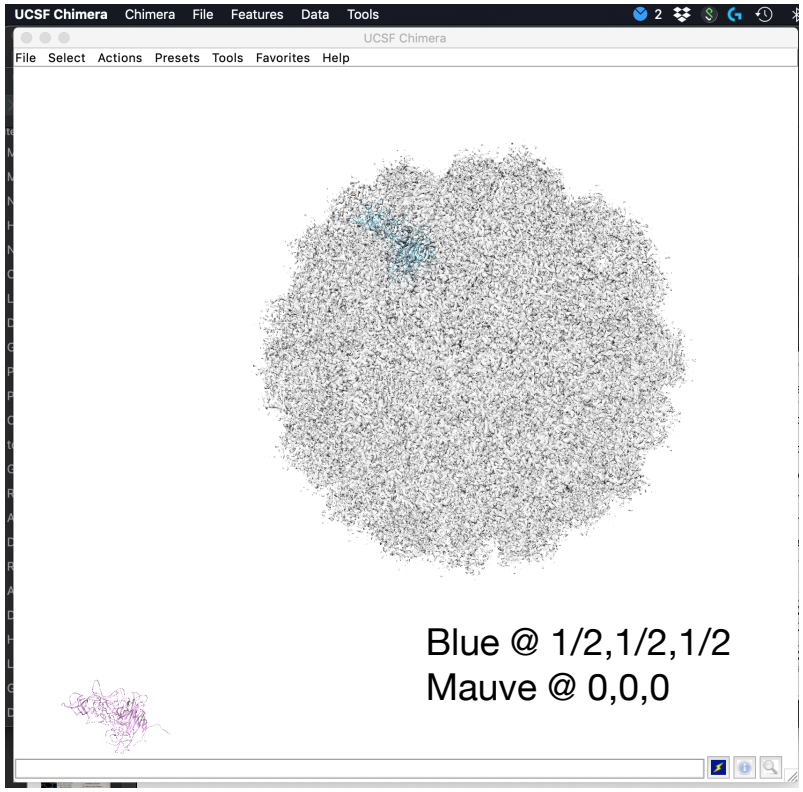
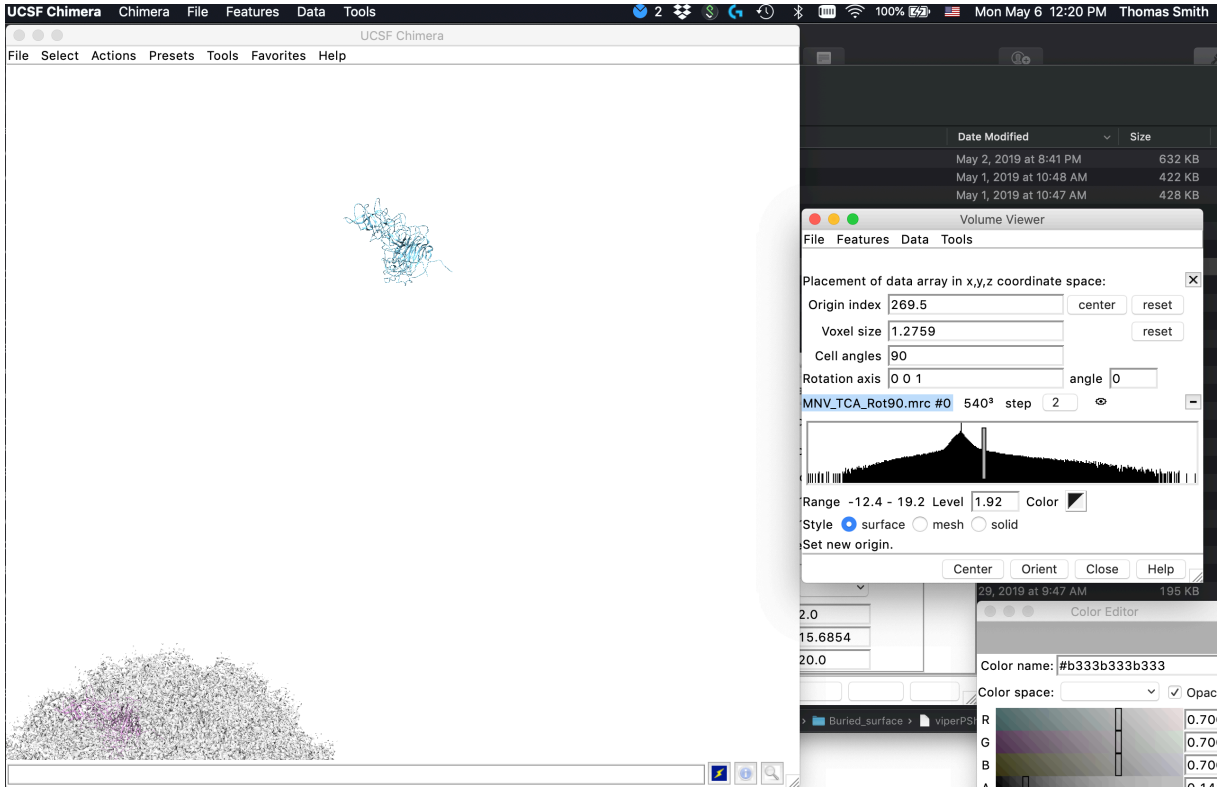
COOT and CryoEM

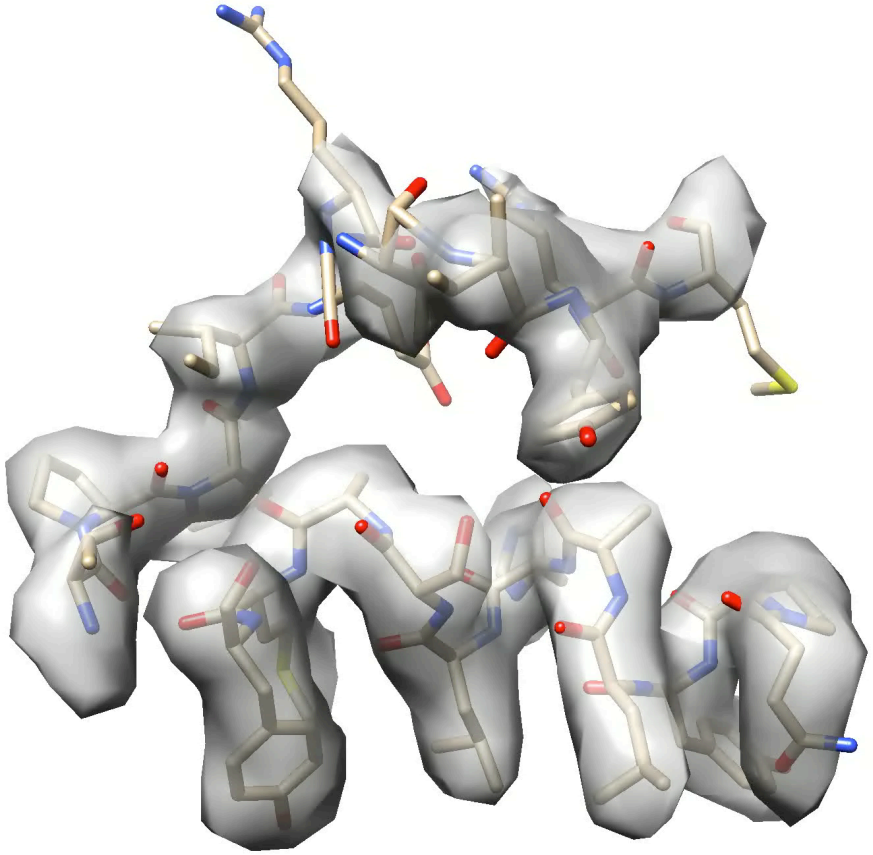
Origin stories….



