

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."

UCSF Chimera Home Page

https://www.cgl.ucsf.edu/chimera/

about projects people publications
resources visit us search

UCSF CHIMERA

an Extensible Molecular Modeling System

UCSF Chimera is 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. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, nonprofit, and personal use. Chimera is developed by the [Resource for Biocomputing, Visualization, and Informatics](#) (RBVI), supported in part by the [National Institutes of Health](#) (P41-GM103311).

[UCSF ChimeraX](#) (or simply ChimeraX) is the next-generation molecular visualization program from the RBVI, following UCSF Chimera.

Quick Links

- [Documentation](#)
- [Getting Started](#)
- [User's Guide](#)
- [Command Index](#)
- [Tutorials and Videos](#)
- [Guide to Volume Data](#)
- [Release Notes](#)
- [Download](#)
- [What's New in Daily Builds](#)
- [Map of Download Locations](#)
- [Galleries](#)
- [Image Gallery](#)
- [Animation Gallery](#)
- [Publications and Talks](#)
- [Related Databases and Software](#)
- [Citing Chimera](#)
- [Contact Us](#)

Recent Citations

[A compact synthetic pathway rewires cancer signaling to therapeutic effector release.](#) Chung HK, Zou X *et al. Science*. 2019 May 3;364(6439). pii: eaat6982.

[eIF2B-catalyzed nucleotide exchange and phosphoregulation by the integrated stress response.](#) Kenner LR, Anand AA *et al. Science*. 2019 May 3;364(6439):491-495.

[Designing a chemical inhibitor for the AAA protein spastin using active site mutations.](#) Cupido T, Pisa R *et al. Nat Chem Biol*. 2019 May;15(5):444-452.

[Architecture of the heteromeric GluA1/2 AMPA receptor in complex](#)

Chimera Search

Go

Google™ Search

News

November 17, 2018
Chimera production release 1.13.1 is now [available](#); see the [release notes](#) for what's new. The Mac version requires OS 10.10 or later.

October 22, 2018
Mac users: the 1.13.1 release candidate and recent daily builds contain a fix for Mojave (OS 10.14). These versions require OS 10.10 or later.

September 21, 2018
Mac users are advised to hold off upgrading to Mojave until we find a fix for Chimera buttons not being shown until the windows containing them are resized. ([Previous news...](#))

Upcoming Events

Feature Highlight

Showing ConSurf Results

The [ConSurf Server](#) provides results as [Chimera Web data](#); after [browser configuration](#), a single click displays the color-coded query structure and multiple sequence alignment with phylogenetic tree and custom headers in a locally installed copy of Chimera ([details](#)).

Special thanks to Elana Erez and the Ben-Tal and Pupko groups at Tel Aviv University, and to Fabian Glaser at the Technion.

([More features...](#))

