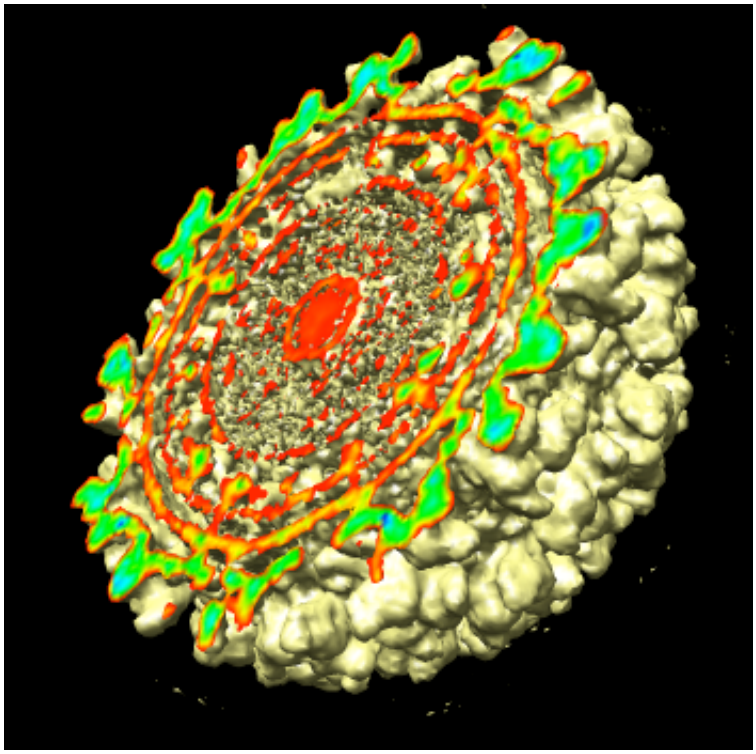
Semliki Forest Virus Chimera Demo

Demonstration of Chimera display capabilities for density maps and Protein Data Bank (PDB) models.

Look at Semliki Forest Virus density map emd_1015.map and PDB model of nucleocapsid protein 1DYL fit into the density map. The density map has 9 angstrom resolution.

