation.
`cofr spec`	Set the center of rotation.
`turn y 30`	Rotate 30 degrees about the y axis.
`move x 5`	Translate 5 Å along the x axis.
`zoom 1.25`	Magnify by a factor of 1.25.
`clip front 0 position ligand`	Place front clip plane at ligand center.
`clip back 6`	Place a back plane 6 Å behind front.
`clip front off`	Turn off the front clipping plane.
`clip back off`	Turn off the back clipping plane.
`clip model #!1 false`	Exclude model #1 from clipping.

MODEL OPERATIONS & COMPARISON

COMMAND / PATTERN	PURPOSE / EXAMPLE
`hbonds ligand reveal true`	Find H-bonds involving ligand and reveal partners.
`distance atom1 atom2`	Measure and display an interatomic distance.
`contacts spec`	Find close contacts involving a target.
`clashes spec`	Find steric clashes involving a target.
`rename #1 BRAF`	Rename model #1 as BRAF.
`split #1 ligands`	Split each ligand into a separate submodel.
`crystalcontacts #1 distance 5`	Find contacts ≤5 Å between crystal-symmetry copies.
`matchmaker #2 to #1`	Sequence-align and fit proteins/nucleic acids; protein matching can use secondary structure.
`align spec1 to spec2`	Least-squares fit any molecule using equal, paired atom sets.

LIGHTING & GRAPHICS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`lighting soft`	Soft multidirectional lighting and shadows.
`lighting full`	Soft lighting plus a key light.
`lighting flat`	Flat, low-shading illustration style.
`lighting simple`	Basic directional lighting.
`lighting depthCue false`	Disable front-to-back depth cueing.
`lighting depthCue true`	Enable depth cueing.
`graphics silhouettes true`	Turn silhouette edges on (true) or off (false)

Selecting precisely

ATOM SPECIFICATIONS (spec)

Build a target from model → chain → residue → atom

SELECT COMMAND — START HERE

COMMAND / PATTERN	PURPOSE / EXAMPLE
`select spec`	Select spec, or replace selection with spec.
`select add spec`	Add spec to the selection.
`select subtract spec`	Remove spec from the selection.
`select clear`	Clear the current selection.

IMPORTANT Type **select spec** to select the items described by **spec**. At the start of a command, **sel** abbreviates the command **select**; used as an atom specification, **sel** means the current selection.

CORE HIERARCHY

COMMAND / PATTERN	PURPOSE / EXAMPLE
`#1`	Atomic model #1.
`#1.2`	Submodel #1.2.
`/A`	Chain A in all atomic models.
`:1230`	All residues numbered 1230.
`:VGH`	All residues named VGH.
`@CA`	All atoms named CA.
`#1/A:1230@CA`	CA atom of residue 1230, chain A, model #1.

LISTS, RANGES & WILDCARDS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`#1,2`	Models 1 and 2.
`/A,C`	Chains A and C.
`:1211,1230`	Residues 1211 and 1230.
`:1200-1230`	Inclusive range, for example residues 1211 to 1230.
`@N,CA,C,O`	Named backbone atoms.
`:GL*`	Residue names beginning with GL.
`@C?`	Two-character atom names starting with C.

READ LEFT TO RIGHT #1/A:1230@CA narrows progressively. Omitted levels remain unrestricted; for example, /A:50 means residue 50 in chain A across all open atomic models.

BUILT-IN SPECS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`protein`	Protein residues.
`nucleic`	Nucleic-acid residues.
`ligand`	Residues classified as ligands.
`solvent`	Solvent residues, commonly water.
`ions`	Residues classified as ions.
`HC`	Hydrogens bonded to carbon (apolar hydrogens).
`main`	Main-chain atoms.
`sidechain`	Amino-acid side-chain atoms.
`backbone`	Polymer backbone atoms.
`helix / strand / coil`	Residues by secondary structure.

LOGICAL COMBINATIONS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`spec1 & spec2`	Intersection: items matching both.
`spec1 | spec2`	Union: items matching either.
`~ spec`	Negation: everything except spec.
`/A & protein`	Protein residues in chain A.
`ligand | ions`	Ligands or ions.
`protein & ~ /B`	Protein excluding chain B.
`(:ASP | :GLU) & /A`	Asp or Glu residues in chain A.

PARENTHESES AND SPACES Use parentheses when mixing union and intersection. Put spaces around &, |, and ~ so the expression is parsed unambiguously.

ATTRIBUTE TESTS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`@@bfactor>50`	Atoms with B-factor above 50.
`@@element=C`	Carbon atoms.
`@@occupancy<1`	Atoms with occupancy below 1.
`protein & @@bfactor>=30`	Protein atoms passing a numeric test.

ATTRIBUTE PREFIX @@ tests atom attributes, :: tests residue attributes, and ## tests model attributes. Attribute names and availability depend on the data and prior calculations.

ZONES & MOLECULAR NEIGHBORHOODS

COMMAND / PATTERN	PURPOSE / EXAMPLE
`select spec :<5`	Select whole residues within 5 Å of spec, including **spec**.
`select spec @<5`	Select atoms within 5 Å of **spec**, including **spec**.
`select zone ligand 5`	Atoms within 5 Å of ligand; ligand excluded.
`select zone sel 5`	Atoms within 5 Å of the current selection.
`select zone :1230 10`	Atoms within 10 Å of residue 1230.
`select zone :1230 10 protein`	Restrict proximity selection to protein atoms.
`... residues true`	Select whole residues touched by the zone.
`... extend true`	Also include the reference atoms.

Examples

COMMAND / PATTERN	PURPOSE / EXAMPLE
`select zone ligand 5 protein residues true`	Whole protein residues with some atoms ≤5 Å from any ligand atom.
`select ligand :<5 & protein`	Whole protein residues with some atoms ≤5 Å from any ligand atom.

SELECTION WITH MOUSE & KEYBOARD

COMMAND / PATTERN	PURPOSE / EXAMPLE
Ctrl + click	Select a displayed atom; background clears selection.
Ctrl + Shift + click	Add or toggle another displayed atom.
Ctrl + drag	Select atoms in a screen rectangle.
Up arrow	Broaden selection through structural levels.
Down arrow	Narrow selection through structural levels.

RELIABLE SELECTION WORKFLOW

COMMAND / PATTERN	PURPOSE / EXAMPLE
1 Start broad	Use model, chain, residue, or a named selector.
2 Refine	Add atom names, logical terms, attributes, or a zone.
3 Inspect	Confirm the green outline and selection counts.
4 Act	Use sel in display, color, analysis, or save commands.
5 Clear	Run select clear before the next independent task.

COMMON PITFALLS

CHECK BEFORE ACTING Model IDs depend on open order; chain case can matter; residue insertion codes may occur. Hidden atoms remain selectable, and a command targets the current selection only when given sel. When no selection is made, the next command will target everything.