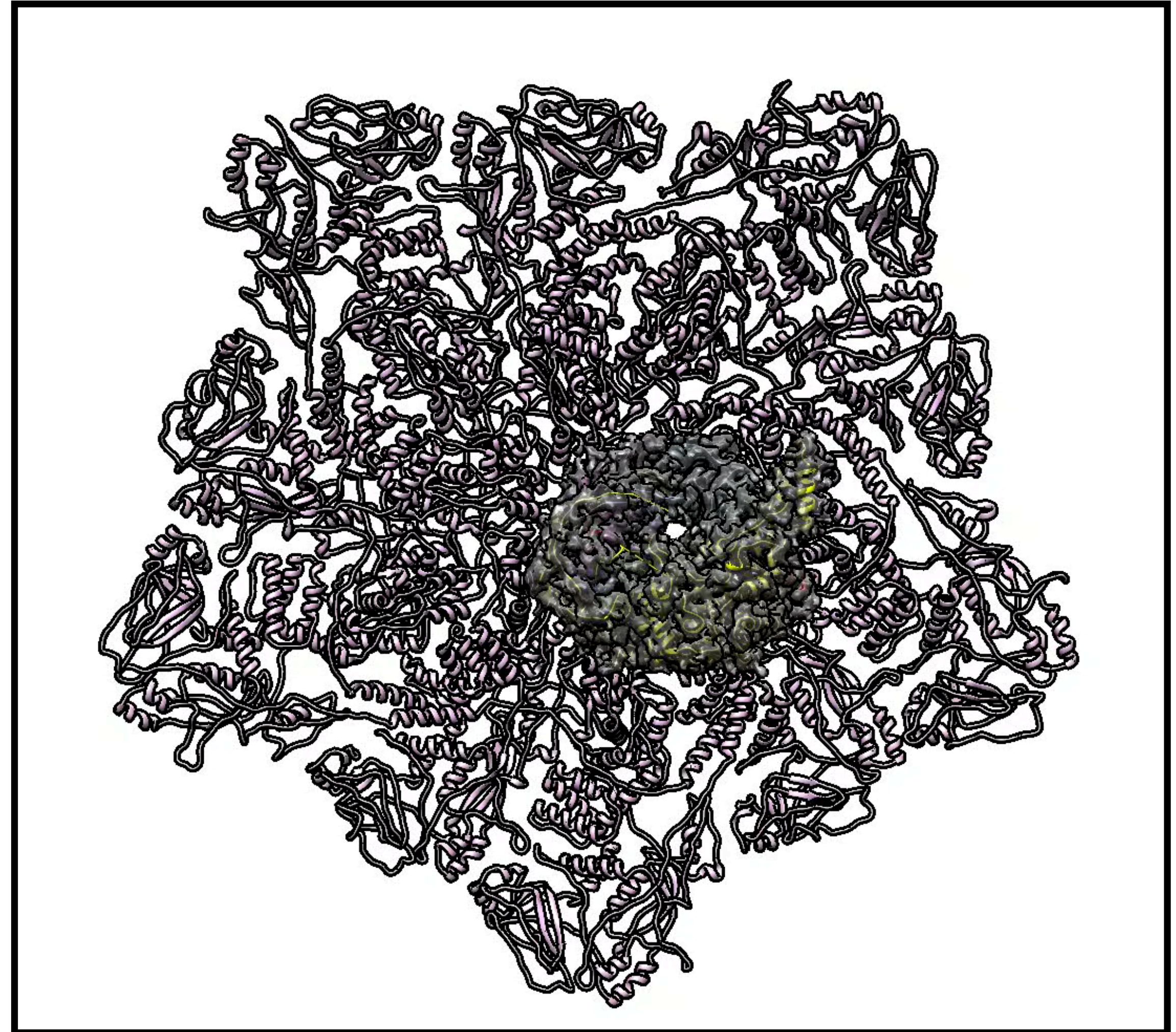
Gallery Sample

Peroxiredoxin Wreath

Peroxiredoxins are enzymes that help cells

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/>



THE BASICS: PART 1

File: Open, Save, Sessions, Screenshots

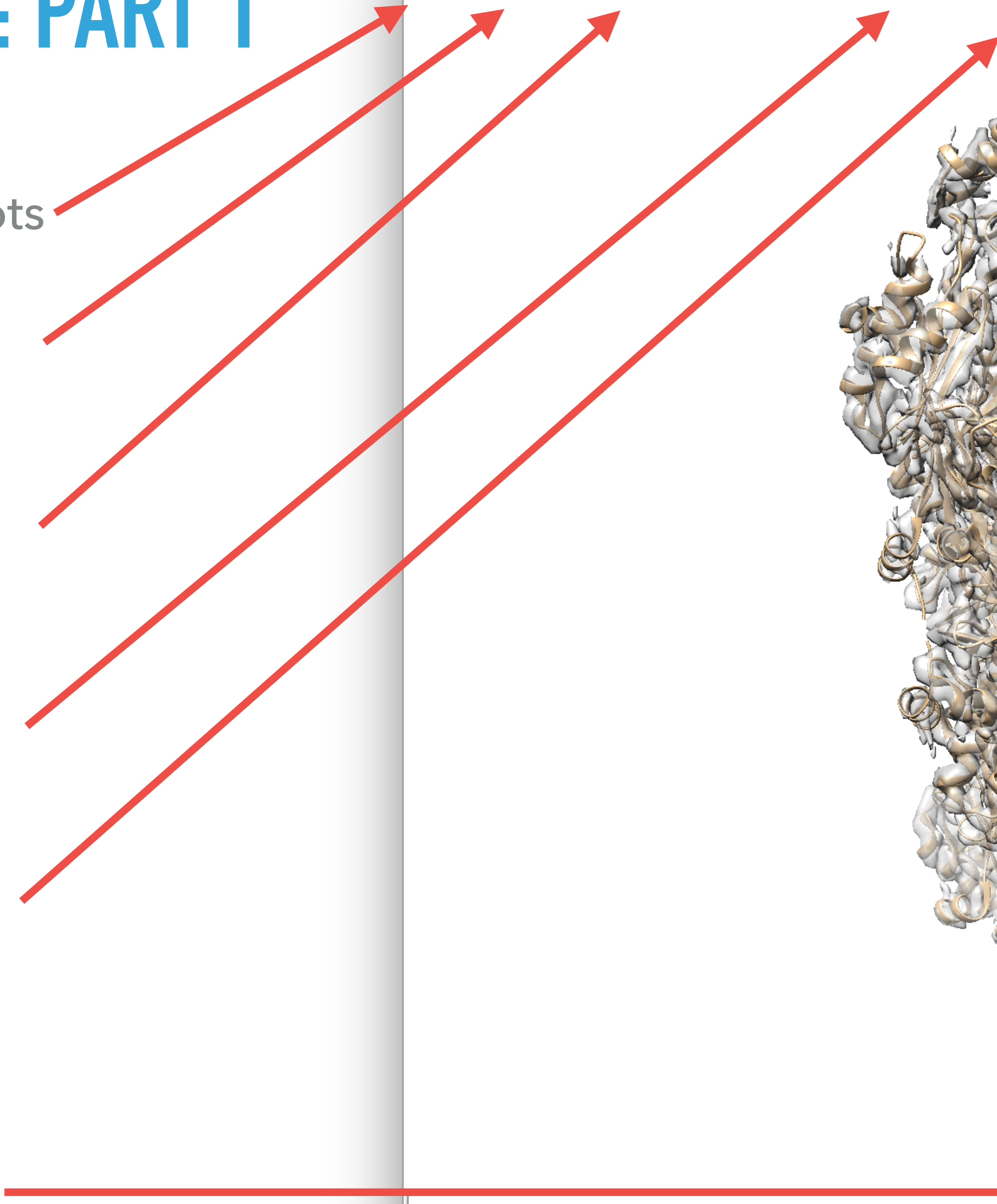
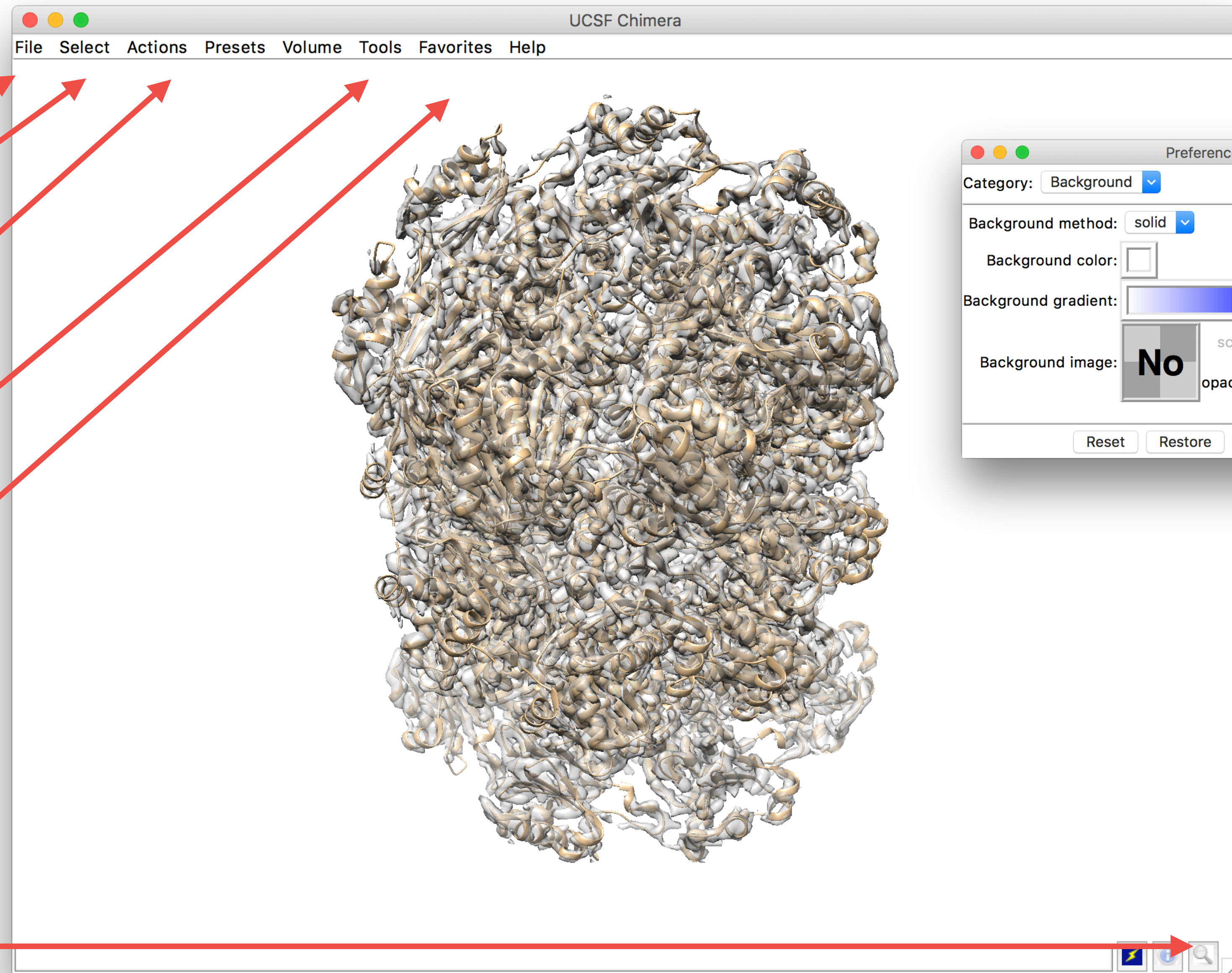
Select: Select atom objects