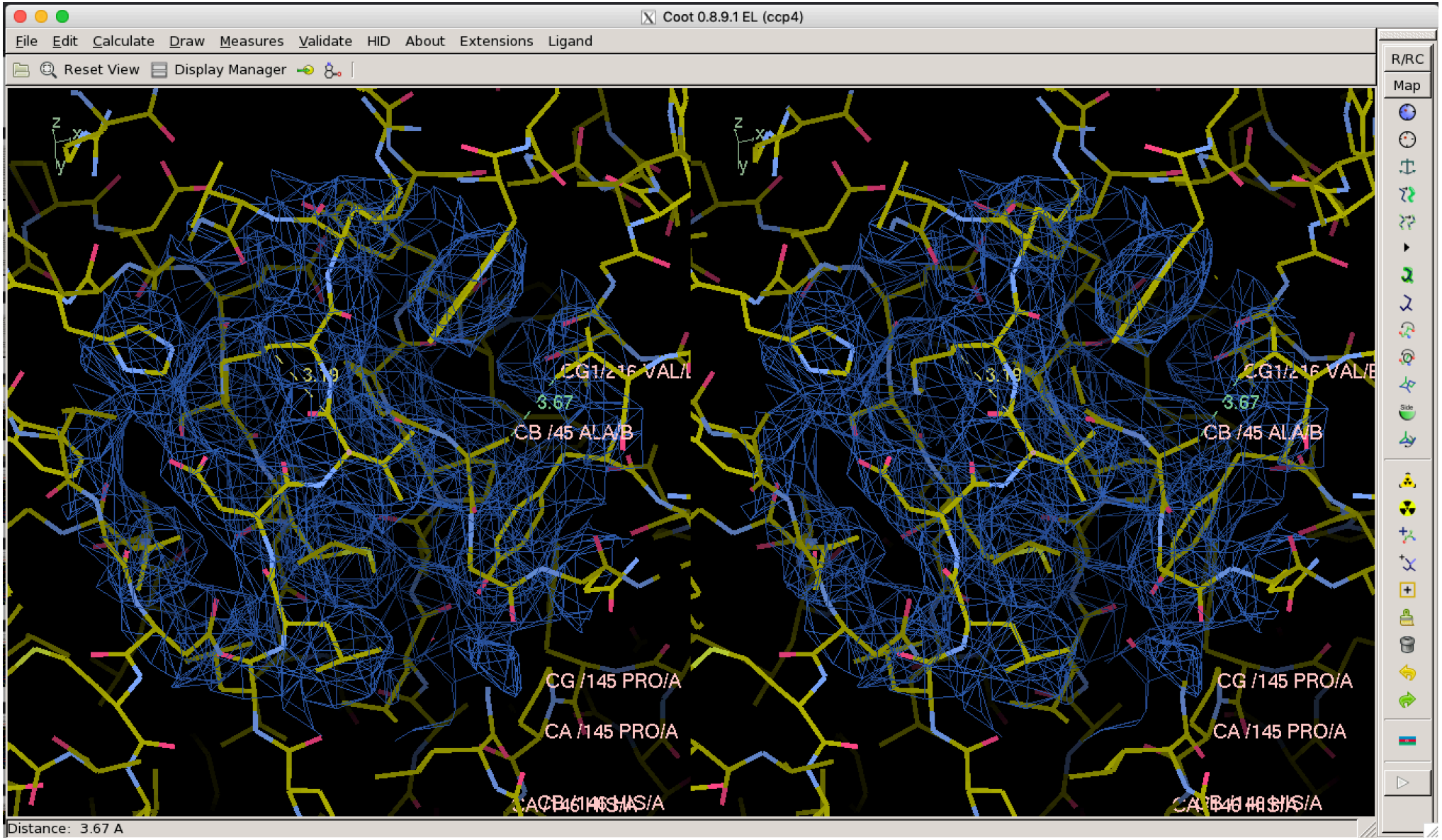


Maps are centered at 1/2,1/2,1/2 in EM. Viruses, in particular, are centered at 0,0,0 for icosahedral symmetry operations. If you 'center' the map in Chimera it looks fine with 0,0,0. If you try to move the origin in EMAN2, it might look fine in Chimera but it does not match in COOT. COOT and PHENIX are in sync with how map origins/headers are (not) read. Therefore, if you open the map and model in COOT and they do not match, PHENIX will not work. We translate the atomic model to an origin at 1/2,1/2,1/2, build, and translate back to find icosahedral partners using the online tools at http://viperdb.scripps.edu/oligomer_multi.php

General Building Notes



At EM resolutions of ~3Å the quality of the main chain atoms are quite good but do not expect to see all of the side chains. Many are absent or highly truncated. In Phenix refinement, you will often see them curled back on themselves as the refinement is trying to get them into density. Because of the truncated density, heavily rely on the large TYR and TRP residues as fiducial marks to make sure you stay in register. For building, rely on chemistry such as interactions and favored rotamer positions for side chains.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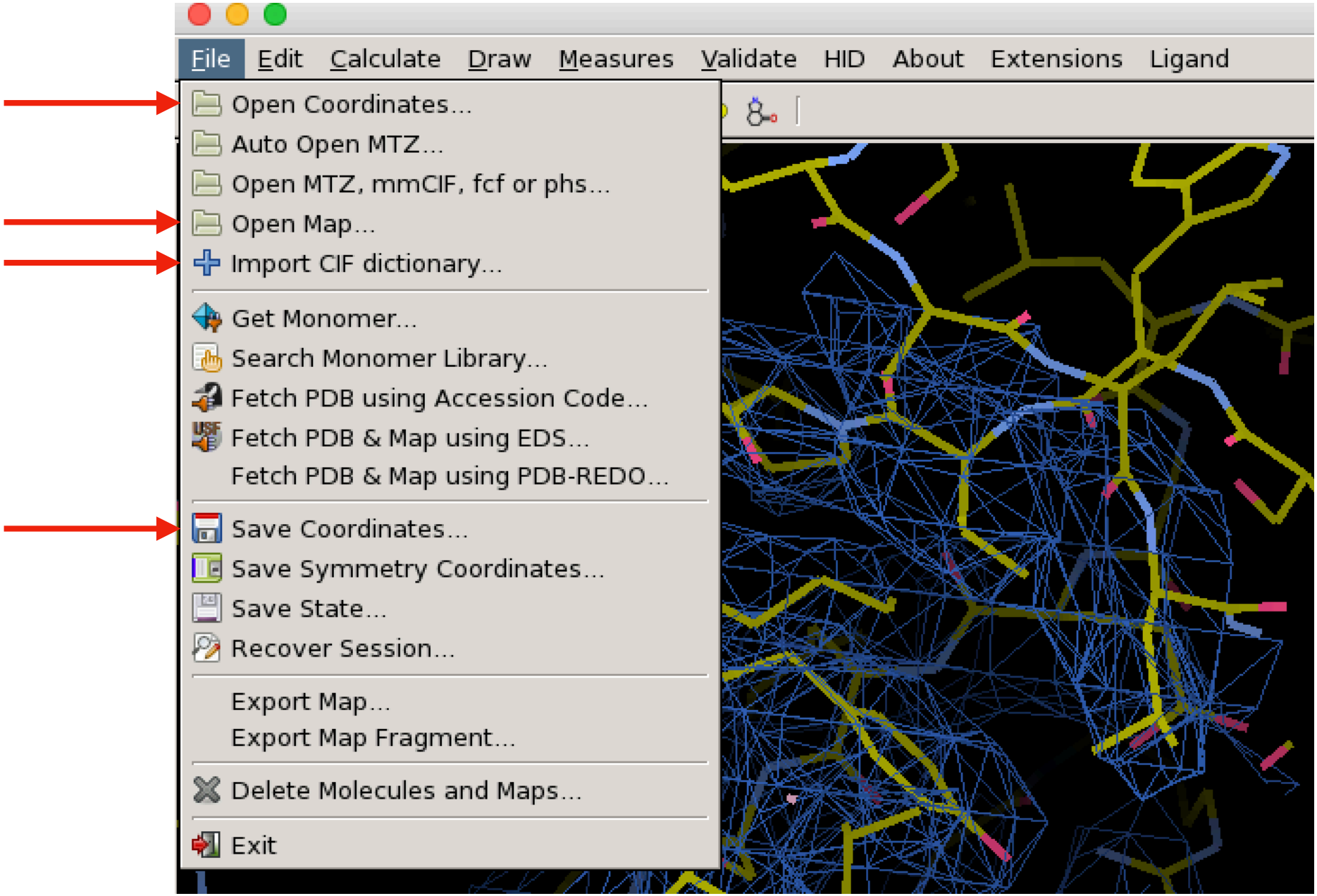
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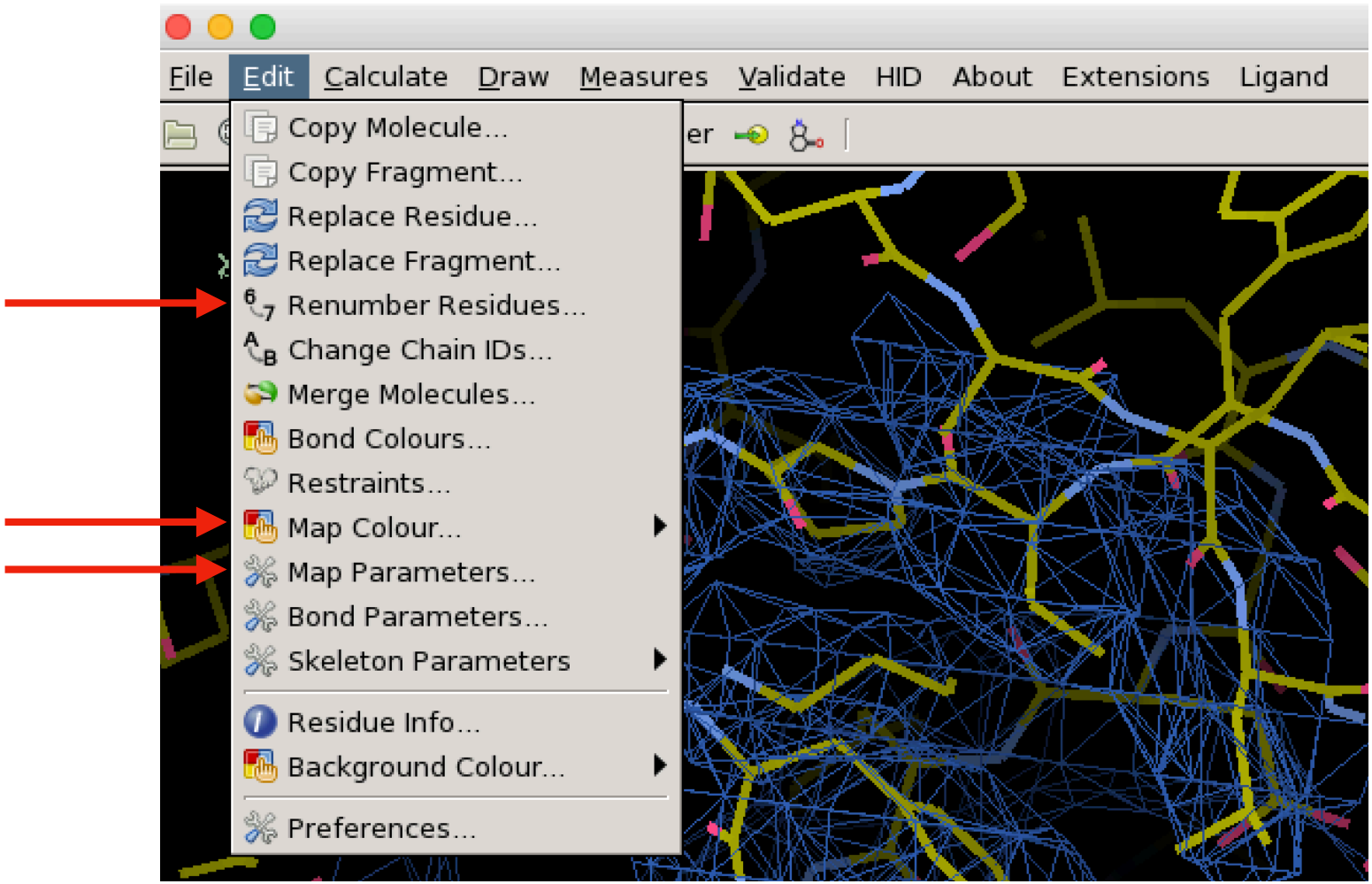
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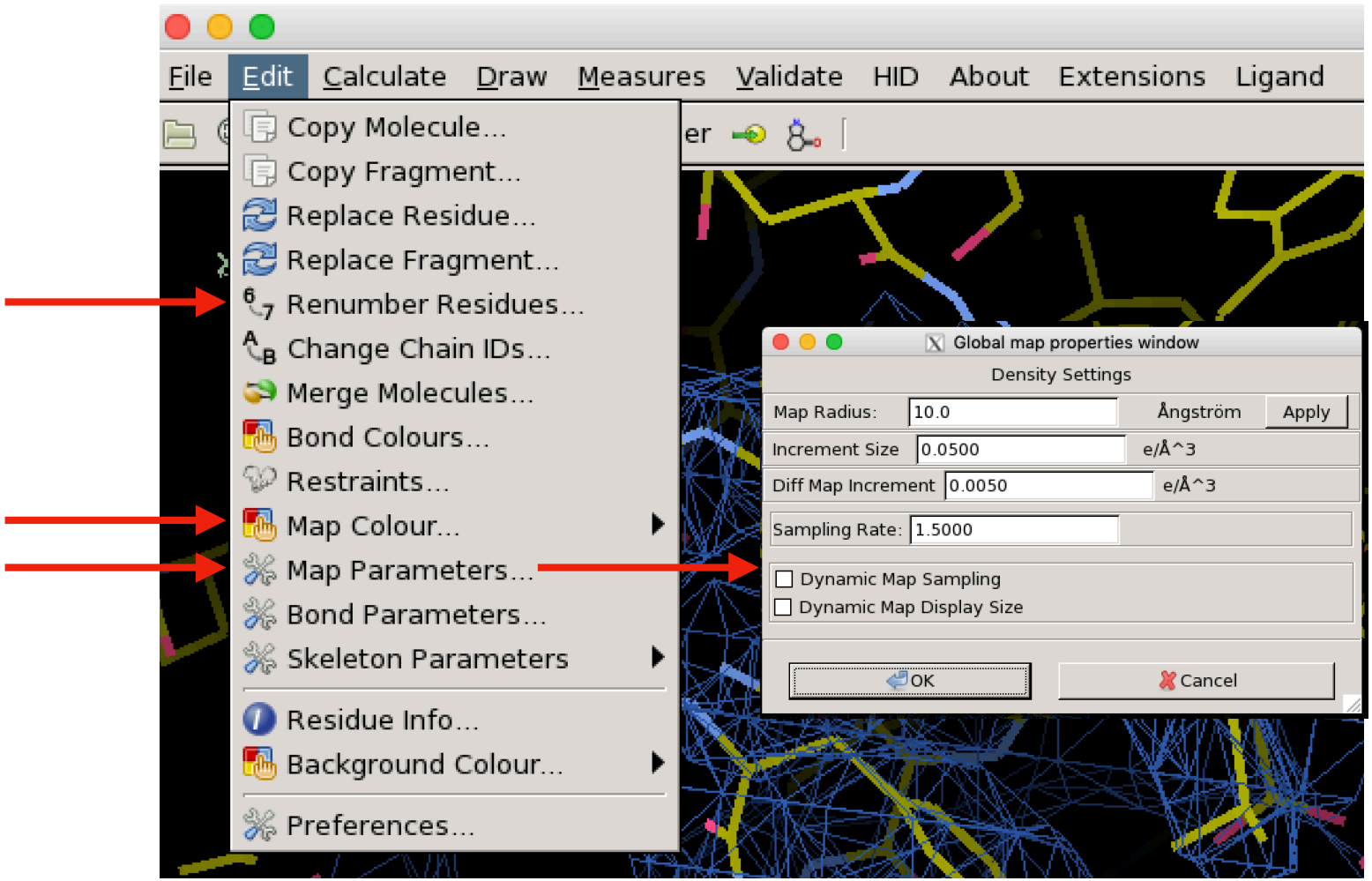
