Chimera Tutorial for EMAN Workshop

Tom Goddard
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Here is a sketch of the Chimera tutorial for the EMAN 2011 Workshop.

For full details view the screen capture video version of the tutorial.

Video tutorial

Outline

Data:

- Rous sarcoma virus EM capsid construct EMDB 1862.
- N-terminal domain, PDB 1em9.
- C-terminal domain, PDB 1eoq.
- HIV capsid pentamer, PDB 3p05.

We look at results from

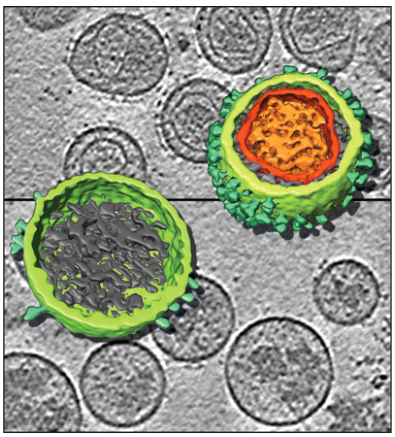
Visualization of a missing link in retrovirus capsid assembly.
Cardone G, Purdy JG, Cheng N, Craven RC, Steven AC.
Nature. 2009 Feb 5;457(7230):694-8.

Steps:

- Set contour level.
- Radial coloring.
- Fitting crystal structure.
- Symmetric placing of molecules.
- Map region coloring.
- Comparing HIV to RSV pentamer.

Using Chimera version 1.5.2.

Rous Sarcoma Virus



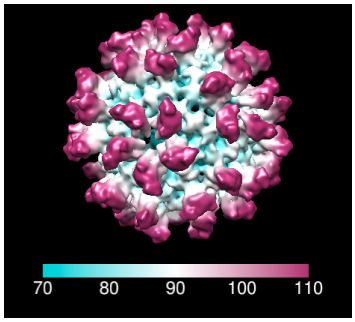
The map is an in vitro construction of empty virus capsids made from 60 copies of the Rous sarcoma virus capsid protein. Actual virus capsids have about 20 times more capsid proteins and are irregular polyhedra. Capsid protein is very similar in HIV.

Set contour level

Open map **emd_1862.map** using menu **File / Open...**. Or fetch map from web (slow) using menu **File / Fetch by Id** entering 1862 in EMDB entry field.

Set contour level in volume dialog so that enclosed volume of surface is 1.8 x 10^6 Å^3, the expected volume for 60 copies of 25 kDalton capsid protein with ~1.2 Å^3 per Dalton. Use volume dialog menu **Tools / Measure Volume and Area**.

Radial coloring



Color map radially using volume dialog menu **Tools / Surface Color**, press **Color** button. Can change colors and create color key using options shown by pressing **Options** button.

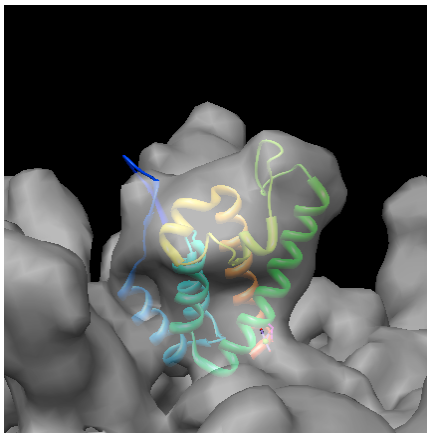
Fitting crystal structure

Fit crystal structure of N-terminal domain (NTD) of capsid protein into map.

Open 1em9.pdb using menu **File / Open...** or use menu **File / Fetch by Id** to fetch from web.

Hide map with eye button in volume dialog next to step size above histogram.

Use menu **Presets / Interactive 1 (ribbons)** to color chains. 1em9 is a dimer. Delete red chain B by selecting one residue (ctrl-click) then press up-arrow keyboard key to select whole chain, then menu **Actions / Atoms and Bonds / delete**. Use **Presets / Interactive 1 (ribbons)** again to color single chain as rainbow.



Move model to approximately correct location in map. Use **Model Panel** (Favorites menu), show map with checkbutton in **S** column, freeze map with checkbutton in **A** (active) column. Move 1em9 with mouse into pentamer lobe of density map. Use ctrl-key with middle mouse button to move 1em9 in or out of screen.

