

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



Phenix Introduction

Dorothee Liebschner

Lawrence Berkeley Laboratory

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 **E**Nvironment for **I**ntegrated **X**tallography



The Phenix Project

Lawrence Berkeley Laboratory

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



University of Cambridge

Randy Read, Airlie McCoy



Los Alamos National Laboratory New Mexico Consortium

Tom Terwilliger, Li-Wei Hung



UTHealth

Matt Baker



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



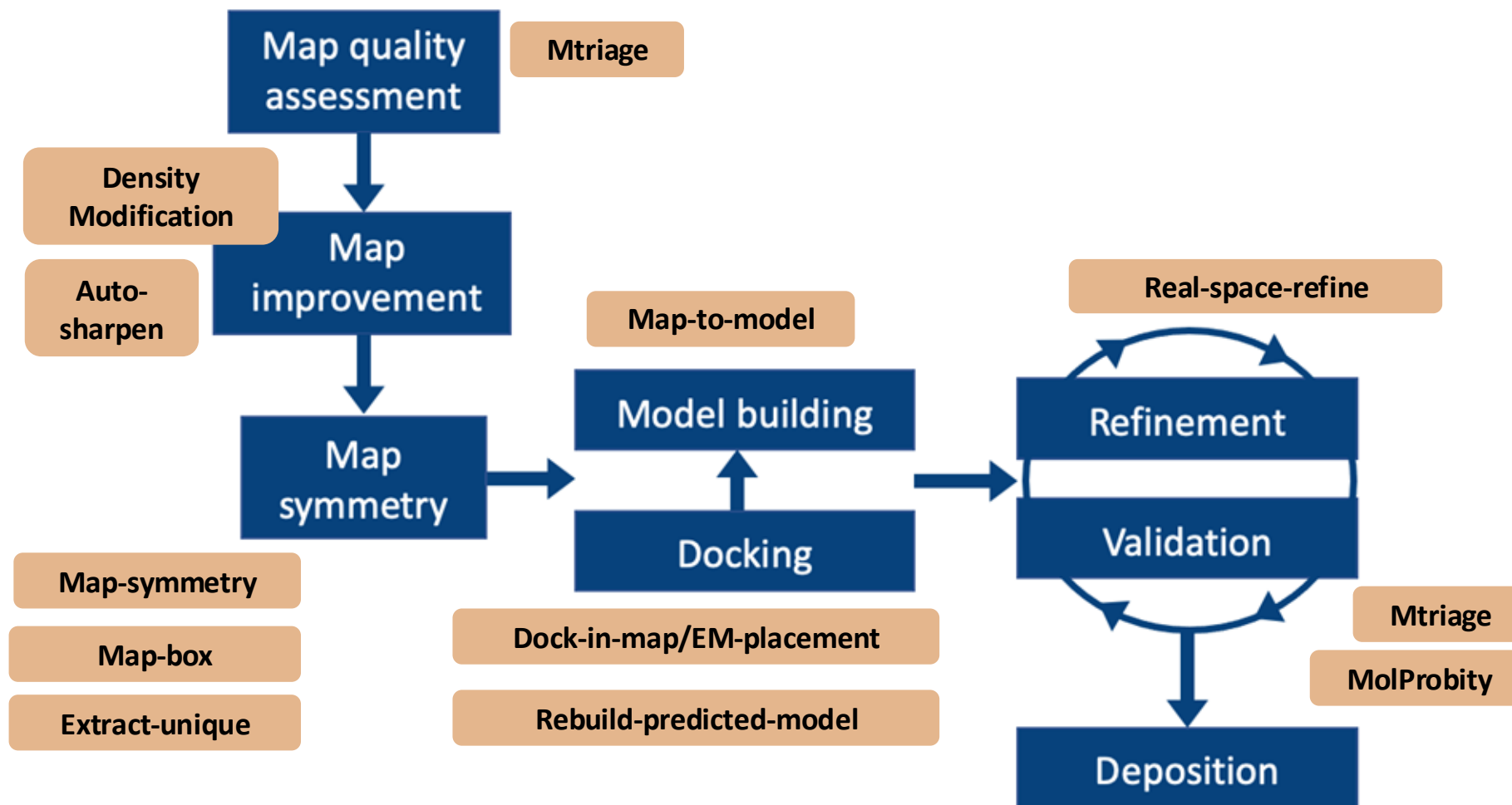
(Phenix)