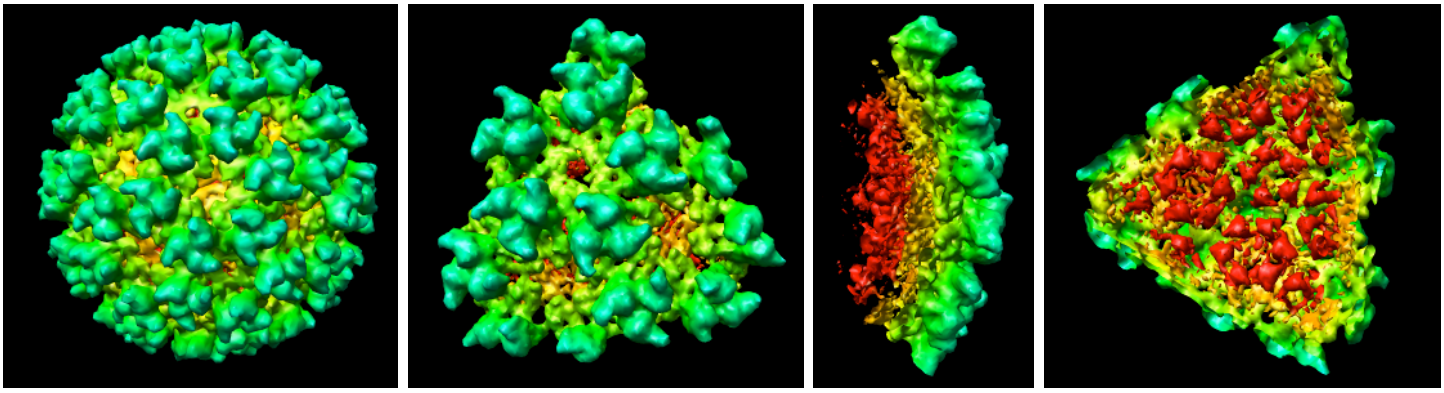
Slicing density map

- Open emd_1080.map.
- Note map size 301 x 301 x 301, subsampling 4x.
- Adjust threshold.
- Turn off volume outline box.
- Color yellow.
- Enveloped virus, glycoproteins embedded in outer membrane enclose nucleocapsid core which surrounds single stranded RNA genome (11.4 kbase).
- Slice to see layers.
- Turn off depth cueing.
- See inside surface -- confusing. Draw cap. Color white.
- Color according to density on cap.
- Move clip plane, translate and rotate with mouse.



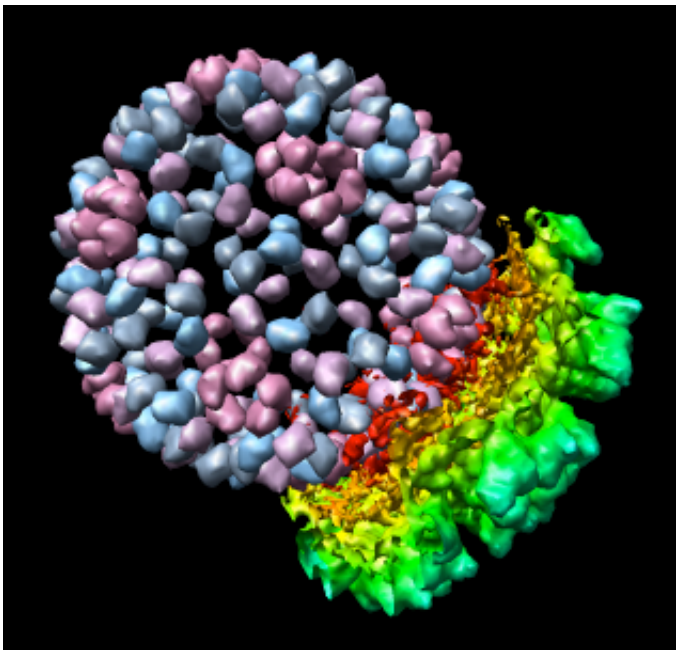
Color radially

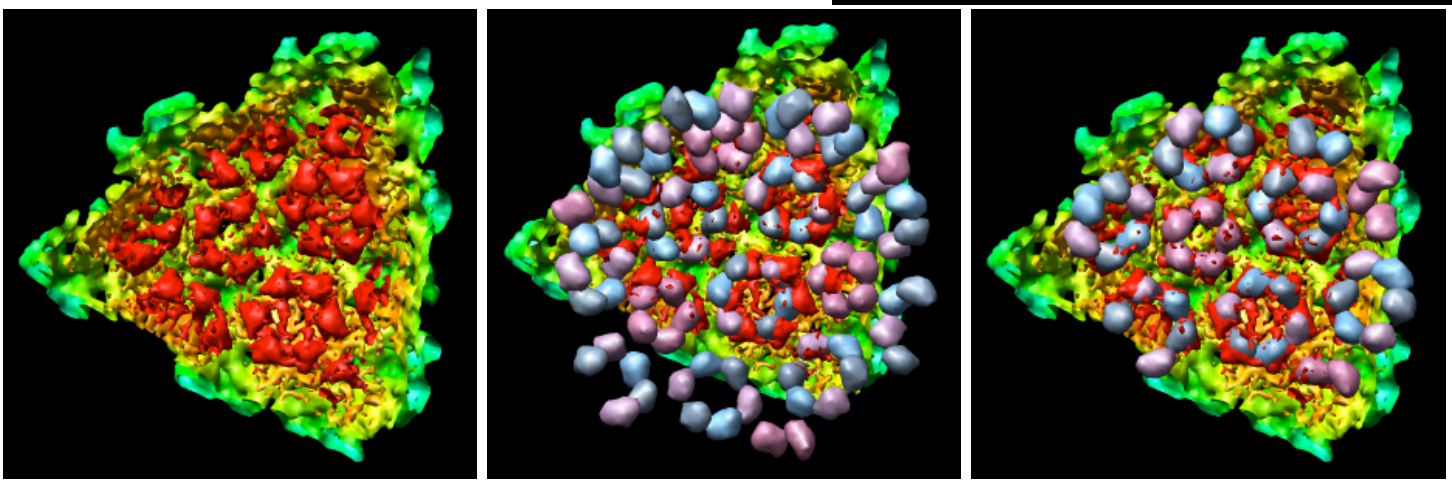
- Turn off coloring, clipping and capping.
- Crop to octant. Orient and select octant with mouse.
- Color radially to show layers. Load radius map, color by radius.
- Adjust color thresholds 200,250,300,350,400.



Show PDB model fit to density

- Open 1dyl, crystal structure fit into map.
- Show icosahedral shell. Each surface represents a protein.
- Unshow density map with model panel.
- Set rotation mode to fixed.
- Reshow density map.
- Hide 1dyl copies away from density map.
- Show density and PDB models separately pointing out 5 protein and 6 protein rings to show misalignment. Common problem.
- Freeze density and hand align PDB.
- Hide and show PDB to show match more clearly.

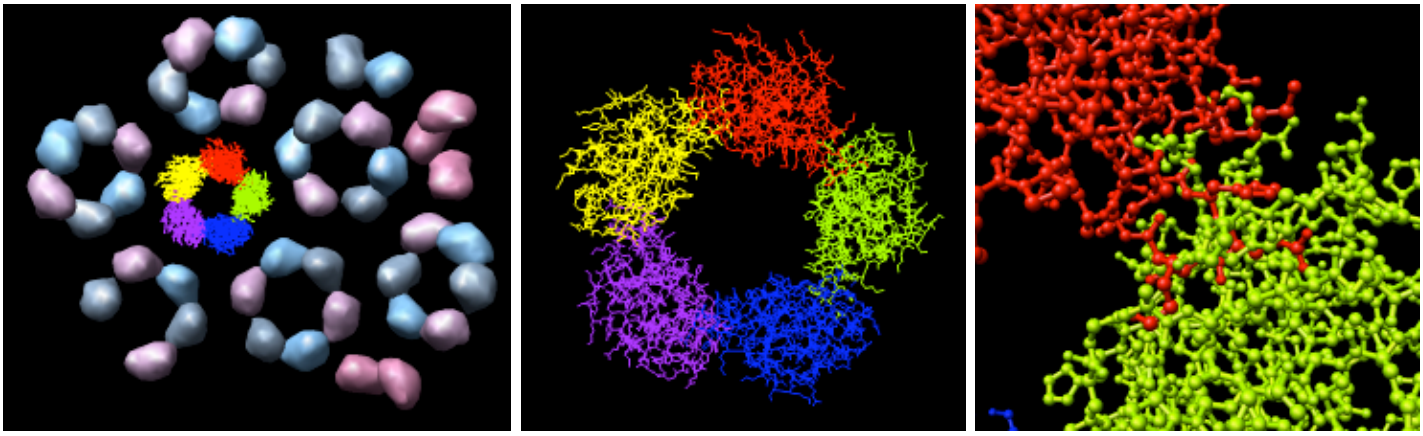




Steric clash

- Unshow density map.
- Show atoms of 5-ring in wire style.

- Hide other chains.
- Change rotation mode to center of models.
- Switch to ball and stick and show clash between to proteins.



Coloring atomic model by density

- Select all chains, show surfaces, zoom out.
- Select loaded atoms, show original copy of 1dyl. Atoms for all copies not loaded.
- Hand select original 1dyl chains, hide others, switch to ribbon.
- Show render by attribute from model panel.
- Color residues by average b-factor.
- Show b-factor as worm thickness.
- Point out two protein-protein contacts (6-ring).
- Reshow all chains, select loaded, hand select worm chains, hide surfaces.
- Turn on depth cueing, adjust clip planes to dim far chains.