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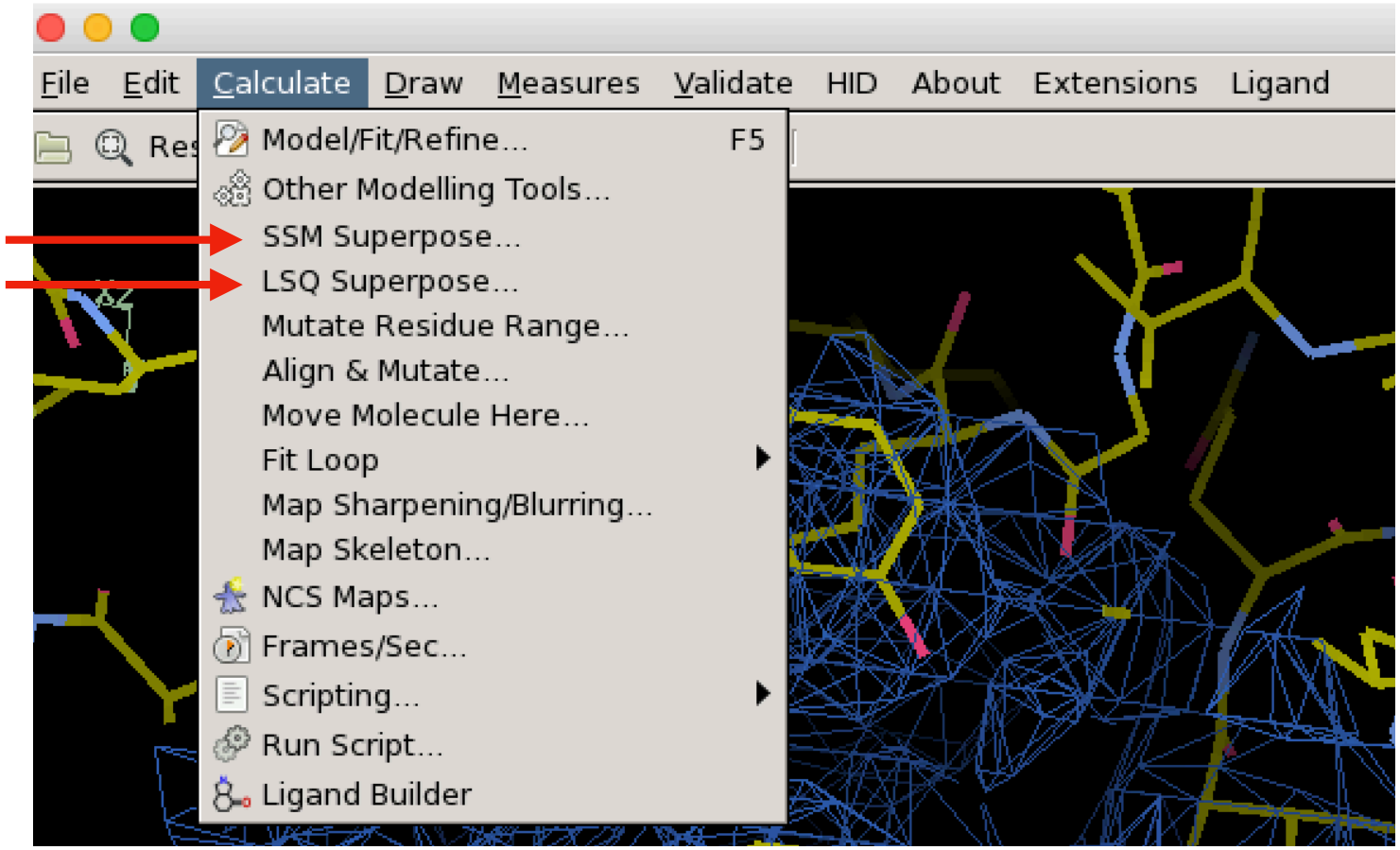
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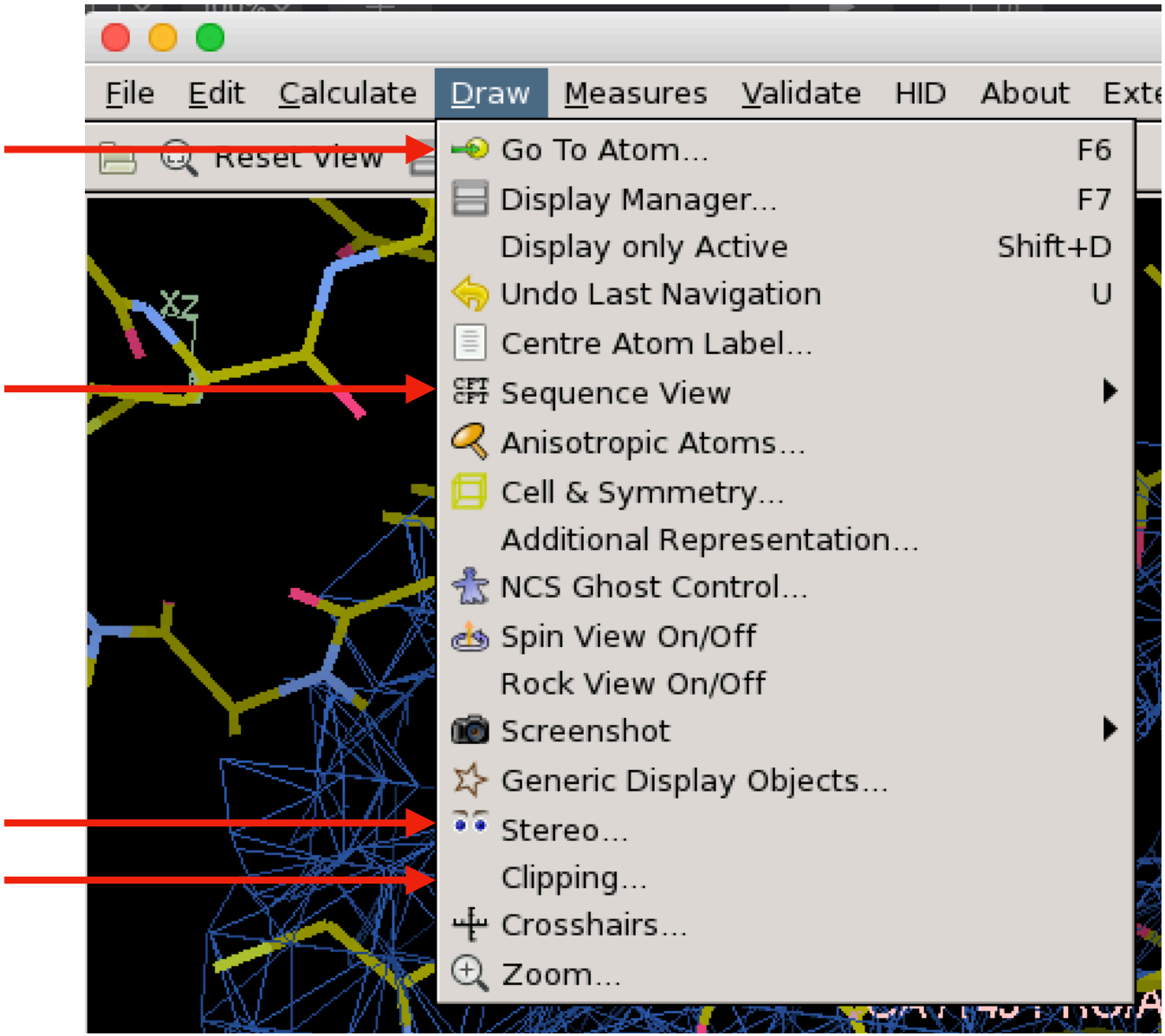
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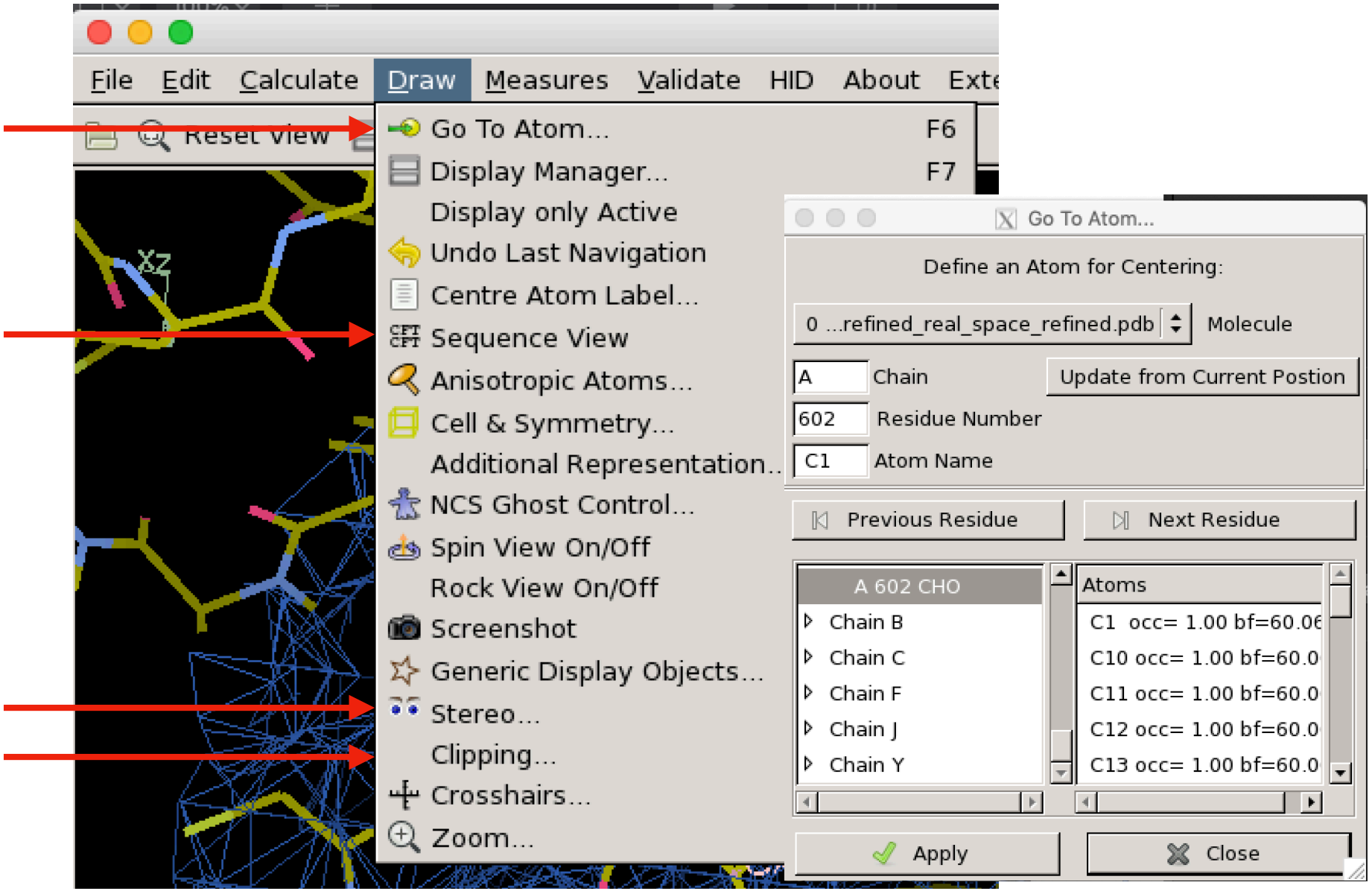
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C10 occ= 1.00 bf=60.0
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C13 occ= 1.00 bf=60.0
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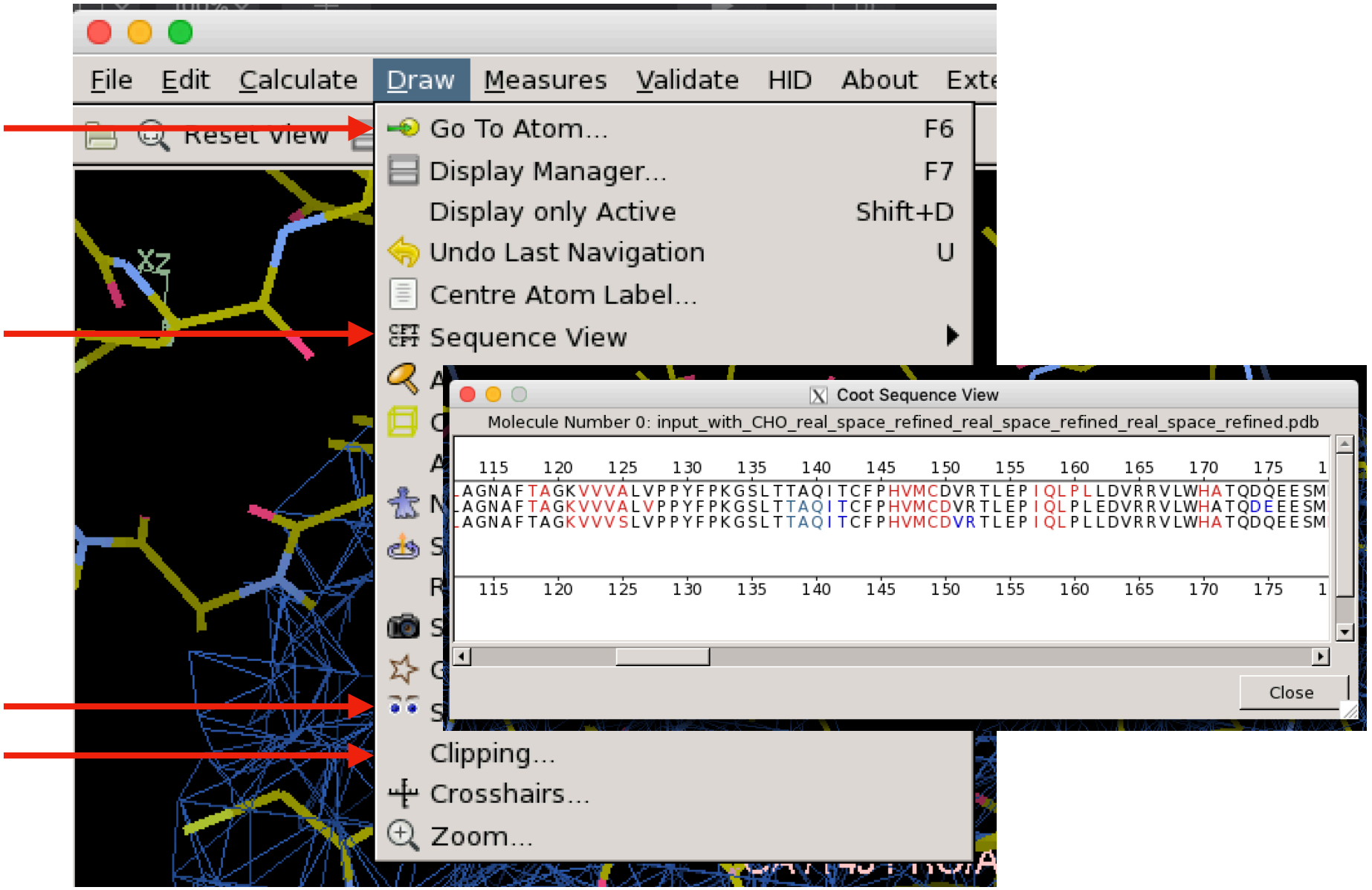
