National Center for CryoEM Access and Training

Virtual Classroom: Intro to Model Building & Refinement. December 7 & 10, 2020.

Please complete this pre-tutorial checklist <u>before</u> the tutorial. Some of these steps may be time consuming:

- ❏ Download tutorial files (models and maps) here: https://drive.google.com/file/d/1hlDNsOJJuDmQ4Y3pFIaHjQNiYxPUguGP/view?usp=sharing
- ❏ Install ChimeraX (downloads are here: https://www.cgl.ucsf.edu/chimerax/download.html)
- ❏ Launch ChimeraX and open a model file (Menu: File>Open then choose any model (.pdb) in the tutorial files you downloaded)
- ❏ Open a map file in ChimeraX (Menu: FIle>Open then choose the map (.map) in the tutorial files)
- ❏ Install Coot
  - ❏ for Linux download from https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/.
  - ❏ For Mac download from http://scottlab.ucsc.edu/xtal/wiki/index.php/Installing_Coot_on_OS_X.
  - ❏ For windows download from https://bernhardcl.github.io/coot/wincoot-download.html.
  - ❏ You can use any version of Coot for this tutorial. I recommend version 0.9. It is significantly updated for lower resolution maps and is the future! Experienced coot users have been known to not like it, so if you must (or are using WinCoot) you can use version 0.8).
- ❏ Launch Coot and open a model file (Menu: File>Open Coordinates then choose any model (.pdb) in the tutorial files)
- ❏ Open a map file in Coot (Menu: File>Open Map then choose the map (.map) in the tutorial files).
- ❏ Install Phenix (downloads are here: https://www.phenix-online.org/)
- ❏ Launch Phenix and create a new project that points to a directory where you will save output files. (We won't use Phenix the first day and can address installation problems then).

If you can check all of these boxes, you're ready to start!

This tutorial will take place over two days. On **day one** we will use **ChimeraX** and **Coot** to assemble a starting model from existing publicly available structures and fit it into an experimental CryoEM map.

On **day two** we will use **Phenix** to perform real space refinements to improve both the fit of the model into the map and the chemical bond geometries of the model. We will use Coot to visually assess the output of the refinements and do some minor model adjustments by hand.

The aim of this tutorial is to provide familiarity with available software tools and techniques used for model generation and refinement. We will cover basic features and uses. This will not provide a comprehensive overview or advanced use of any particular software (this would require a much longer course!). We hope this introduction prepares you to work with your own data or attend more advanced tutorials in the future.