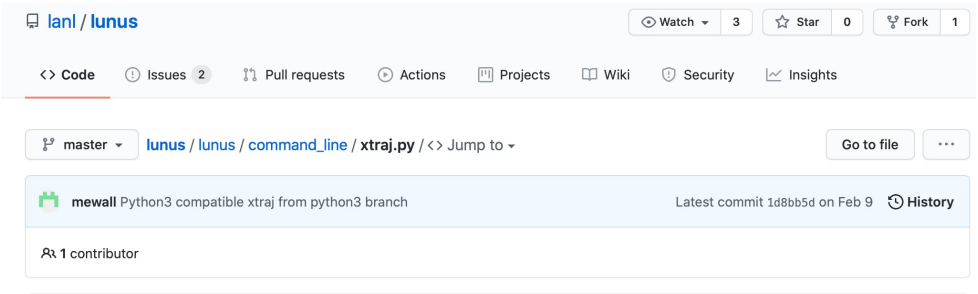
Things you need

- MDTraj, cctbx (The Computational Crystallography Toolbox)
- https://github.com/lanl/lunus/blob/master/lunus/command_line/xtraj.py
- A reference structure (PDB)



Align your trajectory to the reference structure

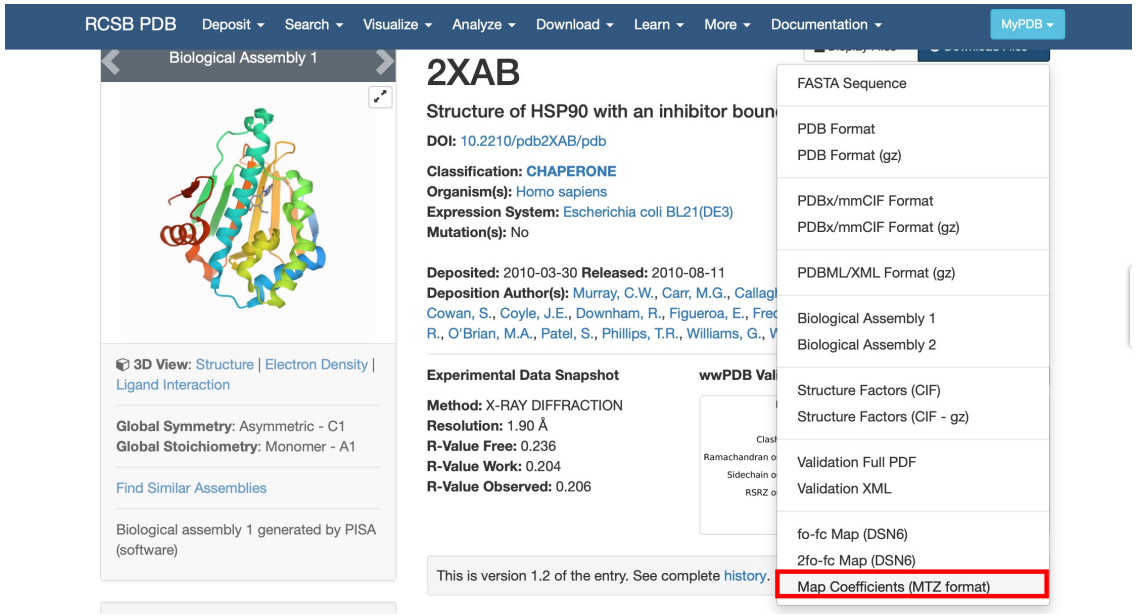
- Use MDTraj (superpose function) to align the trajectory to the reference structure (e.g., crystal structure).
- Optional: only using a subset of the structure (e.g., heavy atoms, backbone).
- Save the first frame as a separate PDB file (after alignment).