Close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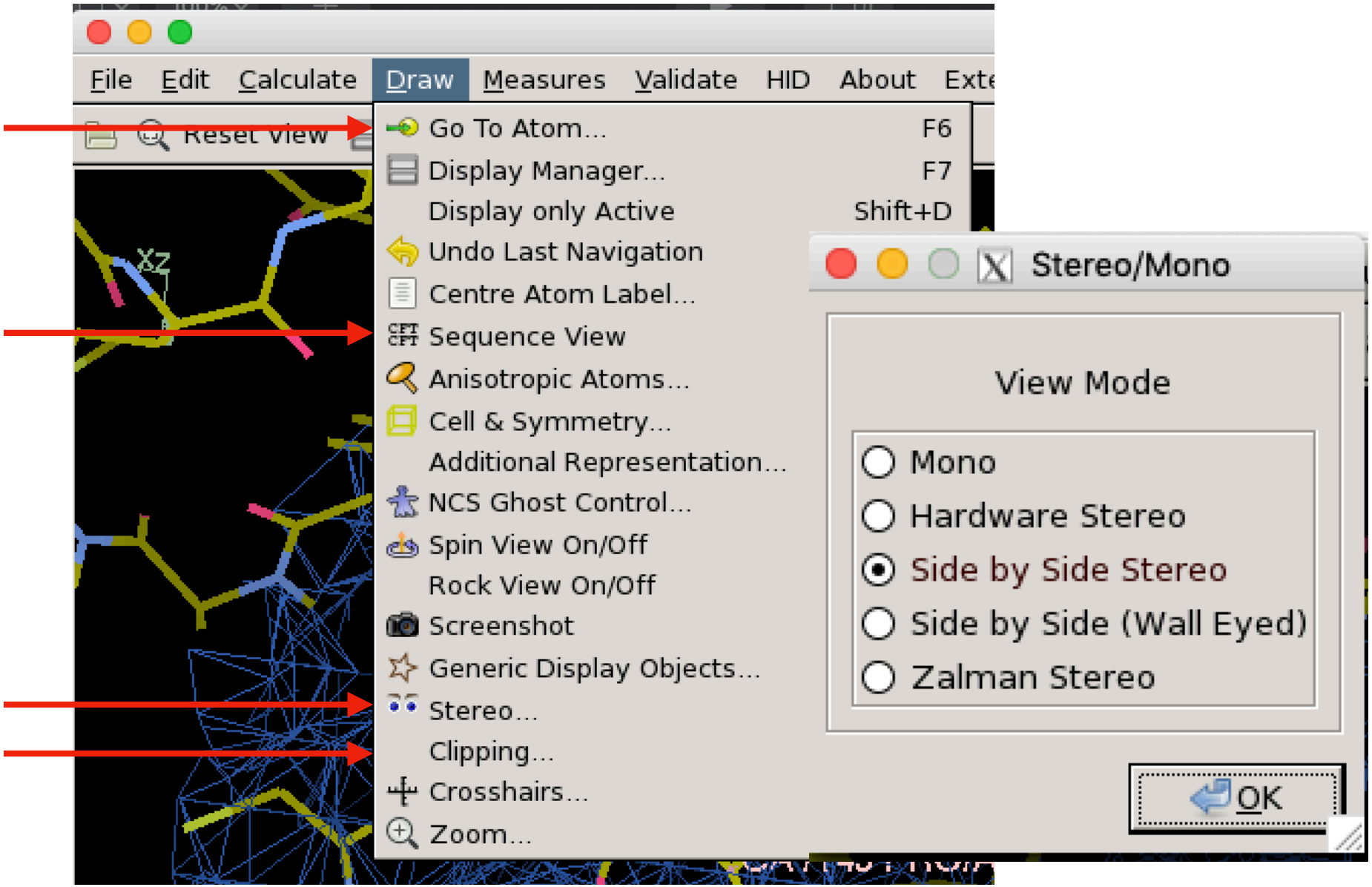
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Rock View On/Off
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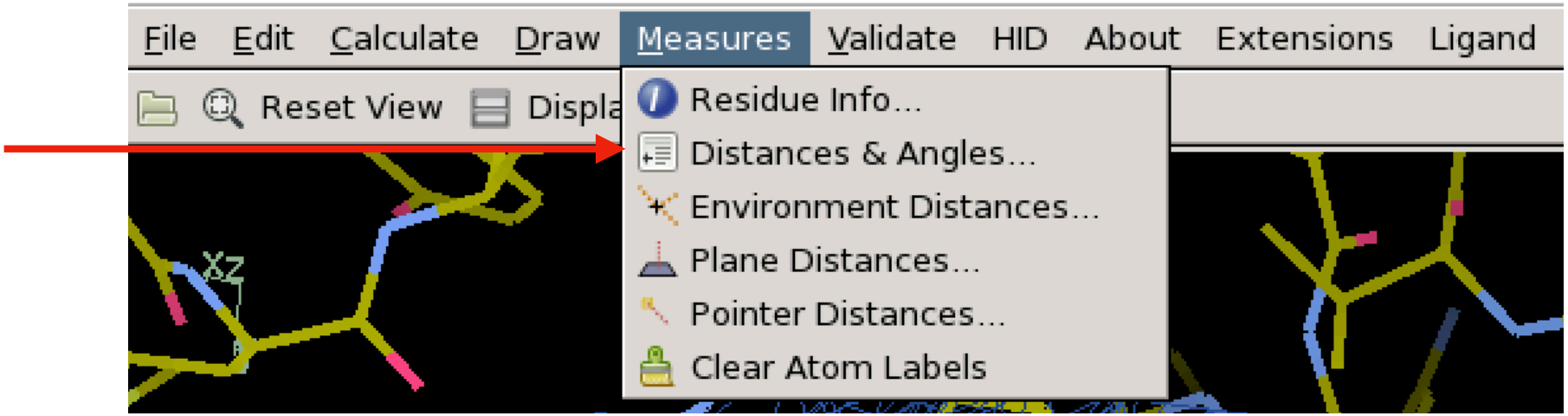
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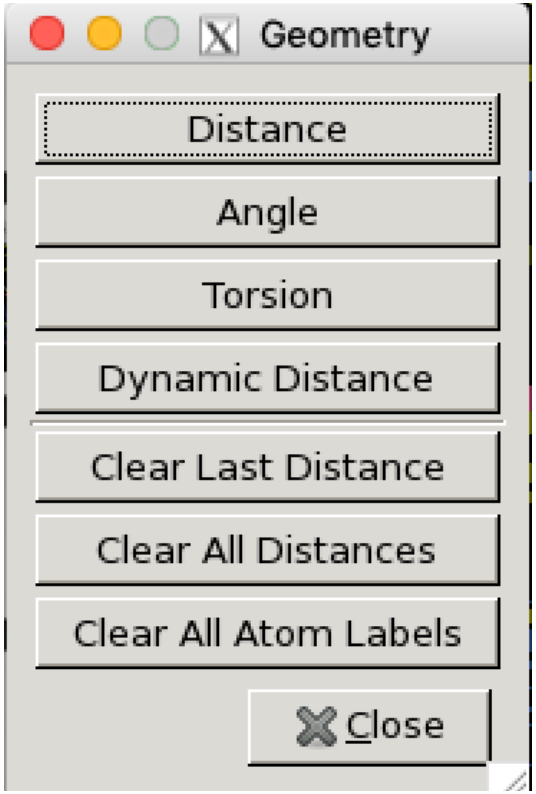
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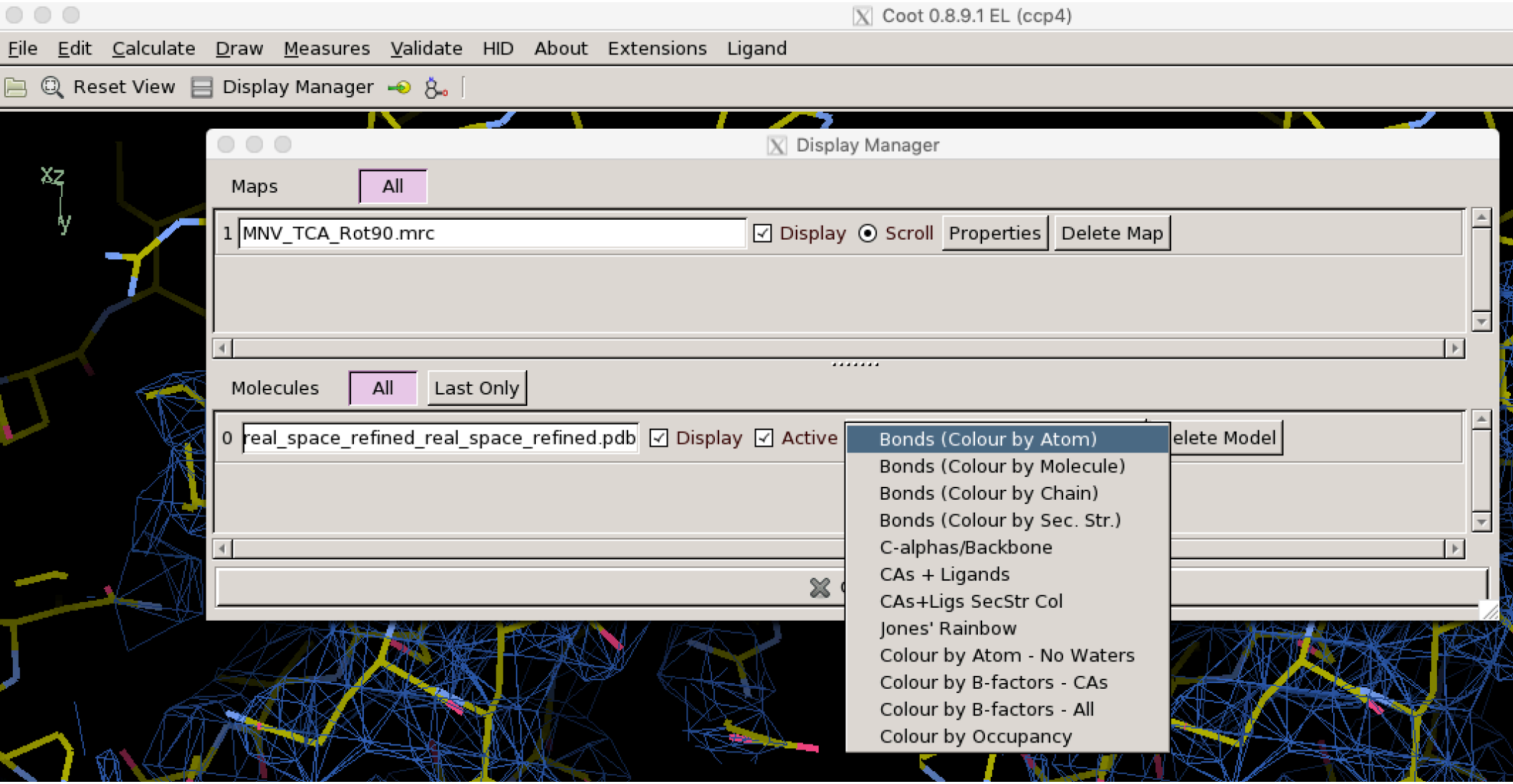
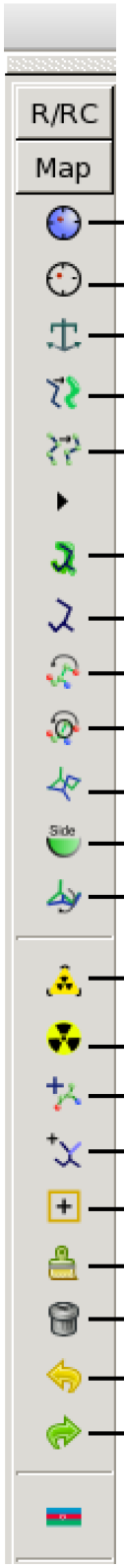


Display Manager - allows you…

1) Hide/display maps and models
2) Turn off/on active
3) For maps, you can control contrast with mouse scroll
4) For models, you can display in various ways (colors, backbones, ligands, etc)



- Click on 2 atoms and it tries to refine the zone according to geometry and density (real space refinement)
- Click on 2 atoms and it tries to refine the zone according to geometry only
- Allows you to fix atoms in the zone for some control over the regularization routines.
- Click on 2 atoms and it will use that zone for rigid body refinement into the density.
- Rotate/translate zone, molecule, or atom depending upon selection.

- Automatically fit the best side chain rotamer into the density.
- Display all of the possible rotamers, one by one, to pick out the best one.
- Rotate about the various bonds in the side chain.
- Torsion general; select 3 atoms and rotate about any bond.
- Flip the carbonyl plane.
- Flip the carbonyl plane. Click on an ‘C’ atom in backbone and it flips the entire plane.
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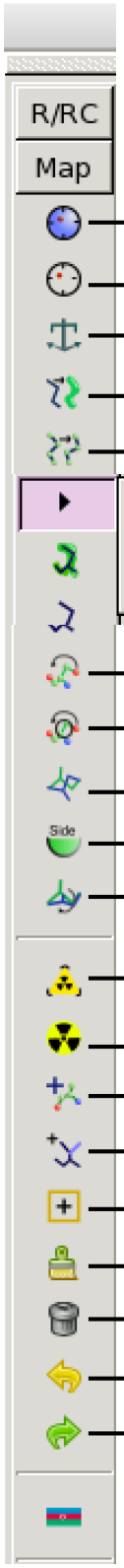
- Mutate the amino acid to a different type of residue and fit into the density.
- Just mutate the amino acid and the user fits it by hand.
- Add an amino acid to the end (either N or C termini) of the chain. Starts off as an ALA and you then mutate.
- Side chains can have 2 conformations. This allows you to add a second conformation.
- Move the cursor to a position and add an atom: HOH, Na, Ca, Cl, Br, SO4, PO4, or other…
- Clear all of the pending picks - i.e. you got confused…
- Delete atoms/residues.
- Undo last action
- Undo last Undo



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Rotate/translate zones of the protein, entire chains, or individual molecules. Redundant with the menu item above.

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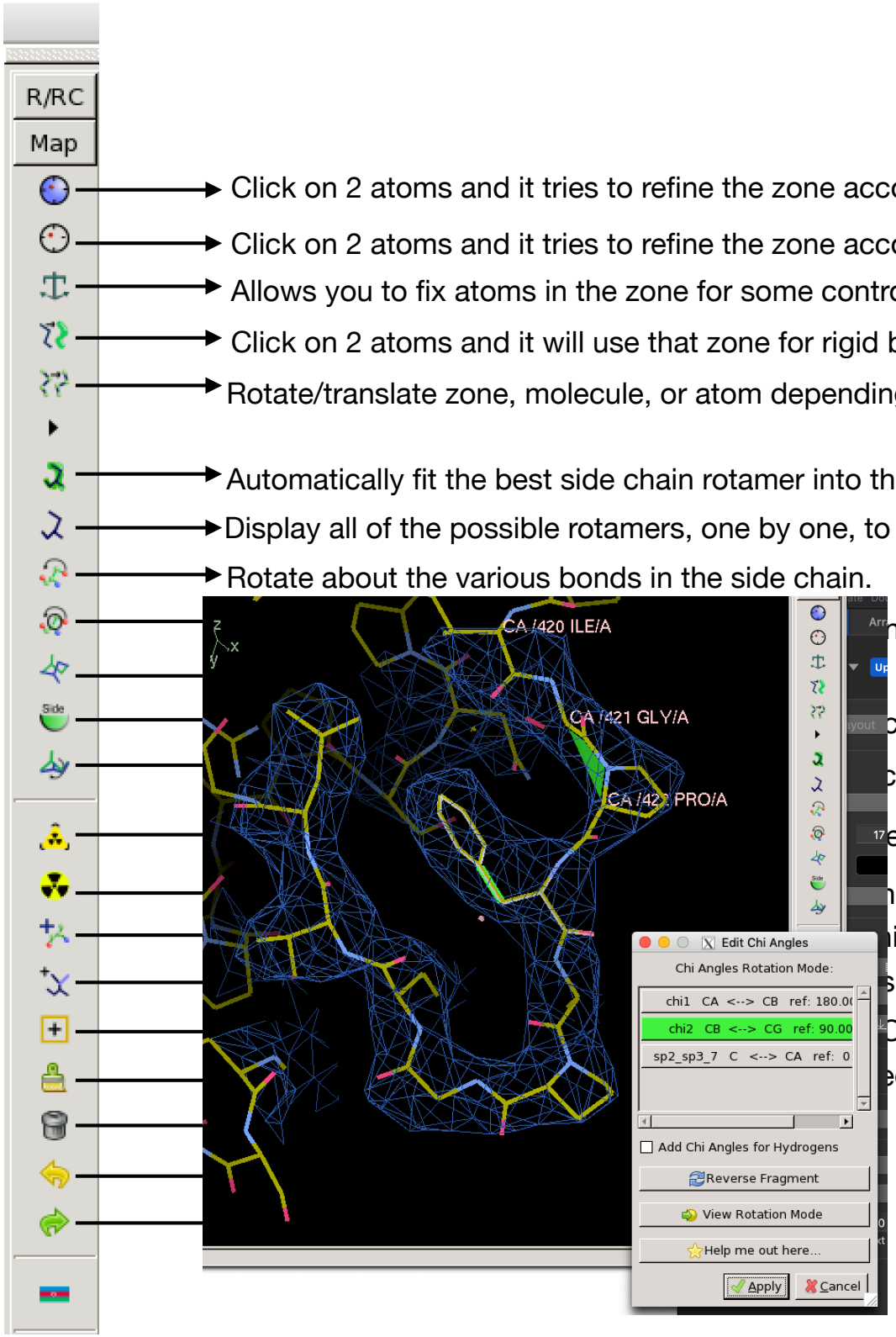

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