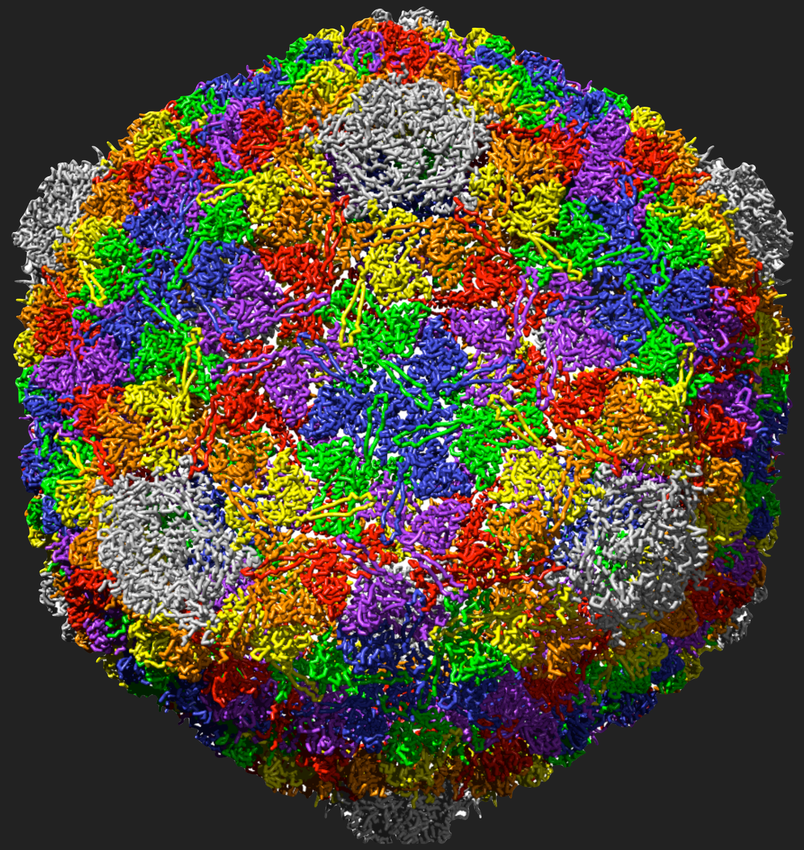


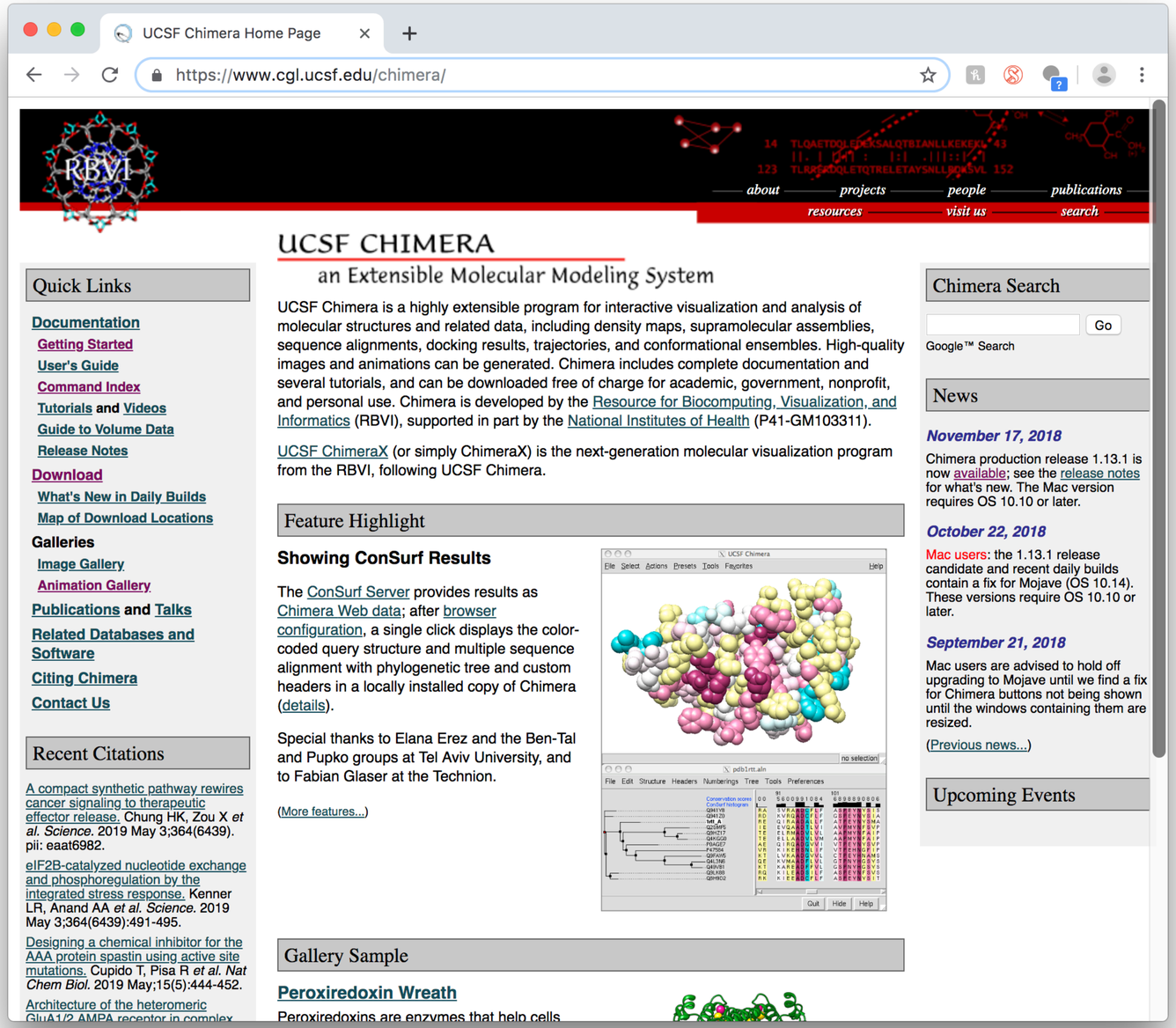
UTMB CRYO-EM WORKSHOP

UCSF CHIMERA

Matthew Baker, Ph.D
Baylor College of Medicine

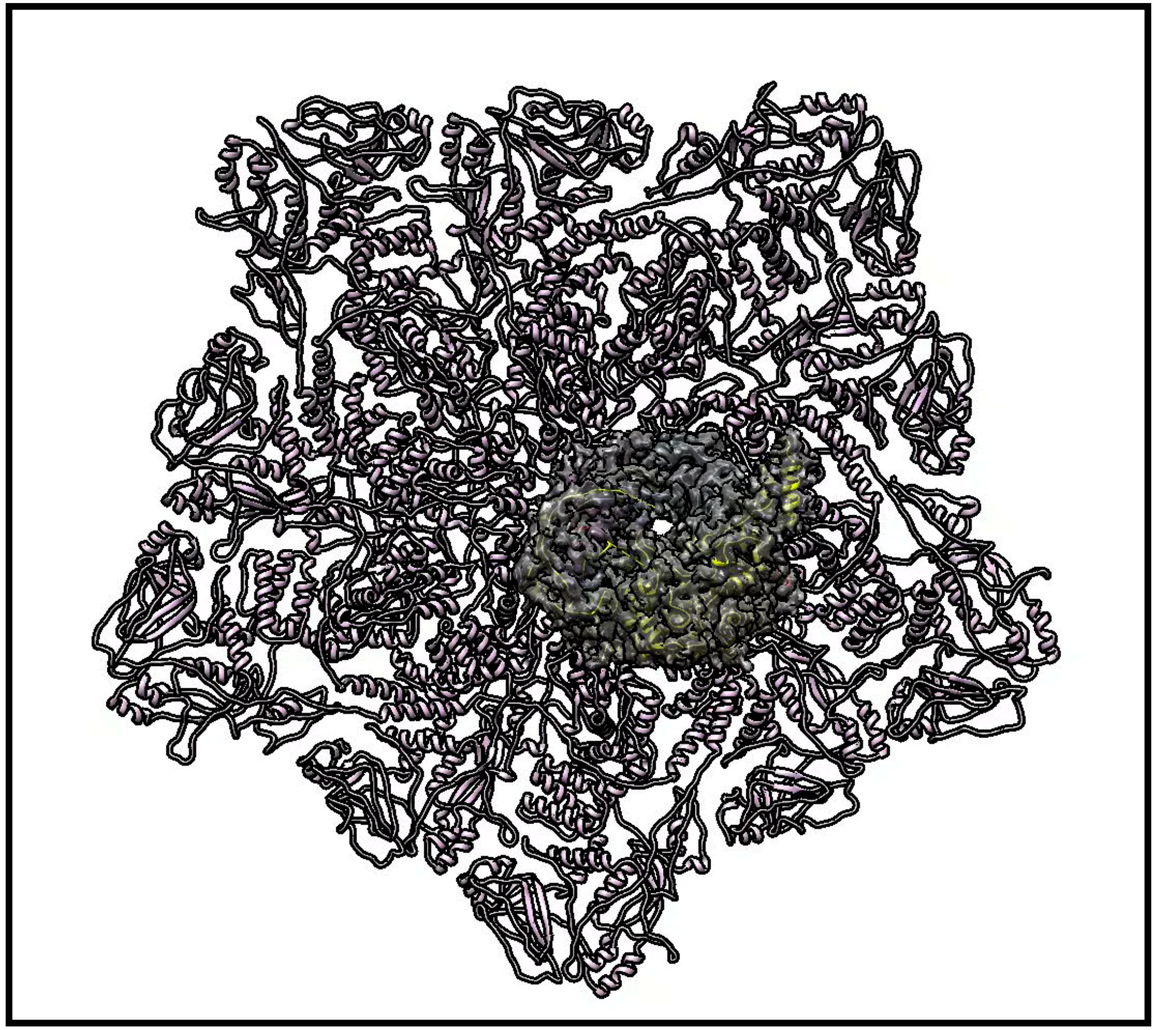
WHAT IS CHIMERA

- "… a highly extensible program for interactive visualization and analysis of molecular structures and related data, including **density maps**, **supramolecular assemblies**, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. "



WHERE TO GET CHIMERA

- Download: https://www.cgl.ucsf.edu/chimera/download.html
- Tutorials: https://www.rbvi.ucsf.edu/chimera/tutorials.html
- Commands: https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/framecommand.html
- ChimeraX: https://www.cgl.ucsf.edu/chimerax/



UCSF Chimera--a visualization system for exploratory research and analysis. Pettersen EF, Goddard TD, Huang CC, Couch GS, Greenblatt DM, Meng EC, Ferrin TE. *J Comput Chem*. 2004 Oct;25(13):1605-12.

THE BASICS: PART 1

File: Open, Save, Sessions, Screenshots

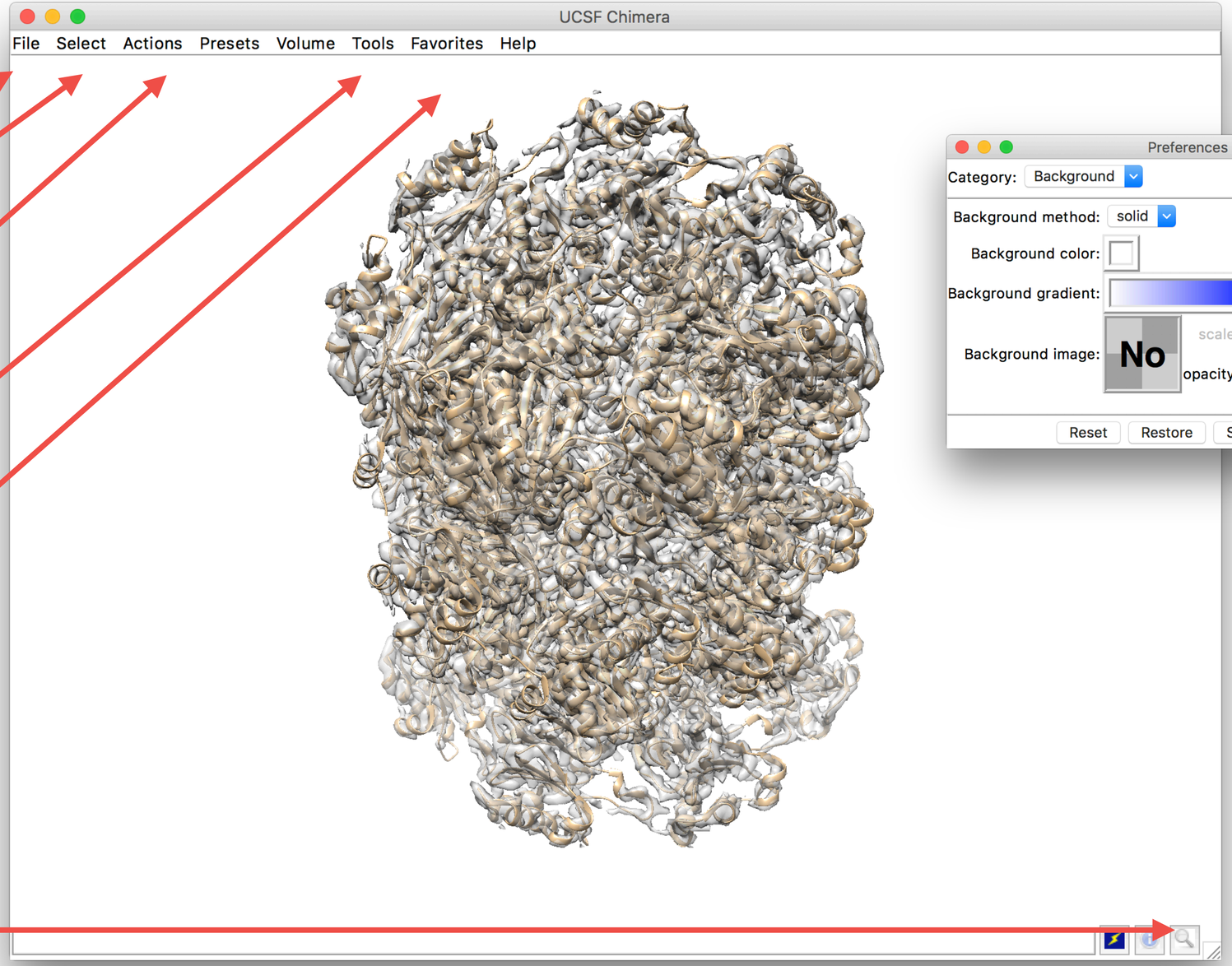
Select: Select atom objects

Actions: Display behaviors, colors, labels, surfaces

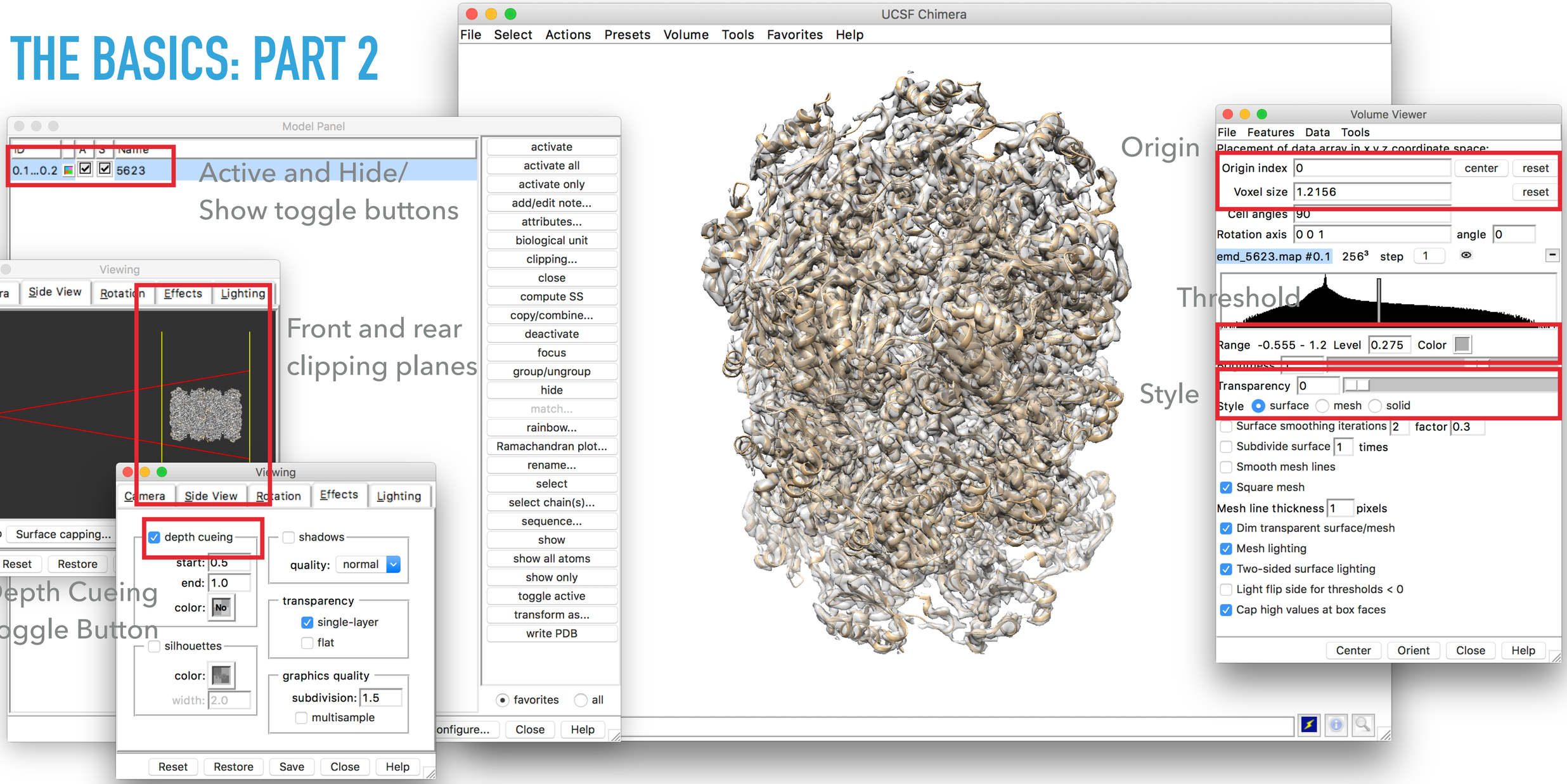
Tools: All utilities

Favorites: Quick access to Model panel, Side View, Preferences and Command line

Inspector: Shows selected molecule attributes

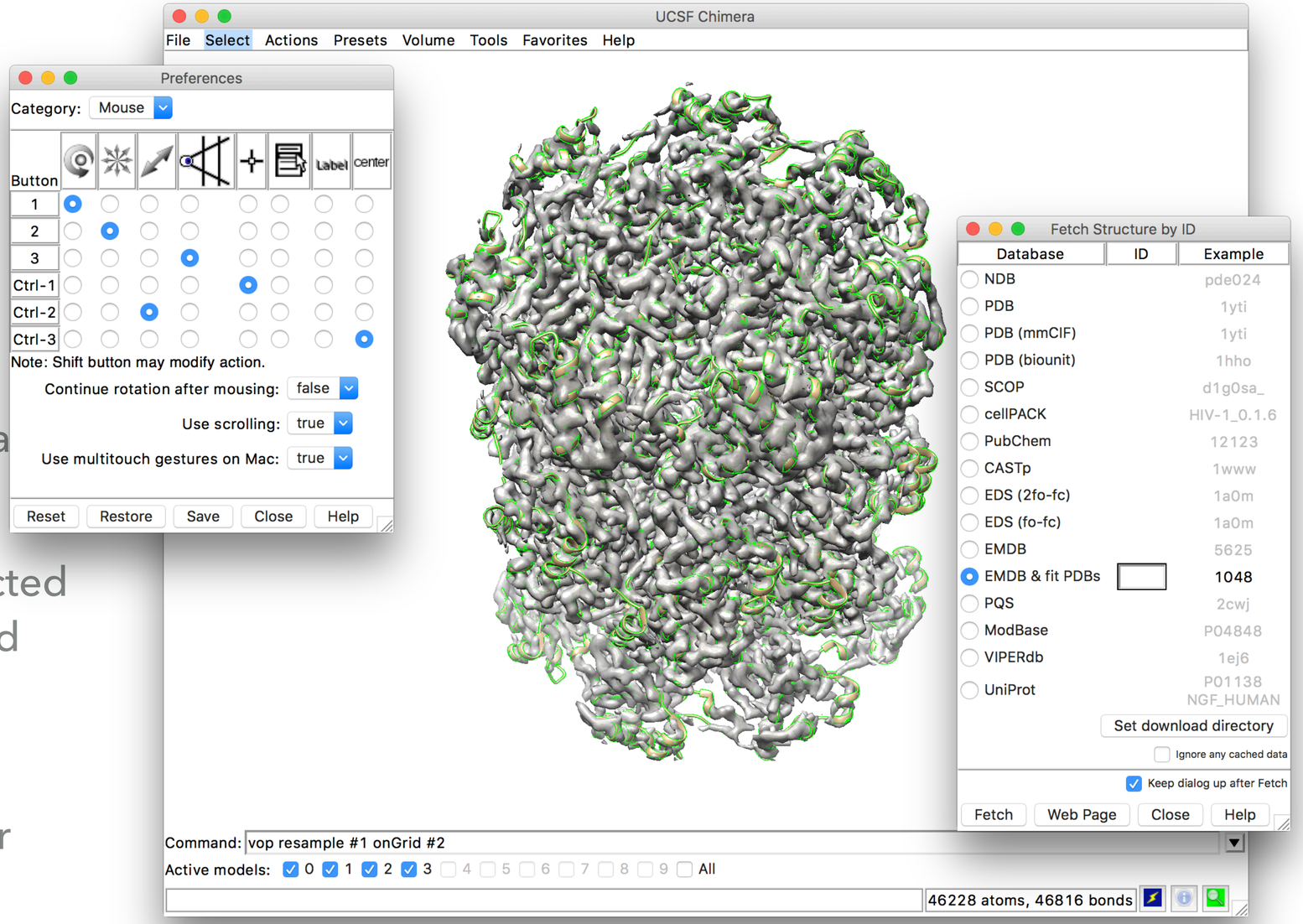


THE BASICS: PART 2



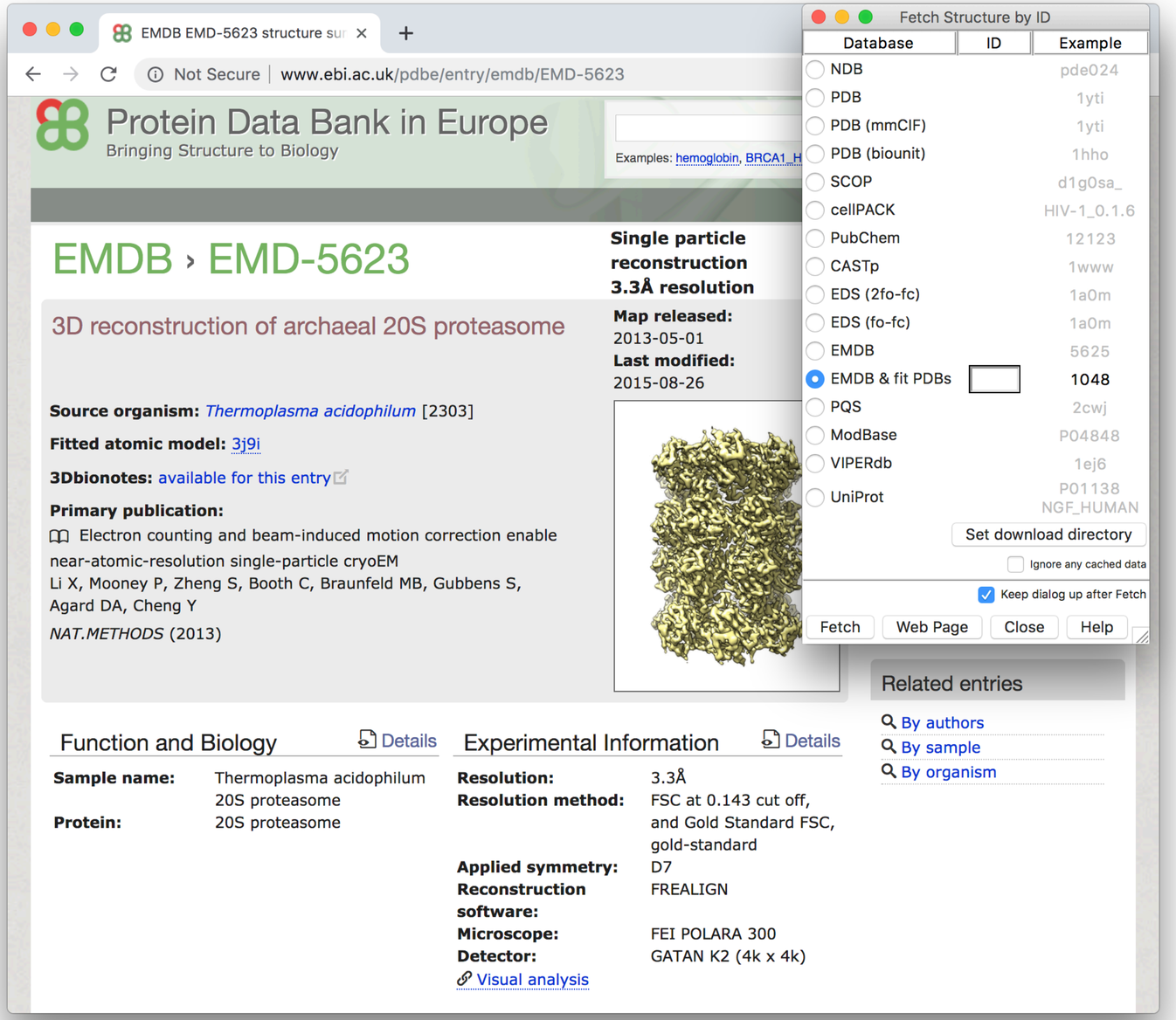
INTERACTING WITH CHIMERA

- Command line (i.e. vop resample #1 onGrid #0)
- Interactive
  - 3-button mouse to rotate, translate a zoom view
  - Select object: Ctrl+left mouse (selected items turn green) Tip: use the up and down arrows to increase/decrease selection
- Load supported files from local drive or remotely from databases



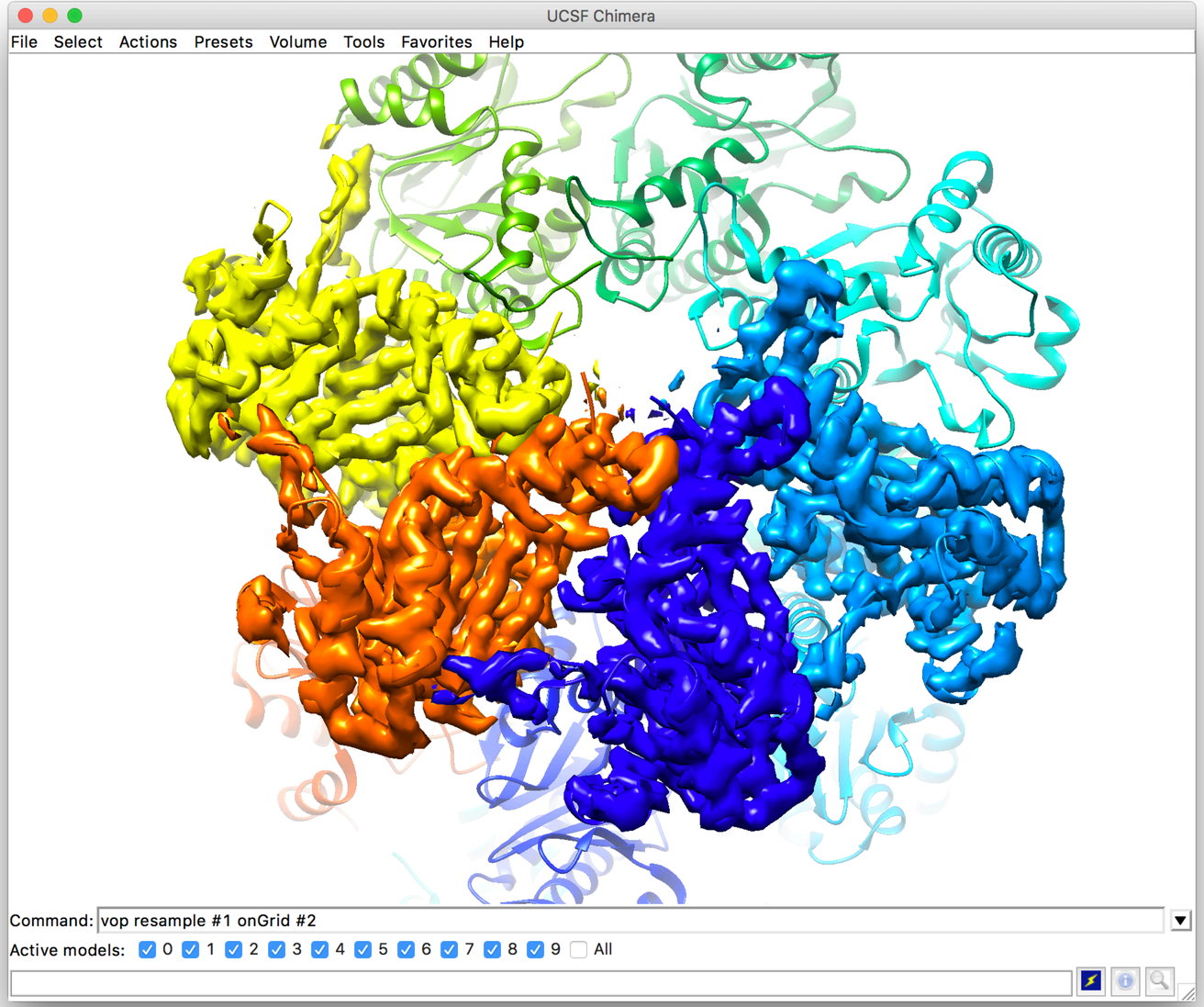
TEST DATA: 20S PROTEASOME

- EMDB 5623 (http://www.ebi.ac.uk/pdbe/entry/emdb/EMD-5623)
- Load map and model directly from EMDB
  - In File Menu, select “Fetch by ID”
  - Select EMDB & fit PDBs
  - Press Fetch
  - Map and Model will appear on screen and in the Model Panel (left click on the ID and the select “group/ungroup” to separate map and models



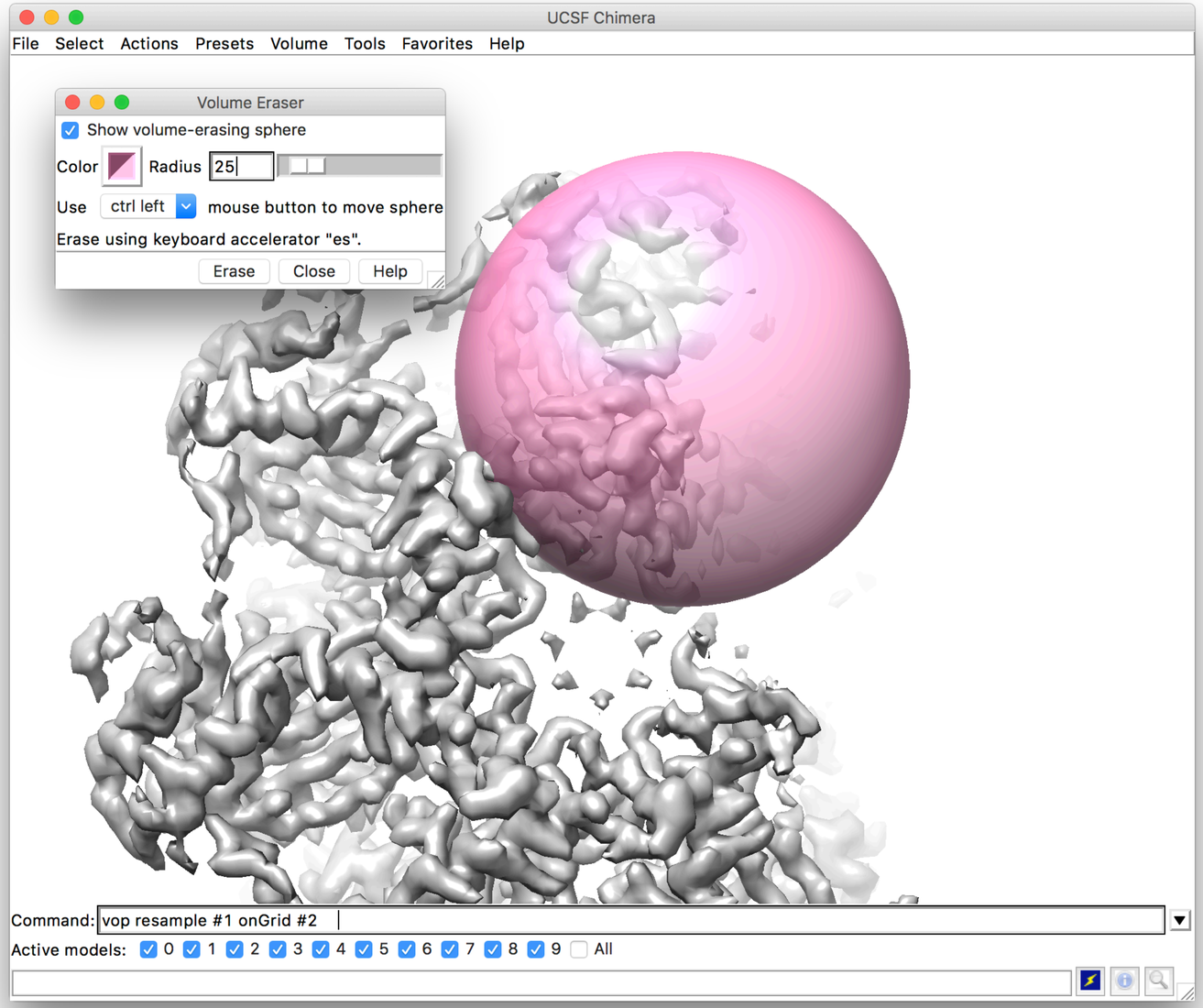
SEGMENTATION #1

- Model-based segmentation
  - Select model
  - Color all chains 1 color
  - Select individual chains and assign unique color to each chain
  - Re-select all chains
  - In Volume Viewer open “Color Zone”
  - Select map and provide a coloring radius
  - Press “Color”
  - If coloring looks good, press “Split Map”



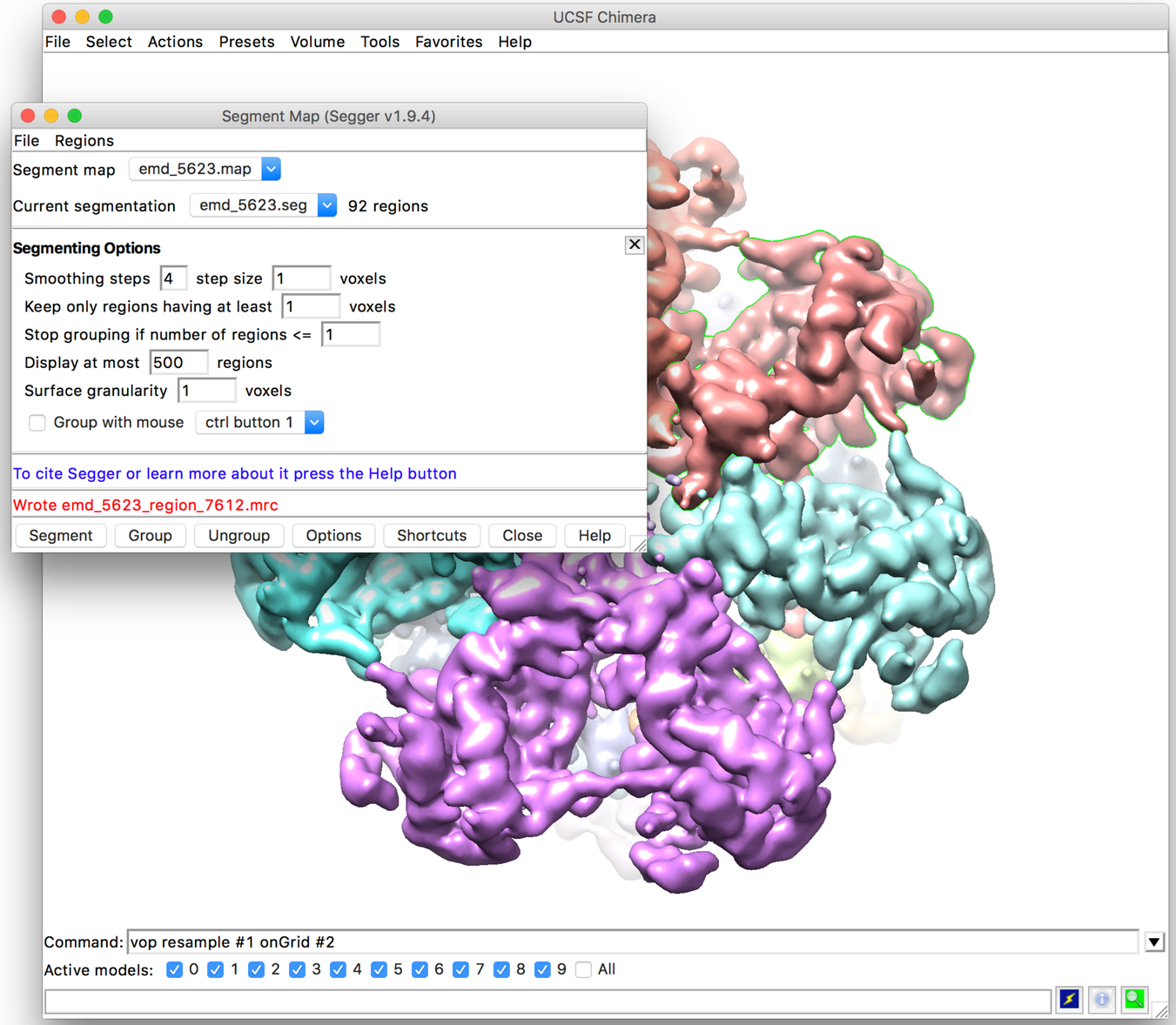
SEGMENTATION #2

- Volume Eraser segmentation
  - Select “Volume Eraser” from the Tools menu in Volume Viewer
  - A semi-transparent sphere will be displayed along with a new widget (the pink sphere in the viewer is your eraser)
  - Start with a largish radius (1~5-25) and set “use” to Ctrl-left
  - Hold Ctrl-left and move the pink sphere eraser; press “Erase” in widget to remove density (a new map is created with erased portions
  - Remove density, progressively shrinking the radius until ROI is obtained
  - This is 3D; you will need to rotate your volume
  - Surface is shown at a specific threshold. Adjust threshold to make sure subunit boundary is defined



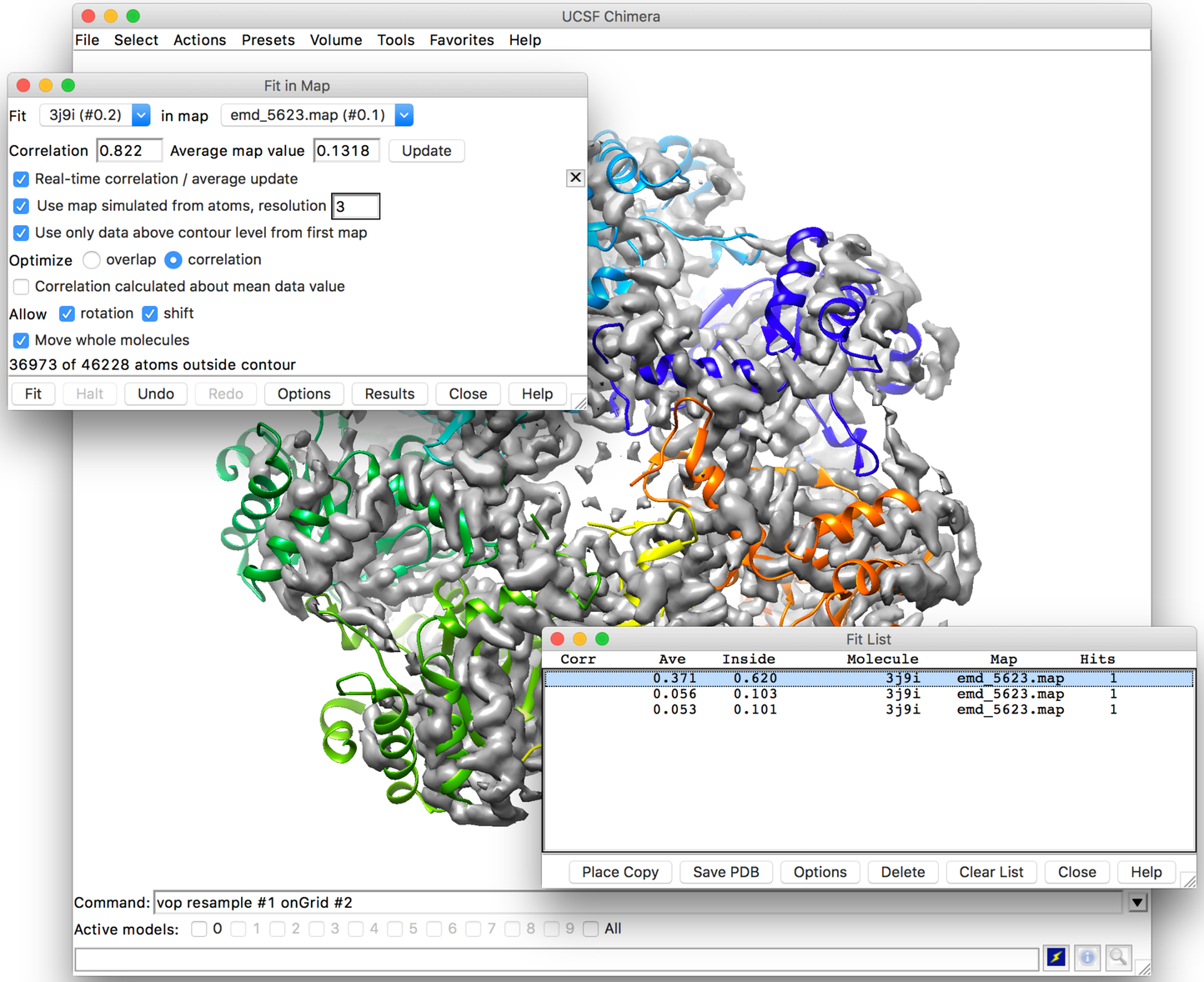
SEGMENTATION #3

- Segger
  - In Volume Viewer, select “Segment Map” from Tools menu
  - Select map and press Options to expand
  - Press Segment to auto segment
  - A set of colored masks will appear
  - Group masks by selecting the masks of a “related” segment (Ctrl+left)
  - Press Group to combine
  - Iterate until you have selected your ROI or entire molecule
  - Extract Density using “Save all/selected Regions to .mrc file”
  - https://www.rbvi.ucsf.edu/chimera/docs/ContributedSoftware/segger/segment.html

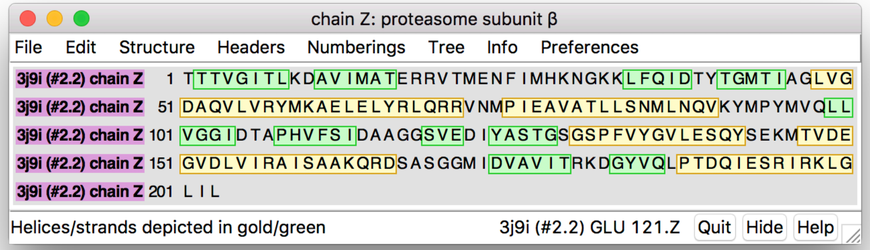


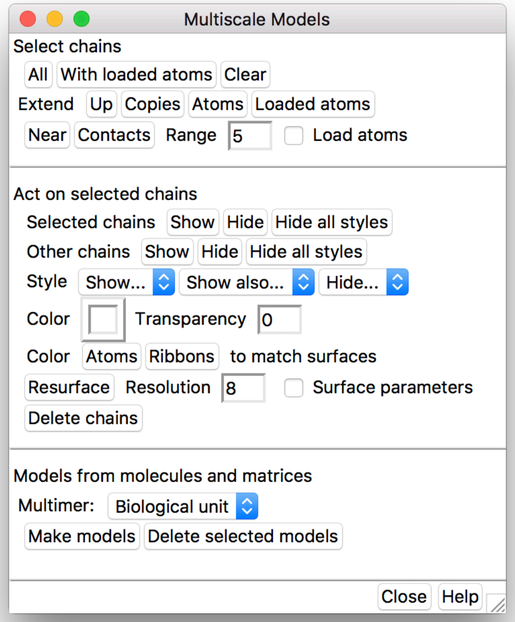
FITTING A MODEL TO A MAP

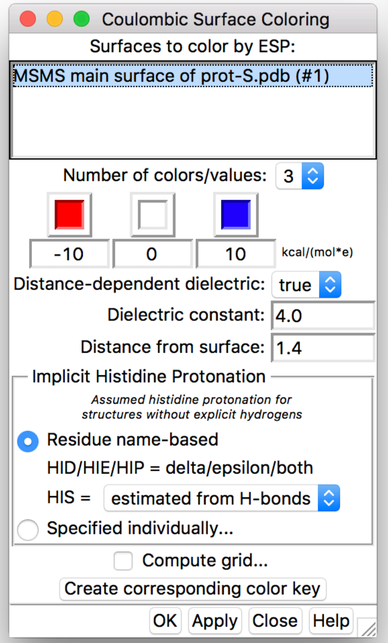
- Simple correlation-based or density overlap fitting
  - Good for quick local, fits when model is “close” to the right fit
  - Volume Viewer –> Tools–> “Fit in Map”
- Global search
  - Global cross correlation-based search that provides
  - Command line: fitmap #0.2 #0.1 search 10
  - Generates an interactive list of top fits
- Multi-model fitting
  - Can handle symmetry
  - Volume Viewer –> Tools–> “Multi-fit”

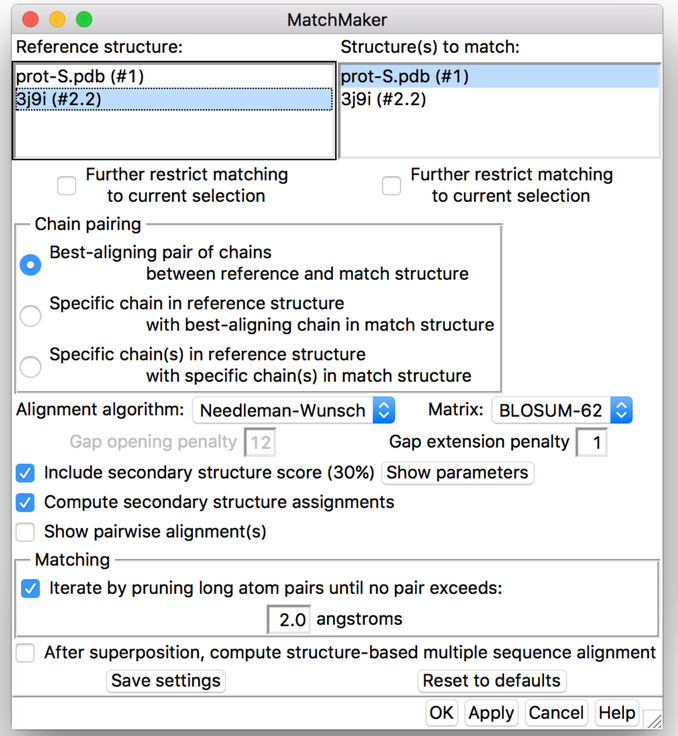


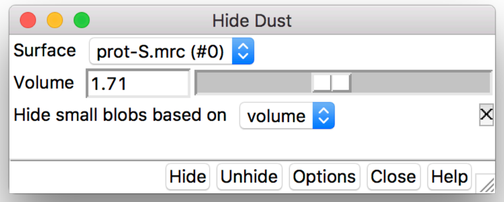
MORE USEFUL TOOLS

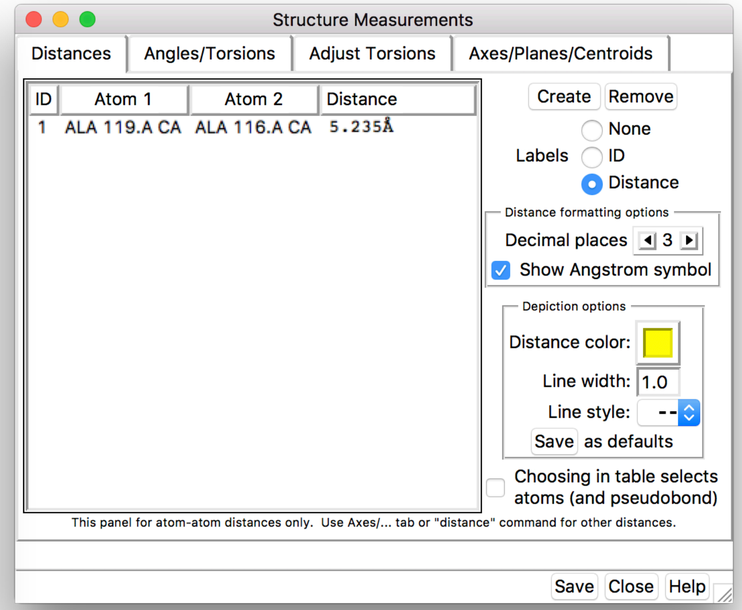


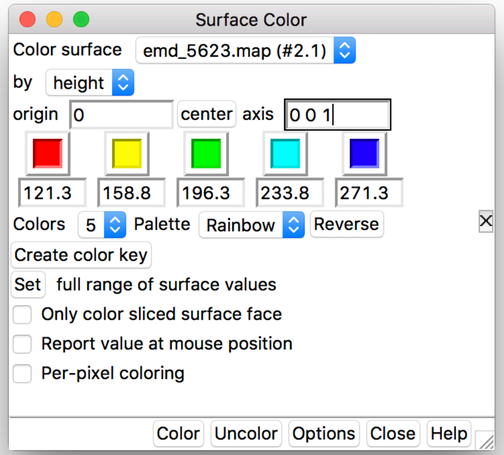






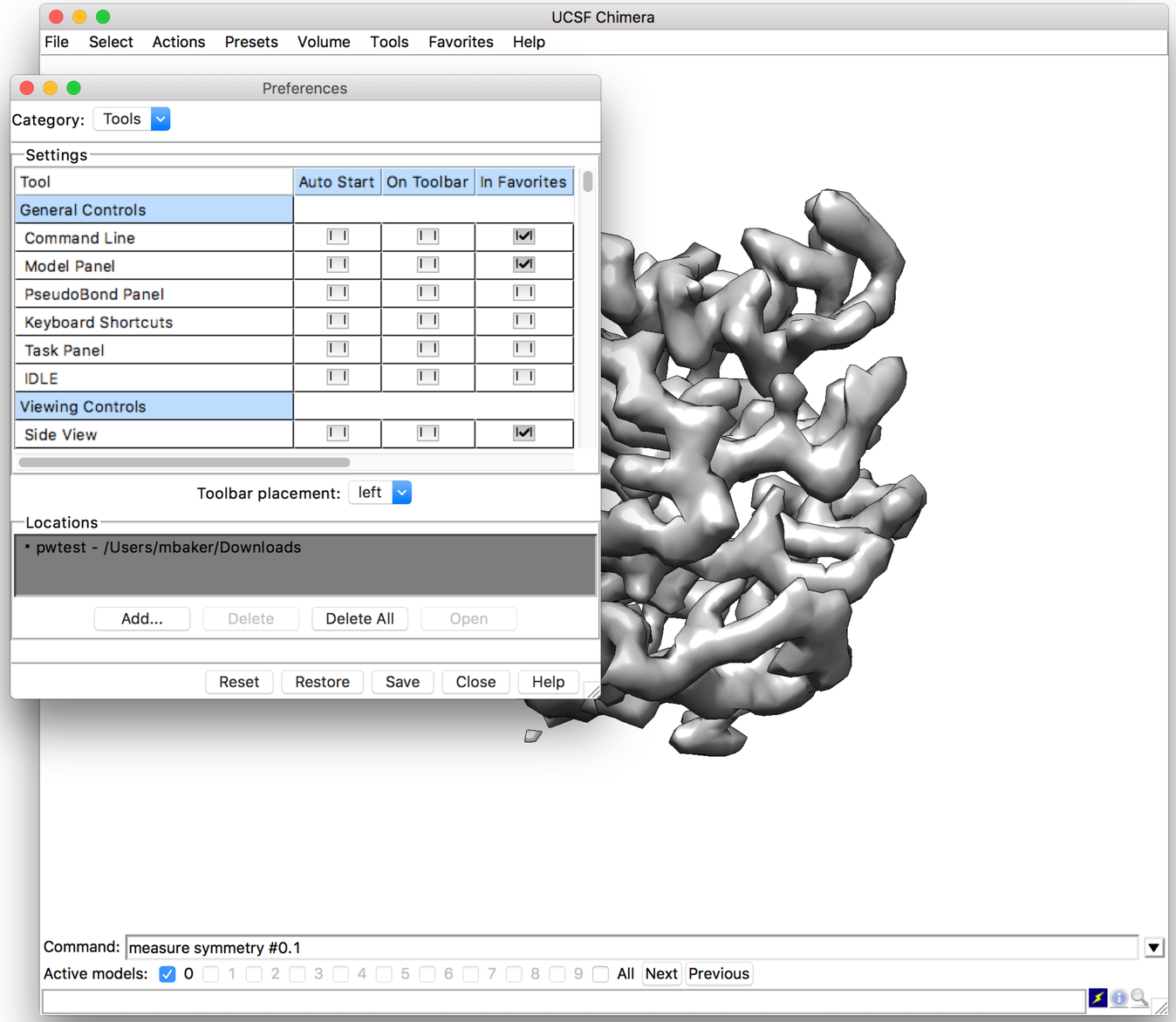






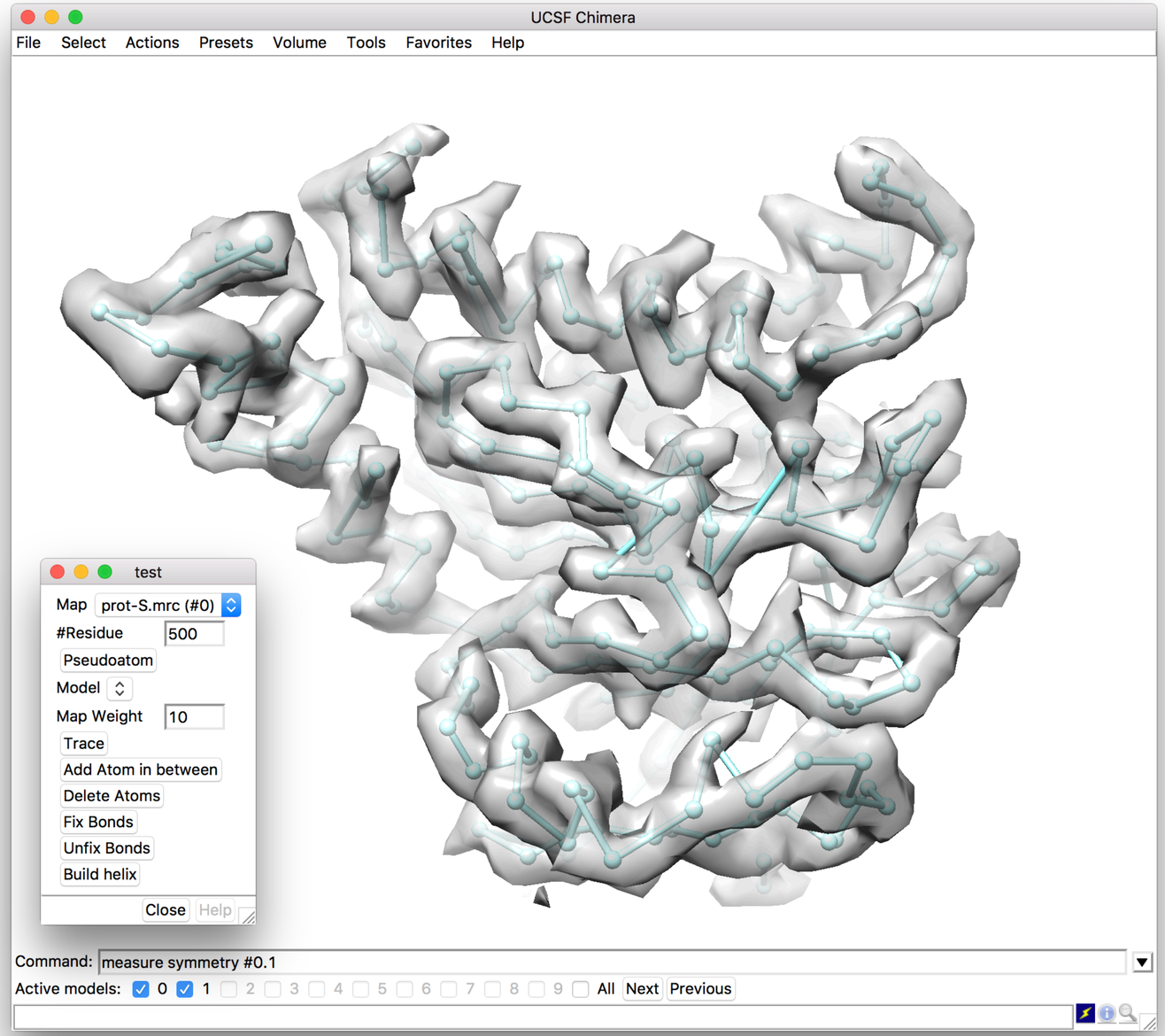
MODIFYING CHIMERA

- In Favorites, select “preferences”
- Select “Tools” from Category menu
- Select tools to Auto-start tools, add quick links to side panel of viewer or add items to Favorites
- Add Chimera Extensions by selecting “Add..” in locations panel
- Save preferences



CHIMERA EXTENSION: PATHWALKING

- Automated Model building with Pathwalking
  - After adding Extension location, “pwtest” appears in Volume Viewer Tools menu
  - Adjust the map threshold in volume viewer and set the number of residues in pwtest. Press pseudo-atom to generate nodes and then Trace to generate path.
- https://blake.bcm.edu/emanwiki/Pathwalker



FOR MORE INFORMATION

- User Guide: https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/
- Getting Started: https://www.cgl.ucsf.edu/Outreach/Tutorials/GettingStarted.html