BERKELEY LAB

U.S. DEPARTMENT OF ENERGY

UNIVERSITY OF CALIFORNIA

Phenix workshop at UT Southwestern Medical Center,
May 20, 2026

Phenix Introduction

Dorothee Liebschner

Lawrence Berkeley Laboratory

UTHealth The University of Texas Health Science Center at Houston

Los Alamos NATIONAL LABORATORY EST. 1943

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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

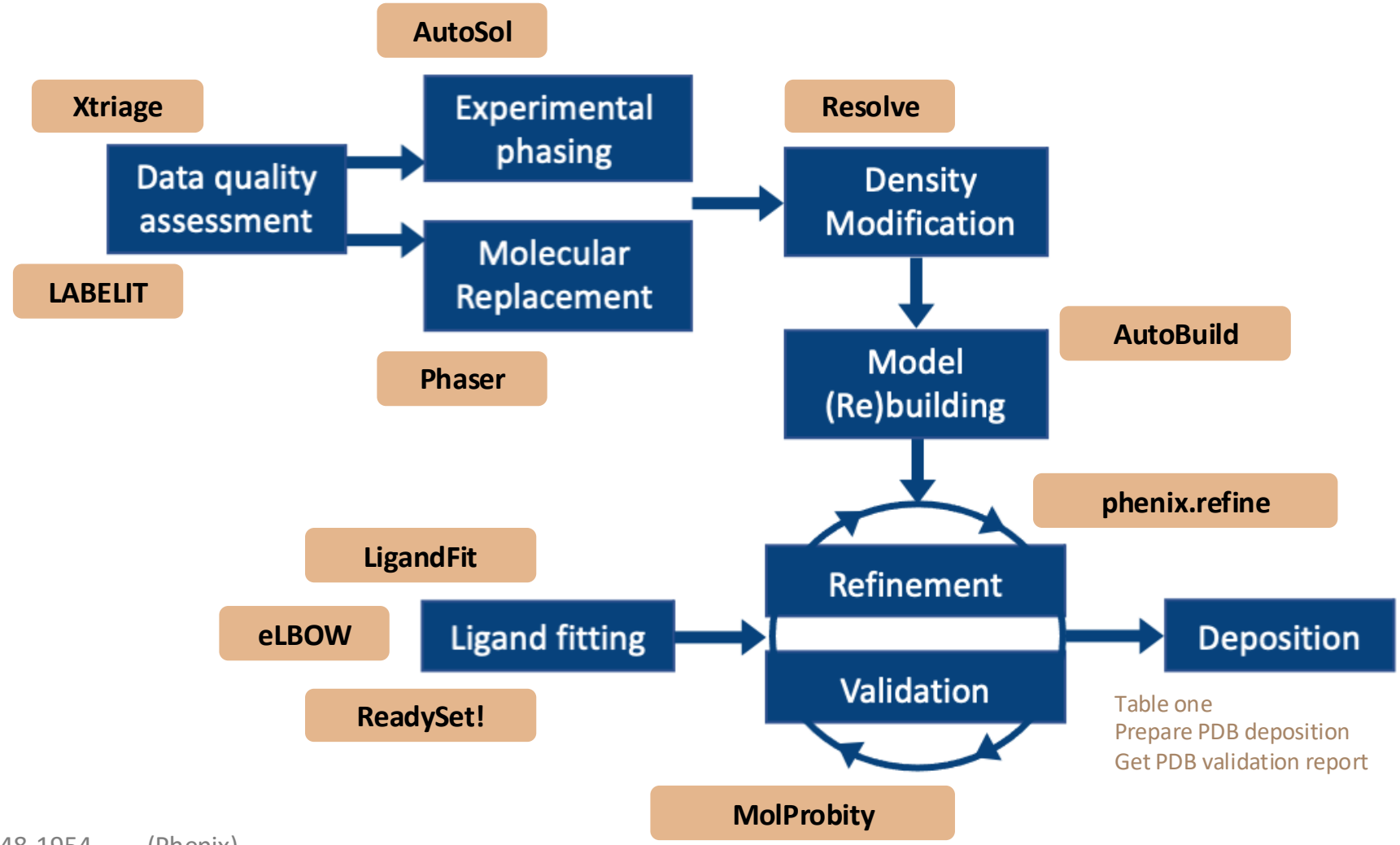
Duke University

Jane Richardson, Vincent Chen

An NIH/NIGMS funded Program Project

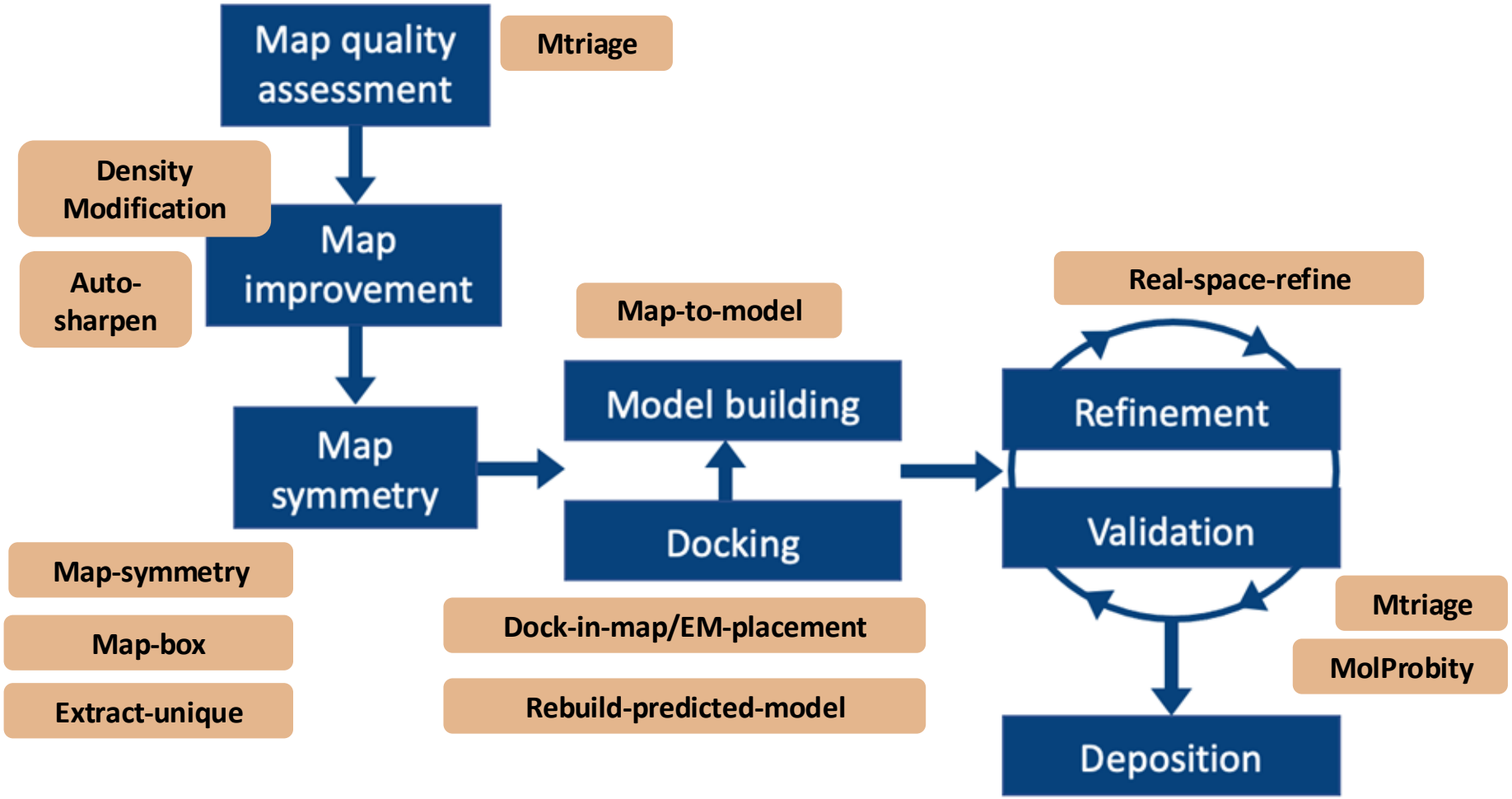
Liebschner D, *et al.*, Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in *Phenix*. Acta Cryst. 2019 **D75**:861–877

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)

Tools for cryo-EM



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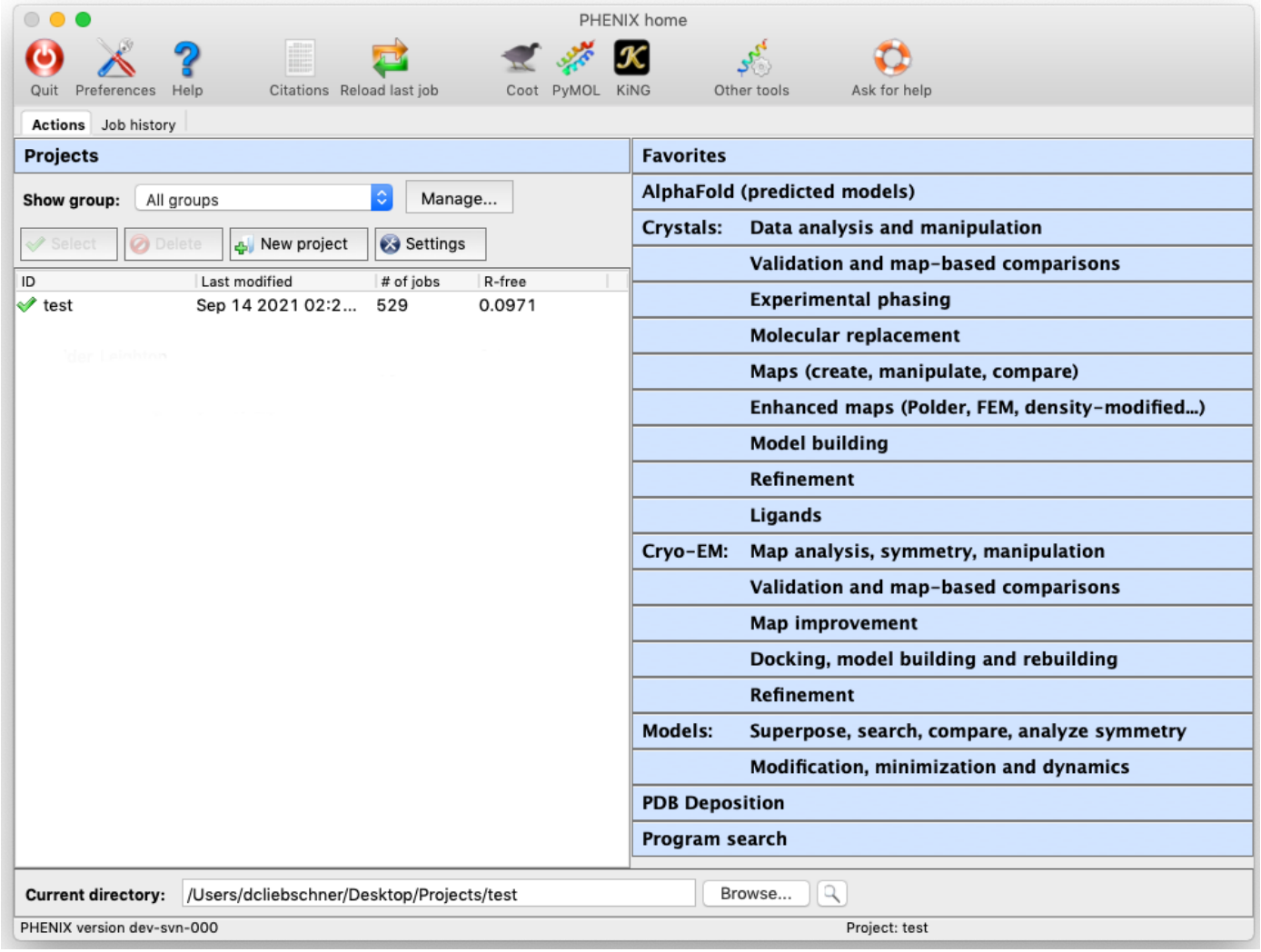
Phenix Graphical User Interface (GUI)

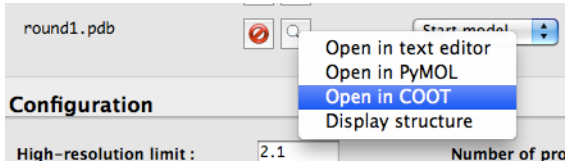
Central GUI for job control and to launch new jobs



Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps

- Any PDB file listed in GUI can also be opened

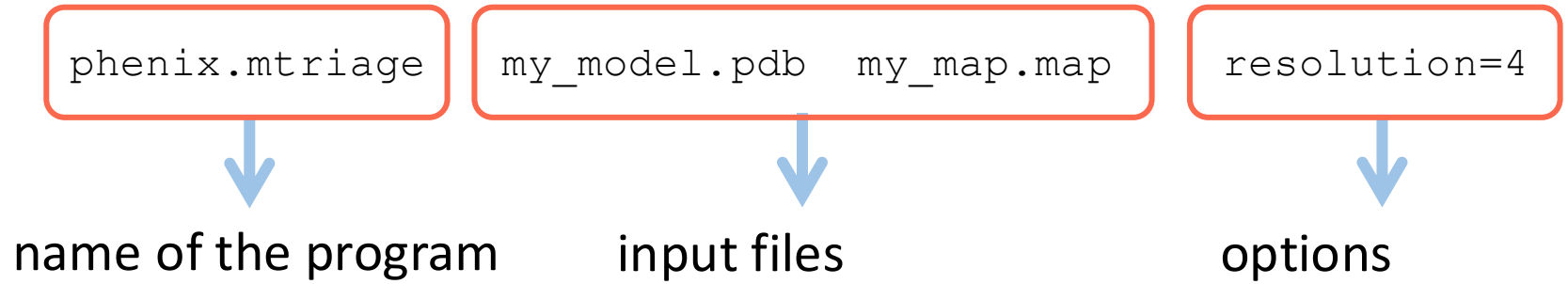


- Specific paths to executables usually required on Linux

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

Command Line

Run on the terminal

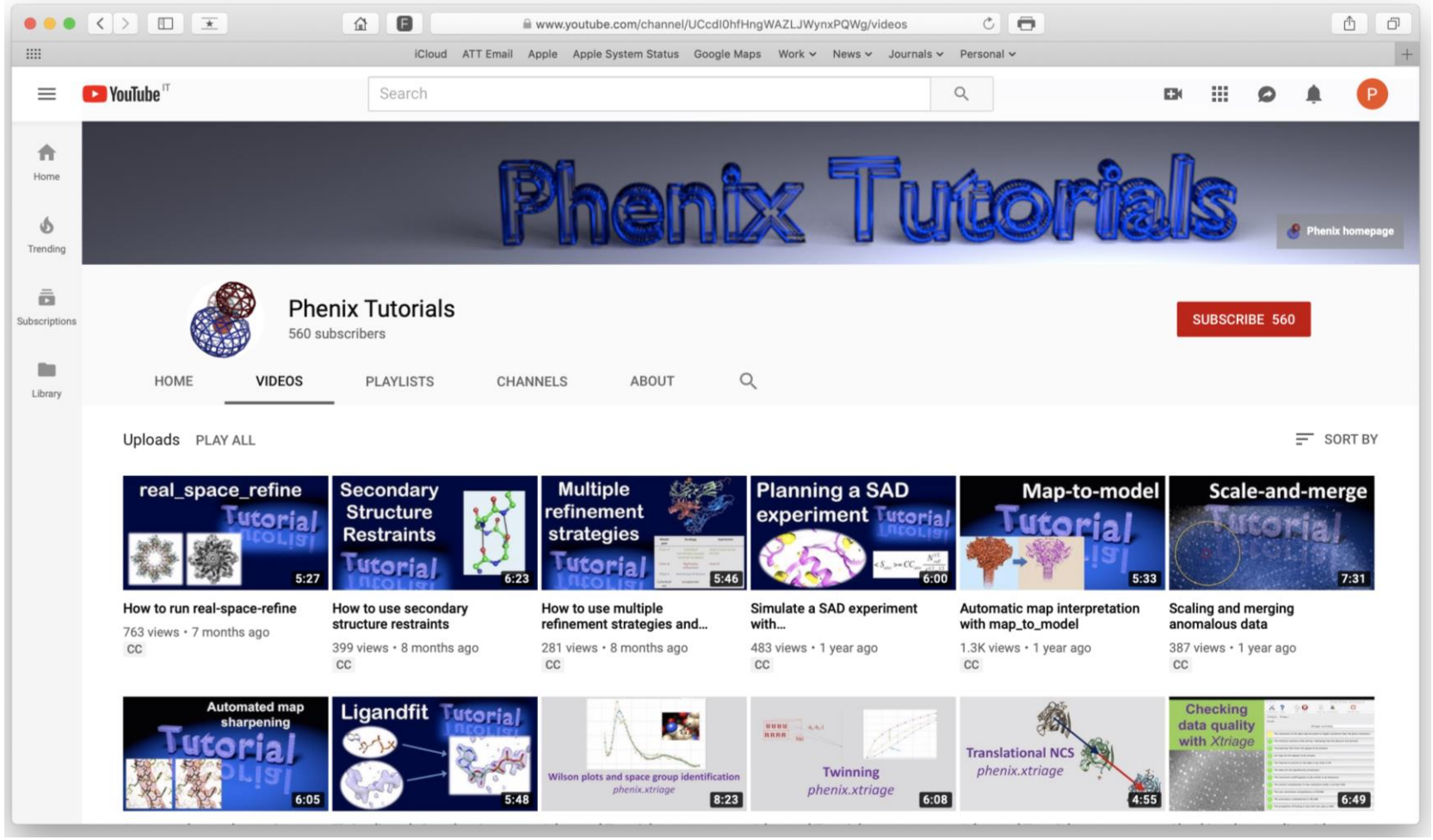


Run in a python script

```
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

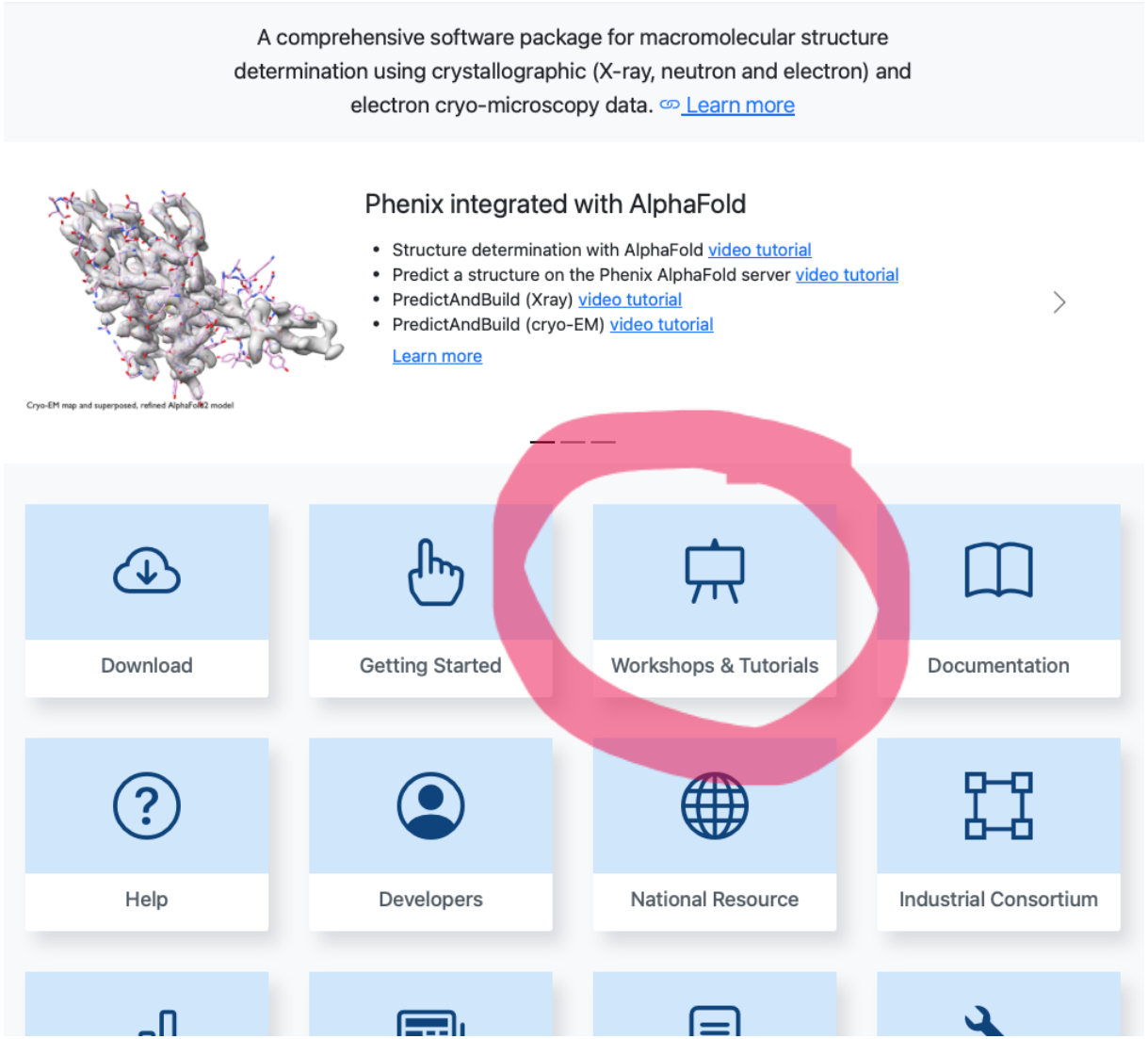
https://www.youtube.com/c/phenixtutorials



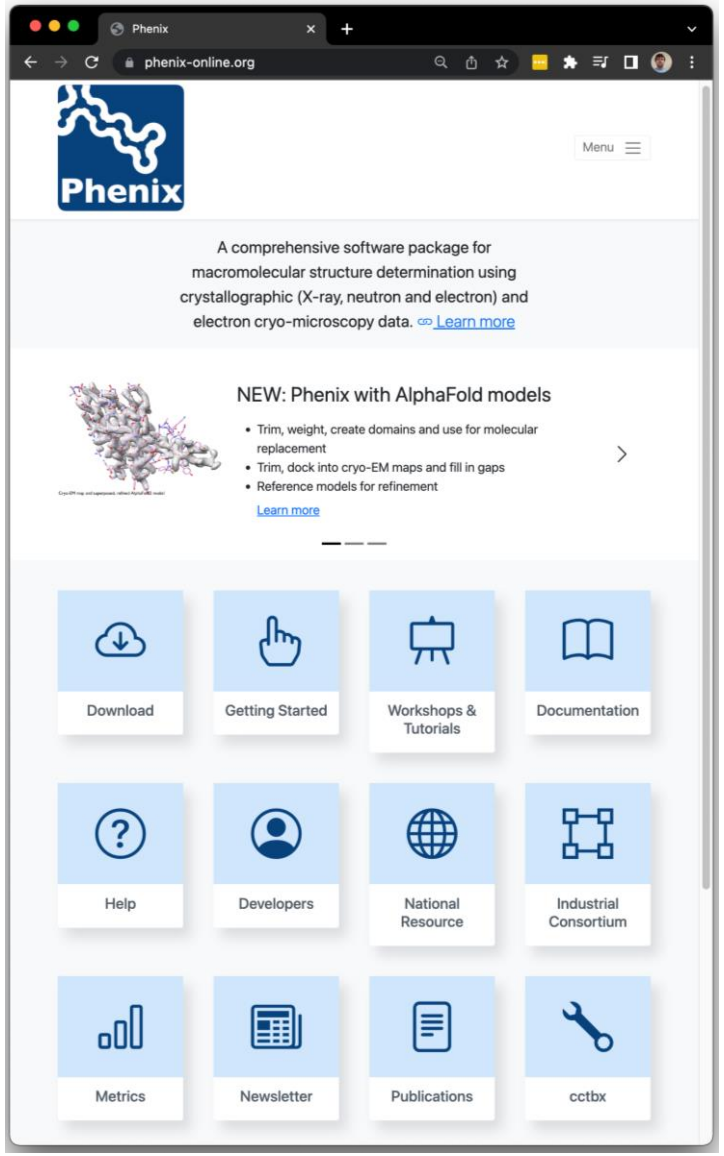
Dorothee Liebschner, Tom Terwilliger, Nigel Moriarty, Christopher Schlicksup, Vincent Chen

Presentation slides

https://phenix-online.org



Phenix resources



Phenix paper

Video tutorials (YouTube)

Documentation

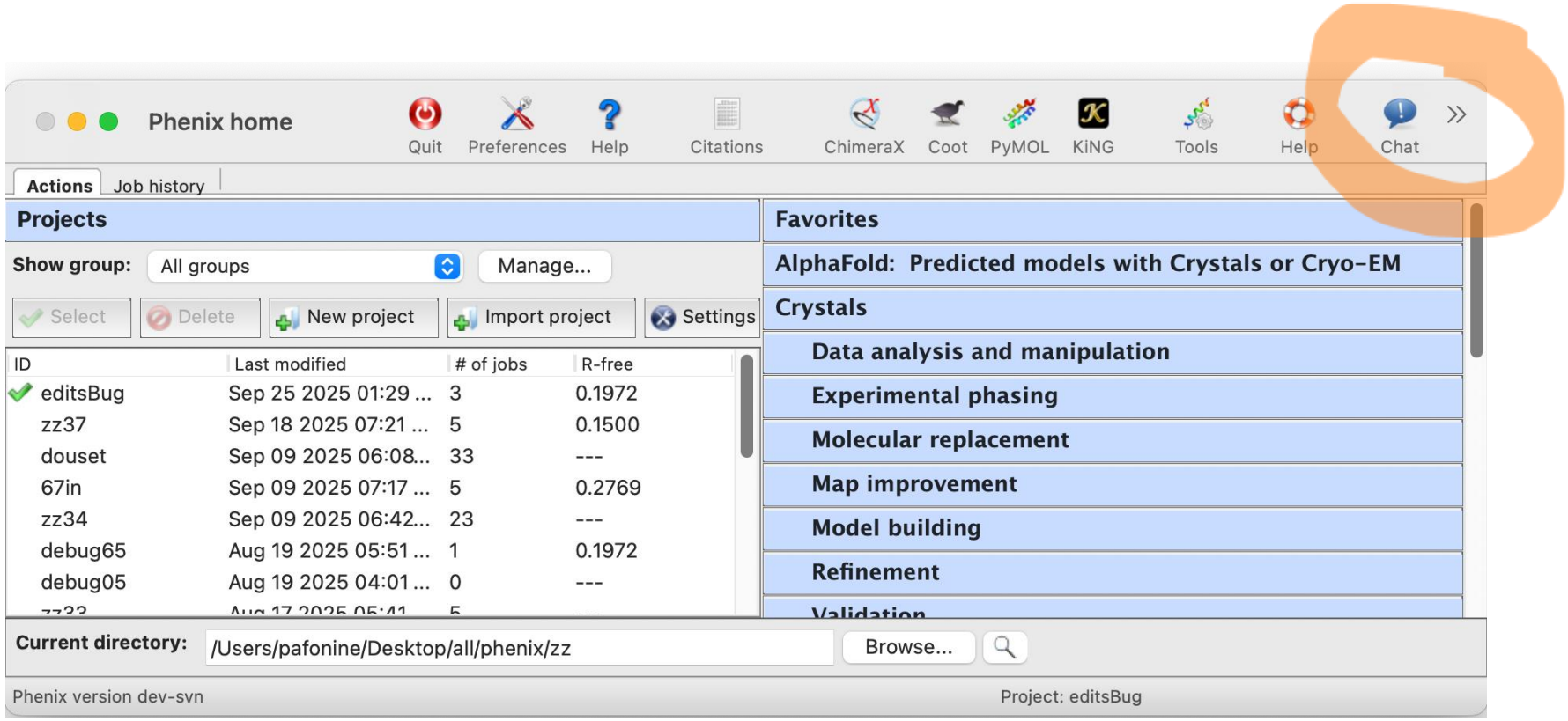
Relevant papers

Bi-annual newsletters

PDFs with slides from workshops

NEW: AI tools in Phenix - Chatbot

phenix-online.org/chatbot



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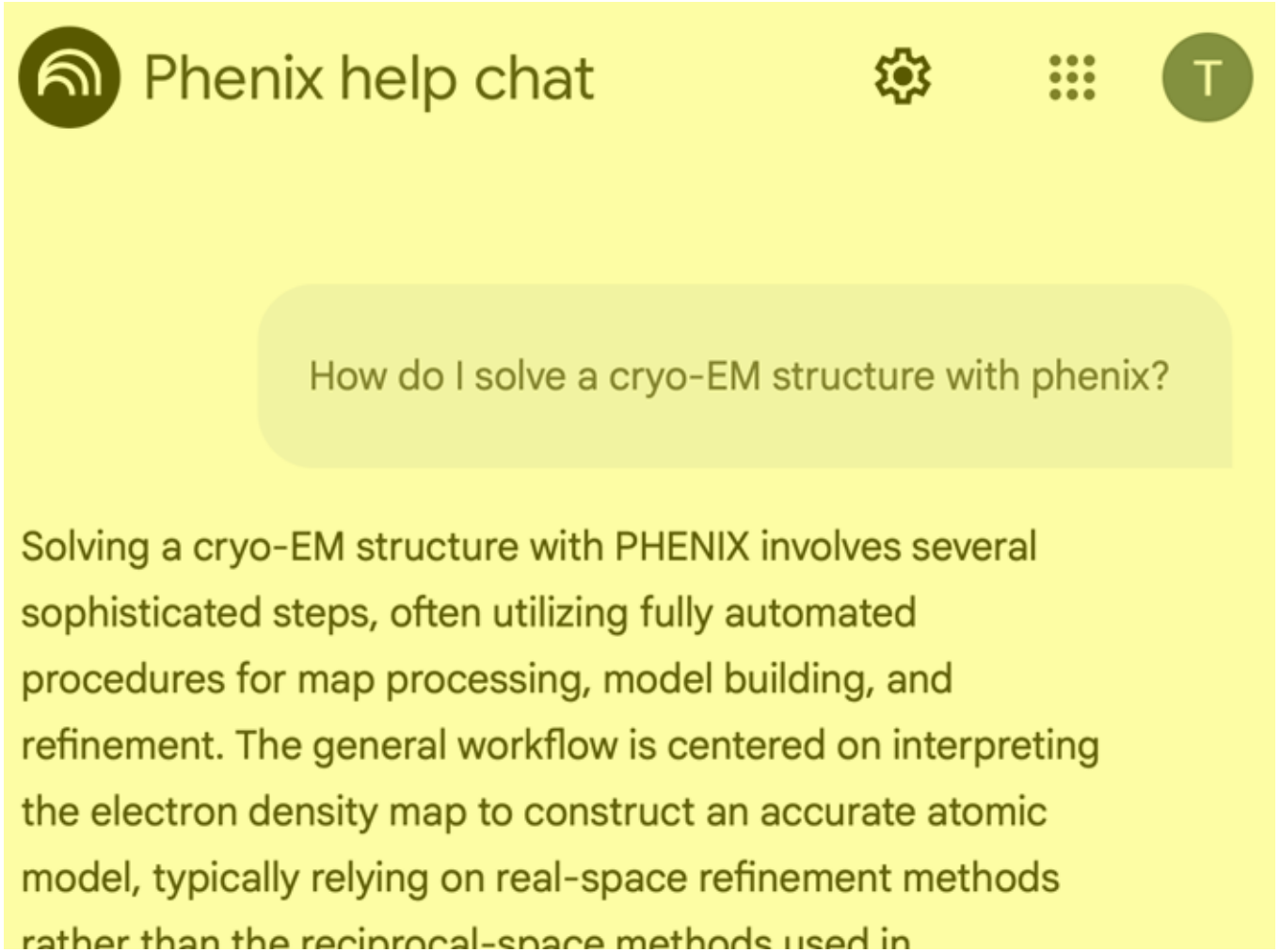
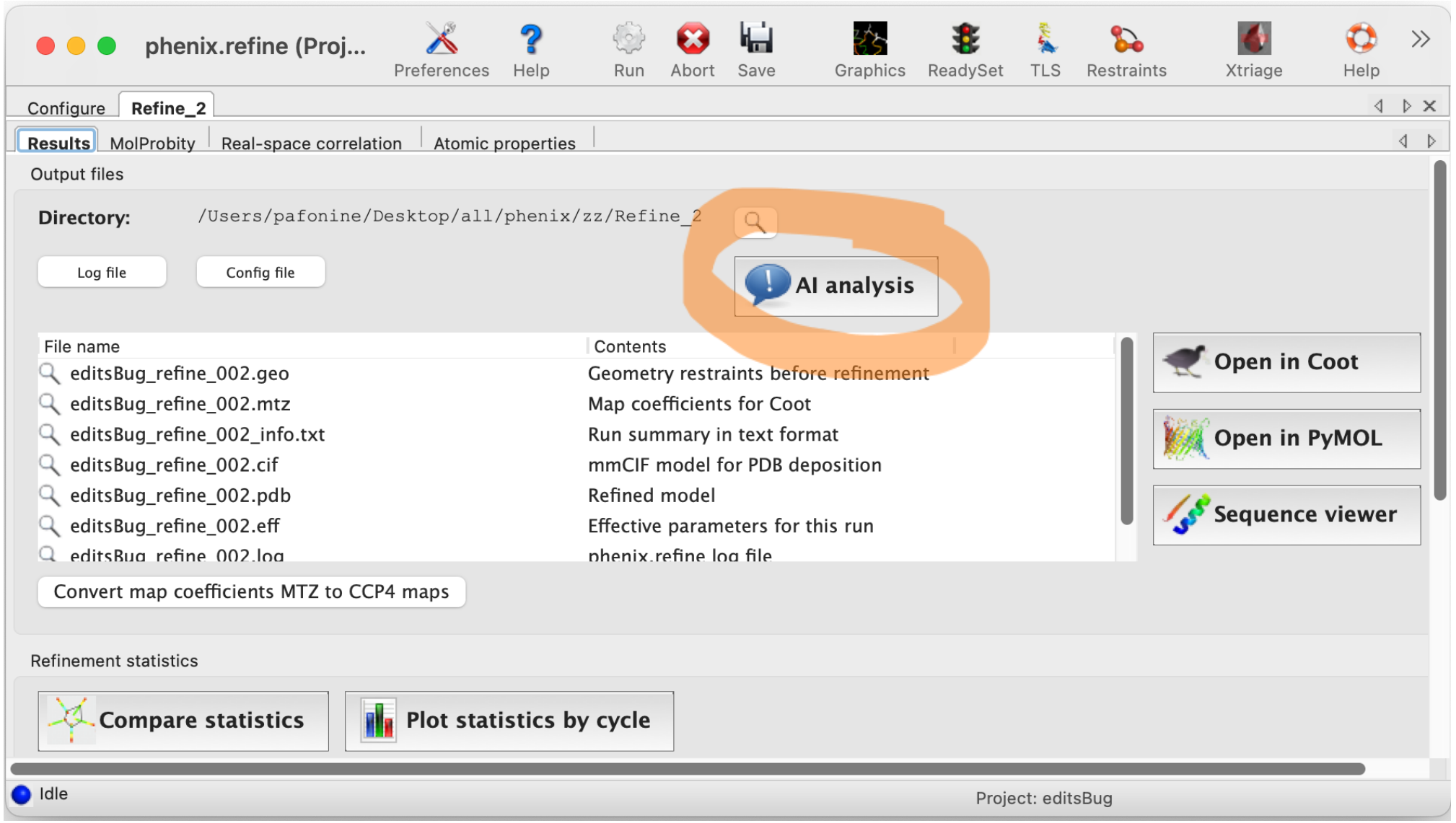


NEW: AI tools in Phenix – AI analysis



NEW: AI tools in Phenix – AI analysis

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

Crystallography courses in the US

CSHL course: Macromolecular Crystallography

Cold Spring Harbor Laboratory

October 11-27, 2026

Home | Meetings | Courses

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

Macromolecular Crystallography

October 11 - 27, 2026

Key Dates:
Application Deadline: July 17, 2026
Arrival: October 11th by 6pm EST
Departure: October 27th

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

Rapidata (May)

SLAC NATIONAL ACCELERATOR LABORATORY

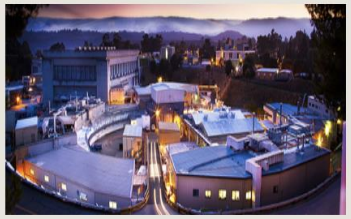
U.S. DEPARTMENT OF ENERGY | Office of Science

RapiData 2026 at SSRL

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

May 4-9 2026

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



Stanford Synchrotron Radiation Lightsource

Event Information

Course dates: May 4-9, 2026

Applications opens: November 17, 2025

Application deadline: We extended the dealine to February 14, 2026! Applications received after the deadline will be placed in a stand-by list.

Event Coordinators

CCP4 school Argonne (June)

CCP4

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

Argonne NATIONAL LABORATORY

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

2026 School

The next CCP4/APS School will be held at the APS on our now traditional late June/early July dates, along with GMCA and NE-CAT. The proposed dates are July 7th to 14th. For more details and application information please visit the 2026 school website.

School Details

Dates: July 7 - July 14, 2025

The first three days will be dedicated to data collection and processing. The rest of the workshop will focus on structure solution, refinement and validation, majoring on crytallography but including electron microscopy.

Acknowledgements

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David Abrahams
Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory