

*Phenix workshop at the University of Nebraska Lincoln,
April 30, 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

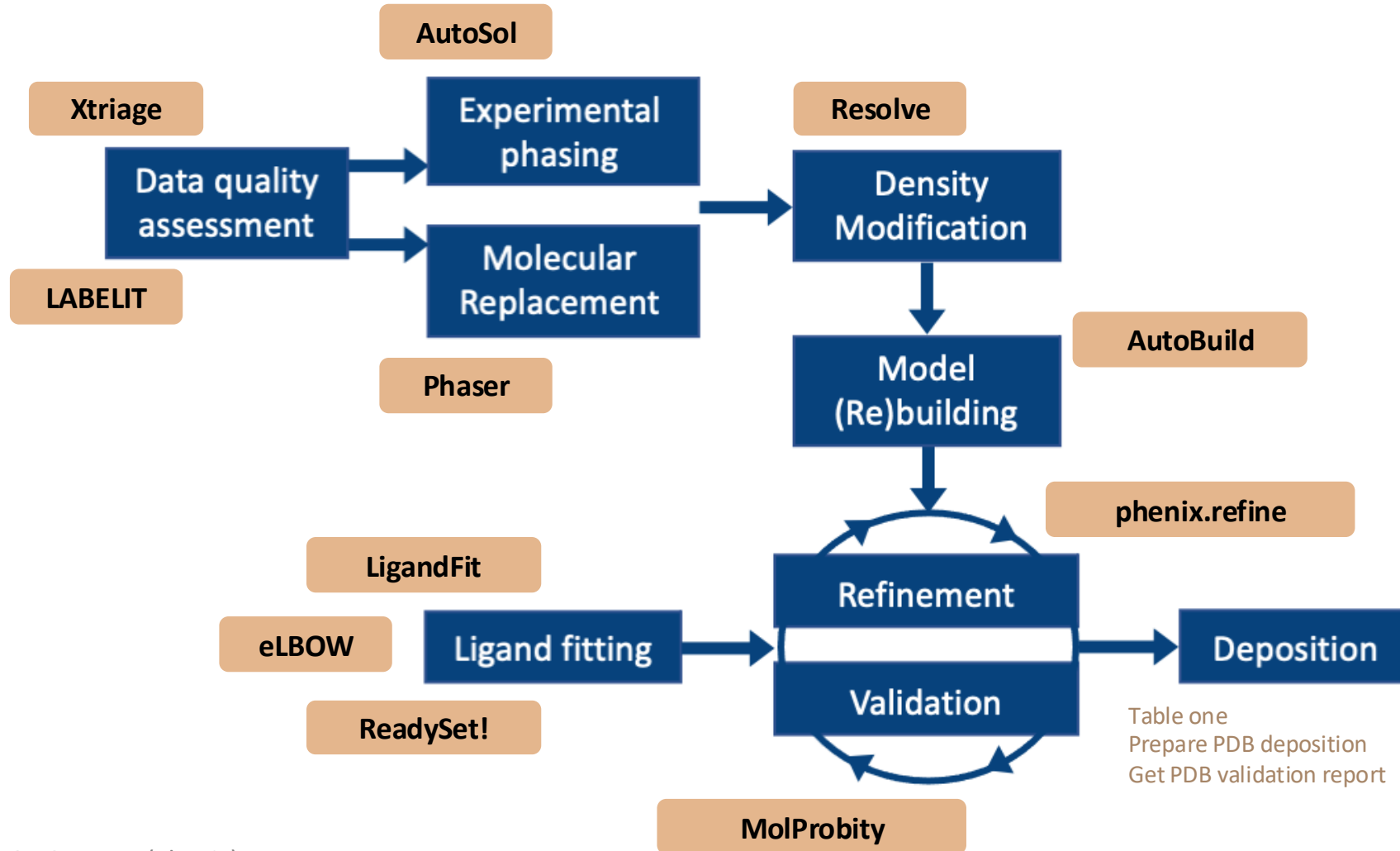


Duke University

Jane Richardson, Vincent Chen



Tools for Crystallography



Acta Cryst. 2002, D58:1948-1954

(Phenix)