(cctbx)

(Phenix)

(Phenix)

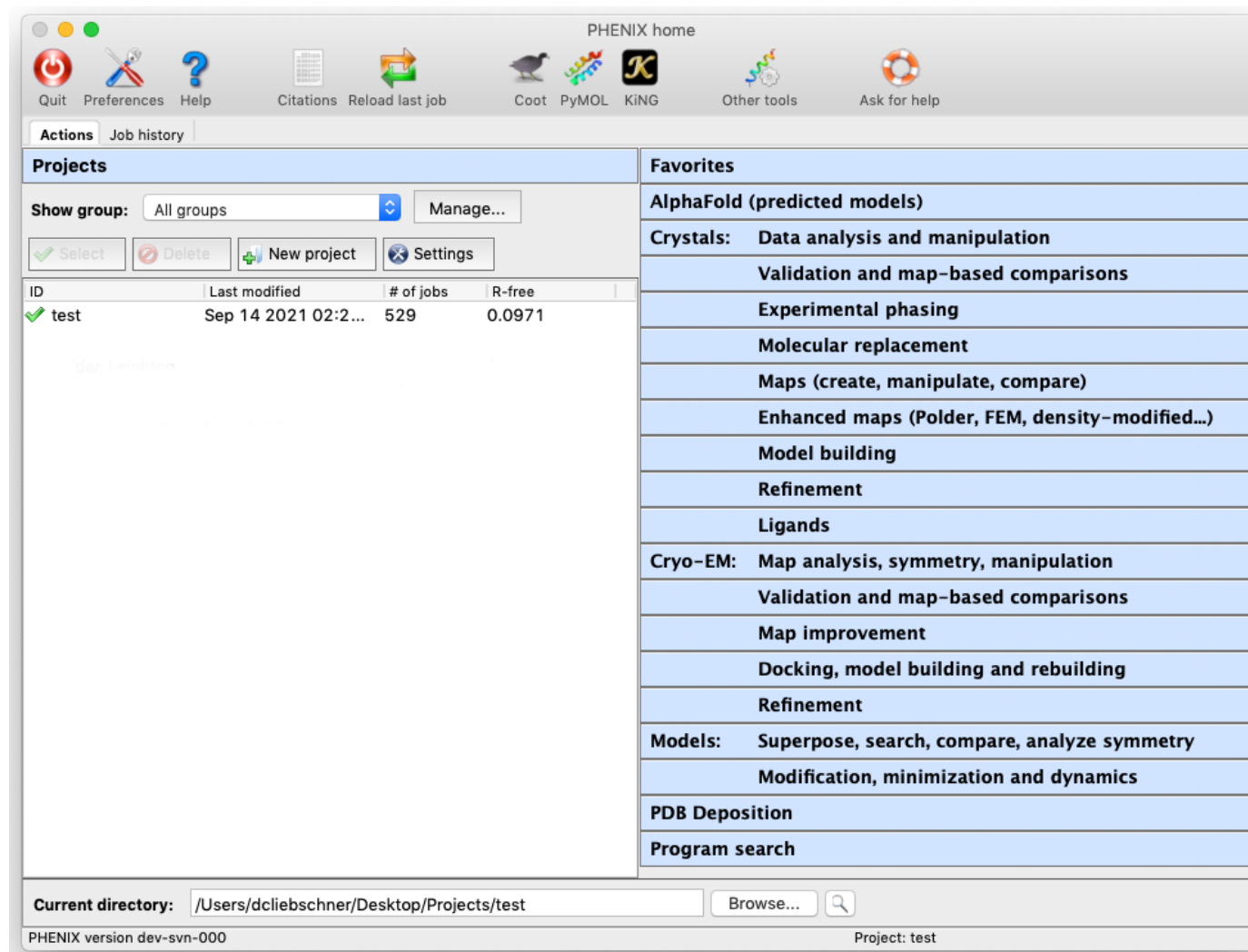
Tools for cryo-EM



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

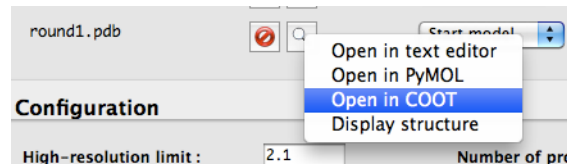


Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps



- Any PDB file listed in GUI can also be opened

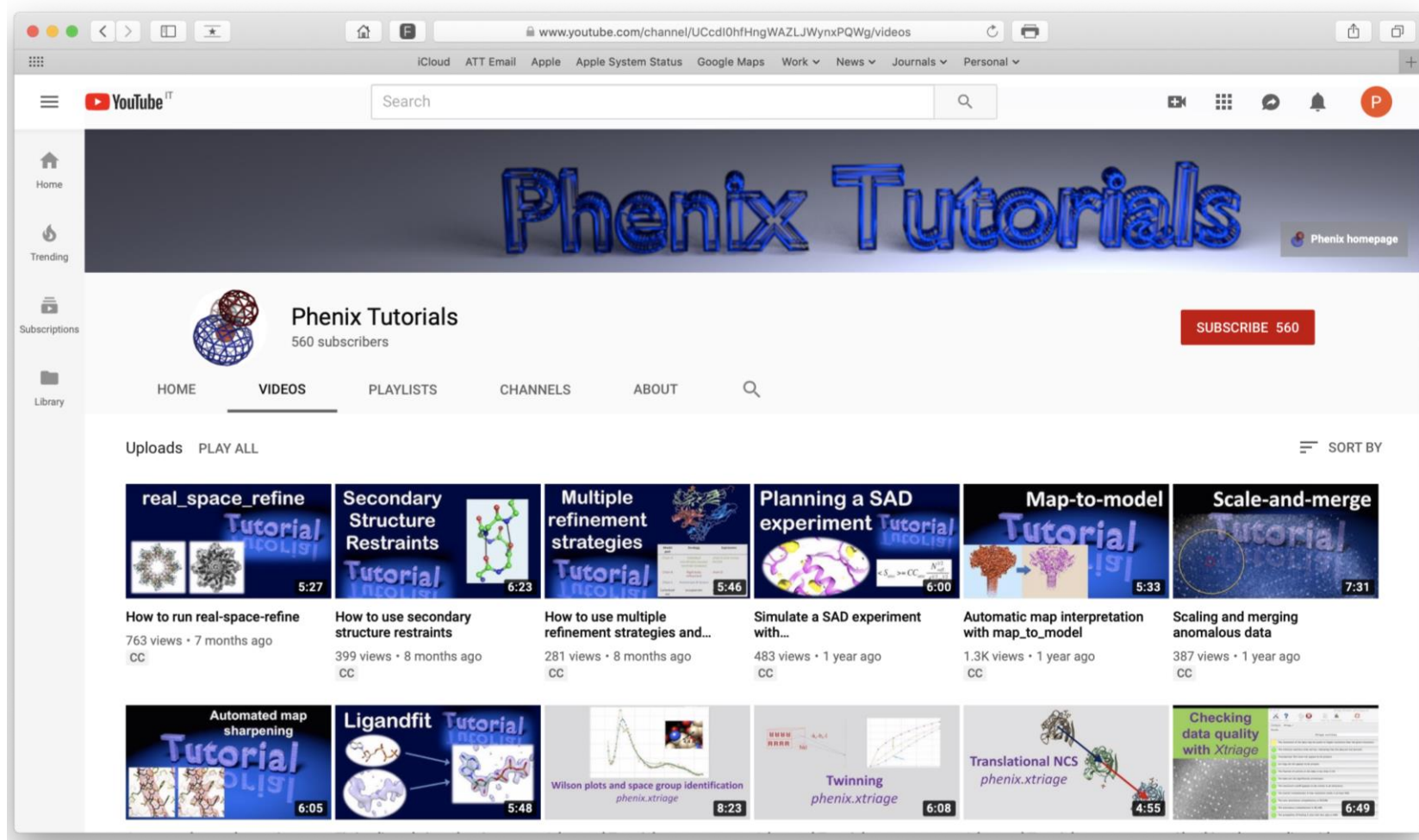


- Specific paths to executables usually required on Linux

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

Video Tutorials

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

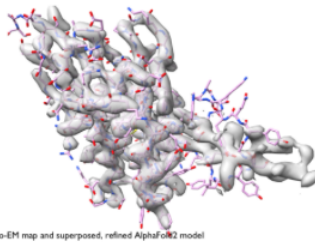


Dorothee Liebschner, Tom Terwilliger, Nigel Moriarty, Christopher Schlicksup, Vincent Chen

Presentation slides

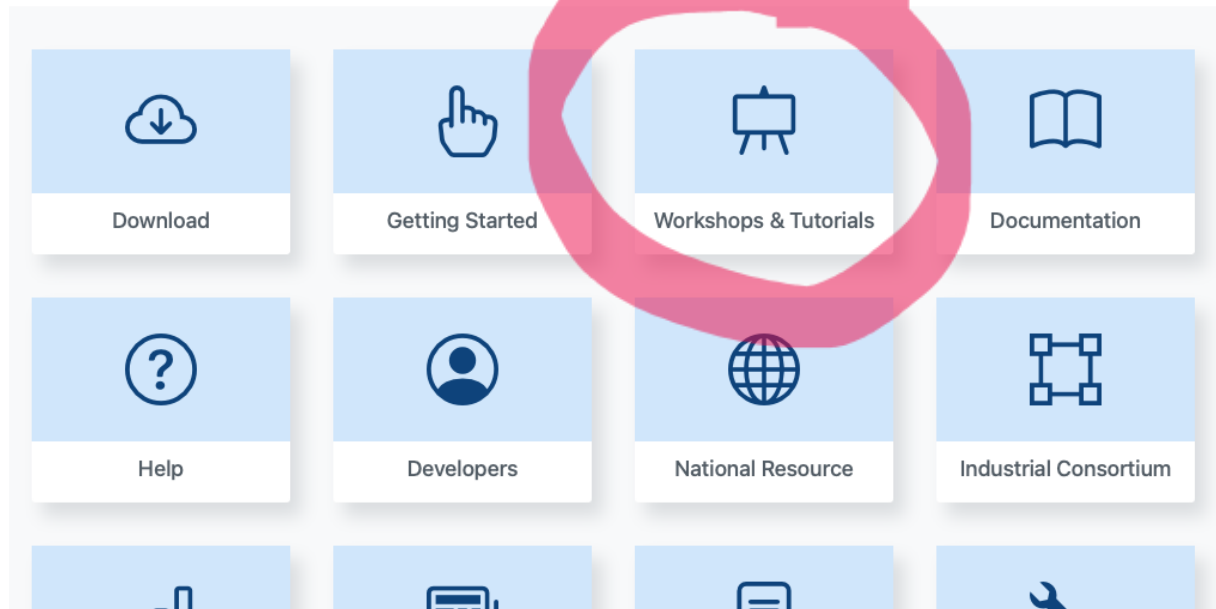
<https://phenix-online.org>

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

