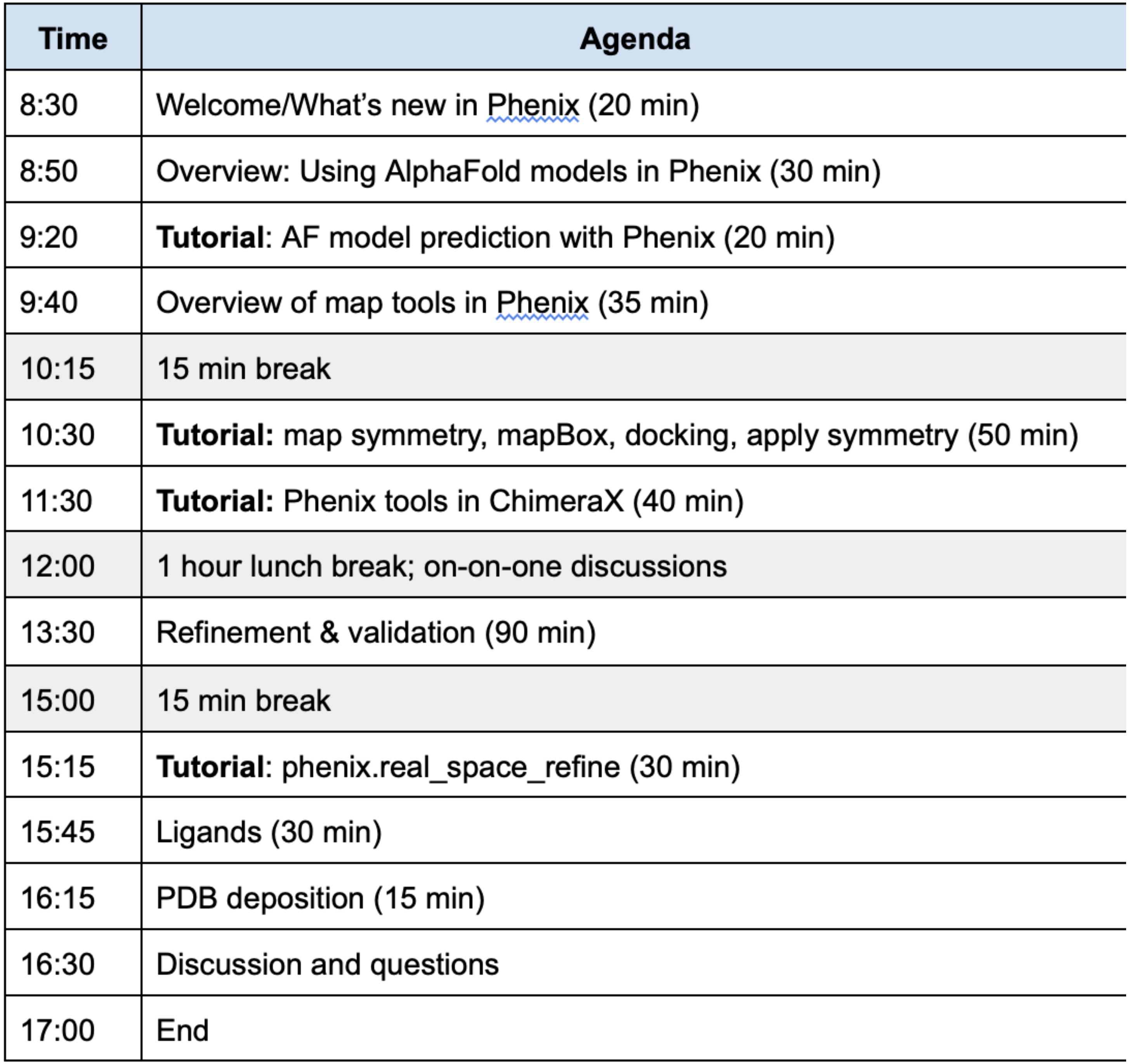
UTMB,
October 2025

Phenix Introduction

Dorothee Liebschner

Lawrence Berkeley Laboratory



Time	Agenda
8:30	Welcome/What's new in Phenix (20 min)
8:50	Overview: Using AlphaFold models in Phenix (30 min)
9:20	**Tutorial**: AF model prediction with Phenix (20 min)
9:40	Overview of map tools in Phenix (35 min)
10:15	15 min break
10:30	**Tutorial:** map symmetry, mapBox, docking, apply symmetry (50 min)
11:30	**Tutorial:** Phenix tools in ChimeraX (40 min)
12:00	1 hour lunch break; on-on-one discussions
13:30	Refinement & validation (90 min)
15:00	15 min break
15:15	**Tutorial**: phenix.real_space_refine (30 min)
15:45	Ligands (30 min)
16:15	PDB deposition (15 min)
16:30	Discussion and questions
17:00	End

What is *Phenix*?

- Package for **automated structure solution** (crystallography, cryo-EM)
- Apply modern programming concepts to develop new algorithms
- Designed to be used by **both novices and experienced users**
- Long-term development and support
- Why is it called *Phenix*?

Python **H**ierarchical **EN**vironment for **I**ntegrated **X**tallography

The Phenix Project

Lawrence Berkeley Laboratory

Paul Adams, Pavel Afonine, Dorothee Liebschner, Nigel Moriarty, Billy Poon, Oleg Sobolev

Los Alamos National Laboratory
New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

UTHealth

Matt Baker

University of Cambridge

Randy Read, Airlie McCoy

Duke University

Jane Richardson, Vincent Chen

An NIH/NIGMS funded Program Project

Liebschner D, *et al.*, Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in *Phenix*. Acta Cryst. 2019 **D75**:861–877

