

Segger Tutorial – Segmenting with Fitted Models

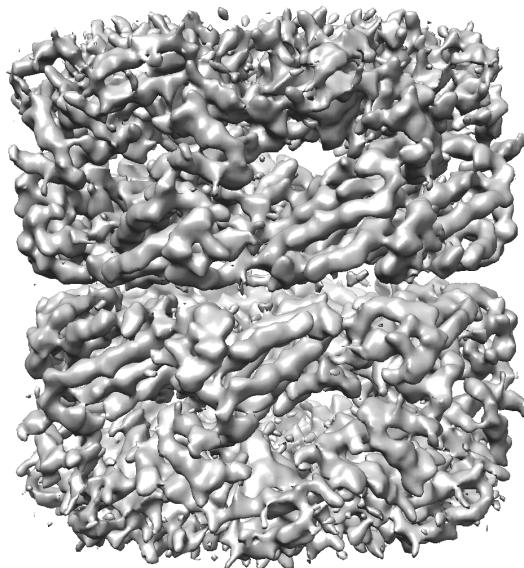
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This tutorial shows how Segger can be used to segment a map based on fitted models. This is a bit different than using the Color Zone (Tools... Volume Data... Color Zone) tool, which simply splits voxels based on proximity to different proteins/molecules in the model. Instead, the boundaries will follow the low-density contours in the density map, and may include smaller adjoining features not in the model better, e.g ligands. The Extract tool in Segger can then be used to mask the density map with the resulting regions (see the Extract tutorial).

1. Opening the map

- In the Chimera main window, select File -> Fetch by ID...
- Select EMDB, and enter code 5001. You should see the map as below, after turning it 90° around the x axis, and lowering the contour level.

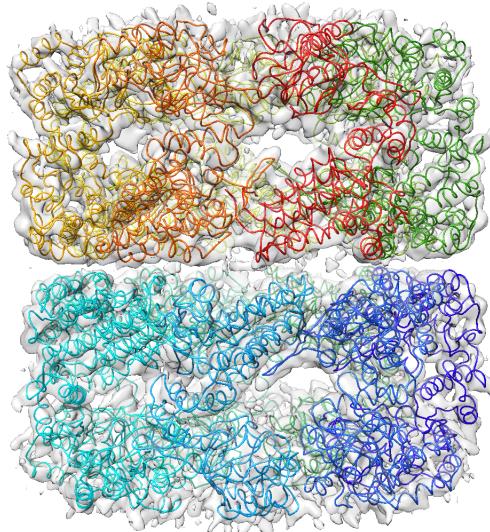


As you may have seen in the previous tutorial, we can segment this map without a model to get the 16 proteins in the complex, but the boundaries are not exactly right. Let's use a fitted model to segment it to get more correct segments:

2. Opening the fitted model

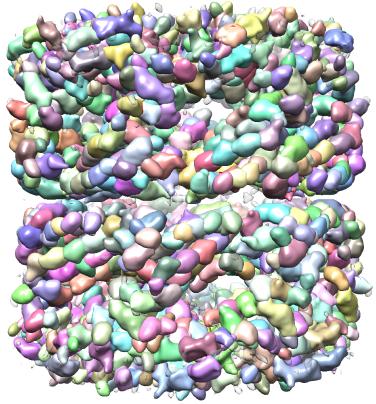
- In the Chimera main window, select File -> Fetch by ID...

- Select PDB, and enter 3cau.
- If you lower the transparency of the map's surface color, and then change the color of each protein with Tools -> Depiction -> Rainbow, select 'chain', Apply, you will see the fitted model as below.

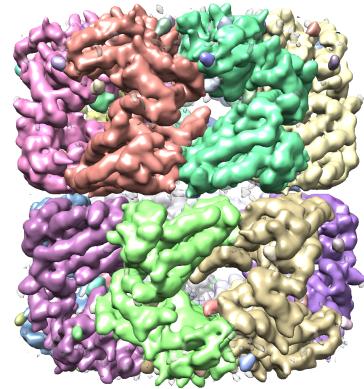


3. Segmenting with the fitted model

- Open the Segger dialog (Tools -> Volume Data -> Segger)
- Select the map in the Segger field if not already selected.
- Press Options at the bottom of the dialog.
- Enter 0 for smoothing steps.
 - This will prevent automatic smoothing and grouping, to get the smallest segments possible.
- Press Segment at the bottom of the dialog.
 - You will see many regions, as shown below on the left.
- Press 'Shortcuts' in the Segger dialog.
- Press the 'Fit' button next to Other tools.
- Make sure no other open models are shown, i.e. only the model to be used for segmenting should be visible in the main Chimera window.
- In the SegFit dialog, select Fit -> Group regions by chains in visible (Molecule) models.
 - This will first generate 14 maps, one for each chain.
 - Then, each segment is checked for overlap with each of the 14 maps, and assigned to the map that it overlaps the most.
 - Finally, the segments assigned to each map are grouped together.
 - If any segments do not overlap any of the maps, they are left as they are.
 - You will see the resulting segments as shown below on the right.



All watershed regions in the map



Regions grouped based on fitted models.

The other option in the Fit menu, Group regions by visible (Molecule) models does something similar, but each map spans an entire model rather than separate chains in the model.

From here, you can use the Extract module to mask out each segment - see Extract tutorial, or just give it a shot, it's somewhat explanatory – open it from the Segger dialog, by pressing the Extract button.