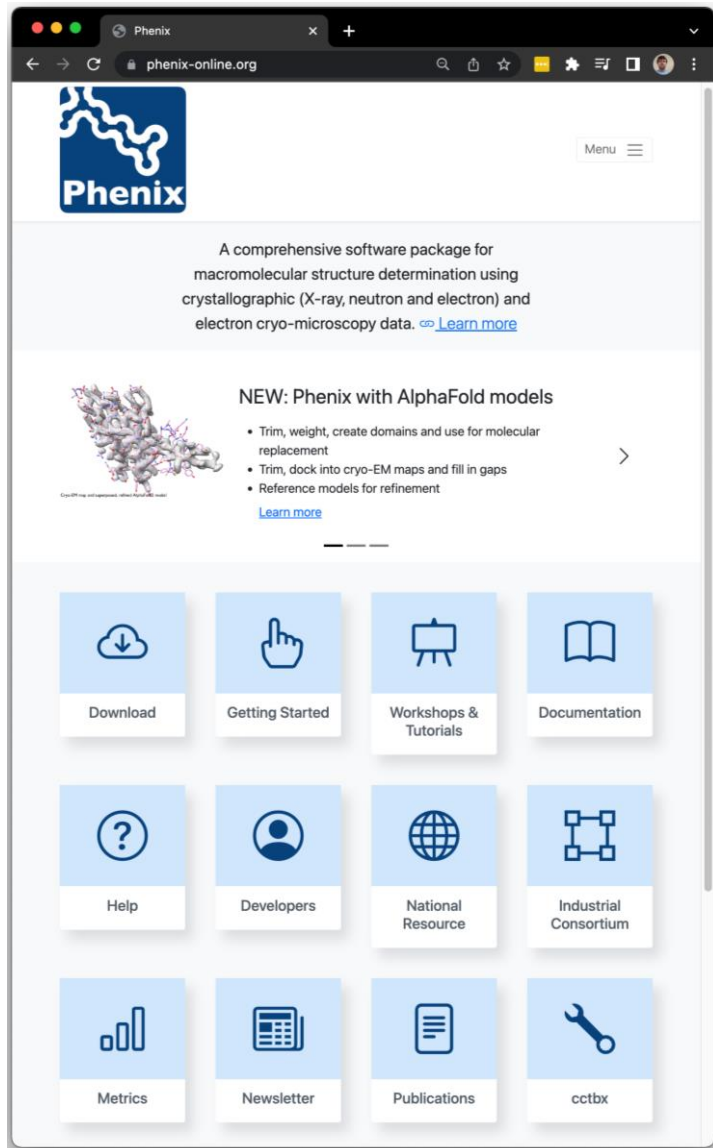


Phenix integrated with AlphaFold

- 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



Phenix paper

Video tutorials (YouTube)

Documentation

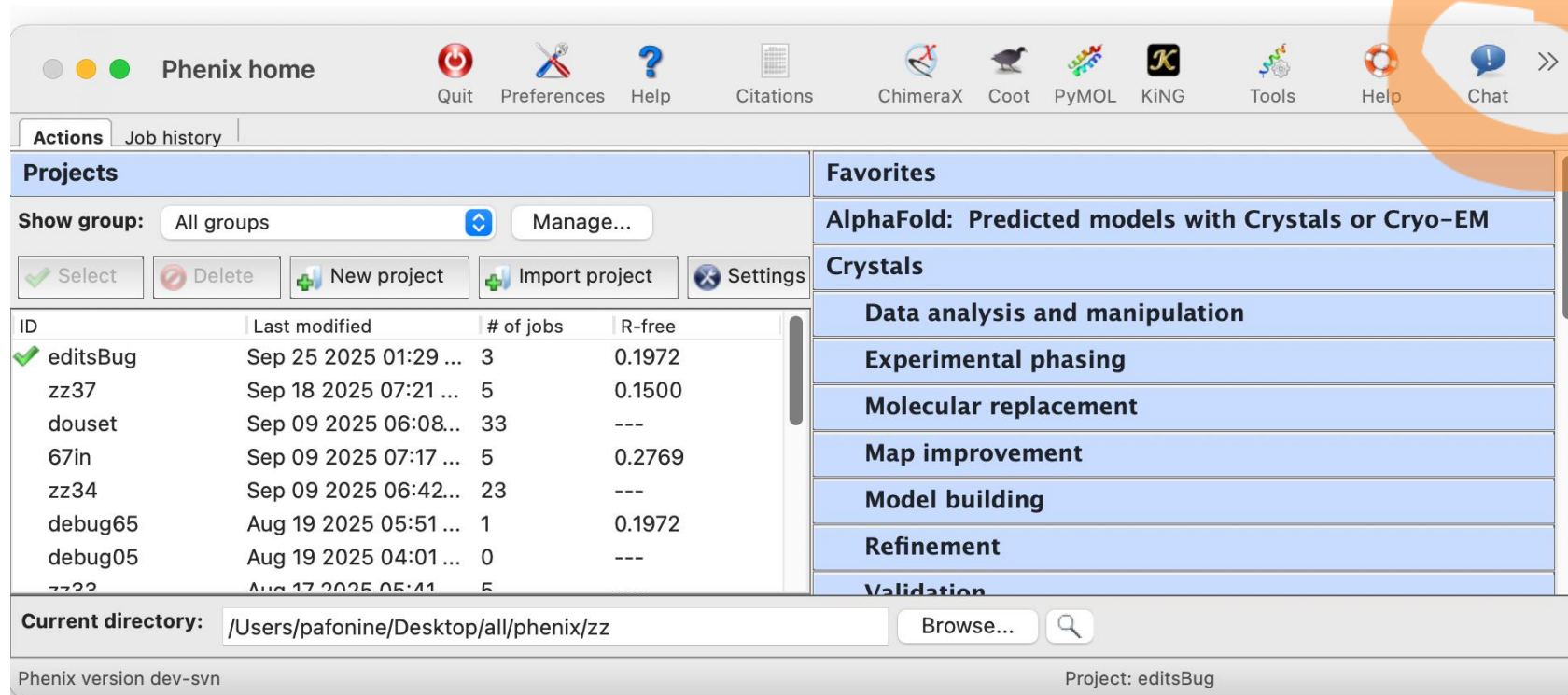
Relevant papers

Bi-annual newsletters

PDFs with slides from workshops

NEW: AI tools in Phenix - Chatbot

phenix-online.org/chatbot



The screenshot shows the Phenix web interface. The top navigation bar includes links for Quit, Preferences, Help, Citations, ChimeraX, Coot, PyMOL, KiNG, Tools, Help, and Chat. The Chat button is highlighted with an orange circle. Below the navigation bar, there are tabs for Actions and Job history. The main content area is divided into two panels: Projects and Favorites. The Projects panel shows a table of projects with columns for ID, Last modified, # of jobs, and R-free. The Favorites panel shows a list of favorite projects, including AlphaFold: Predicted models with Crystals or Cryo-EM, Crystals, Data analysis and manipulation, Experimental phasing, Molecular replacement, Map improvement, Model building, Refinement, and Validation. The current directory is shown as /Users/pafonine/Desktop/all/phenix/zz.

Phenix home

Quit Preferences Help Citations ChimeraX Coot PyMOL KiNG Tools Help Chat

Actions Job history

Projects

Show group: All groups Manage...

Select Delete New project Import project Settings

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	---
zz33	Aug 17 2025 05:41 ...	5	---

Favorites

AlphaFold: Predicted models with Crystals or Cryo-EM

Crystals

Data analysis and manipulation

Experimental phasing

Molecular replacement

Map improvement

Model building

Refinement

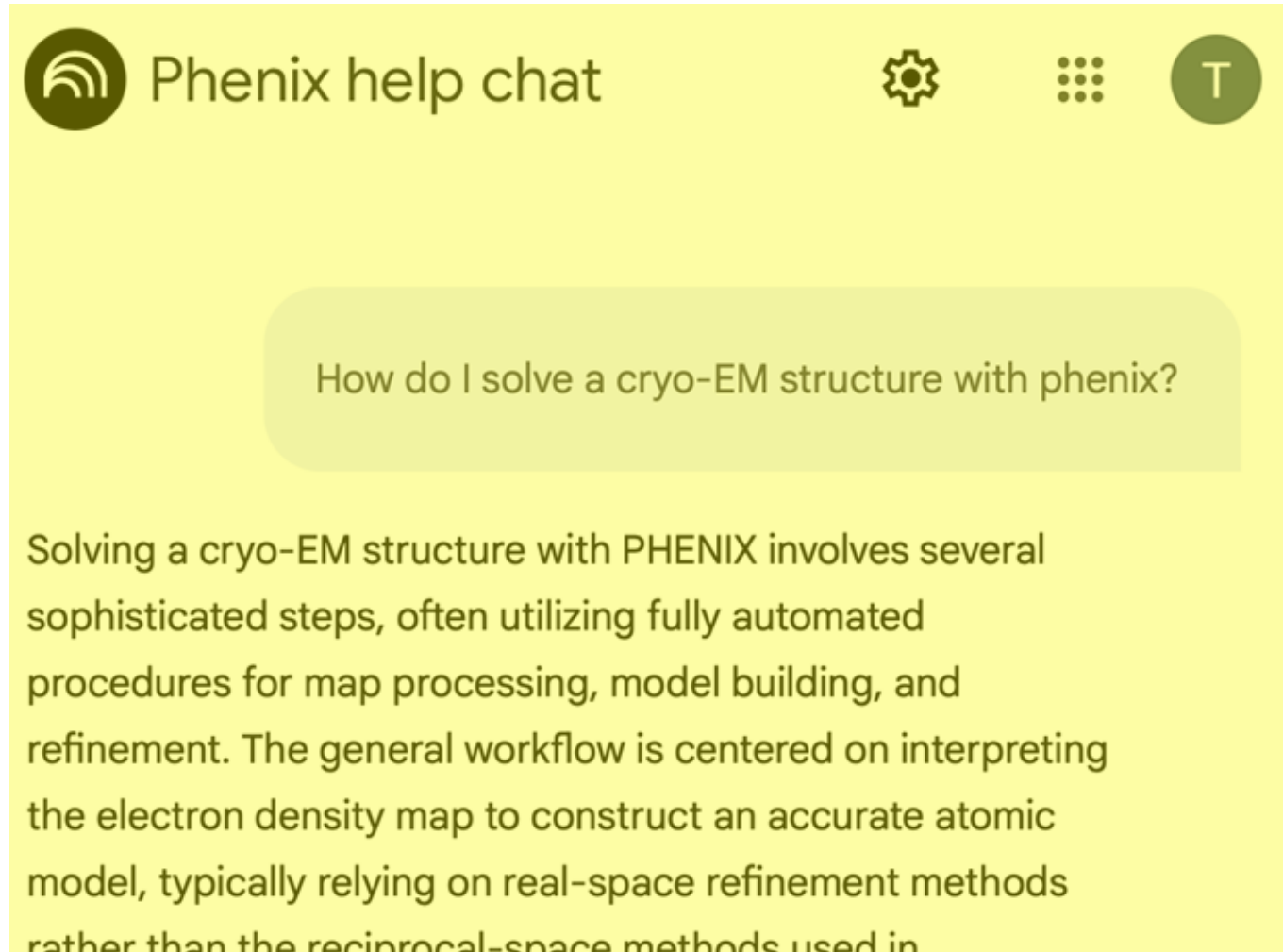
Validation

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

Phenix version dev-svn Project: editsBug

NEW: AI tools in Phenix - Chatbot

phenix-online.org/chatbot



NEW: AI tools in Phenix – AI analysis

The screenshot displays the Phenix software interface, specifically the 'Results' tab. The window title is 'phenix.refine (Proj...'. The menu bar includes 'Preferences', 'Help', 'Run', 'Abort', 'Save', 'Graphics', 'ReadySet', 'TLS', 'Restraints', 'Xtriage', and 'Help'. The 'Results' tab is active, showing 'Output files' and 'Refinement statistics'.

Output files

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

Log file Config file

AI analysis (highlighted with an orange circle)

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

Convert map coefficients MTZ to CCP4 maps

Refinement statistics

Compare statistics Plot statistics by cycle

Open in Coot Open in PyMOL Sequence viewer

Project: editsBug

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 acceptable ranges, suggesting a good fit to the experimental data.
 - **RMSD (0.27 Å)** indicates a high level of structural accuracy.
 - **Map-model CC 2mFo-DFc (0.78)** and **Map-model CC mFo-DFc (0.65)** indicate a strong correlation between the model and the electron density map.
 - **pLDDT (95.48)** indicates high confidence in the predicted structure.
- These metrics suggest that the goals of the program, to generate a high-quality structural model, were largely achieved.

4. Suggested Next Steps:

- **Refinement with 'phenix.refine':**
 - **Input:** The best overall predicted model ('Predicted Model') and the experimental data ('Experimental Data').

Crystallography courses in the US

CSHL course: Macromolecular Crystallography



Cold Spring Harbor Laboratory

October 11-27, 2026

Meetings & Courses Program

Crossroads of Biology



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

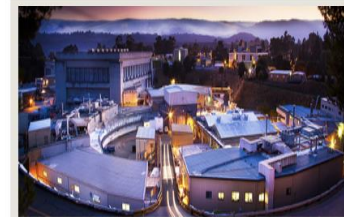
Departure: October 27th

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

Rapidata (May)



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

Event Coordinators

CCP4 school Argonne (June)



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

Argonne
NATIONAL LABORATORY

[Home](#)[About the School](#)[2026 School](#)[Publications](#)[Location](#)[Contact us](#)[Sponsors](#)

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 crystallography but including electron microscopy.

Acknowledgements

Berkeley Laboratory

Pavel Afonine, Youval Dar, Nat Echols, Jeff Headd, Richard Gildea, Ralf Grosse-Kunstleve, Dorothee Liebschner, Nigel Moriarty, Nader Morshed, Billy Poon, Ian Rees, Nicholas Sauter, Oleg Sobolev, Peter Zwart

Los Alamos Laboratory/New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

Baylor College of Medicine

Matt Baker

Cambridge University

Randy Read, Airlie McCoy, Gabor Bunckozi, Tristan Croll, Rob Oeffner, Kaushik Hatti, Massimo Sammito, Duncan Stockwell, Laurent Storoni

Duke University

Jane Richardson & David Richardson, Ian Davis, Vincent Chen, Jeff Headd, Chris Williams, Bryan Arendall, Bradley Hintze, Laura Murray

UC San Francisco

Ben Barad, Yifan Cheng, Jaime Fraser

University of Washington

Frank DiMaio, Ray Wang, David Baker

Oak Ridge National Laboratory

Marat Mustyakimov, Paul Langan

Other Collaborators

Corey Hryc, Zhao Wang, Wah Chiu
Pawel Janowski, David Case
Dale Tronrud, Donnie Berholz, Andy Karplus
Alexandre Urzhumtsev & Vladimir Lunin
Garib Murshudov & Alexi Vagin
Paul Emsley, Bernhard Lohkamp, Kevin Cowtan
David Abrahams
Phenix Testers & Users

Funding

- NIH/NIGMS: P01GM063210, P50GM062412, P01GM064692, R01GM071939
- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory