

*Phenix User Workshop, Missoula, Montana*



# Introduction to Phenix

Dorothee Liebschner  
Lawrence Berkeley Laboratory

# What is *Phenix*?

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- 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 Project



## Lawrence Berkeley Laboratory

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



## University of Cambridge

Randy Read, Airlie McCoy,  
Alisia Fadini



## Los Alamos National Laboratory New Mexico Consortium

Tom Terwilliger, Li-Wei Hung



## UTHealth

Matt Baker



## Duke University

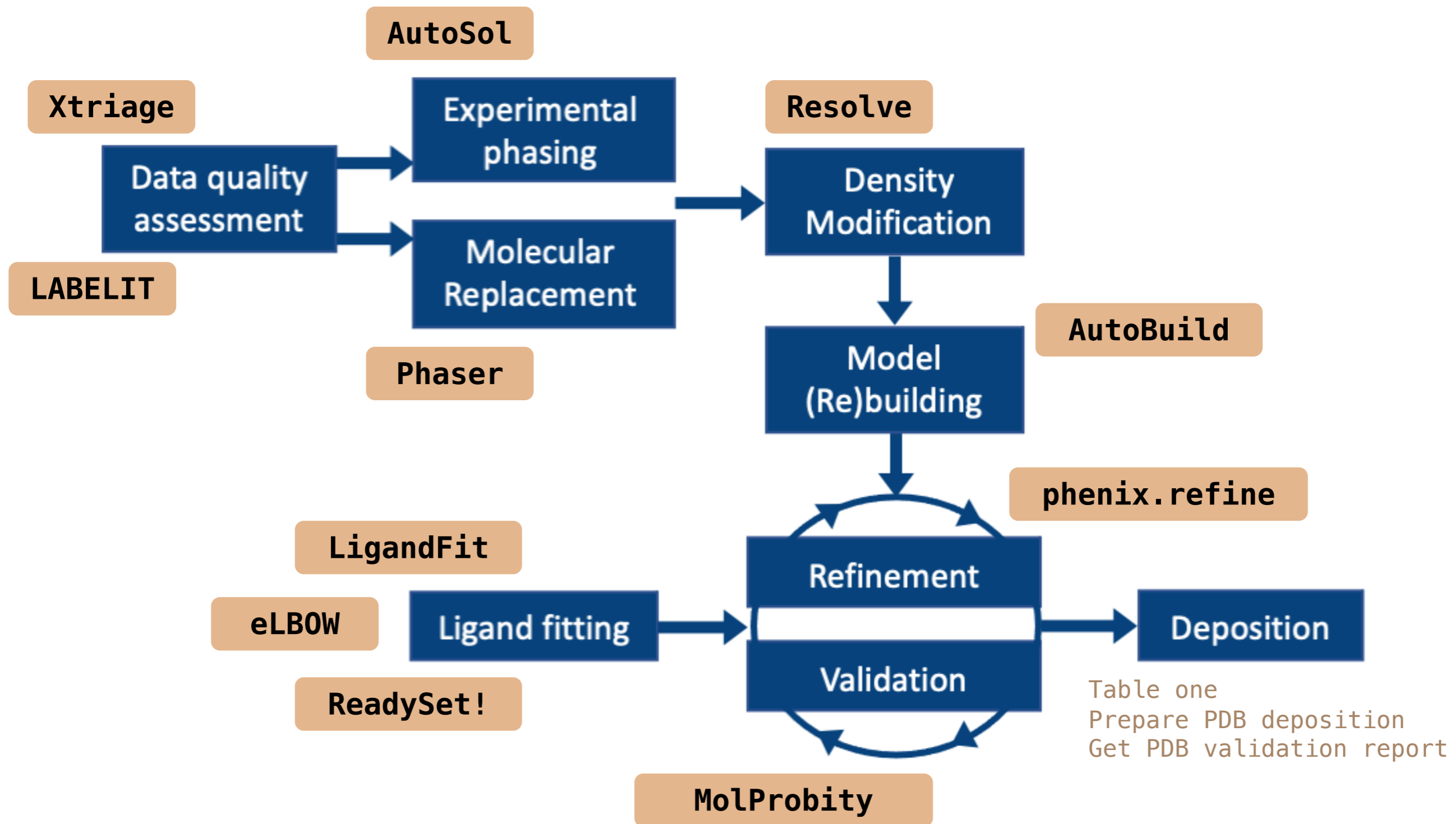
Jane & David Richardson,  
Christopher Williams,  
Vincent Chen