Actions: Display behaviors, colors, labels, surfaces

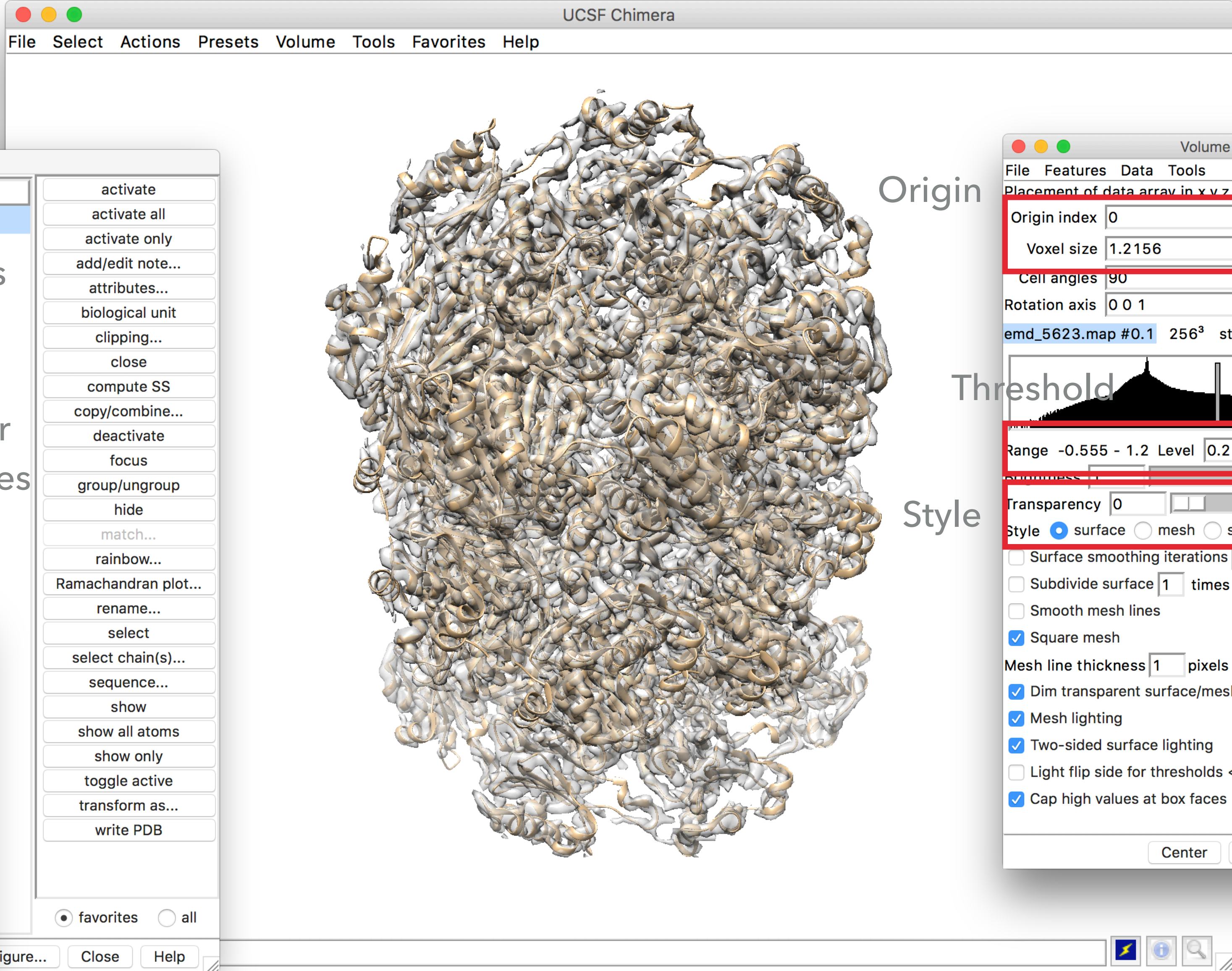
Tools: All utilities

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

Inspector: Shows selected molecule attributes



THE BASICS: PART 2



Model Panel

ID	A	S	Name
0.1...0.2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	5623

Active and Hide/
Show toggle buttons

Viewing

Camera Side View Rotation Effects Lighting

Front and rear clipping planes

Viewing

Camera Side View Rotation Effects Lighting

depth cueing

start: 0.5 end: 1.0 color: No

silhouettes color: width: 2.0

shadows quality: normal

transparency single-layer flat

graphics quality subdivision: 1.5 multisample

Depth Cueing Toggle Button

Origin

Volume Viewer

File Features Data Tools

Placement of data array in x y z coordinate space:

Origin index 0 center reset

Voxel size 1.2156 reset

Threshold

Cell angles 90

Rotation axis 0 0 1 angle 0

emd_5623.map #0.1 256³ step 1

Range -0.555 - 1.2 Level 0.275 Color

Style

Transparency 0

Style surface mesh solid

Surface smoothing iterations 2 factor 0.3

Subdivide surface 1 times

Smooth mesh lines

Square mesh

Mesh line thickness 1 pixels

Dim transparent surface/mesh

Mesh lighting

Two-sided surface lighting

Light flip side for thresholds < 0

Cap high values at box faces

Center Orient Close Help

INTERACTING WITH CHIMERA

- ▶ Command line (i.e. vop resample #1 onGrid #0)
- ▶ Interactive
 - ▶ 3-button mouse to rotate, translate and 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

The screenshot displays the UCSF Chimera software interface. The main window shows a protein structure rendered in a grey surface representation with green and orange highlights. Overlaid on the interface are two dialog boxes: 'Preferences' and 'Fetch Structure by ID'. The 'Preferences' dialog is set to 'Mouse' and shows various mouse button actions. The 'Fetch Structure by ID' dialog lists several databases, with 'EMDB & fit PDBs' selected and a search box containing '1048'. At the bottom, the command line shows 'vop resample #1 onGrid #2' and the status bar indicates '46228 atoms, 46816 bonds'.

