ChimeraX

Cheat Sheet

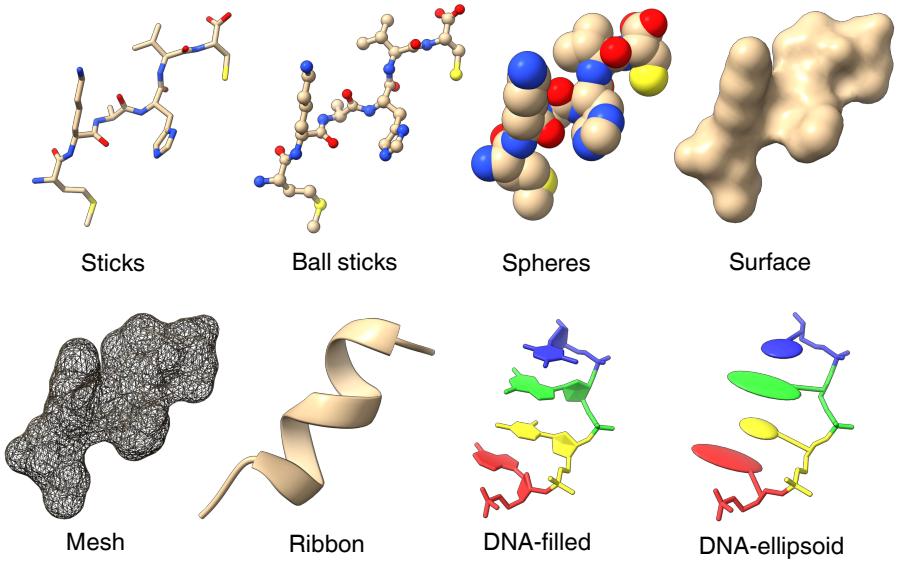
Created by: Alejandro Pereira[a]

[a]Department of Microbiology, University of Georgia, Athens, Georgia, USA

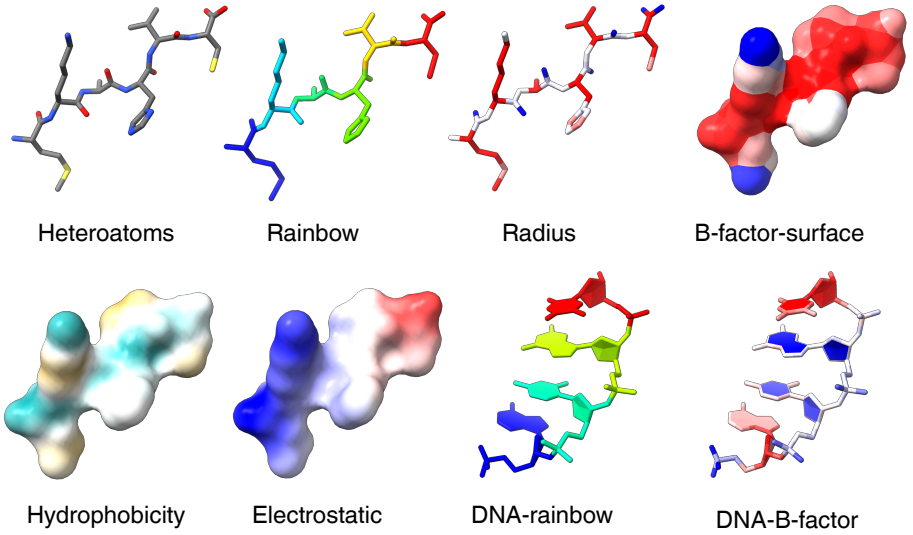
Description of application

UCSF ChimeraX is a tool for viewing and analyzing molecular structures. It supports common structure and data formats such as PDB, CIF, JSON, and NumPy (.npz) files. You can use ChimeraX to look at sequences, make high-quality images, run protein-prediction tools (like AlphaFold and Boltz), and extend functionality through the community driven ToolShed. ChimeraX is free for academic, nonprofit, government, and personal use. To download the software, find documentation, or explore new features, visit the official homepage: https://www.cgl.ucsf.edu/chimerax/. This cheat sheet was done on version 1.10.1 on macOS.

Different ways to represent your molecule



Different ways to describe your molecule



Additional features of ChimeraX

10 useful ChimeraX features

1. MatchMaker – Align and superimpose molecular structures.
2. Rotamers – View and swap amino-acid side-chain rotamers.
3. Surface Clipping – Slice through surfaces to reveal internal features.
4. Contacts – Identify contacts between atoms, residues, or chains.
5. Clashes – Detect steric clashes in models.
6. Distances – Measure distances between atoms or residues.
7. Labeling – Add atom, residue, or chain labels to annotate structures.
8. Movie Making – Create smooth molecular animations to show conformational changes, zoom-ins, or rotations.
9. Model Editing – Delete atoms, mutate residues, or modify structures.
10. High-Quality Rendering – Produce publication-ready images and animations.

Useful commands

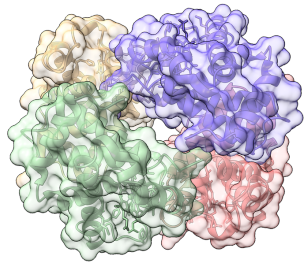
5 useful ChimeraX commands for CLI

1. MatchMaker (mm) – Align two structures.
   Comm: mm #1 to #2 (aligns model 1 to 2)
2. Select (sel) – Select a residue, chain, or model.
   Comm: sel /A:50 (select residue 50, chain A)
3. Deselect (~sel) – Clear selection.
   Comm: ~sel
4. Color (color) – Color specific atoms or regions. You first need to select something.
   Comm: color sel red (color residue 50 red)
5. Show/Hide (show/hide) – Toggle visibility.
   Comm: hide atoms; show cartoon

Publication quality examples

Ex 1: Hemoglobin Tetramer (color chains differently, show ribbon + 50% transparent surface). For this example, enter each step separately in the command-line interface (CLI).

1. Open 1A00
2. Color bychain
3. Surface
4. Transparency 50
5. Graphics silhouettes true
6. Save test.png transparentBackground true



Ex 2: DNA polymerase I (AF-P00582-F1-v6) (download mmCIF and predicted align error [JSON] files, import into ChimeraX, color by pLDDT)

1. Go to https://alphafold.ebi.ac.uk/entry/AF-P00582-F1
2. Download mmCIF and predicted align error files
3. Drag and drop both files into ChimeraX
4. Click “Color pLDDT” in the new window
5. Save test.png transparentBackground true