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

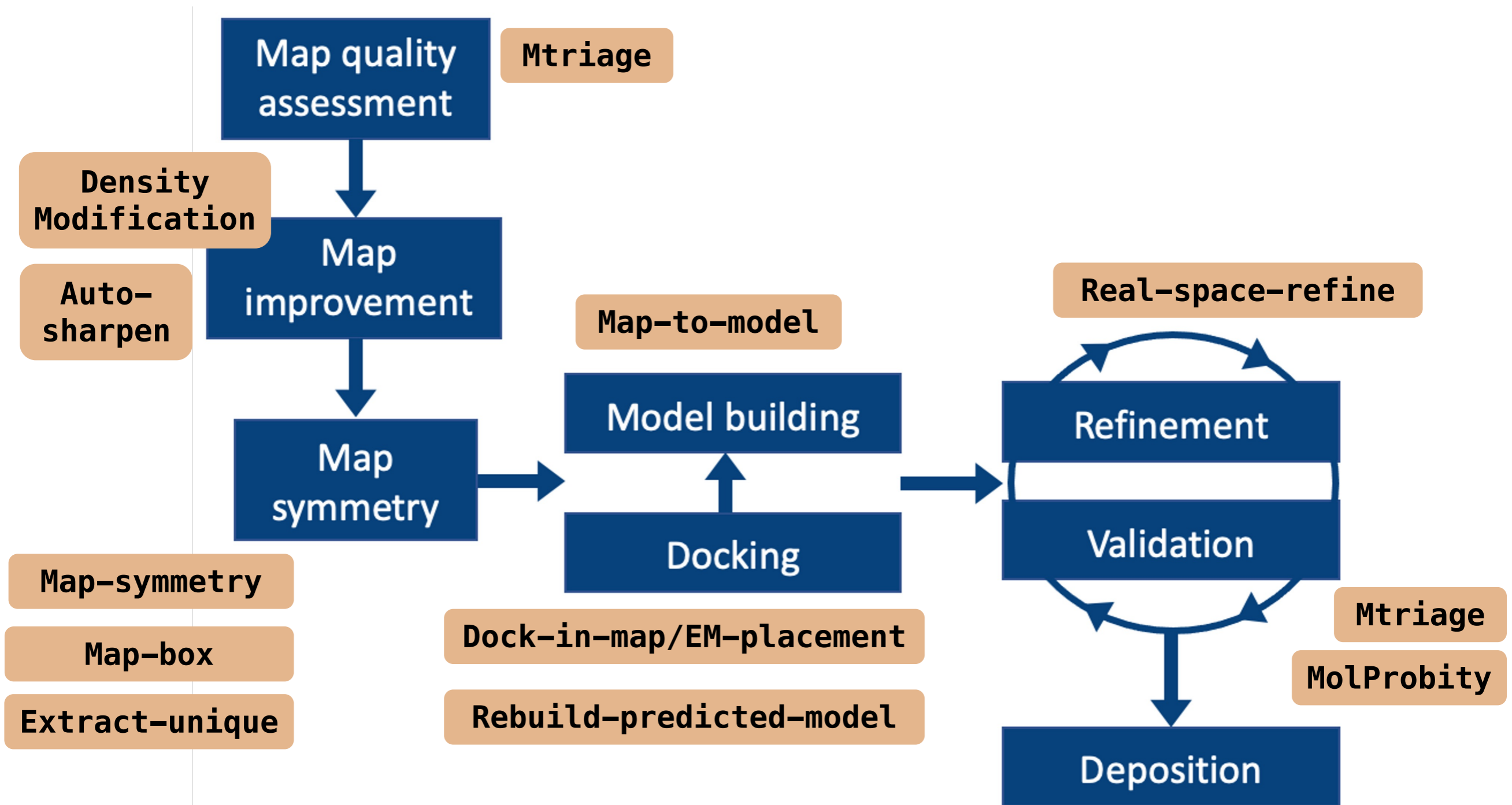


*Acta Cryst.* 2002, D58:1948-1954  
*J. Appl. Cryst.* 2002, 35:126-136  
*Acta Cryst.* 2010, D66: 213-221  
*Acta Cryst.* 2019 D75:861-877

(Phenix)  
(cctbx)  
(Phenix)  
(Phenix)

Table one  
Prepare PDB deposition  
Get PDB validation report

# Tools for Cryo-EM



*Acta Cryst.* 2002, D58:1948-1954  
*J. Appl. Cryst.* 2002, 35:126-136  
*Acta Cryst.* 2010, D66: 213-221  
*Acta Cryst.* 2019 D75:861-877

(Phenix)  
 (cctbx)  
 (Phenix)  
 (Phenix)

Features

# Phenix GUI

Central GUI for job control and to launch new jobs

The screenshot displays the Phenix GUI 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 two tabs: '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 the projects:

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
- 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'.

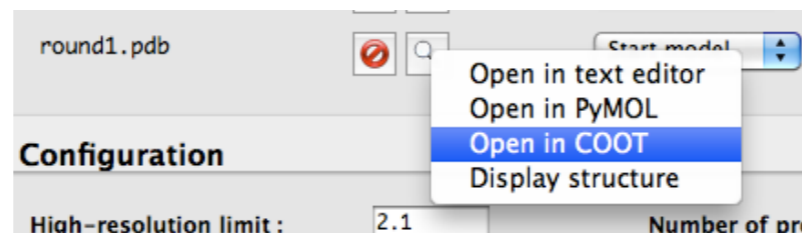
# Coot/PyMOL/ChimeraX integration

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- Most results can be opened directly in graphics apps



- Any PDB file listed in GUI can also be opened



- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running
- Coot must have Python support (default on Mac)
- Specific paths to executables usually required on Linux

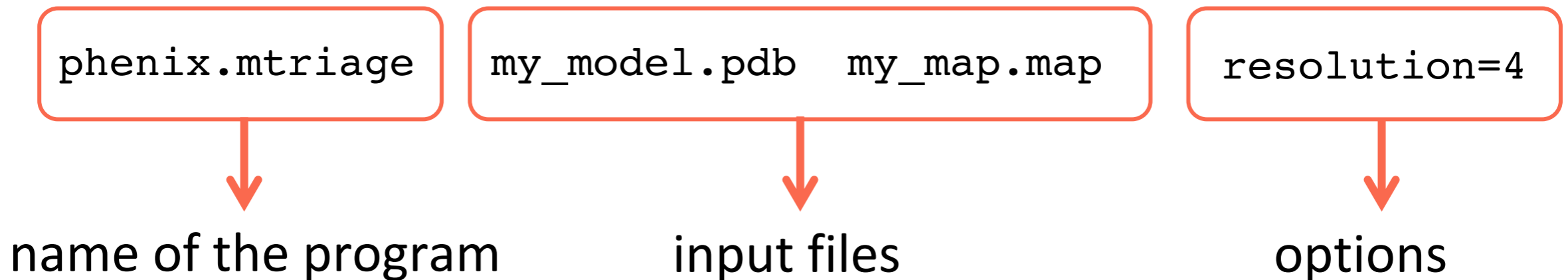
Preferences → Graphics → Full path to Coot [...PyMOL]



# Command Line Tools

---

## 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

www.youtube.com/channel/UCcdl0hfHngWAZLJWynxPQWg/videos

YouTube IT Search

## Phenix Tutorials

Phenix homepage

Phenix Tutorials  
560 subscribers

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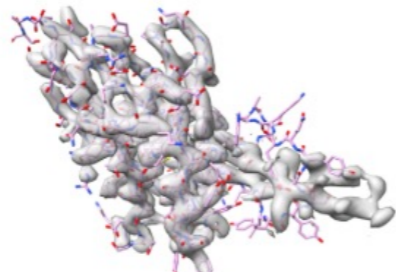
- real\_space\_refine Tutorial** (5:27)  
How to run real-space-refine  
763 views • 7 months ago  
CC
- Secondary Structure Restraints Tutorial** (6:23)  
How to use secondary structure restraints  
399 views • 8 months ago  
CC
- Multiple refinement strategies Tutorial** (5:46)  
How to use multiple refinement strategies and...  
281 views • 8 months ago  
CC
- Planning a SAD experiment Tutorial** (6:00)  
Simulate a SAD experiment with...  
483 views • 1 year ago  
CC
- Map-to-model Tutorial** (5:33)  
Automatic map interpretation with map\_to\_model  
1.3K views • 1 year ago  
CC
- Scale-and-merge Tutorial** (7:31)  
Scaling and merging anomalous data  
387 views • 1 year ago  
CC
- 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, Nigel Moriarty,  
Tom Terwilliger, Christopher Schlicksup, Vincent Chen