Tools for Crystallography

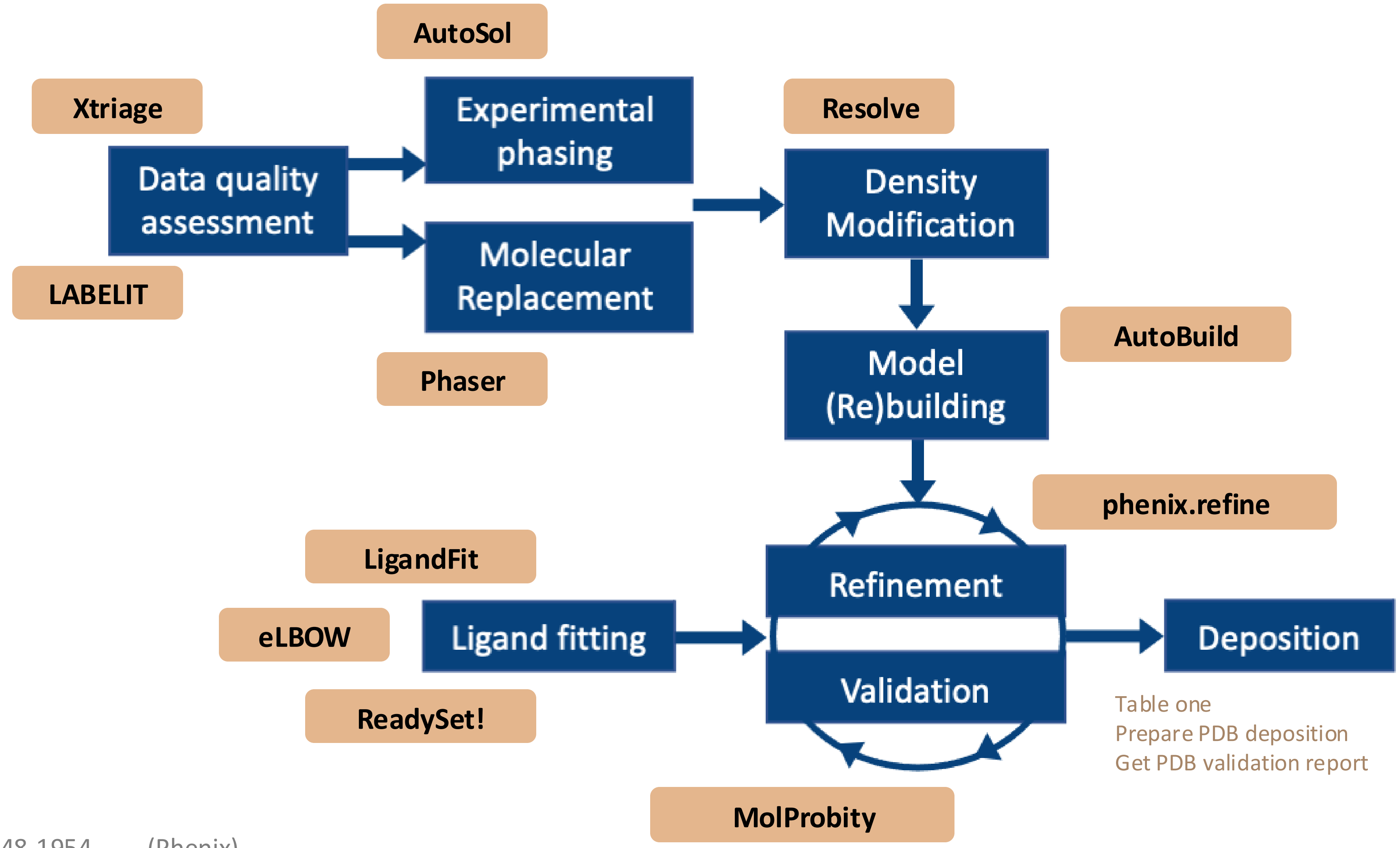
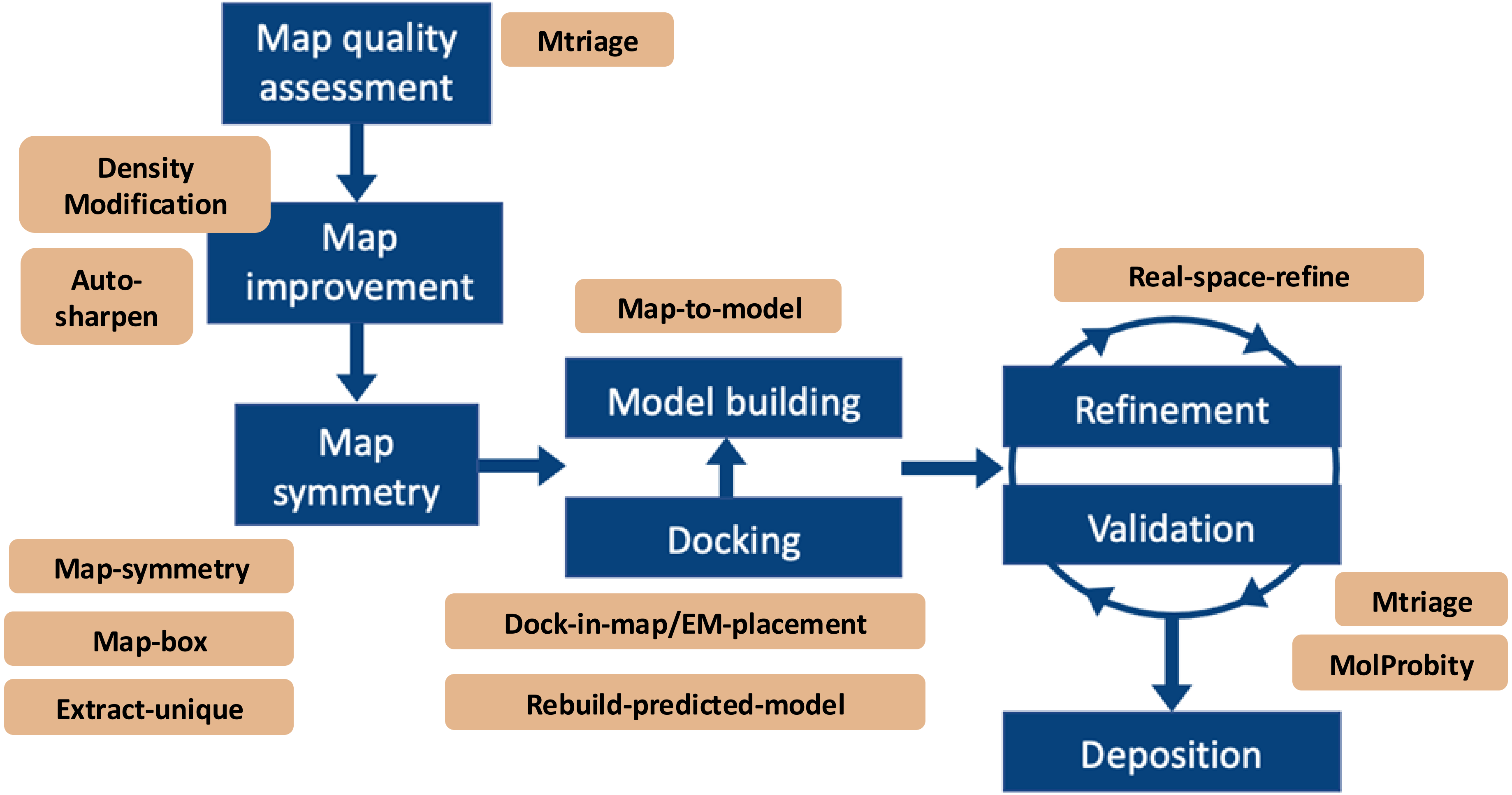


Table one
Prepare PDB deposition
Get PDB validation report

Acta Cryst. 2002, D58:1948-1954	(Phenix)
J. Appl. Cryst. 2002, 35:126-136	(cctbx)
Acta Cryst. 2010, D66: 213-221	(Phenix)
Acta Cryst. 2019 D75:861–877	(Phenix)