Calculate the electron densities

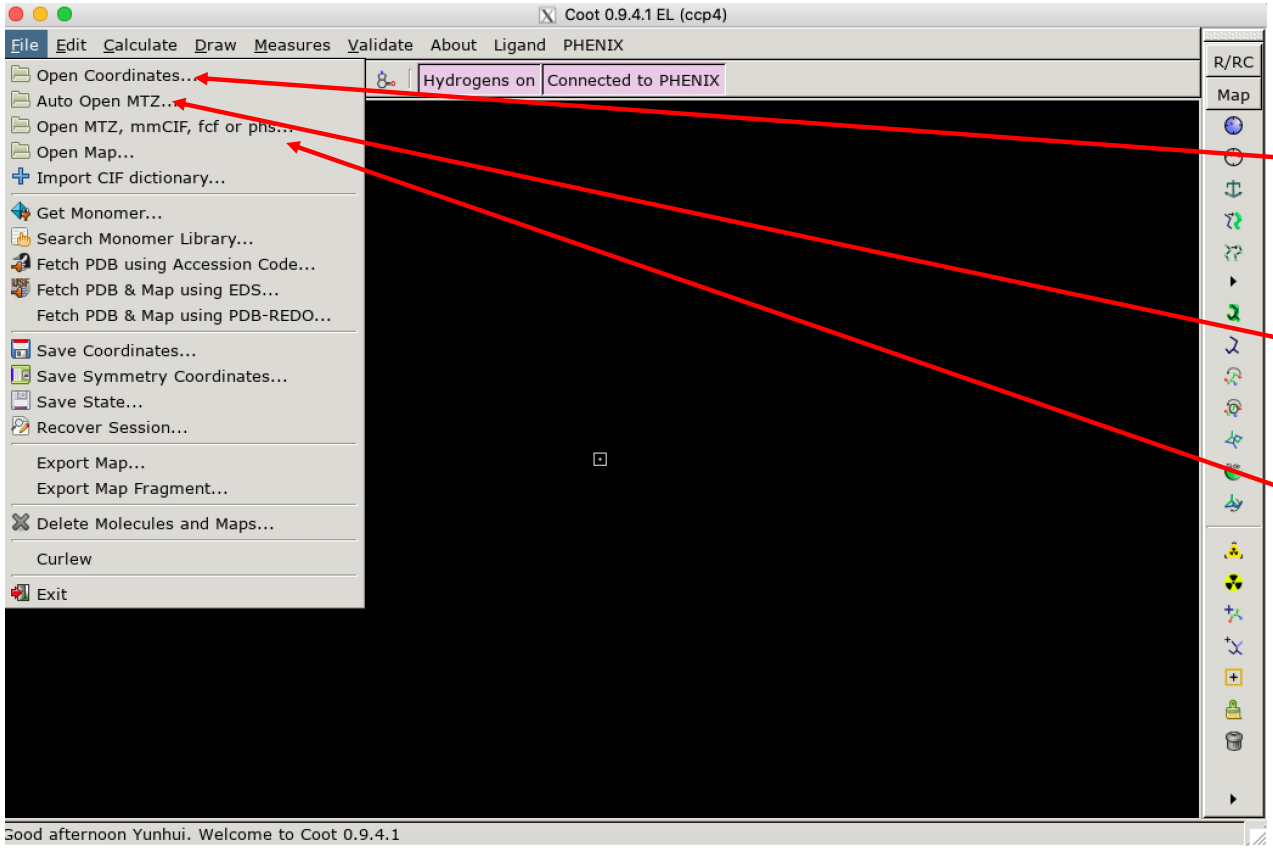
- python xtraj.py traj=aligned.xtc top=first.pdb first=0 last=12000
- Optional:
- python xtraj.py traj=aligned.xtc top=first.pdb selection="water" first=0 last=12000 fcalc=water_fcalc.mtz icalc=water_icalc.mtz diffuse=water_diffuse.hkl
- One more thing: replace “MODEL 0” with “MODEL 1” in the pdb file (required by Coot)

To visualize the results/compare with experiment, you need…

- Coot and/or Phenix **Phenix** *Python-based Hierarchical ENvironment for Integrated Xtallography*
- Crystal structures and electron density