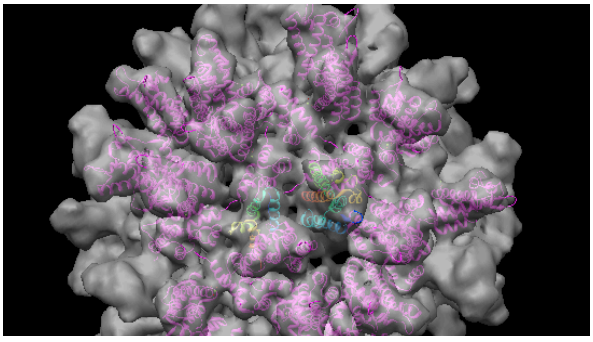
Use volume dialog menu **Tools / Fit in Map**, choose **Fit 1em9.pdb** and press **Fit** button to optimize fit (rigid rotation and translation). Average map value is average density map value over all atom positions.

Make map transparent by pressing **Color** button on volume dialog, adjust 4th slider (alpha), click **Opacity** switch to see 4th slider.

Show correlation coefficient using Fit in Map **Options** button, enable "Use simulated map, resolution 10", press **Update** button. Changing contour level of simulated map changes domain where correlation is calculated and can change correlation values 0.8 to 0.9.

Load tutorial session file **emd_1862_1em9_1eoq_fit.py** using menu **File / Restore session...** to get fit N-terminal and C-terminal domains, or fit C-terminal domain yourself, pdb 1eoq.

Symmetric placing of molecules

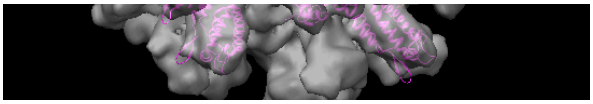


Create symmetric copies of fit crystal structure using **sym** command. Show command-line using menu **Favorites / Command-line**

```
sym #1 group i,222r coord #0 range 100
```

This command copies 1em9 fit model #1 (numbers listed in Model Panel) using icosahedral symmetry with standard reference orientation having 2-fold axes along x,y,z (222r) using

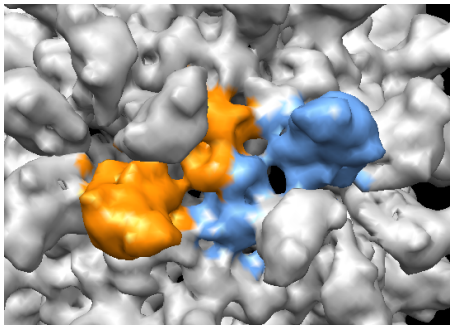
the map (model #0) coordinate system, making copies only within 100 Å.



To copy both N-terminal and C-terminal domains, either repeat command for 1eoq (model #2) or combine domains into one model using:

```
~sym #1
combine #1,2
close #1,2
sym #3 group i,222r coord #0 range 100
```

Map region coloring

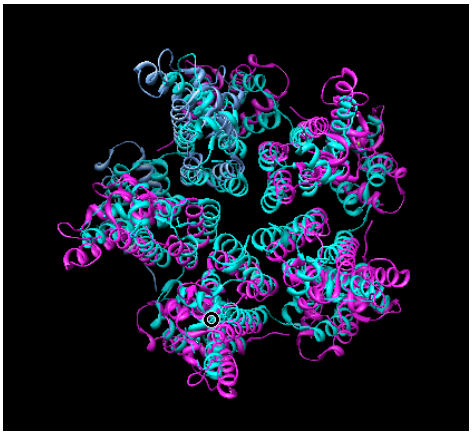


Color map to show two neighboring capsid proteins. Select each protein ctrl-click then press up-arrow key to select entire molecule, then color with menu **Actions / Color / orange**. Color adjoining protein a different color.

Select both colored proteins using ctrl-click, shift-ctrl-click to add to selection, and up-arrow key. Use volume menu **Tools / Color Zone**, set radius to 5 and press **Color** to color map surface to match colors of selected molecules within 5 Å.

Hide all molecule using **Model Panel** (Favorites menu) click density map list entry and press **Show only** button in right column of Model Panel.

Comparing HIV to RSV pentamer



Compare HIV crystal structure pentamer 3p05 to fit Rous sarcoma virus pentamer.

Select Rous sarcoma virus pentamer using ctrl-click and shift-ctrl-click to select one residue in each of 5 molecules, then up-arrow key. Invert selection with menu **Select / Invert (all models)** and hide other molecules using menu **Actions / Ribbon / hide** and **Actions / Atoms and Bonds / hide**.

Open HIV pentamer 3p05.pdb with menu **File / Open...** or **File / Fetch by Id...**.

Move and fit HIV pentamer into Rous sarcoma map. Select 3p05 in Model Panel list and press **Activate only**, move to approximate fit in map, use Fit in Map dialog to optimize fit, use Model Panel **Activate All** button to allow moving all models. Hide map.

HIV pentamer and Rous sarcoma pentamer have very similar folds (same alpha helical bundles) and alignments.