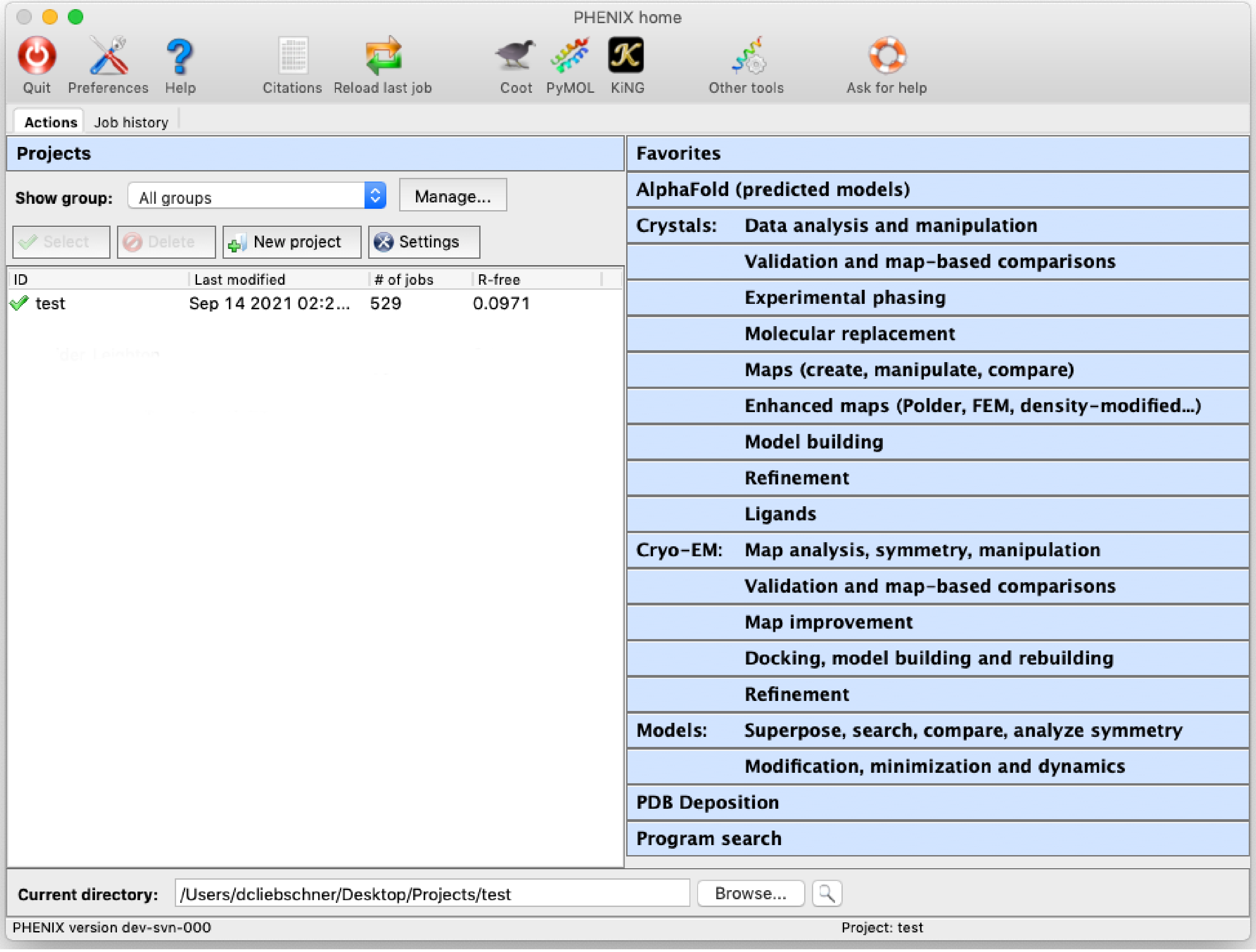
Tool for cryo-EM



Acta Cryst. 2002, D58:1948-1954 (Phenix)
J. Appl. Cryst. 2002, 35:126-136 (cctbx)
Acta Cryst. 2010, D66: 213-221 (Phenix)
Acta Cryst. 2019 D75:861–877 (Phenix)

Phenix Graphical User Interface (GUI)

Central GUI for job control and to launch new jobs



Show group: All groups

ID	Last modified	# of jobs	R-free
✓ test	Sep 14 2021 02:2...	529	0.0971

Current directory: /Users/dcliebschner/Desktop/Projects/test

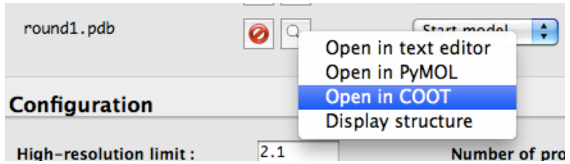
PHENIX version dev-svn-000

Project: test

Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps

- Any PDB file listed in GUI can also be opened



High-resolution limit : 2.1

- Specific paths to executables usually required on Linux

Preferences → Graphics → Full path to Coot […PyMOL]

Command Line

Run on the terminal

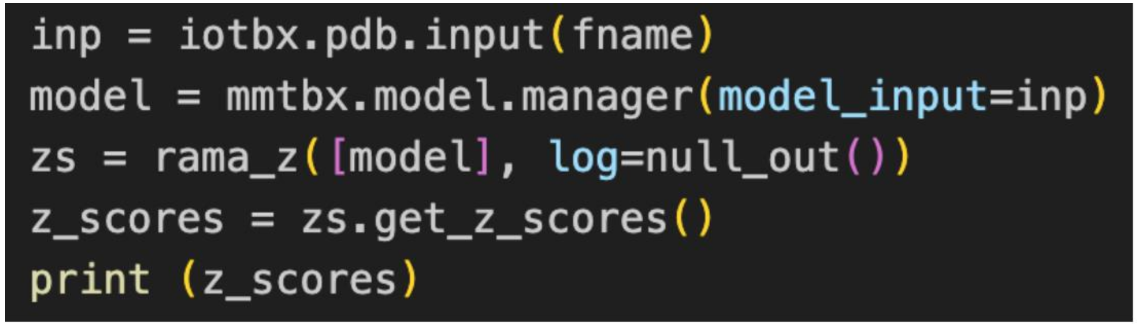
```
phenix.mtriage    my_model.pdb   my_map.map    resolution=4
```