UCSF Chimera

File Select Actions Presets Volume Tools Favorites Help

Preferences

Category: Mouse

Button						
1	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
2	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
3	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Ctrl-1	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>
Ctrl-2	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Ctrl-3	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>

Note: Shift button may modify action.

Continue rotation after mousing: false

Use scrolling: true

Use multitouch gestures on Mac: true

Reset Restore Save Close Help

Fetch Structure by ID

Database	ID	Example
<input type="radio"/> NDB		pde024
<input type="radio"/> PDB		1yti
<input type="radio"/> PDB (mmCIF)		1yti
<input type="radio"/> PDB (biounit)		1hho
<input type="radio"/> SCOP		d1g0sa_
<input type="radio"/> cellPACK		HIV-1_0.1.6
<input type="radio"/> PubChem		12123
<input type="radio"/> CASTp		1www
<input type="radio"/> EDS (2fo-fc)		1a0m
<input type="radio"/> EDS (fo-fc)		1a0m
<input type="radio"/> EMDB		5625
<input checked="" type="radio"/> EMDB & fit PDBs	<input type="text" value="1048"/>	1048
<input type="radio"/> PQS		2cwj
<input type="radio"/> ModBase		P04848
<input type="radio"/> VIPERdb		1ej6
<input type="radio"/> UniProt		P01138 NGF_HUMAN

Set download directory Ignore any cached data Keep dialog up after Fetch

Fetch Web Page Close Help

Command: vop resample #1 onGrid #2

Active models: 0 1 2 3 4 5 6 7 8 9 All

46228 atoms, 46816 bonds

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)

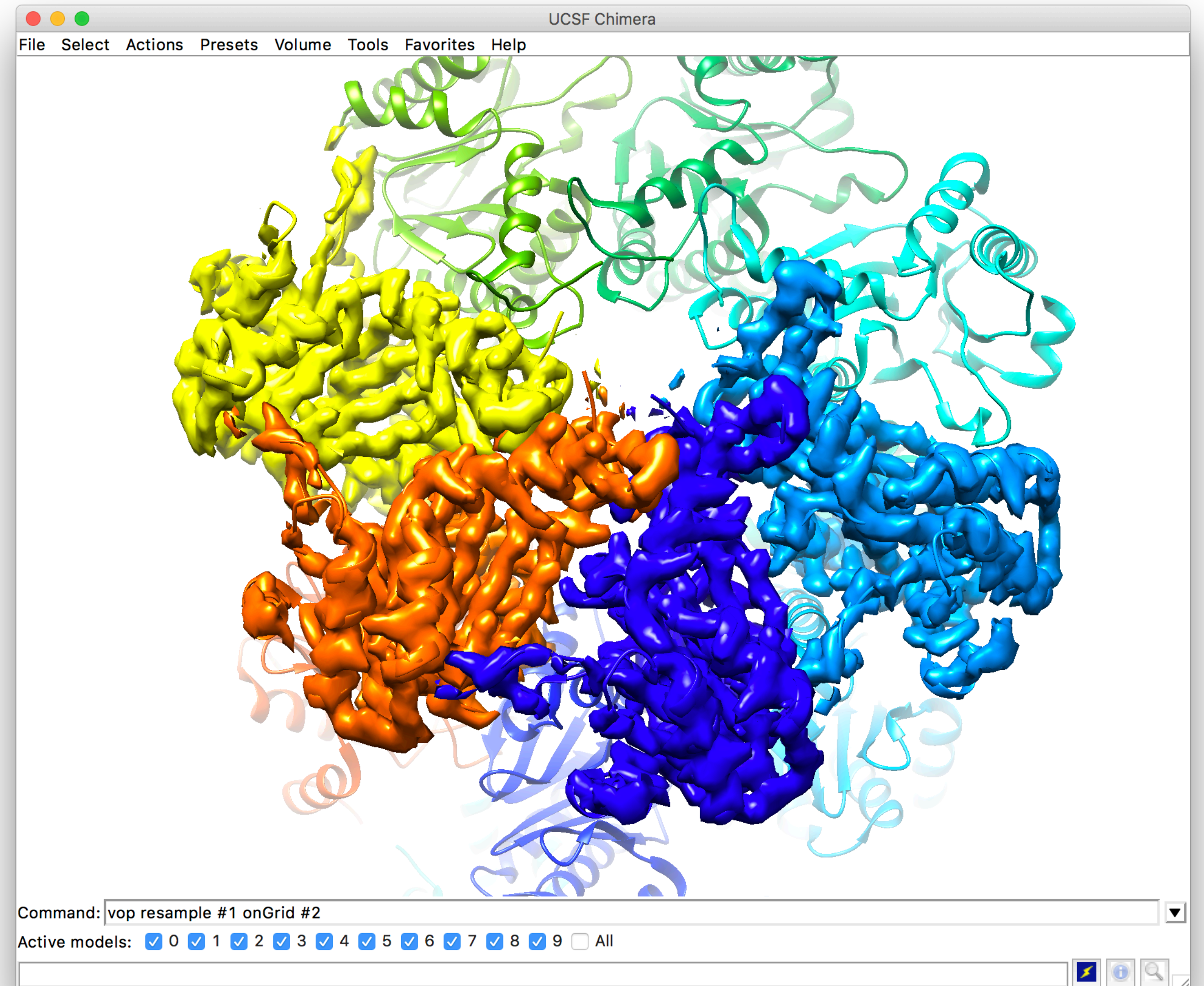
The screenshot shows the Protein Data Bank in Europe website for entry EMD-5623. The page title is "EMDB > EMD-5623" and the subtitle is "3D reconstruction of archaeal 20S proteasome". The main content area includes the source organism (*Thermoplasma acidophilum*), the fitted atomic model (3j9i), and the primary publication information. A 3D reconstruction of the 20S proteasome is shown as a yellow mesh structure. The "Experimental Information" section provides details on resolution (3.3Å), resolution method, applied symmetry (D7), reconstruction software (FREALIGN), microscope (FEI POLARA 300), and detector (GATAN K2).

Overlaid on the right side of the browser window is the "Fetch Structure by ID" dialog box. It features a table with columns for Database, ID, and Example. The "EMDB & fit PDBs" option is selected, and the ID field contains "1048". Other options include NDB, PDB, PDB (mmCIF), PDB (biounit), SCOP, cellPACK, PubChem, CASTp, EDS (2fo-fc), EDS (fo-fc), EMDB, PQS, ModBase, VIPERdb, and UniProt. The dialog also includes a "Set download directory" button, an "Ignore any cached data" checkbox, and a "Keep dialog up after Fetch" checkbox which is checked. Buttons for "Fetch", "Web Page", "Close", and "Help" are at the bottom.