J. Appl. Cryst. 2002, 35:126-136

(cctbx)

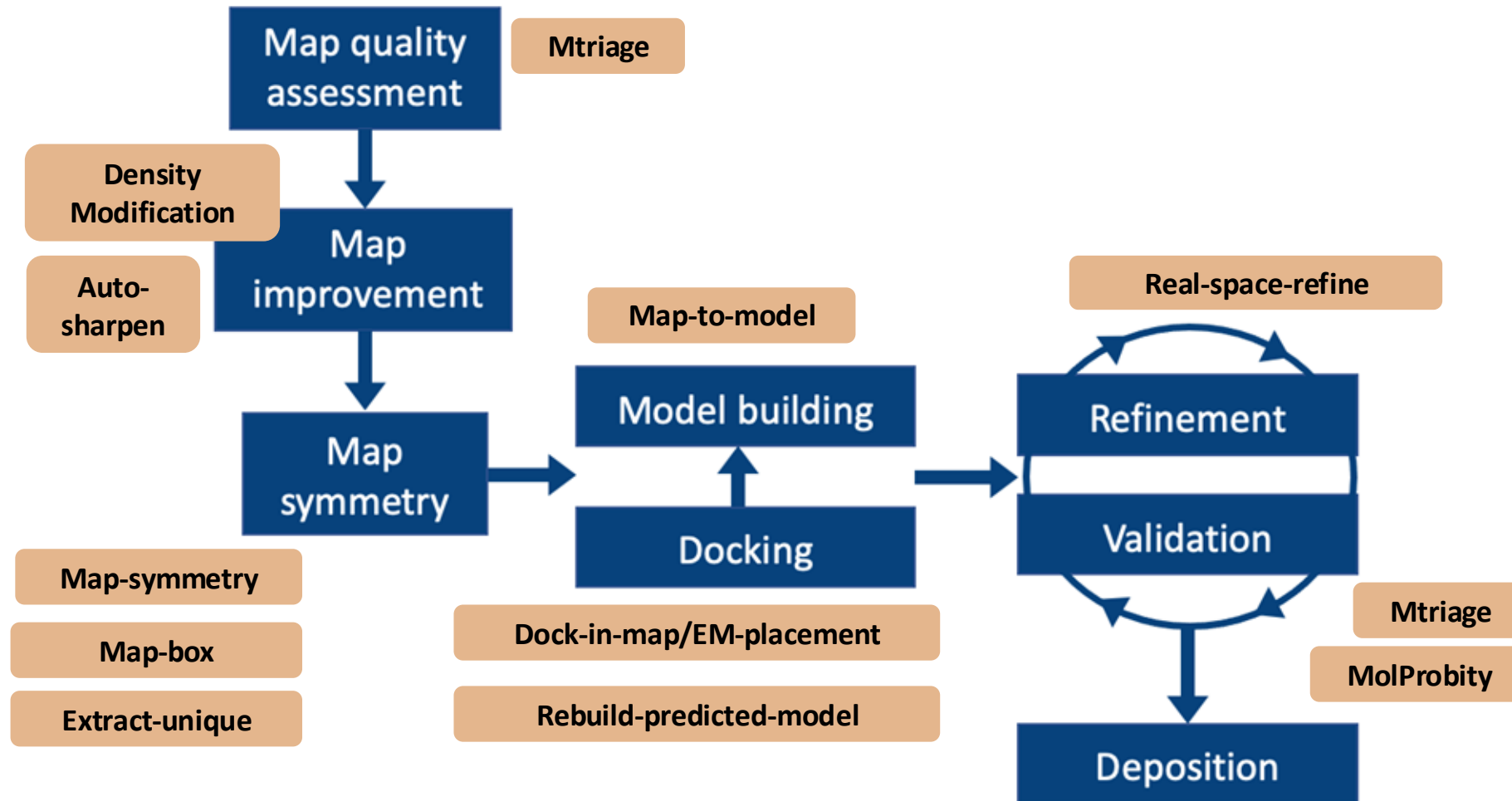
Acta Cryst. 2010, D66: 213-221

(Phenix)

Acta Cryst. 2019 D75:861-877

(Phenix)

Tool for cryo-EM



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



The screenshot displays the PHENIX graphical user interface. At the top, there is a menu bar with icons for Quit, Preferences, Help, Citations, Reload last job, Coot, PyMOL, KING, Other tools, and Ask for help. Below the menu bar, there are tabs for 'Actions' and 'Job history'. The main area is divided into two panels. The left panel, titled 'Projects', contains a 'Show group' dropdown menu set to 'All groups' and a 'Manage...' button. Below this are buttons for 'Select', 'Delete', 'New project', and 'Settings'. A table lists project details:

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

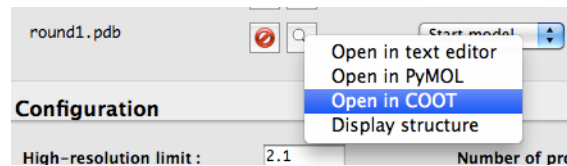
The right panel, titled 'Favorites', lists various tool categories: AlphaFold (predicted models), Crystals: Data analysis and manipulation, Validation and map-based comparisons, Experimental phasing, Molecular replacement, Maps (create, manipulate, compare), Enhanced maps (Polder, FEM, density-modified...), Model building, Refinement, Ligands, Cryo-EM: Map analysis, symmetry, manipulation, Validation and map-based comparisons, Map improvement, Docking, model building and rebuilding, Refinement, Models: Superpose, search, compare, analyze symmetry, Modification, minimization and dynamics, PDB Deposition, and Program search. At the bottom, there is a 'Current directory' field showing '/Users/dcliebschner/Desktop/Projects/test' and a 'Browse...' button. The status bar at the very bottom indicates 'PHENIX version dev-svn-000' and '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

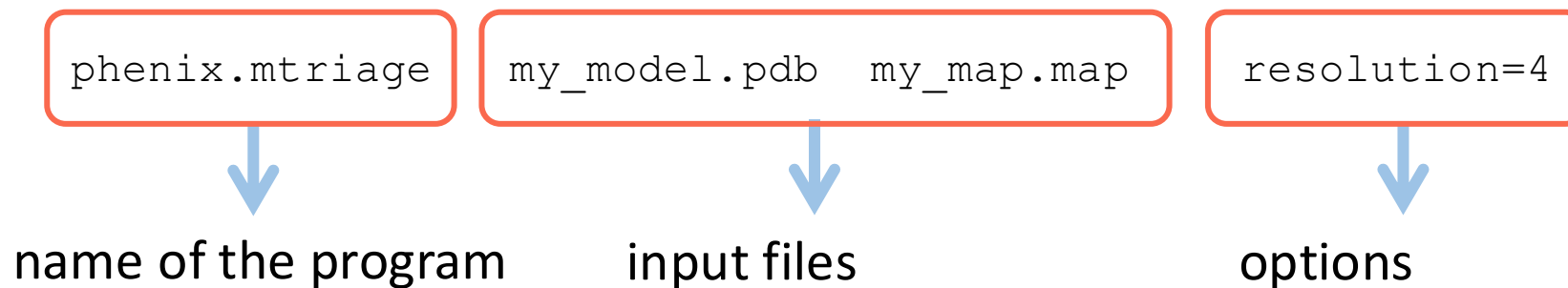


- Specific paths to executables usually required on Linux

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/phenix tutorials>

The screenshot shows the YouTube channel page for Phenix Tutorials. The channel name is "Phenix Tutorials" with 560 subscribers. The page features a grid of video thumbnails, each with a title, description, view count, and upload date. The videos cover various topics in X-ray crystallography, such as real-space refinement, secondary structure restraints, multiple refinement strategies, SAD experiments, map-to-model interpretation, and scaling and merging data.

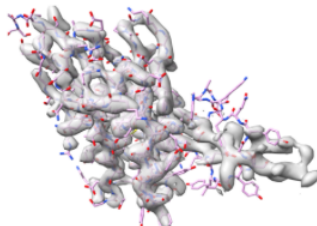
Video Title	Duration	Views	Upload Date
real_space_refine Tutorial	5:27	763 views	7 months ago
Secondary Structure Restraints Tutorial	6:23	399 views	8 months ago
Multiple refinement strategies Tutorial	5:46	281 views	8 months ago
Planning a SAD experiment Tutorial	6:00	483 views	1 year ago
Map-to-model Tutorial	5:33	1.3K views	1 year ago
Scale-and-merge Tutorial	7:31	387 views	1 year ago
Automated map sharpening Tutorial	6:05		
Ligandfit Tutorial	5:48		
Wilson plots and space group identification phenix.xtriage	8:23		
Twinning phenix.xtriage	6:08		
Translational NCS phenix.xtriage	4:55		
Checking data quality with Xtriage	6:49		

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

Presentation slides

<https://phenix-online.org>

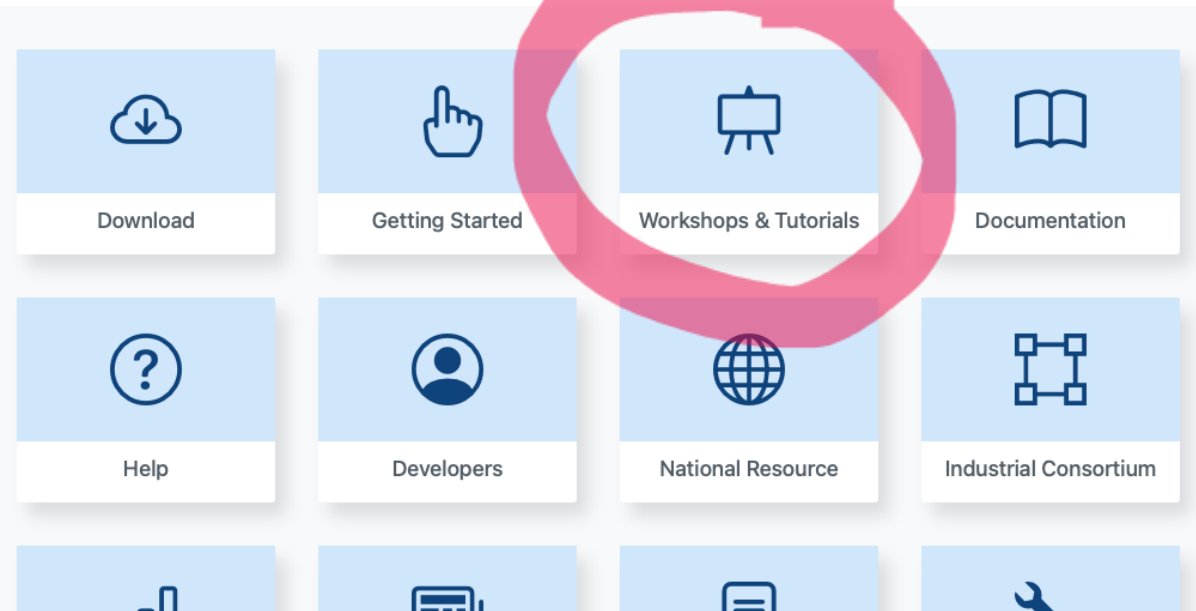
A comprehensive software package for macromolecular structure determination using crystallographic (X-ray, neutron and electron) and electron cryo-microscopy data. [Learn more](#)



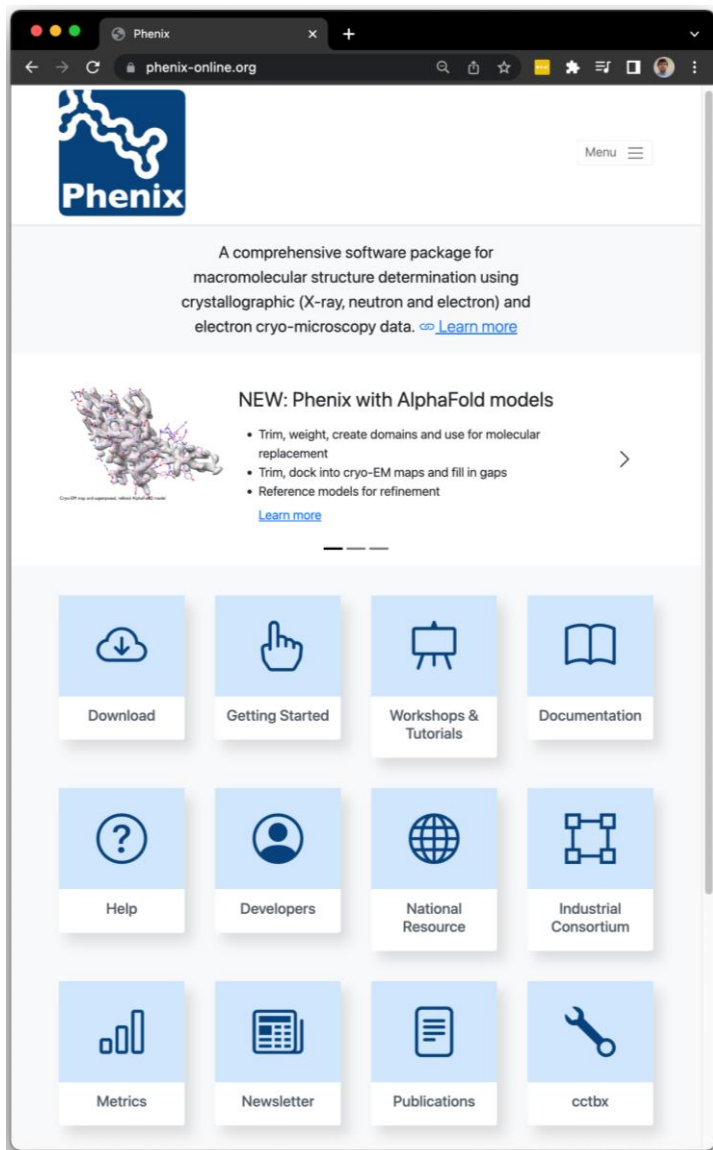
Cryo-EM map and superposed, refined AlphaFold2 model

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](#)

A grid of navigation buttons for the Phenix website. The buttons are arranged in three rows and four columns. The first row contains: Download (cloud with arrow), Getting Started (hand cursor), Workshops & Tutorials (whiteboard with pointer), and Documentation (open book). The second row contains: Help (question mark), Developers (person icon), National Resource (globe), and Industrial Consortium (network diagram). The third row contains: (partially visible bar chart icon), (partially visible calendar icon), (partially visible list icon), and (partially visible wrench icon). A large, hand-drawn pink circle highlights the 'Workshops & Tutorials' button.

Phenix resources



Phenix paper

Video tutorials (YouTube)

Documentation

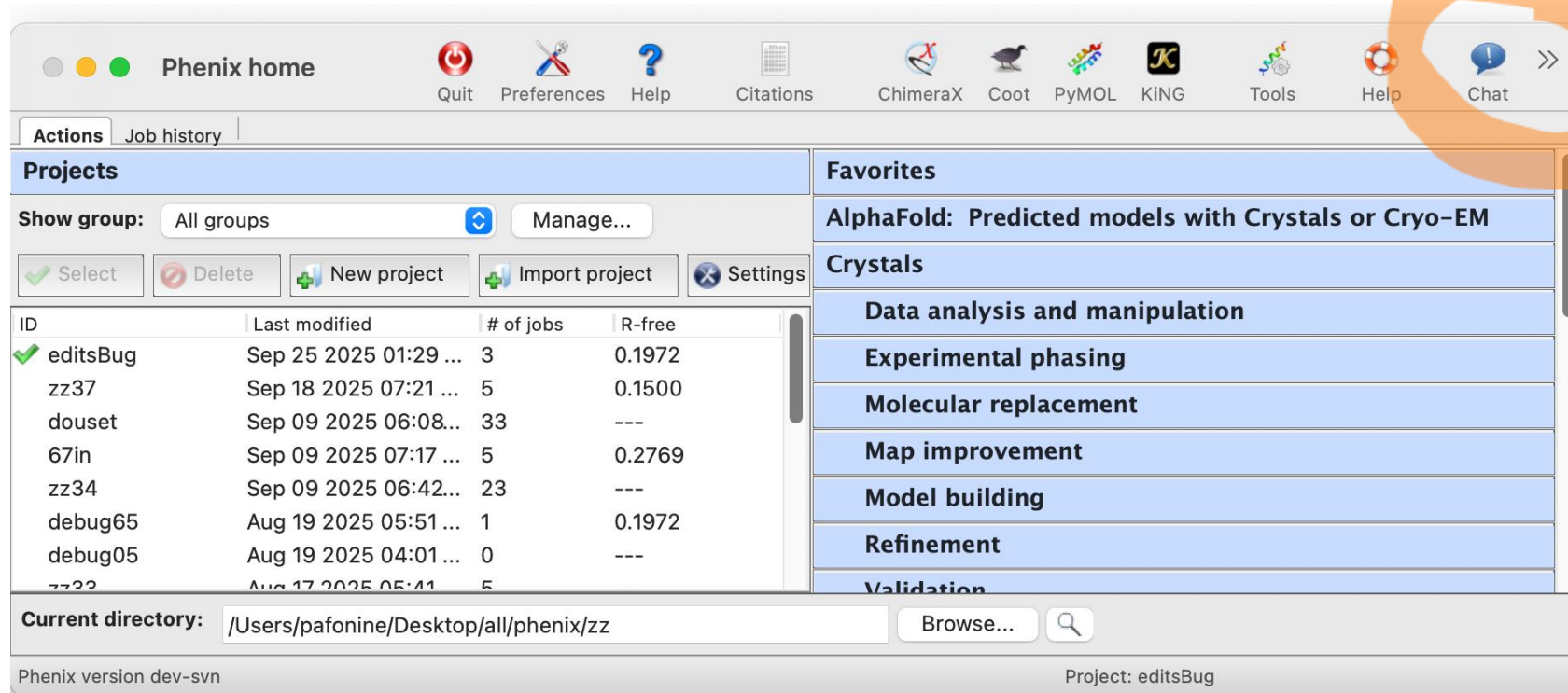
Relevant papers

Bi-annual newsletters

PDFs with slides from workshops

NEW: AI tools in Phenix - Chatbot

phenix-online.org/chatbot

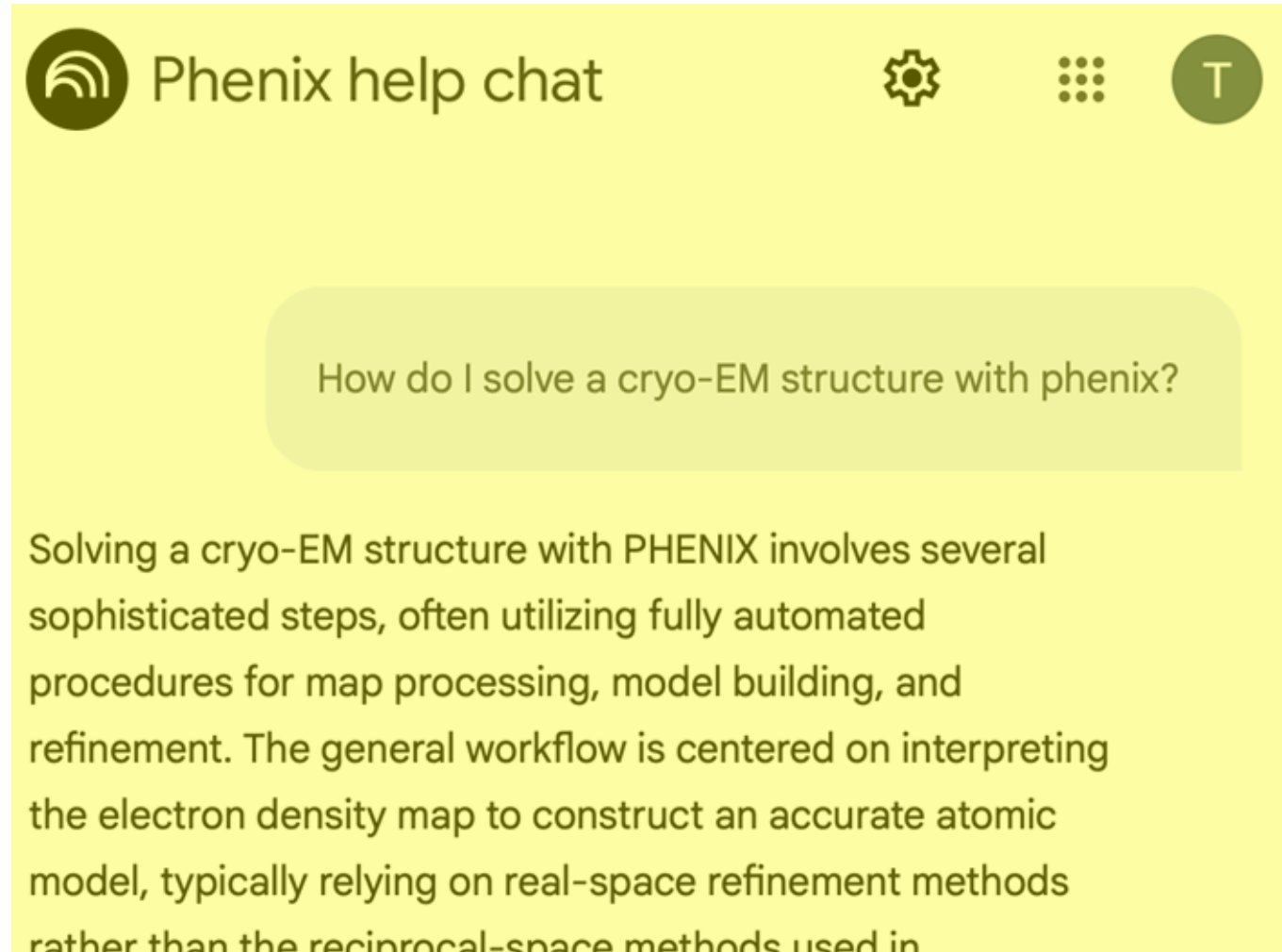


The screenshot shows the Phenix web interface. At the top, there is a navigation bar with icons for Quit, Preferences, Help, Citations, ChimeraX, Coot, PyMOL, KiNG, Tools, Help, and Chat. The Chat icon is circled in orange. Below the navigation bar, there are tabs for Actions and Job history. The main content area is divided into two columns: Projects and Favorites. The Projects column has a 'Show group' dropdown set to 'All groups' and buttons for Select, Delete, New project, Import project, and Settings. Below these buttons is a table with columns for ID, Last modified, # of jobs, and R-free. The Favorites column lists various tools and features like AlphaFold, Crystals, Data analysis and manipulation, Experimental phasing, Molecular replacement, Map improvement, Model building, Refinement, and Validation. At the bottom, there is a 'Current directory' field showing '/Users/pafonine/Desktop/all/phenix/zz' and a 'Project: editsBug' label.