name of the program

input files

options

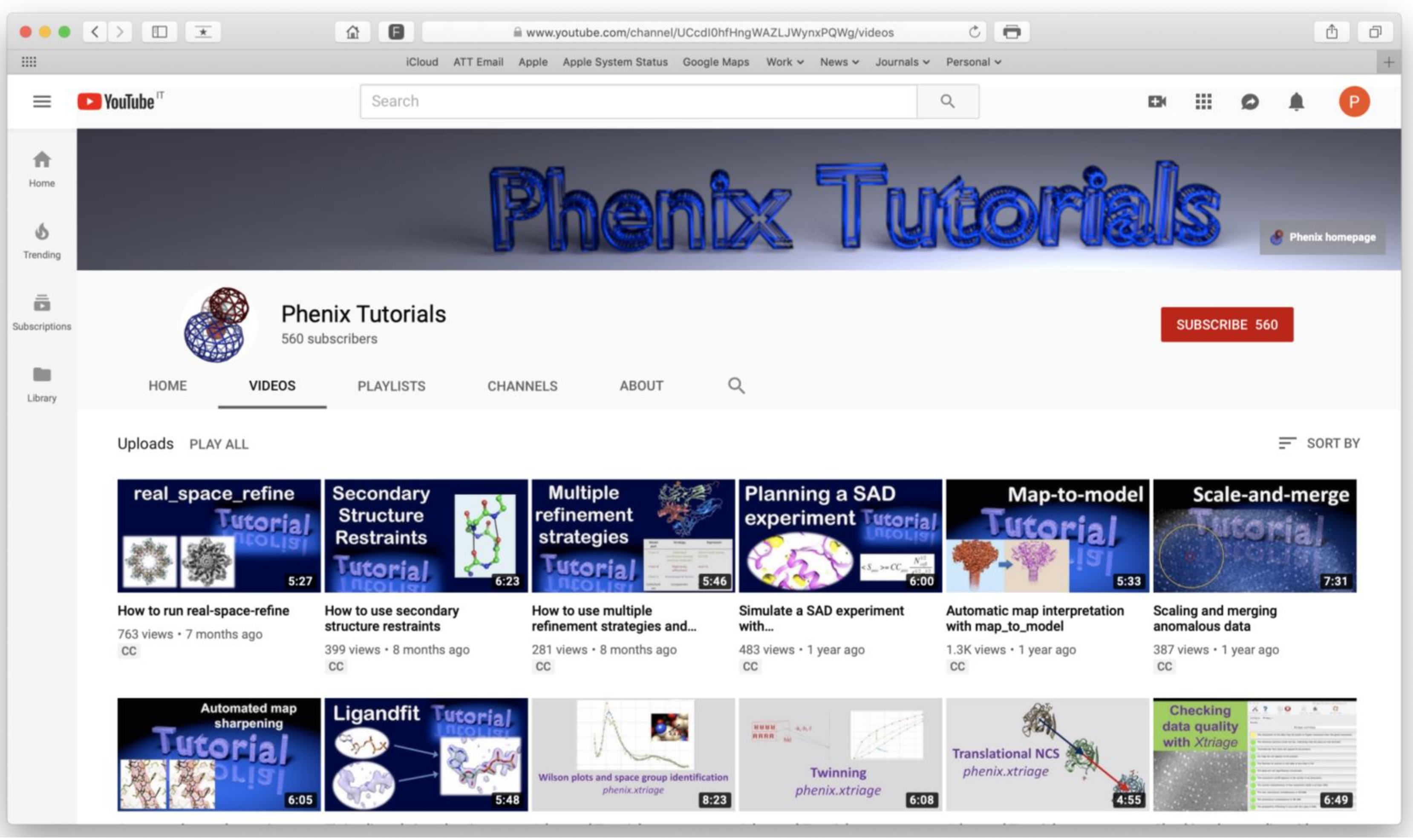
Run in a python script



```
inp = iotbx.pdb.input(fname)
model = mmtbx.model.manager(model_input=inp)
zs = rama_z([model], log=null_out())
z_scores = zs.get_z_scores()
print (z_scores)
```

Video Tutorials

https://www.youtube.com/c/phenixtutorials



Phenix Tutorials
560 subscribers

How to run real-space-refine
763 views • 7 months ago
CC

How to use secondary structure restraints
399 views • 8 months ago
CC

How to use multiple refinement strategies and...
281 views • 8 months ago
CC

Simulate a SAD experiment with...
483 views • 1 year ago
CC

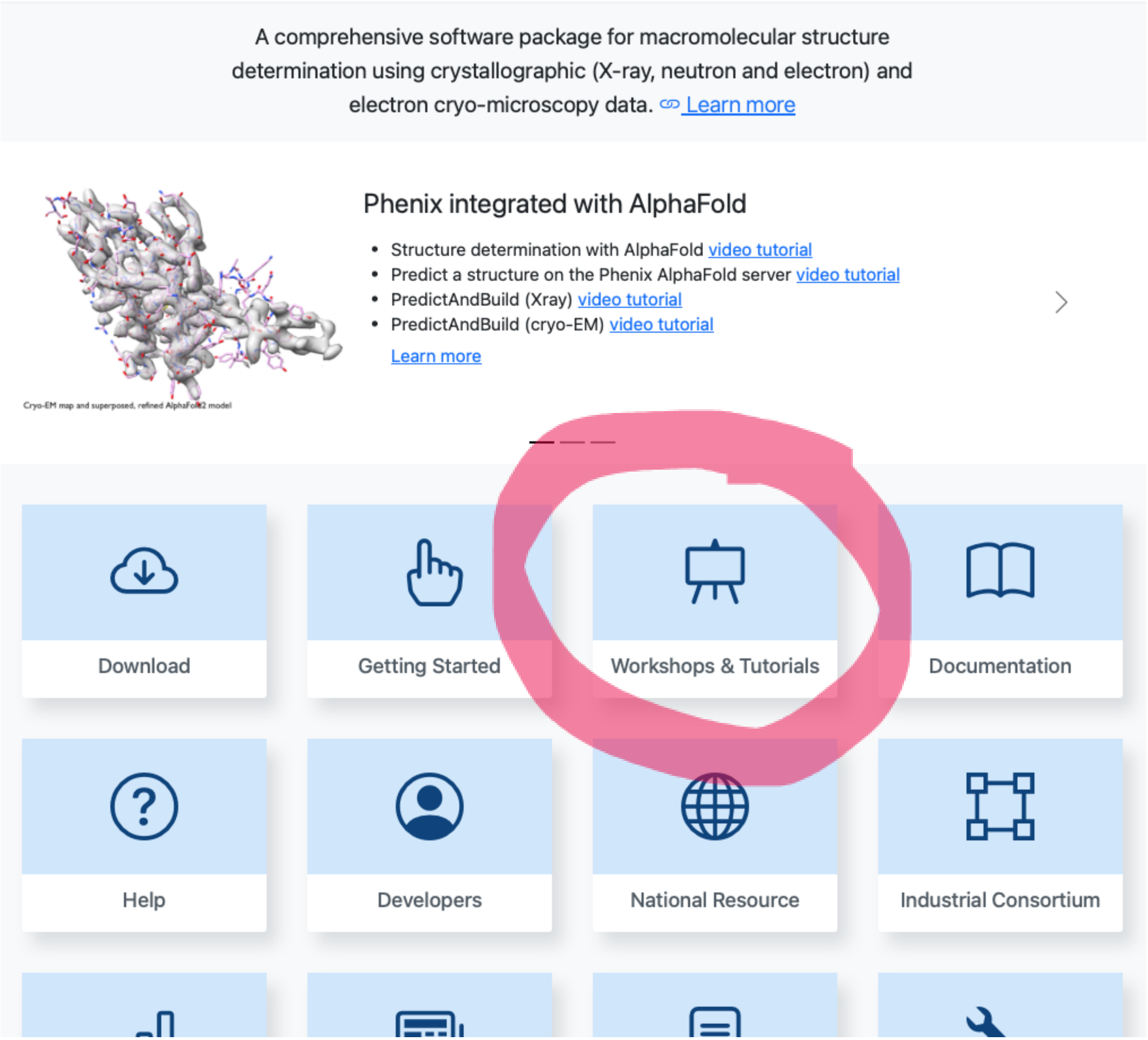
Automatic map interpretation with map_to_model
1.3K views • 1 year ago
CC

Scaling and merging anomalous data
387 views • 1 year ago
CC

Dorothee Liebschner, Tom Terwilliger, Nigel Moriarty, Christopher Schlicksup, Vincent Chen

Presentation slides

https://phenix-online.org



A comprehensive software package for macromolecular structure determination using crystallographic (X-ray, neutron and electron) and electron cryo-microscopy data. Learn more

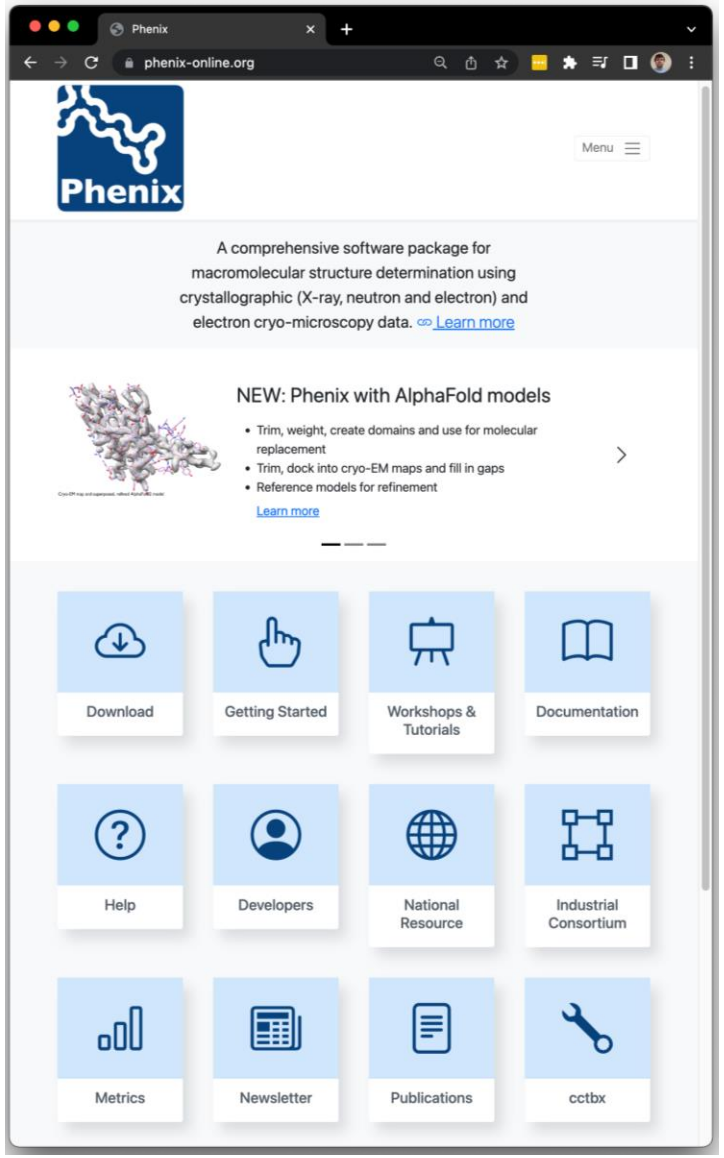
Cryo-EM map and superposed, refined AlphaFold2 model

Phenix integrated with AlphaFold

- Structure determination with AlphaFold video tutorial
- Predict a structure on the Phenix AlphaFold server video tutorial
- PredictAndBuild (Xray) video tutorial
- PredictAndBuild (cryo-EM) video tutorial

Learn more

Phenix resources



A comprehensive software package for macromolecular structure determination using crystallographic (X-ray, neutron and electron) and electron cryo-microscopy data. Learn more

NEW: Phenix with AlphaFold models

- Trim, weight, create domains and use for molecular replacement
- Trim, dock into cryo-EM maps and fill in gaps
- Reference models for refinement

Learn more

Phenix paper

Video tutorials (YouTube)

