BERKELEY LAB

U.S. DEPARTMENT OF ENERGY

UNIVERSITY OF CALIFORNIA

AsCA meeting,
6 December 2025

Phenix Introduction

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Lawrence Berkeley Laboratory

UTHealth The University of Texas Health Science Center at Houston

Los Alamos NATIONAL LABORATORY EST. 1943

BERKELEY LAB

UNIVERSITY OF CAMBRIDGE

Time	Agenda
9:00	Welcome/Introduction to Phenix (15 min)
9:15	Using AlphaFold predictions for structure determination (30 min)
9:45	**Tutorial 1**: AlphaFold structure prediction (15 min)
10:00	Molecular replacement (30 min)
10:30	15 min break
10:45	**Tutorial 2:** Xtriage (30 min)
11:15	**Tutorial 3**: MR with AlphaFold (30 min)
11:45	**Tutorial 4**: cryo-EM docking, fit loops, douse with ChimeraX
12:30	1 hour lunch break; one-on-one discussions
13:30	Refinement (60 min)
14:30	**Tutorial 5**: Refinement (30 min)
15:00	15 min break
15:15	Validation (45 min)
16:00	Ligands (15 min)
16:15	**Tutorial 6**: Polder maps (15 min)
16:30	**Tutorial 7**: Predict and build (20 min)
16:50	FAQ, Discussion and questions, workshop survey
17:00	End