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	---

NEW: AI tools in Phenix - Chatbot

phenix-online.org/chatbot



The screenshot shows a chat interface with a yellow background. At the top left is a circular icon with a signal symbol, followed by the text "Phenix help chat". To the right are three icons: a gear, a 3x3 grid, and a circle with the letter "T". A light green rounded rectangle contains the question: "How do I solve a cryo-EM structure with phenix?". Below this, a larger light green rounded rectangle contains the answer: "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

The screenshot displays the Phenix software interface. At the top, there is a menu bar with icons for Preferences, Help, Run, Abort, Save, Graphics, ReadySet, TLS, Restraints, Xtrriage, and Help. Below the menu bar, the 'Configure' tab is active, and the 'Refine_2' sub-tab is selected. The 'Results' tab is also visible, with sub-tabs for MolProbability, Real-space correlation, and Atomic properties. The main area shows the 'Output files' section with a directory path: /Users/pafonine/Desktop/all/phenix/zz/Refine_2. A search icon is present next to the directory path. Below the directory path, there are buttons for 'Log file' and 'Config file'. A table lists the output files and their contents. The first row is highlighted, and the 'AI analysis' button is circled in orange. To the right of the table, there are three buttons: 'Open in Coot', 'Open in PyMOL', and 'Sequence viewer'. At the bottom, there are buttons for 'Compare statistics' and 'Plot statistics by cycle'. The status bar at the bottom shows 'Idle' and 'Project: editsBug'.

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

Log file Config file

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
editsBua_refine_002.loa	phenix.refine loa file

Convert map coefficients MTZ to CCP4 maps

Refinement statistics

Compare statistics Plot statistics by cycle

Open in Coot Open in PyMOL Sequence viewer

Idle 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 Fo-DFc (0.78)** indicate a strong correlation between the model and the electron density map.
 - **pLDDT (95.48)** indicates high confidence in the model.
- 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')

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”

Crystallography courses in the US

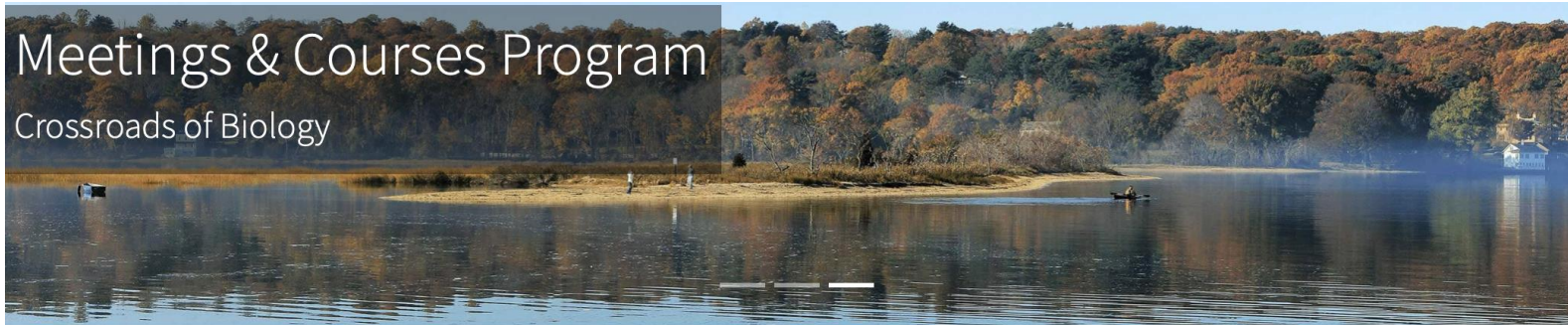
CSHL course: Macromolecular Crystallography



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](#)

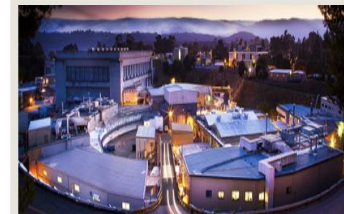
[Announcement](#)

[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



[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