Documentation

Relevant papers

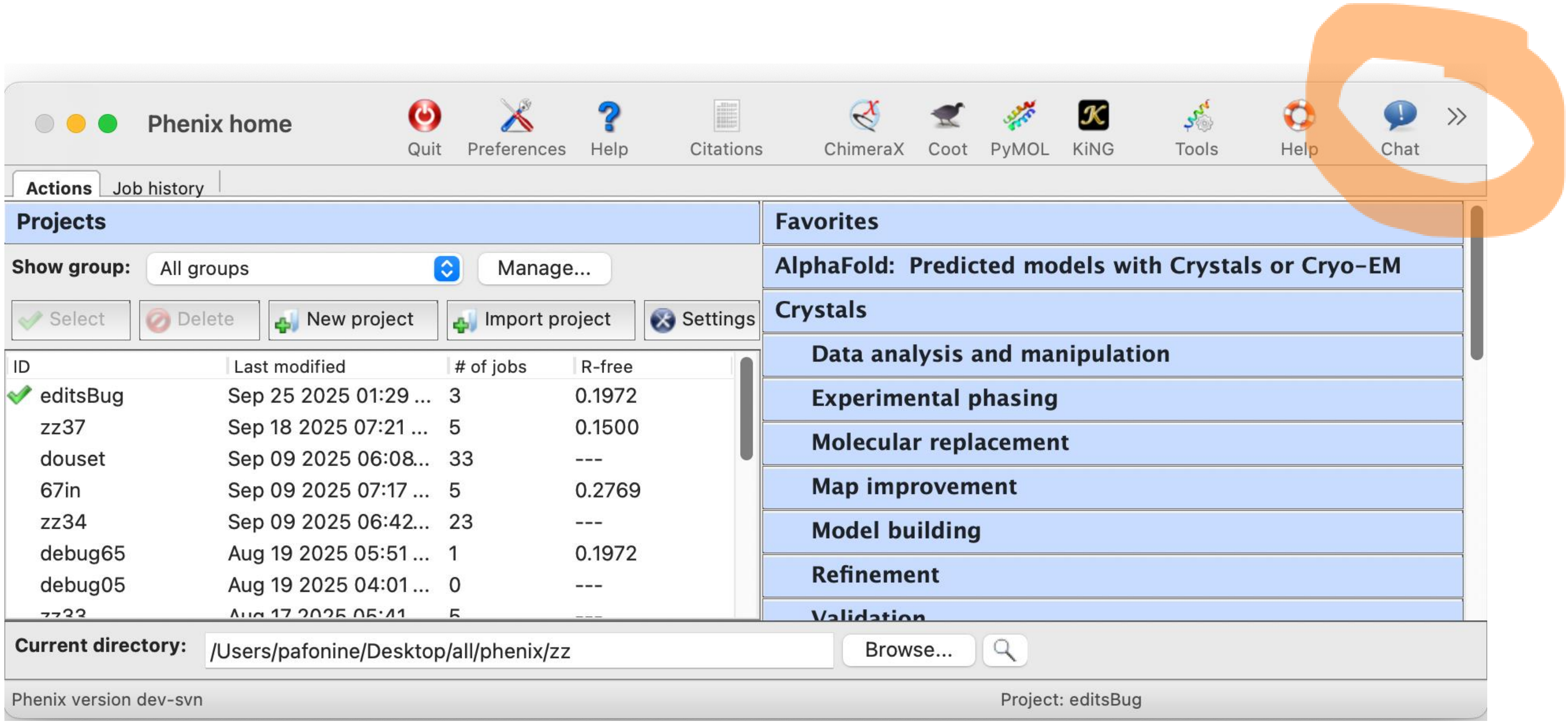
Bi-annual newsletters

PDFs with slides from workshops

NEW: AI tools in Phenix

Phenix chatbot

phenix-online.org/chatbot



Show group: All groups

ID	Last modified	# of jobs	R-free
✓ editsBug	Sep 25 2025 01:29 ...	3	0.1972
zz37	Sep 18 2025 07:21 ...	5	0.1500
douset	Sep 09 2025 06:08...	33	---
67in	Sep 09 2025 07:17 ...	5	0.2769
zz34	Sep 09 2025 06:42...	23	---
debug65	Aug 19 2025 05:51 ...	1	0.1972
debug05	Aug 19 2025 04:01 ...	0	---

Current directory: /Users/pafonine/Desktop/all/phenix/zz

Phenix version dev-svn

Project: editsBug

NEW: AI tools in Phenix

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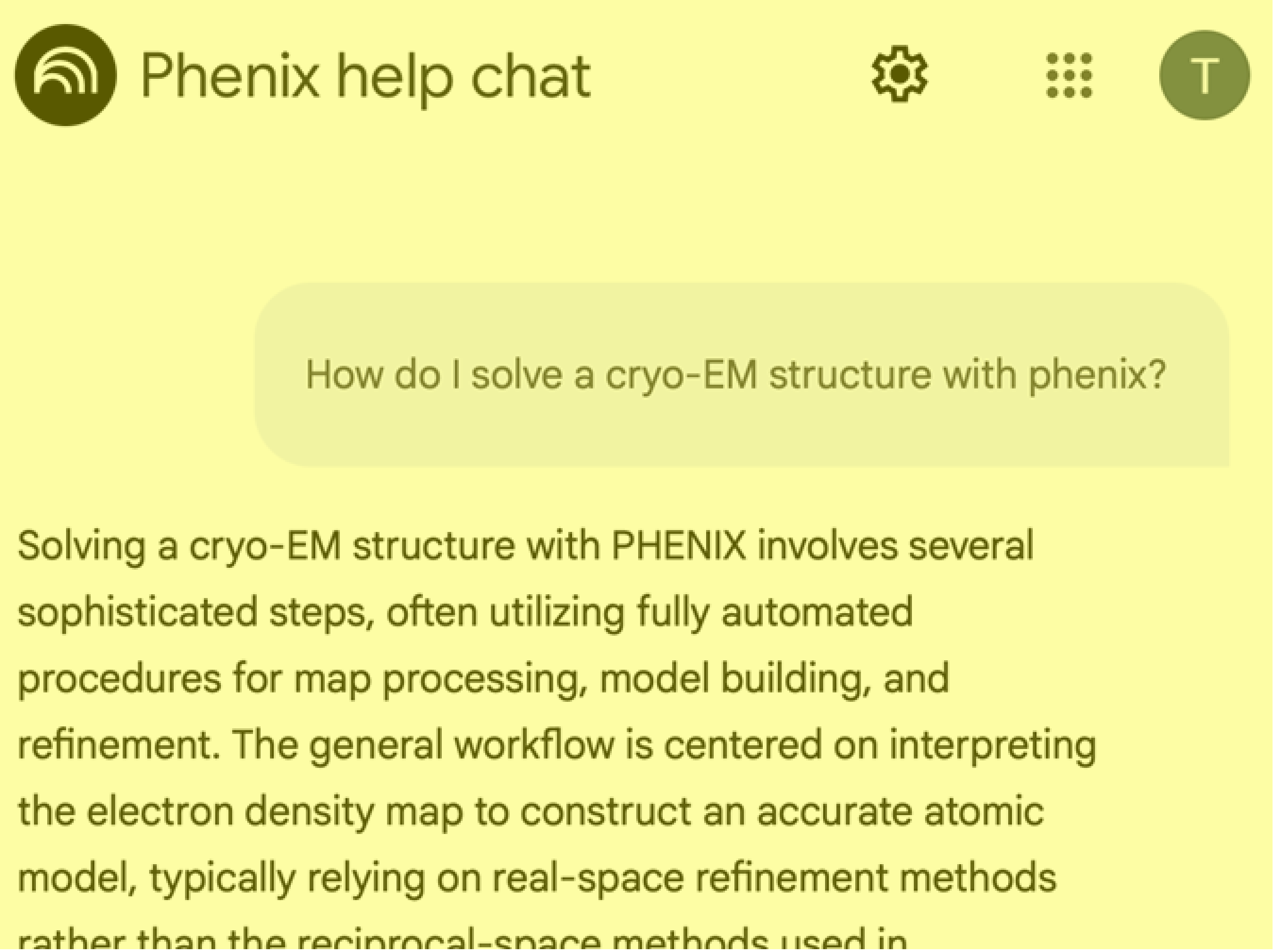
phenix-online.org/chatbot