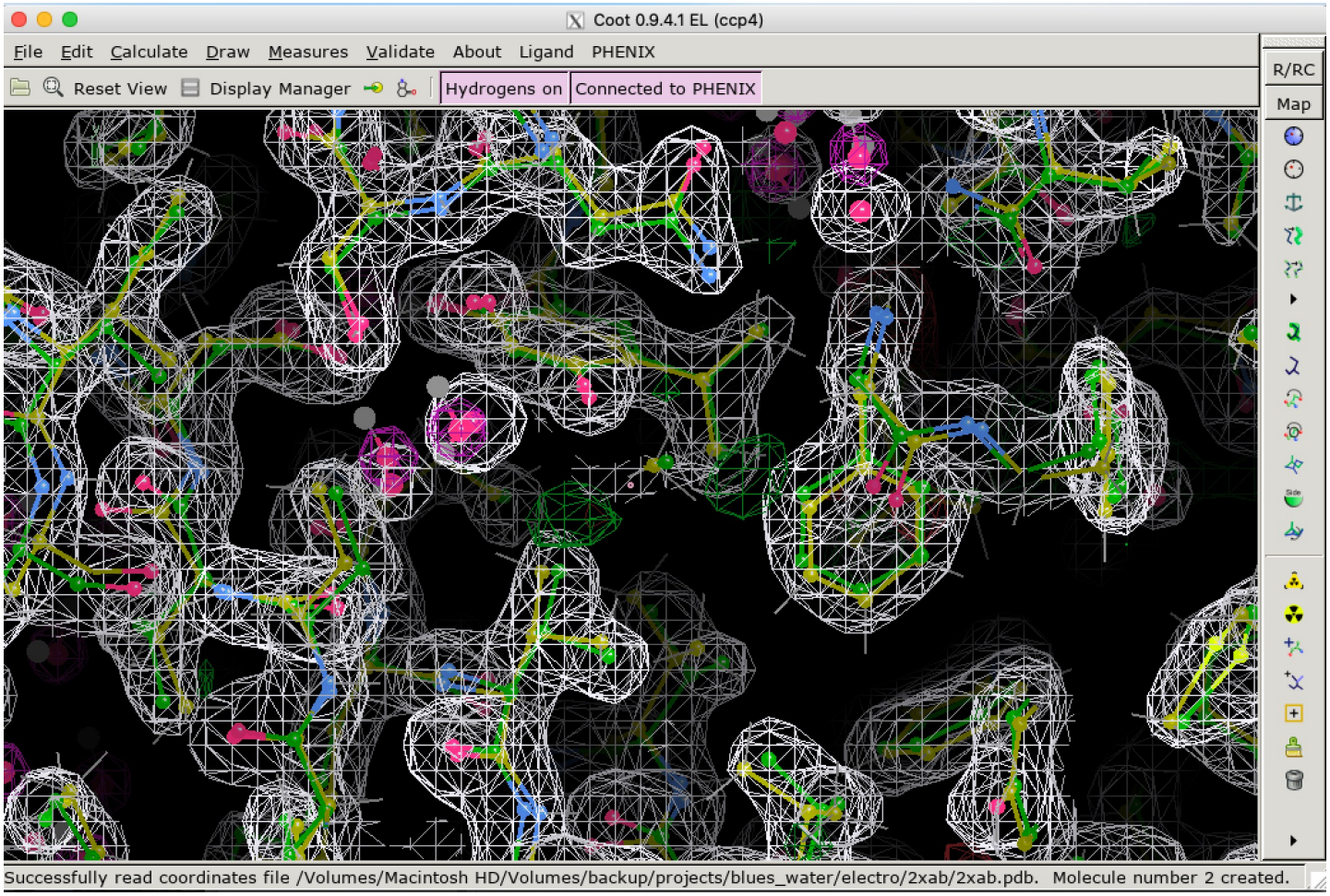
Use Coot to visualize the results



Your reference structure and your aligned PDB file

Downloaded electron density file (PDBcode_phases.mtz)

Your calculated electron density file (water_fcalc.mtz)


Coot 0.9.4.1 EL (ccp4)
File Edit Calculate Draw Measures Validate About Ligand PHENIX
Reset View
Display Manager
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Connected to PHENIX
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