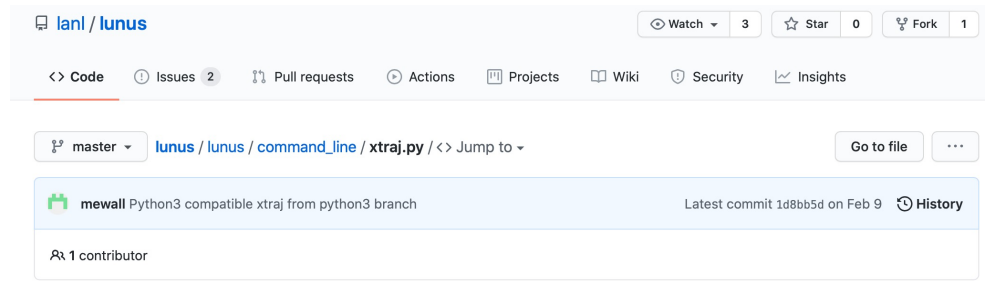


Things you need

- 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
- Crystal structures and electron density

Phenix

*Python-based **H**ierarchical **E**nvironment for **I**ntegrated **X**tallography*

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation MyPDB

Biological Assembly 1

2XAB
Structure of HSP90 with an inhibitor bound

DOI: [10.2210/pdb2XAB/pdb](https://doi.org/10.2210/pdb2XAB/pdb)

Classification: **CHAPERONE**

Organism(s): [Homo sapiens](#)

Expression System: [Escherichia coli BL21\(DE3\)](#)

Mutation(s): No

Deposited: 2010-03-30 Released: 2010-08-11

Deposition Author(s): Murray, C.W., Carr, M.G., Callaghan, S., Cowan, S., Coyle, J.E., Downham, R., Figueroa, E., Freyberger, A., R., O'Brian, M.A., Patel, S., Phillips, T.R., Williams, G., V.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.90 Å

R-Value Free: 0.236

R-Value Work: 0.204

R-Value Observed: 0.206

3D View: [Structure](#) | [Electron Density](#) | [Ligand Interaction](#)

Global Symmetry: Asymmetric - C1

Global Stoichiometry: Monomer - A1

[Find Similar Assemblies](#)

Biological assembly 1 generated by PISA (software)

wwPDB Validation

Structure Factors (CIF)

Structure Factors (CIF - gz)

Validation Full PDF

Validation XML

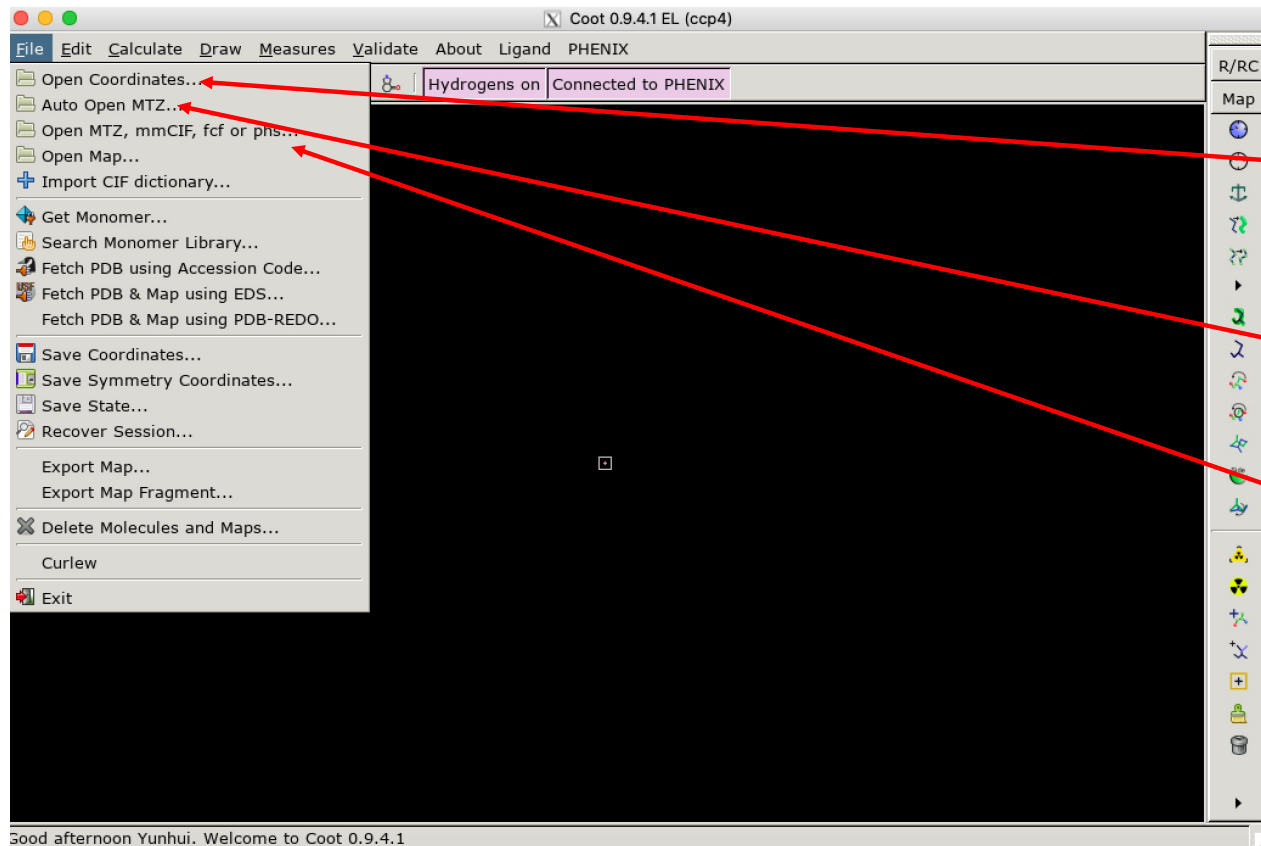
fo-fc Map (DSN6)

2fo-fc Map (DSN6)

Map Coefficients (MTZ format)

This is version 1.2 of the entry. See complete [history](#).

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)