Wifi:
Phenix

Password
20251206

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

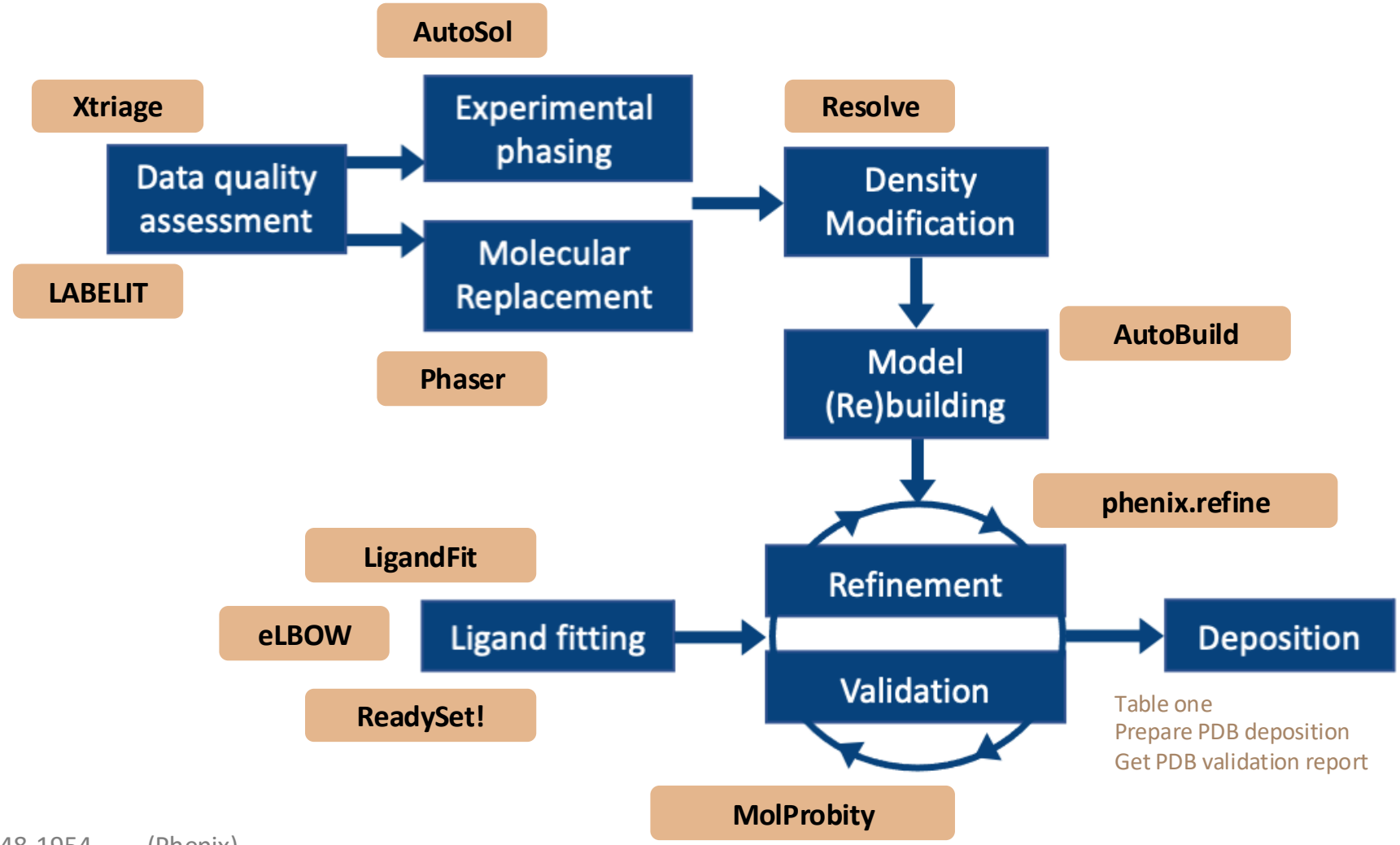
Duke University

Jane Richardson, Vincent Chen

An NIH/NIGMS funded Program Project

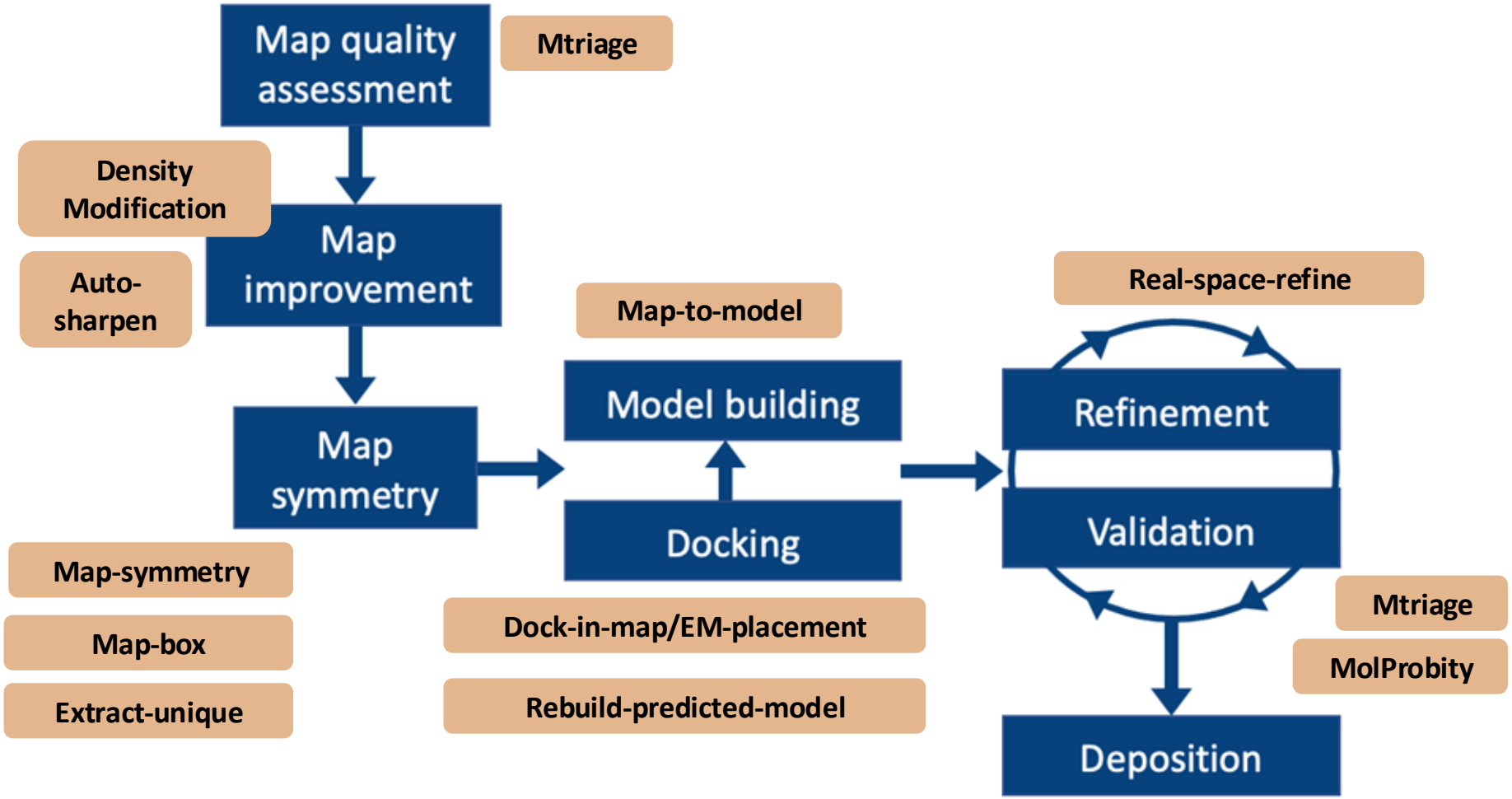
Liebschner D, *et al.*, Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in *Phenix*. Acta Cryst. 2019 **D75**:861–877

Tools for Crystallography



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



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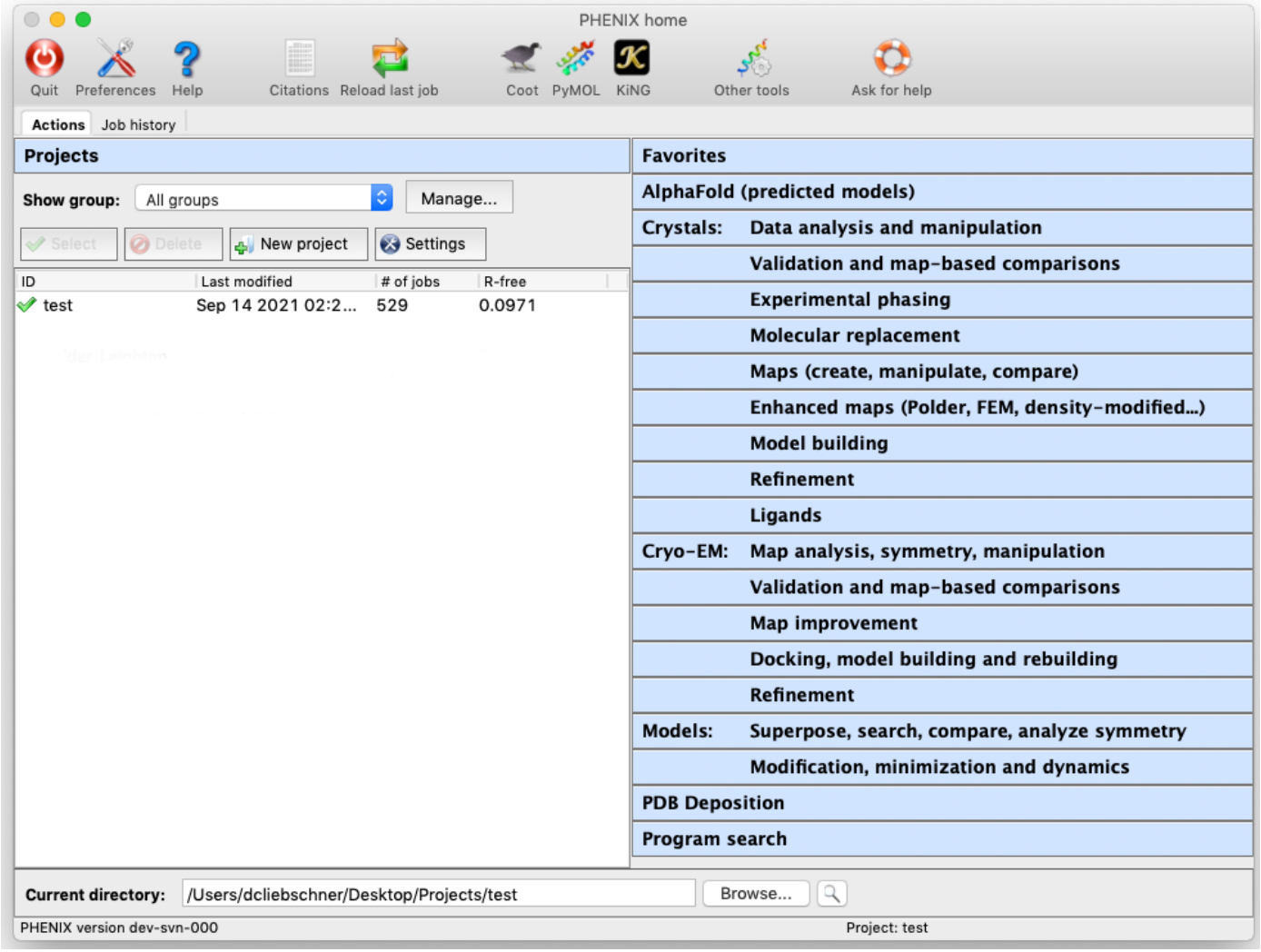
Phenix Graphical User Interface (GUI)

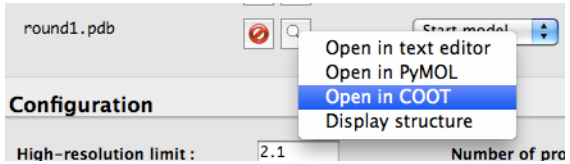
Central GUI for job control and to launch new jobs



Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps

- Any PDB file listed in GUI can also be opened

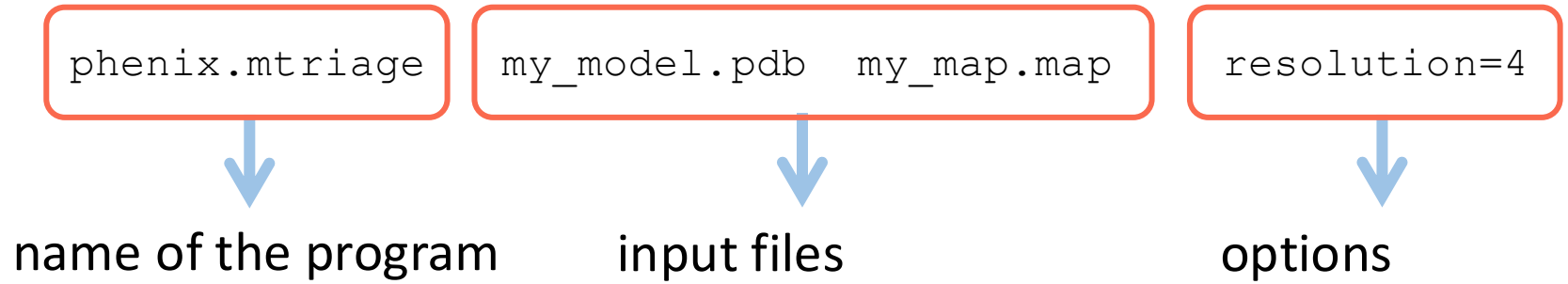


- Specific paths to executables usually required on Linux

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

Command Line

Run on the terminal

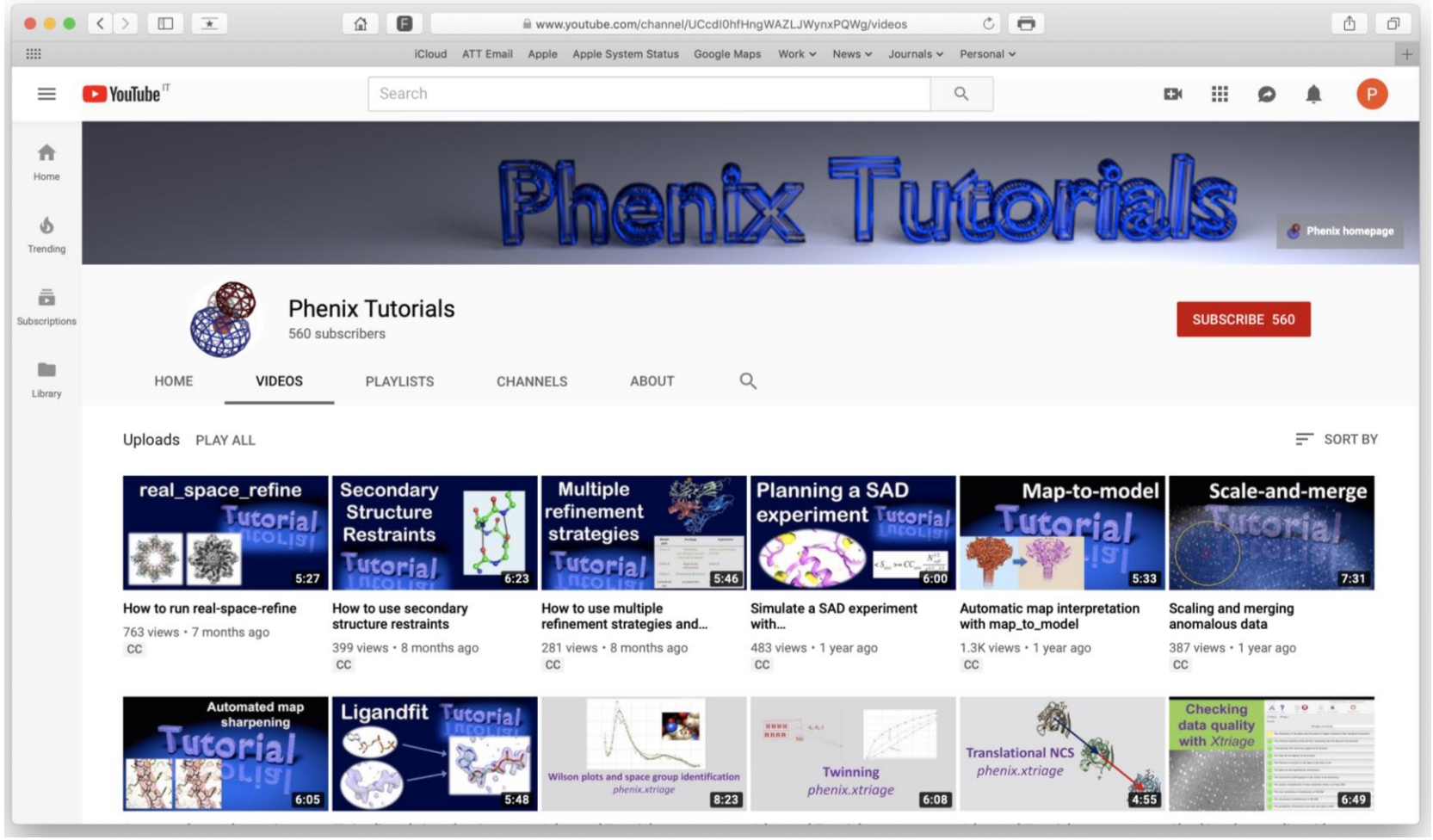


Run in a python script

```
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

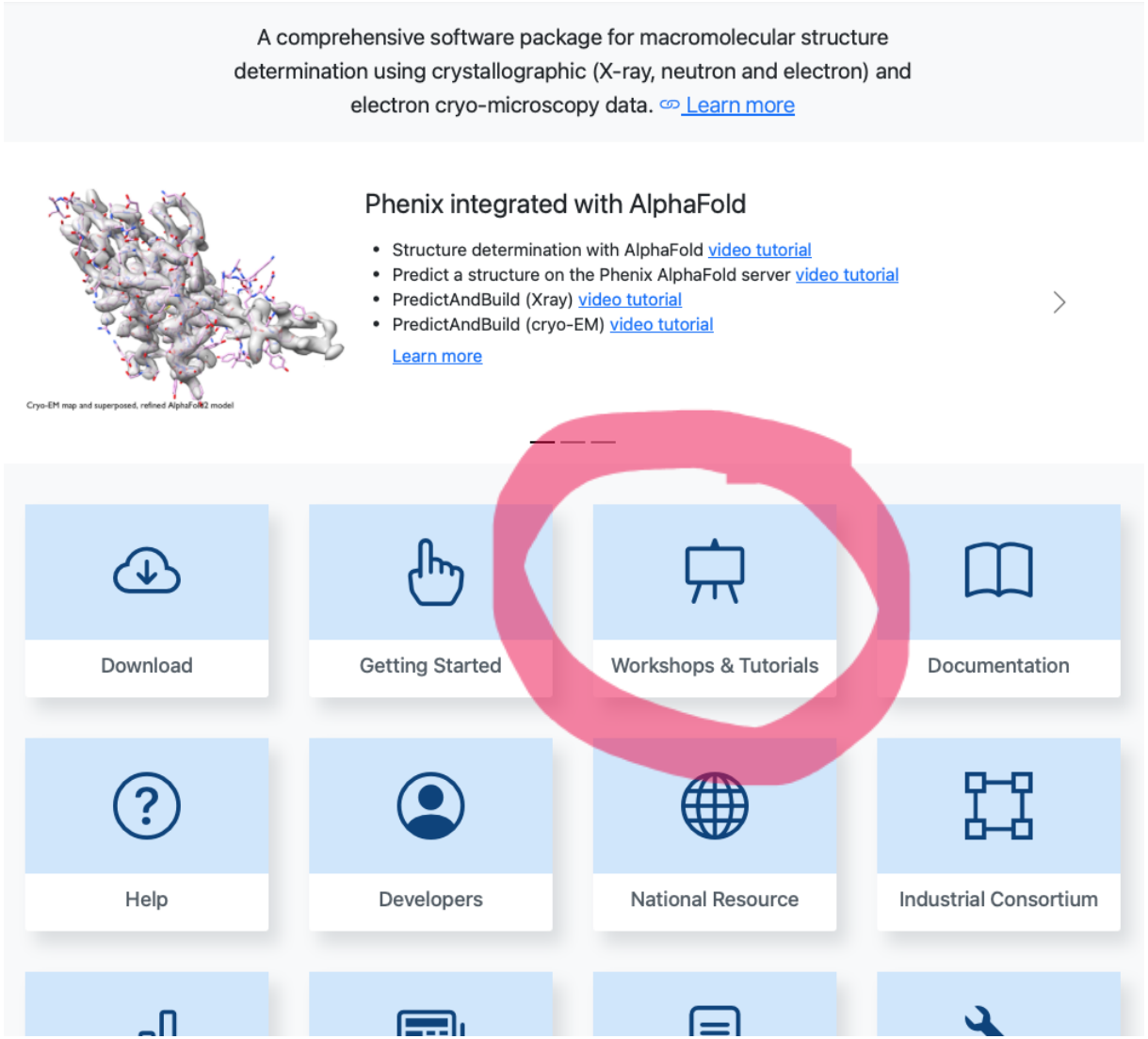
https://www.youtube.com/c/phenixtutorials



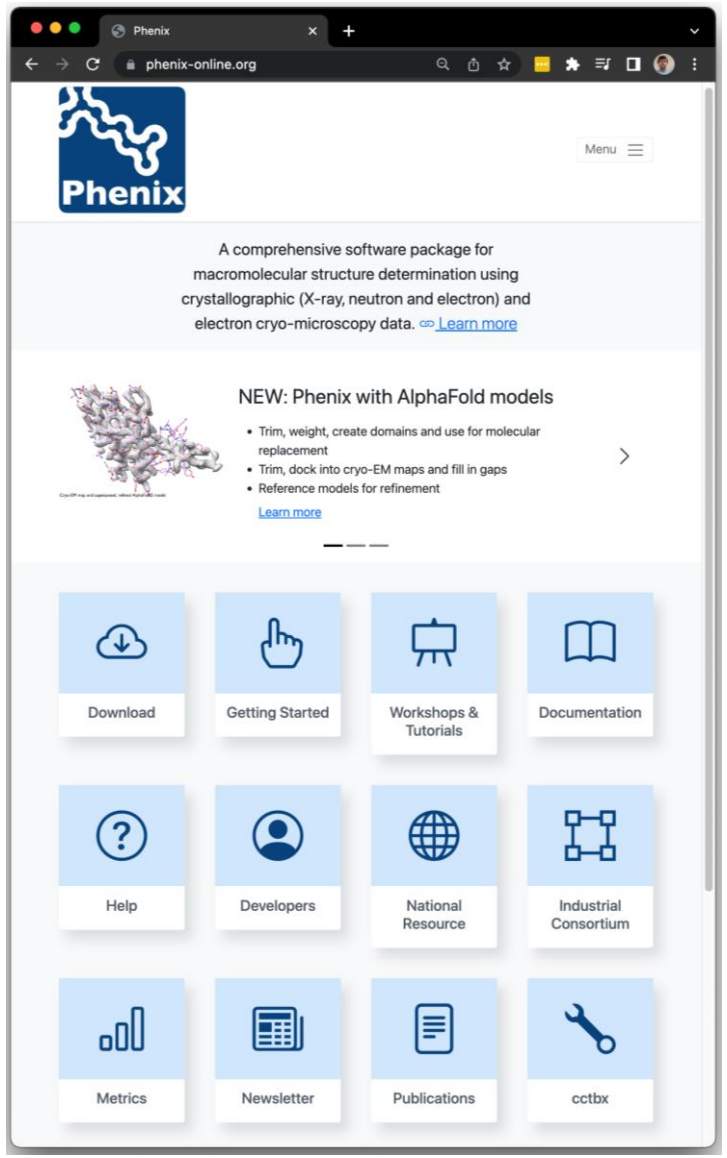
Dorothee Liebschner, Tom Terwilliger, Nigel Moriarty, Christopher Schlicksup, Vincent Chen

Presentation slides

https://phenix-online.org



Phenix resources



Phenix paper

Video tutorials (YouTube)

Documentation

Relevant papers

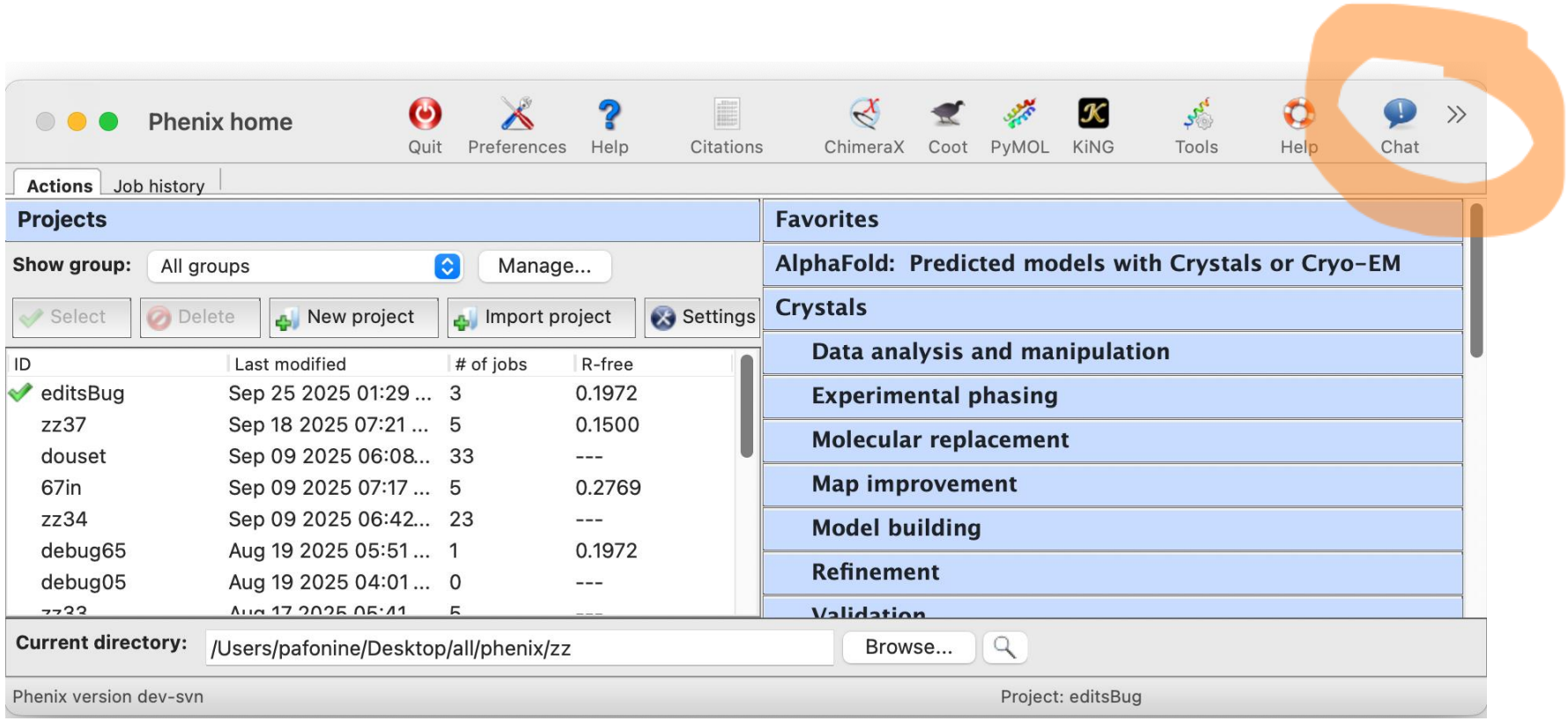
Bi-annual newsletters

PDFs with slides from workshops

NEW: AI tools in Phenix

Phenix chatbot

phenix-online.org/chatbot



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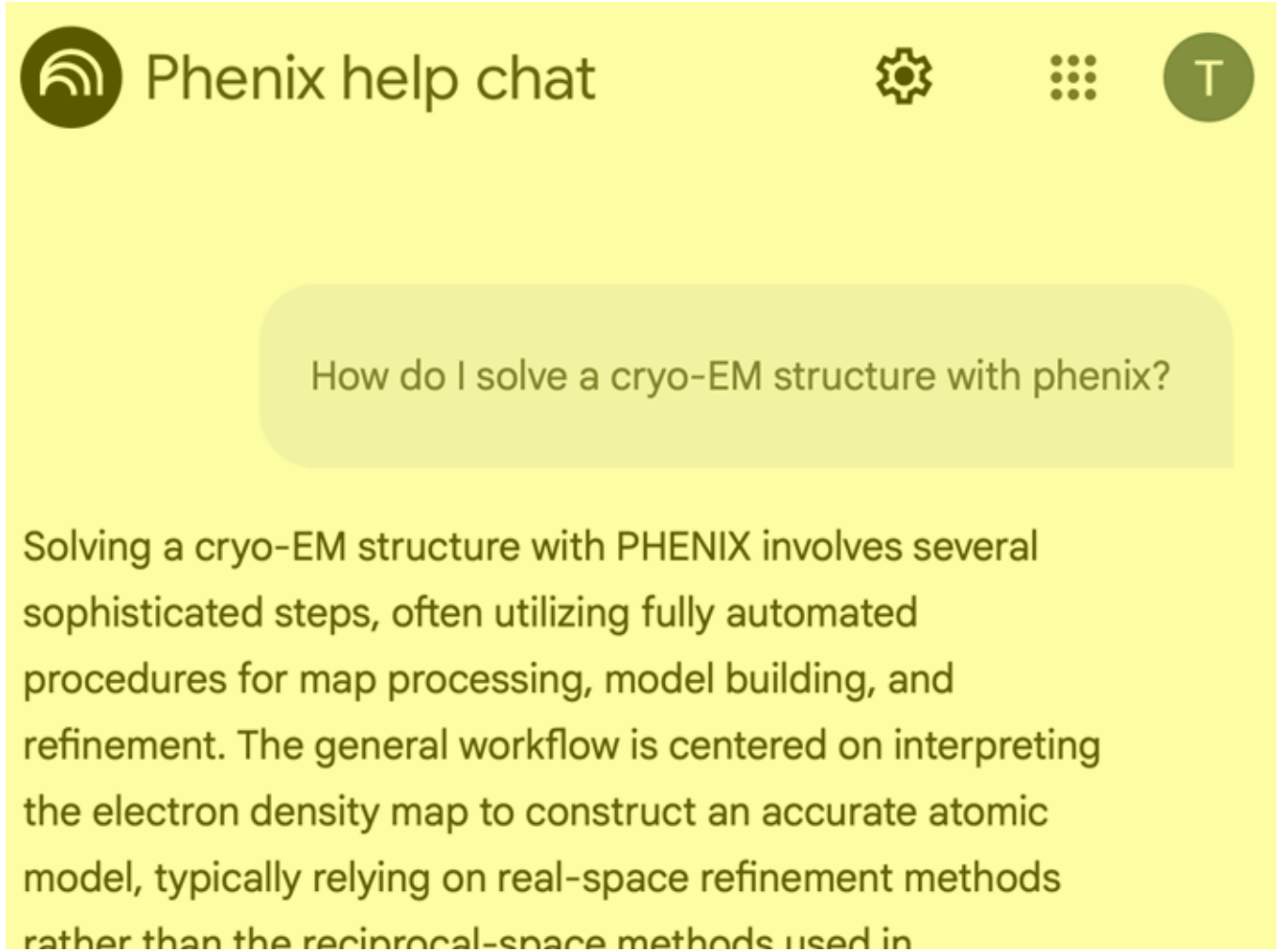
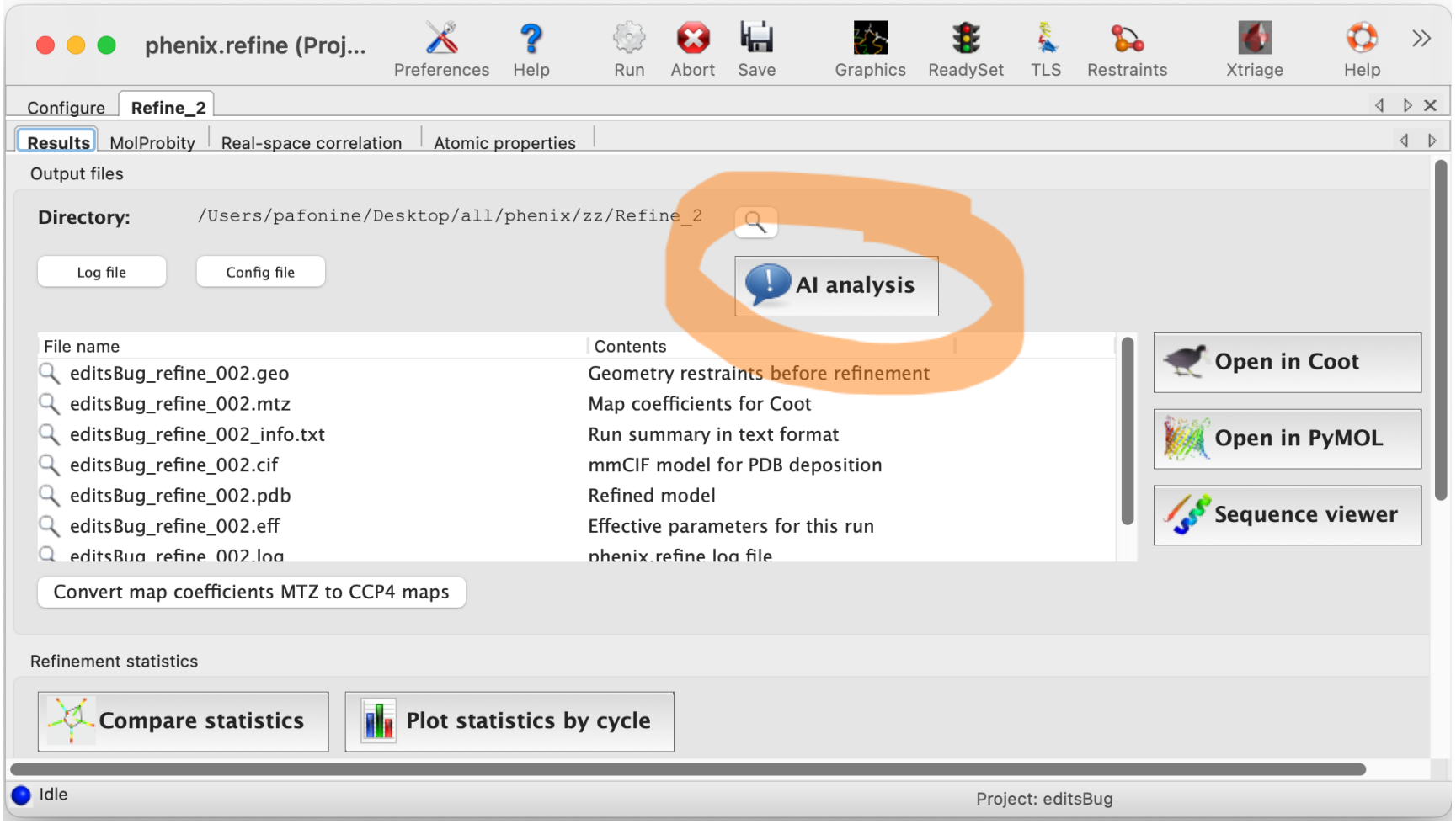


NEW: AI tools in Phenix

AI analysis of results



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)

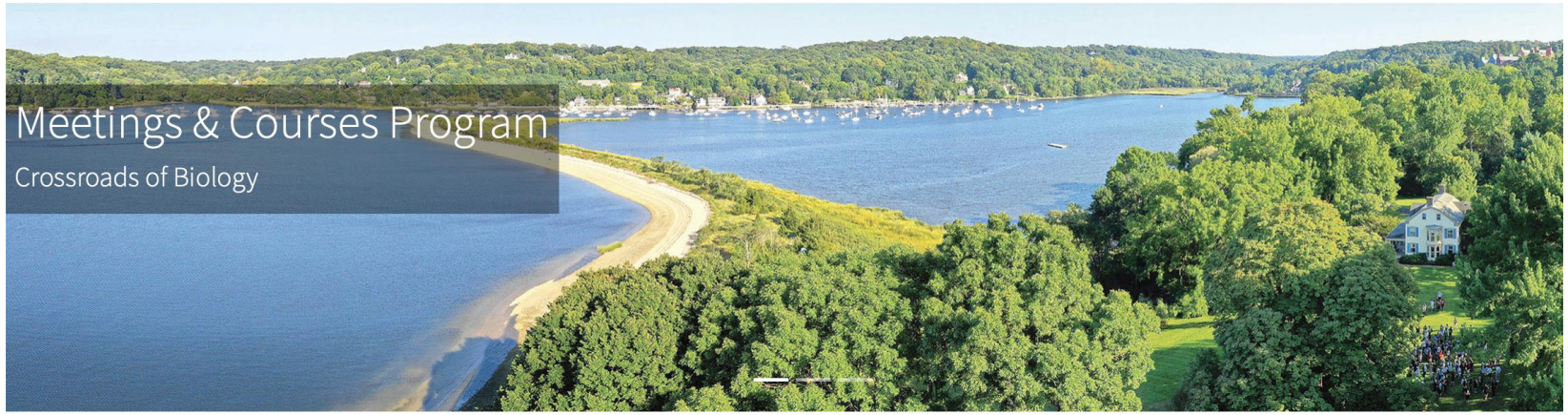
We can update the documentation to give the chatbot the information it needs to give a good answer

Crystallography courses in the US

CSHL course: Macromolecular Crystallography

CSH Cold Spring Harbor Laboratory

October 12-28, 2025



Home | Meetings | Courses

WELCOME | INFO | APPLICATION | TRAVEL | SPONSORS | PAYMENTS | POLICIES

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)

SLAC NATIONAL ACCELERATOR LABORATORY

U.S. DEPARTMENT OF ENERGY | Office of Science

RapiData 2025 at SSRL

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

May 5 - May 10, 2025

Home | Announcement | Application and Registration | Schedule | Participant Information | Transportation

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)

CCP4

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

Argonne NATIONAL LABORATORY

Home | 2025 Home | Program | Course Material | Application | Accommodation | Location | Participants | Contact us | Acknowledgements

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.

Acknowledgements

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Duke University
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University of Washington
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David Abrahams
Phenix Testers & Users

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