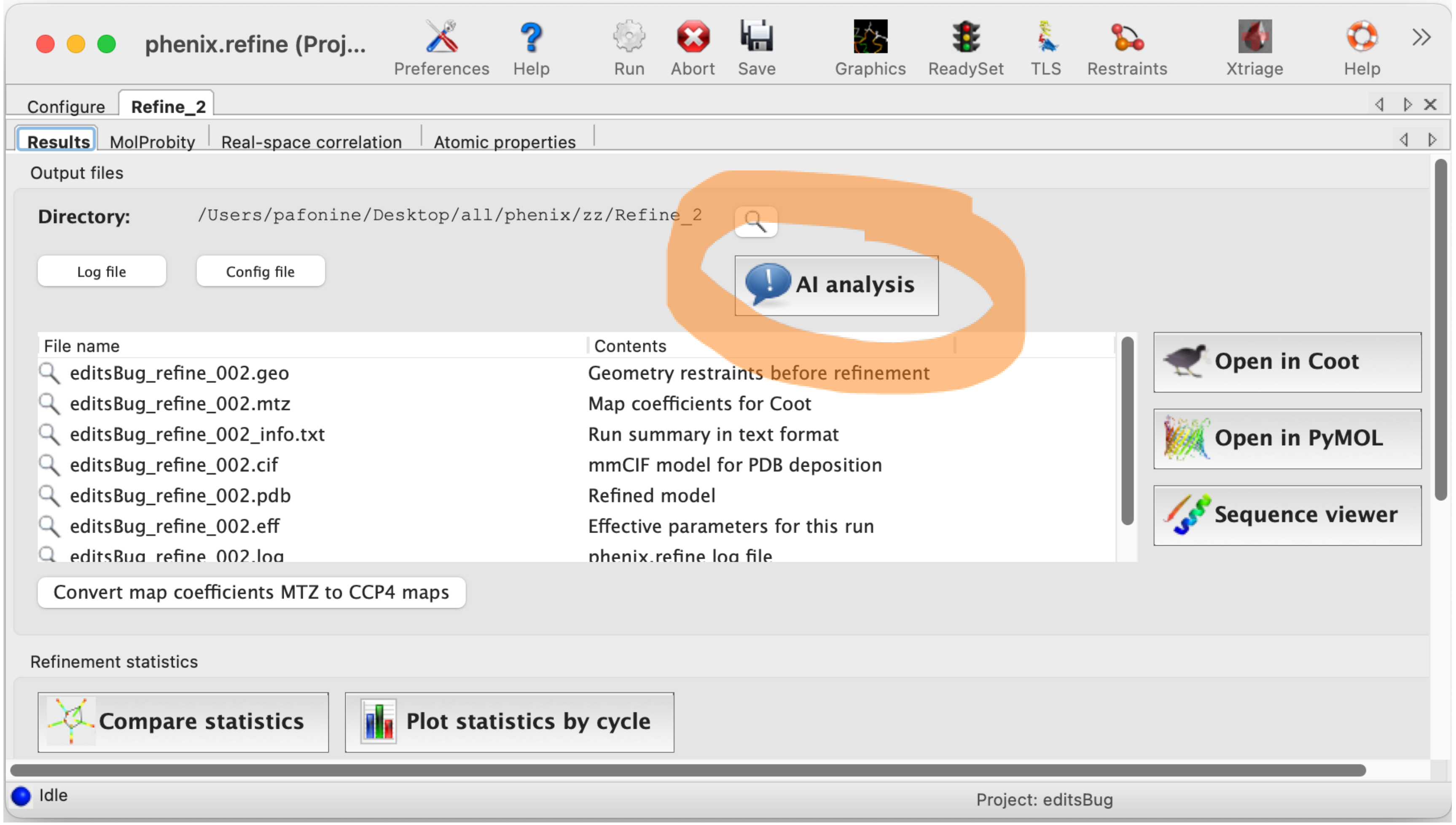


How do I solve a cryo-EM structure with phenix?

Solving a cryo-EM structure with PHENIX involves several sophisticated steps, often utilizing fully automated procedures for map processing, model building, and refinement. The general workflow is centered on interpreting the electron density map to construct an accurate atomic model, typically relying on real-space refinement methods rather than the reciprocal-space methods used in

NEW: AI tools in Phenix

AI analysis of results



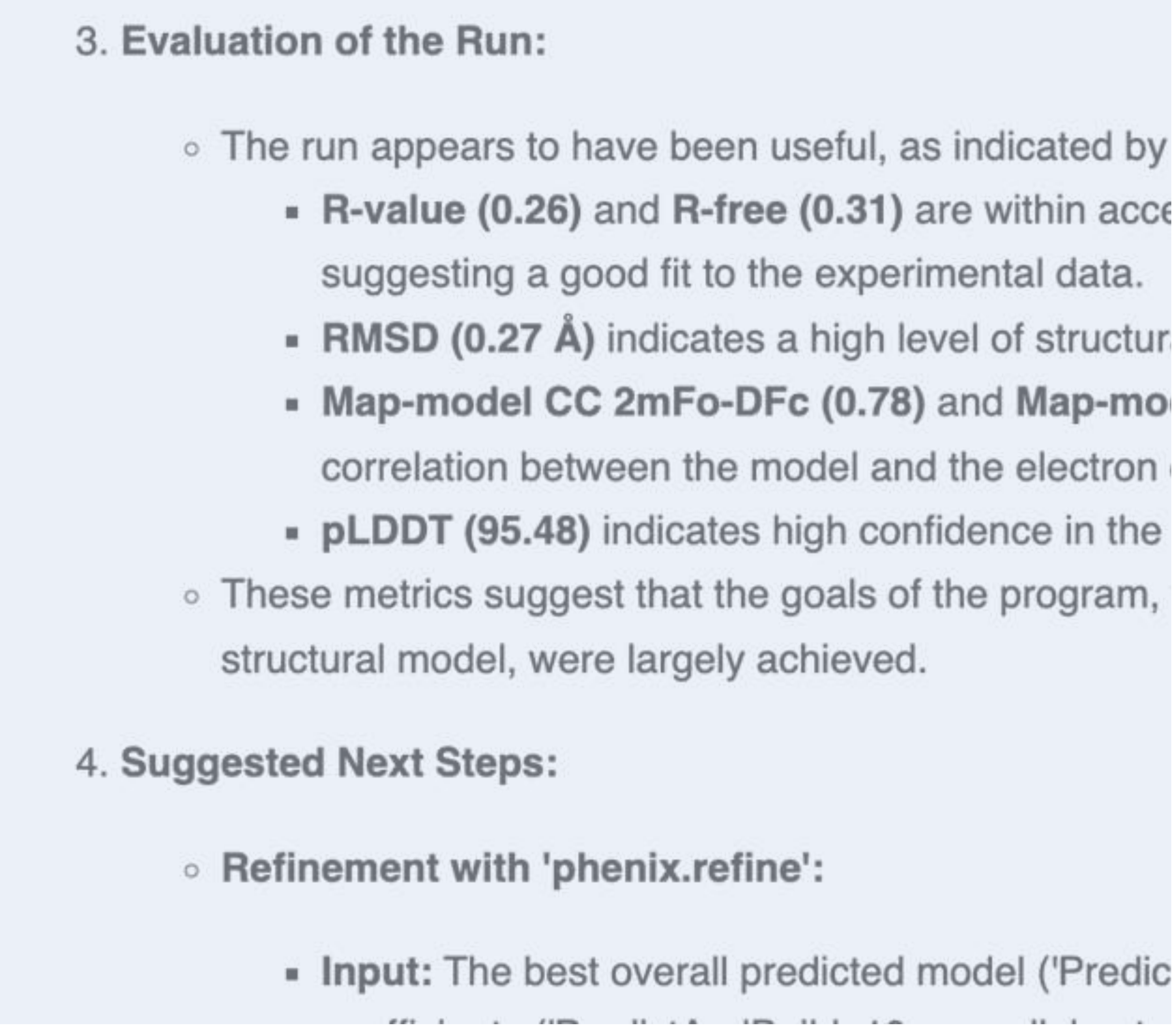
Directory: /Users/pafonine/Desktop/all/phenix/zz/Refine_2

File name	Contents
editsBug_refine_002.geo	Geometry restraints before refinement
editsBug_refine_002.mtz	Map coefficients for Coot
editsBug_refine_002_info.txt	Run summary in text format
editsBug_refine_002.cif	mmCIF model for PDB deposition
editsBug_refine_002.pdb	Refined model
editsBug_refine_002.eff	Effective parameters for this run
editsBug_refine_002.log	phenix.refine log file

Project: editsBug

NEW: AI tools in Phenix

AI analysis of results



3. **Evaluation of the Run:**
    - The run appears to have been useful, as indicated by
        - **R-value (0.26)** and **R-free (0.31)** are within acce
          suggesting a good fit to the experimental data.
        - **RMSD (0.27 Å)** indicates a high level of structur
        - **Map-model CC 2mFo-DFc (0.78)** and **Map-mo**
          correlation between the model and the electron
        - **pLDDT (95.48)** indicates high confidence in the
    - These metrics suggest that the goals of the program,
      structural model, were largely achieved.

4. **Suggested Next Steps:**
    - **Refinement with 'phenix.refine':**
        - **Input:** The best overall predicted model ('Predic

Chatbot: What it can and cannot do

It is good for:

- Summarizing the documentation
- Asking specific questions that can be answered based on the documentation
- Asking follow-up questions

It can make mistakes of give incomplete answers:

Create an atom selection string that will select all the main-chain atoms of the nucleic acid residues in chain A

may yield:

“backbone and chain A”

instead of:

“backbone and (not protein) and chain A”

Chatbot: What is needed to run it

- A Google account
  - Any account will work
  - A paid account will allow you to ask more questions in a day

- You can help us to improve the chatbot:

If the chatbot gives a bad answer…

Let us know (send an email)

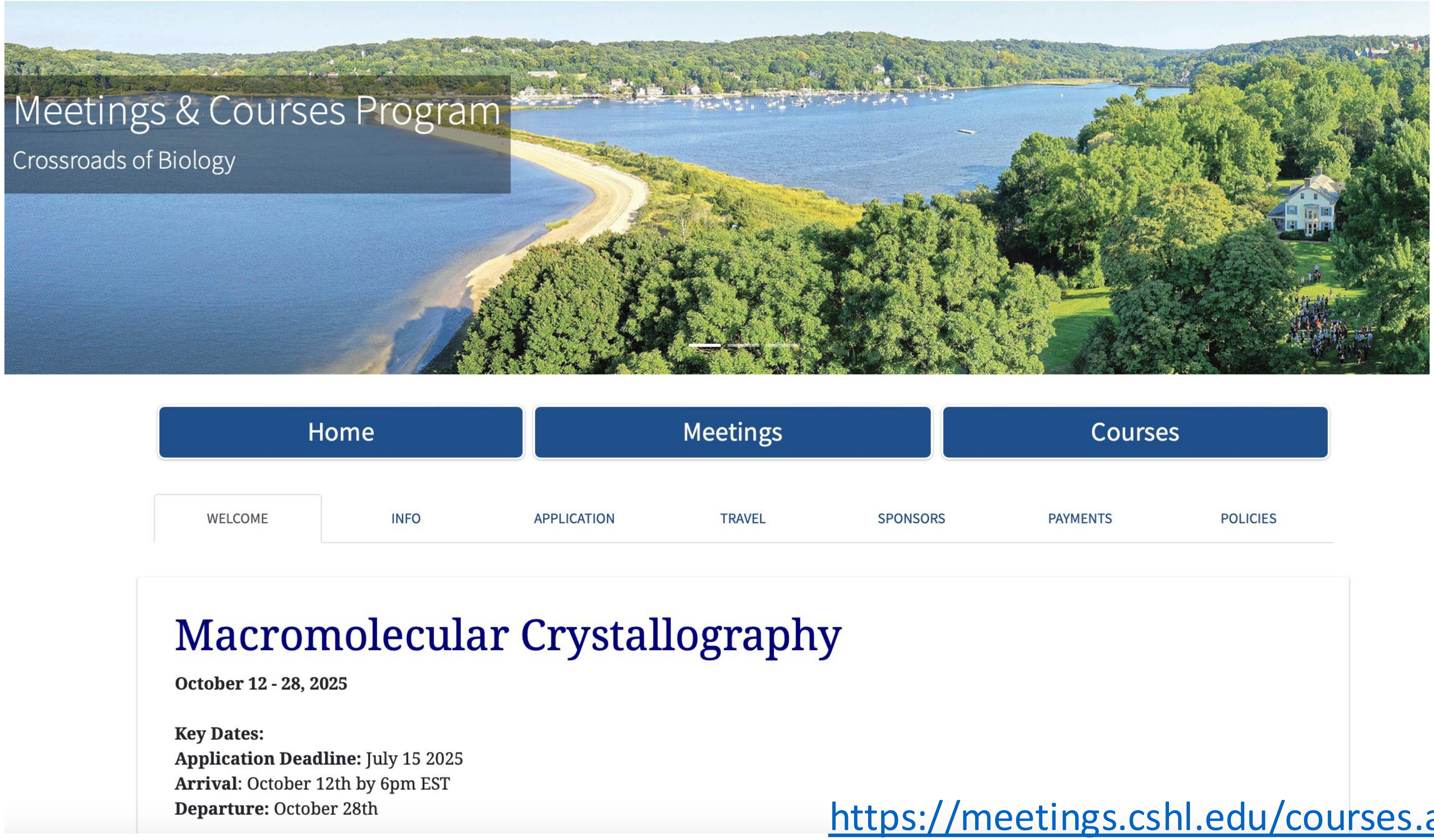
We can update the documentation to give the chatbot the information it needs to give a good answer

Crystallography courses in the US

CSHL course: Macromolecular Crystallography

CSH Cold Spring Harbor Laboratory

October 12-28, 2025



Macromolecular Crystallography

October 12 - 28, 2025

Key Dates:
Application Deadline: July 15 2025
Arrival: October 12th by 6pm EST
Departure: October 28th

https://meetings.cshl.edu/courses.aspx?course=C-CRYS

Rapidata (May)

RapiData 2025 at SSRL

Data Collection and Structure Solving: A Practical Course in Macromolecular X-Ray Diffraction Measurement

May 5 - May 10, 2025

Stanford Synchrotron Radiation Lightsource

Event Information

Course dates: May 5 - May 10, 2025

Applications opens: November 2024

Application deadline: January 31 2025
Applications received after the deadline will be placed in a stand-by list.

CCP4 school Argonne (June)

Collaborative Computational Project No. 4
Software for Macromolecular X-Ray Crystallography

CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond

School Announcement

We are very pleased to announce the 17th annual CCP4 USA Crystallography School organized jointly with the National Institute of General Medical Sciences and National Cancer Institute Structural Biology Facility at the Advanced Photon Source (GM/CA@APS). The 2025 school will take place at the Advanced Photon Source (APS) synchrotron site at Argonne National Laboratory, near Chicago.

School Dates

June 23 – 30, 2025
The first two days will be dedicated to data collection and processing. The rest of the school will focus on structure solution, refinement and validation. The workshop will be proceeded by two virtual introduction days.

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Phenix Testers & Users

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