Database	ID	Example
<input type="radio"/>	NDB	pde024
<input type="radio"/>	PDB	1yti
<input type="radio"/>	PDB (mmCIF)	1yti
<input type="radio"/>	PDB (biounit)	1hho
<input type="radio"/>	SCOP	d1g0sa_
<input type="radio"/>	cellPACK	HIV-1_0.1.6
<input type="radio"/>	PubChem	12123
<input type="radio"/>	CASTp	1www
<input type="radio"/>	EDS (2fo-fc)	1a0m
<input type="radio"/>	EDS (fo-fc)	1a0m
<input type="radio"/>	EMDB	5625
<input checked="" type="radio"/>	EMDB & fit PDBs	1048
<input type="radio"/>	PQS	2cwj
<input type="radio"/>	ModBase	P04848
<input type="radio"/>	VIPERdb	1ej6
<input type="radio"/>	UniProt	P01138 NGF_HUMAN

SEGMENTATION #1

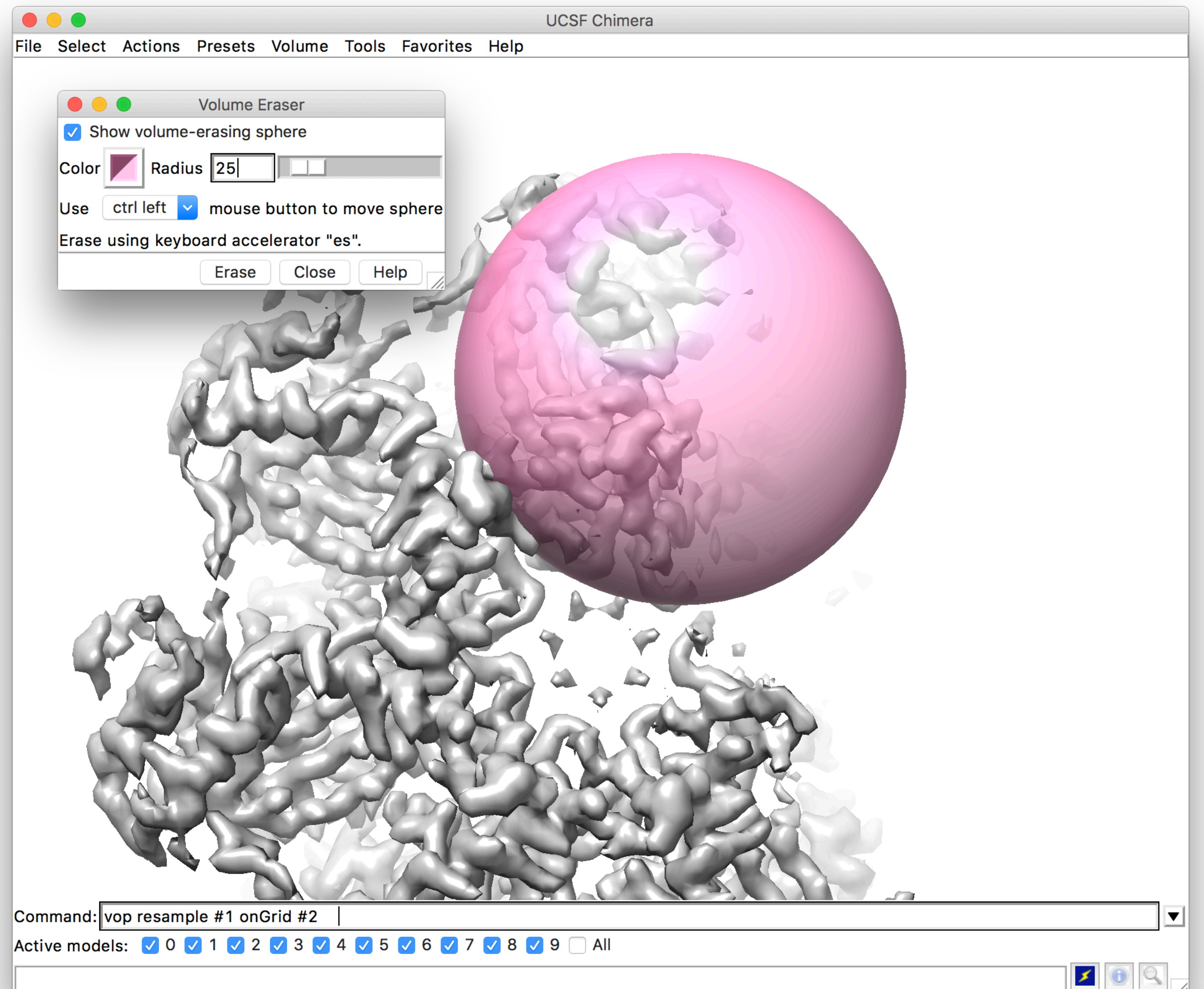
- ▶ Model-based segmentation
 - ▶ Select model
 - ▶ Color all chains 1 color
 - ▶ Select individual chains and assign unique color to each chain
 - ▶ Re-select all chains
 - ▶ In Volume Viewer open "Color Zone"
 - ▶ Select map and provide a coloring radius
 - ▶ Press "Color"
- ▶ If coloring looks good,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

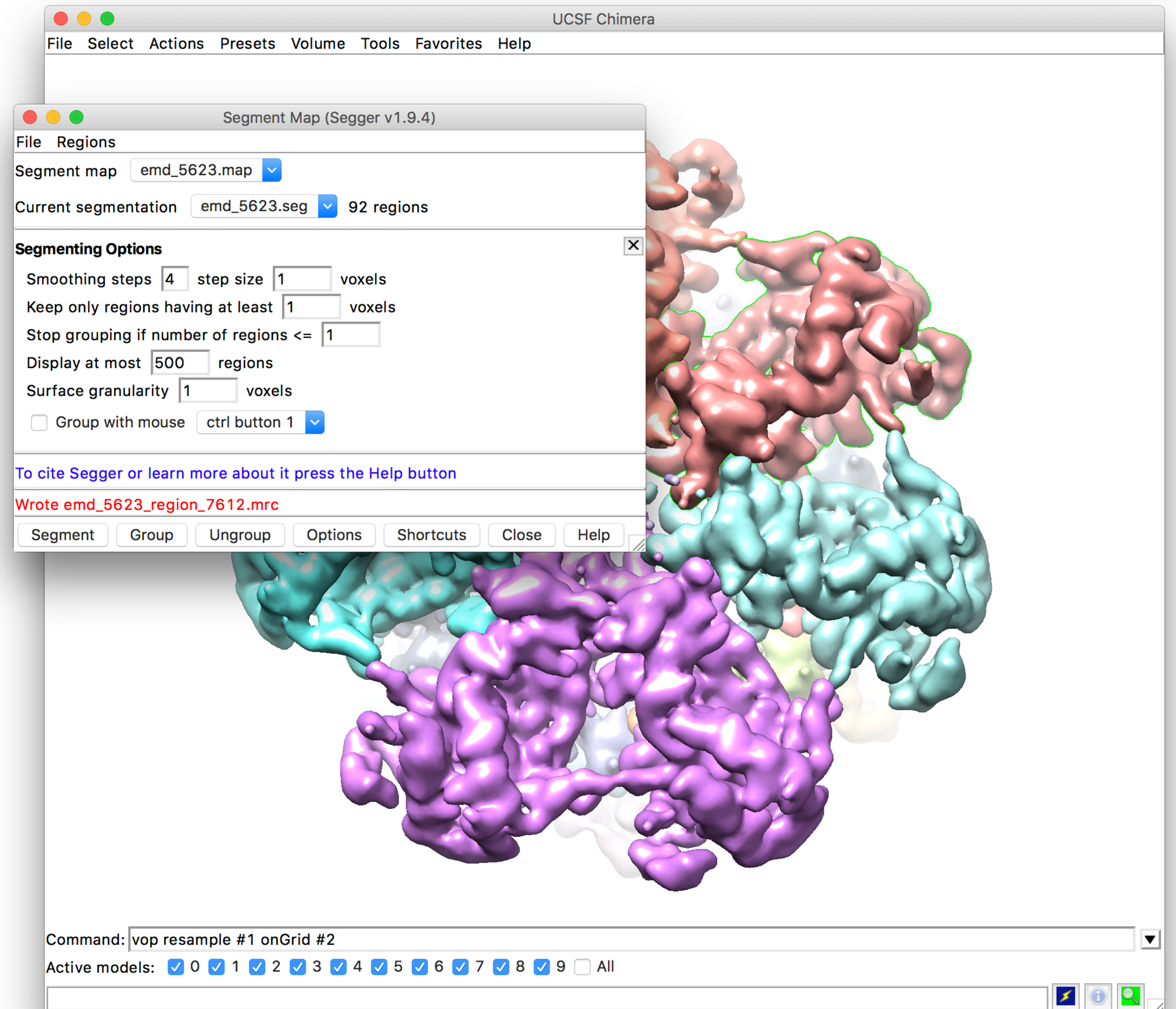


SEGMENTATION #3

▶ Segger

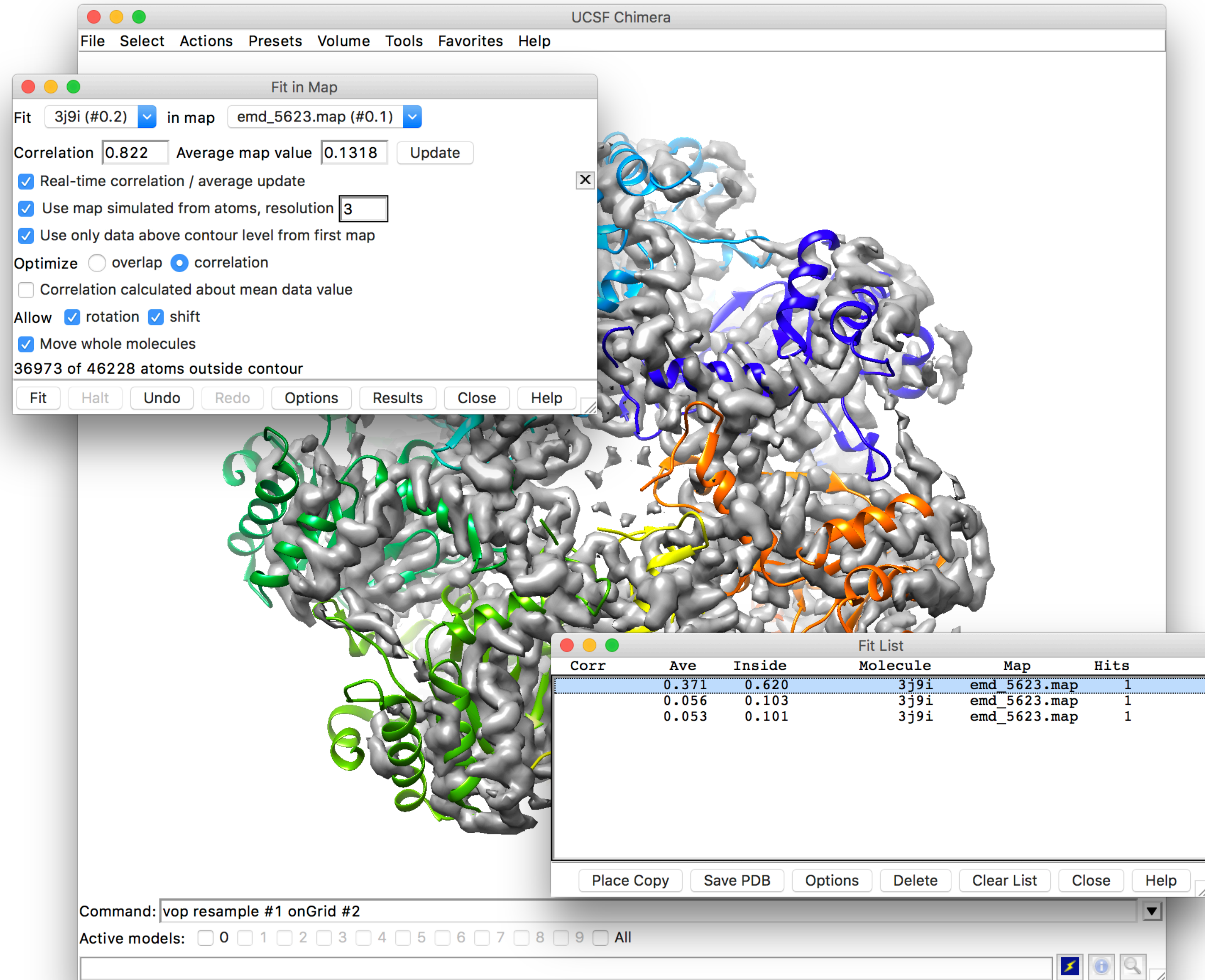
- ▶ In Volume Viewer, select "Segment Map" from Tools menu
- ▶ Select map and press Options to expand
- ▶ Press Segment to auto segment
- ▶ A set of colored masks will appear
- ▶ Group masks by selecting the masks of a "related" segment (Ctrl+left)
- ▶ Press Group to combine
- ▶ Iterate until you have 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

chain Z: proteasome subunit β

File Edit Structure Headers Numberings Tree Info Preferences

```

3j9i (#2.2) chain Z 1 TTTVGITLKDAVIMATERV T M E N F I M H K N G K K L F Q I D T Y T G M T I A G L V G
3j9i (#2.2) chain Z 51 DAQVLVRYMKAELELYRLQRRV N M P I E A V A T L L S N M L N Q V K Y M P Y M V Q L L
3j9i (#2.2) chain Z 101 V G G I D T A P H V F S I D A A G G S V E D I Y A S T G S G S P F V Y G V L E S Q Y S E K M T V D E
3j9i (#2.2) chain Z 151 G V D L V I R A I S A A K Q R D S A S G G M I D V A V I T R K D G Y V Q L P T D Q I E S R I R K L G
3j9i (#2.2) chain Z 201 L I L
    
```

Helices/strands depicted in gold/green 3j9i (#2.2) GLU 121.Z Quit Hide Help

MatchMaker

Reference structure: prot-S.pdb (#1)
3j9i (#2.2)

Structure(s) to match: prot-S.pdb (#1)
3j9i (#2.2)

Further restrict matching to current selection Further restrict matching to current selection

Chain pairing

- Best-aligning pair of chains between reference and match structure
- Specific chain in reference structure with best-aligning chain in match structure
- Specific chain(s) in reference structure with specific chain(s) in match structure

Alignment algorithm: Needleman-Wunsch Matrix: BLOSUM-62

Gap opening penalty 12 Gap extension penalty 1

Include secondary structure score (30%) Show parameters

Compute secondary structure assignments

Show pairwise alignment(s)

Matching

Iterate by pruning long atom pairs until no pair exceeds: 2.0 angstroms

After superposition, compute structure-based multiple sequence alignment

Save settings Reset to defaults OK Apply Cancel Help

Structure Measurements

Distances Angles/Torsions Adjust Torsions Axes/Planes/Centroids

ID	Atom 1	Atom 2	Distance
1	ALA 119.A CA	ALA 116.A CA	5.235Å

Create Remove

Labels None ID Distance

Distance formatting options

Decimal places 3

Show Angstrom symbol

Depiction options

Distance color:

Line width: 1.0

Line style: --

Save as defaults

Choosing in table selects atoms (and pseudobond)

This panel for atom-atom distances only. Use Axes/... tab or "distance" command for other distances.

Save Close Help

Multiscale Models

Select chains

All With loaded atoms Clear

Extend Up Copies Atoms Loaded atoms

Near Contacts Range 5 Load atoms

Act on selected chains

Selected chains Show Hide Hide all styles

Other chains Show Hide Hide all styles

Style Show... Show also... Hide...

Color Transparency 0

Color Atoms Ribbons to match surfaces

Resurface Resolution 8 Surface parameters

Delete chains

Models from molecules and matrices

Multimer: Biological unit

Make models Delete selected models

Close Help

Coulombic Surface Coloring

Surfaces to color by ESP:

MSMS main surface of prot-S.pdb (#1)

Number of colors/values: 3

-10 0 10 kcal/(mol*e)

Distance-dependent dielectric: true

Dielectric constant: 4.0

Distance from surface: 1.4

Implicit Histidine Protonation

Assumed histidine protonation for structures without explicit hydrogens

- Residue name-based
- HID/HIE/HIP = delta/epsilon/both
- HIS = estimated from H-bonds
- Specified individually...

Compute grid...

Create corresponding color key

OK Apply Close Help

Hide Dust

Surface prot-S.mrc (#0)

Volume 1.71

Hide small blobs based on volume

Hide Unhide Options Close Help

Surface Color

Color surface emd_5623.map (#2.1)

by height

origin 0 center axis 0 0 1

121.3 158.8 196.3 233.8 271.3

Colors 5 Palette Rainbow Reverse

Create color key

Set full range of surface values

Only color sliced surface face

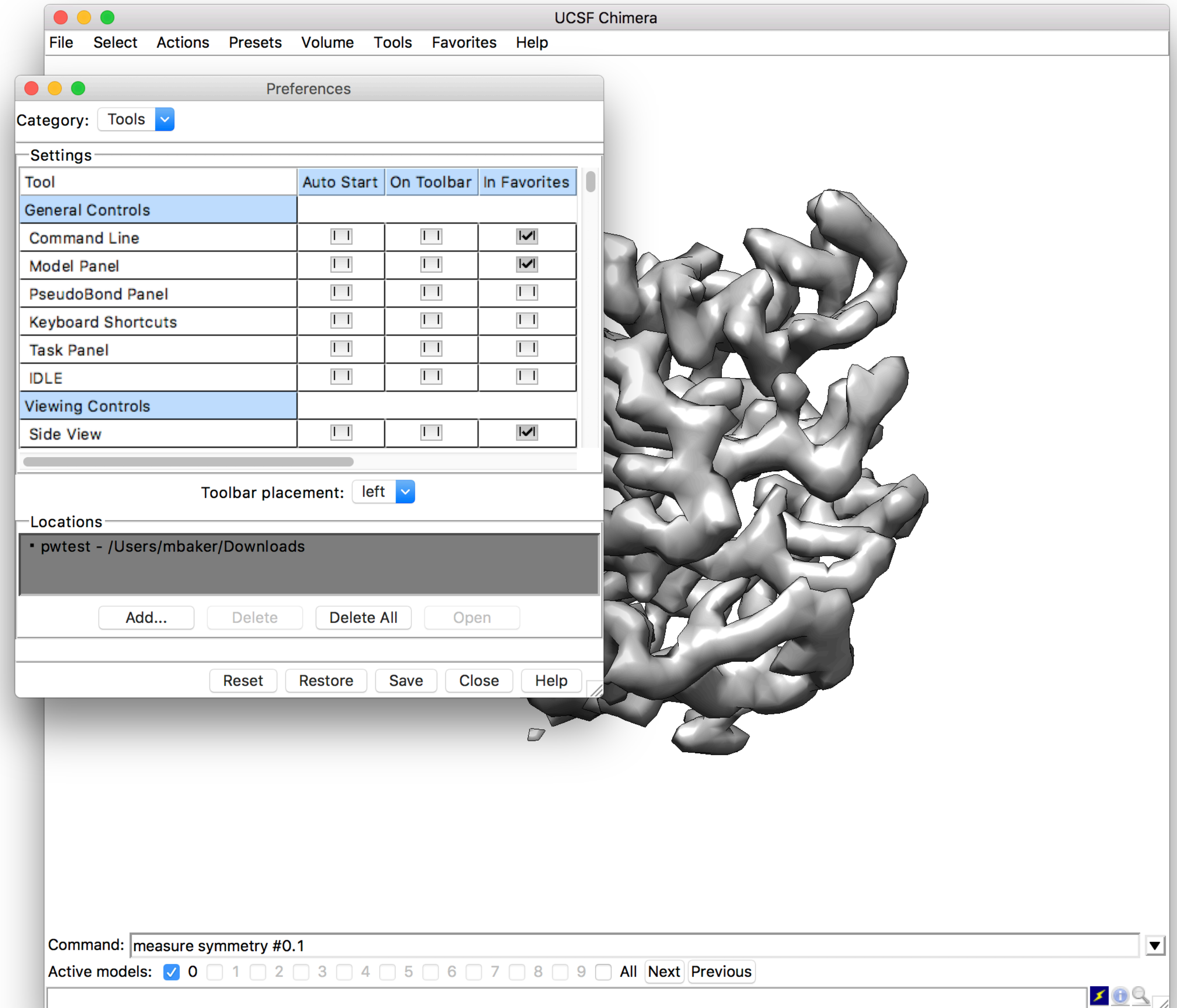
Report value at mouse position

Per-pixel coloring

Color Uncolor Options Close Help

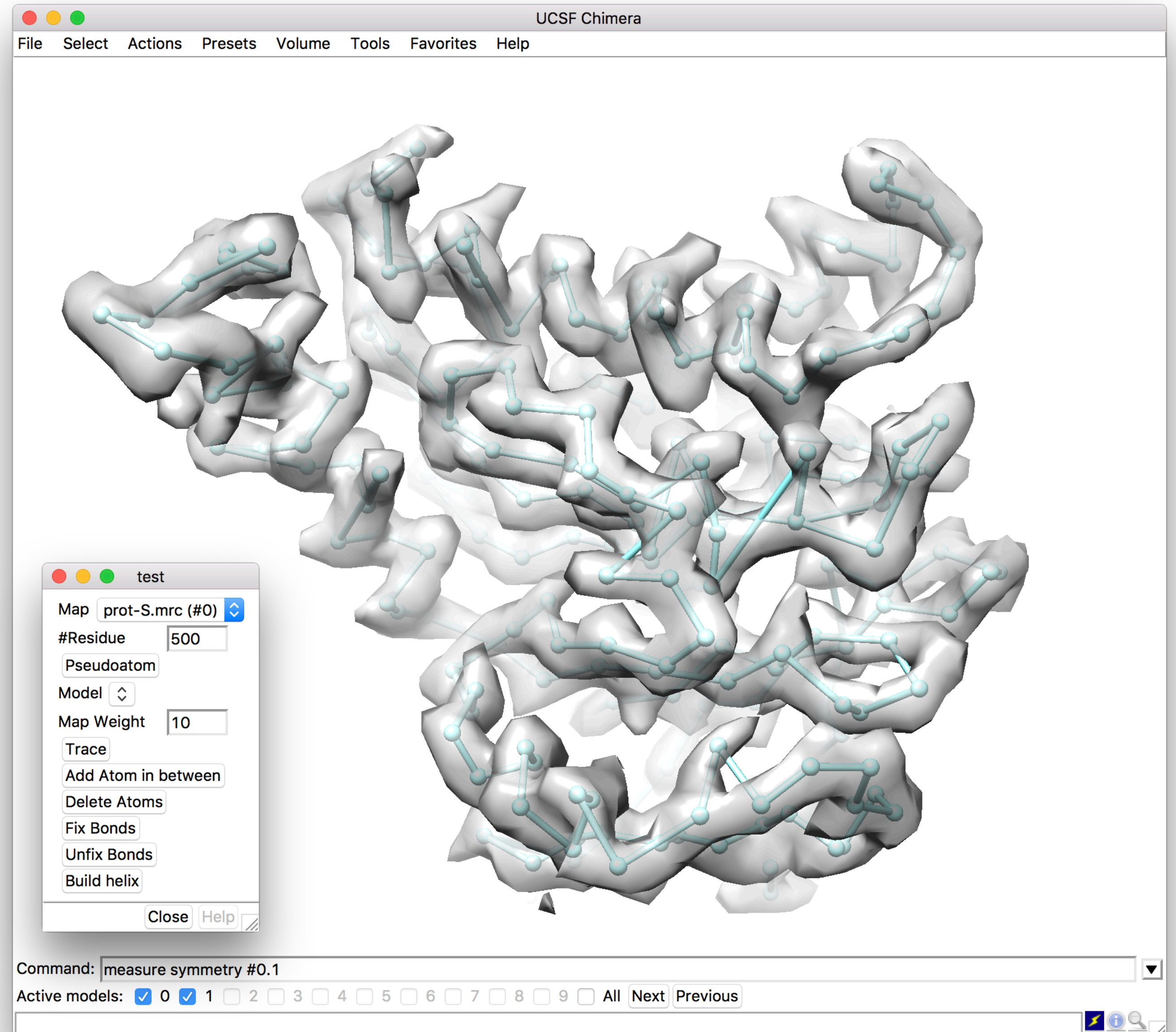
MODIFYING CHIMERA

- ▶ 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>

Getting Started with UCSF Chimera x
+

← → ↻
https://www.cgl.ucsf.edu/Outreach/Tutorials/GettingStarted.html#MenuMouse
☆ 🔍 🌐 ?

UCSF Chimera - Getting Started

This tutorial provides an overview of basic features in Chimera. You can interact with Chimera using menus and/or commands. The basic features of Chimera are available either way, but not all command functions are available in menus or graphical interfaces, and not all menu or graphical interface functions are available in commands. Thus, it is useful to become familiar with both ways of interacting with Chimera.

The **Working with menus** and **Working with commands** sections are independent of each other and (for the most part) cover identical operations, accomplished in different ways. If you go through both sections, you can skip portions that cover issues you already understand. You can also go back and forth between the sections to see the correspondence between menu and command operations.

Outline:

- [Working with menus - Part 1](#)
 - [Getting started](#)
 - [Opening a structure](#)
 - [Side View](#)
 - [Using the mouse](#)
 - [Selection with the mouse](#)
 - [Selection/Action](#)
 - [Models and model status](#)
- [Working with menus - Part 2](#)
 - [Setup](#)
 - [Representations](#)
 - [Surfaces](#)
- [Front image how-to \(menu\)](#)
- [Working with commands - Part 1](#)
 - [Getting started](#)
 - [Opening a structure](#)
 - [Side View](#)
 - [Using the mouse](#)
 - [Selection with the mouse](#)
 - [Command/Target](#)
 - [Models and model status](#)
- [Working with commands - Part 2](#)
 - [Setup](#)
 - [Representations](#)
 - [Surfaces](#)



DNA helix with bound netropsin

Typographical Conventions		
Item	Example	Description
Keyboard key	Ctrl	The control key
Mouse key	Btn1	Mouse button 1 (left button)
Menu action	File→Open	File Menu bar pulldown, followed by Open