# Presentation slides

- **Lectures**  
<https://phenix-online.org>

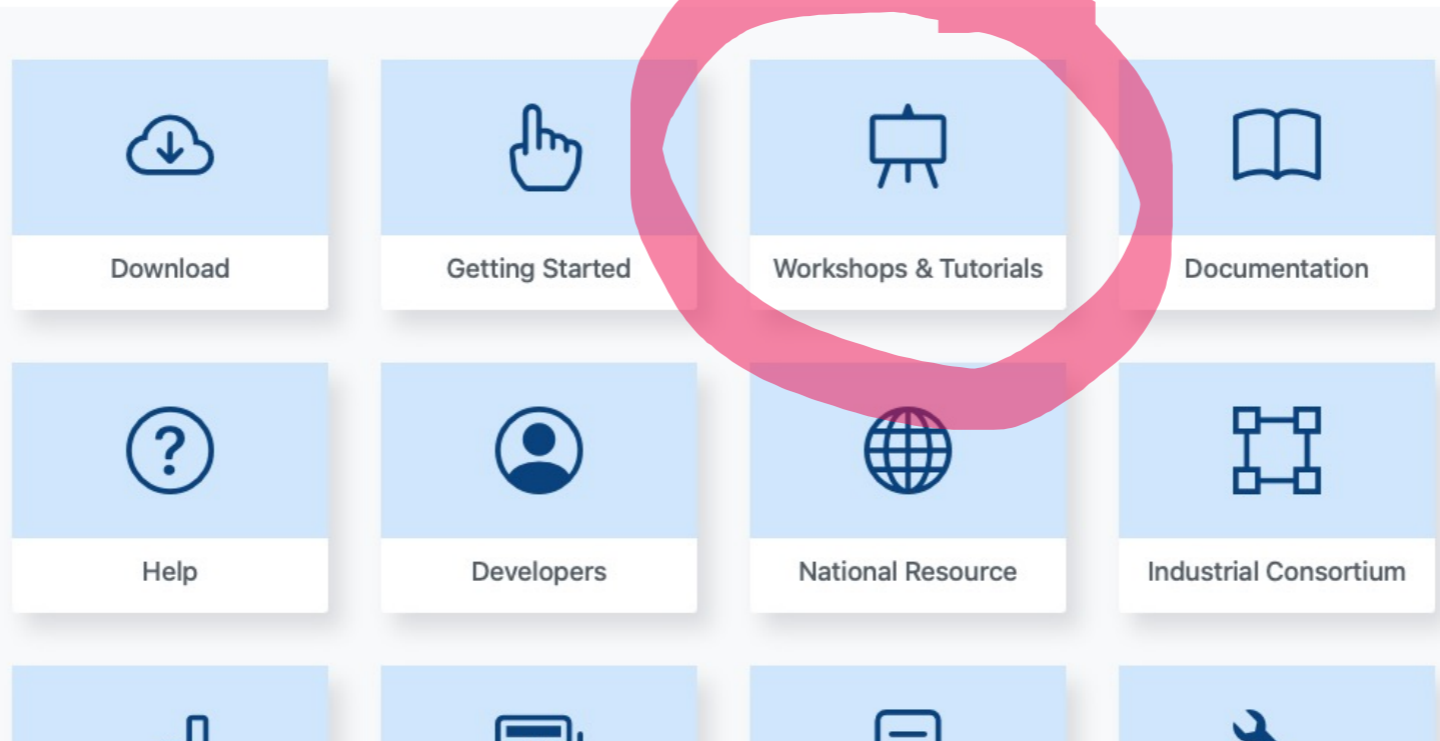
A comprehensive software package for macromolecular structure determination using crystallographic (X-ray, neutron and electron) and electron cryo-microscopy data. [Learn more](#)



Cryo-EM map and superposed, refined AlphaFold2 model

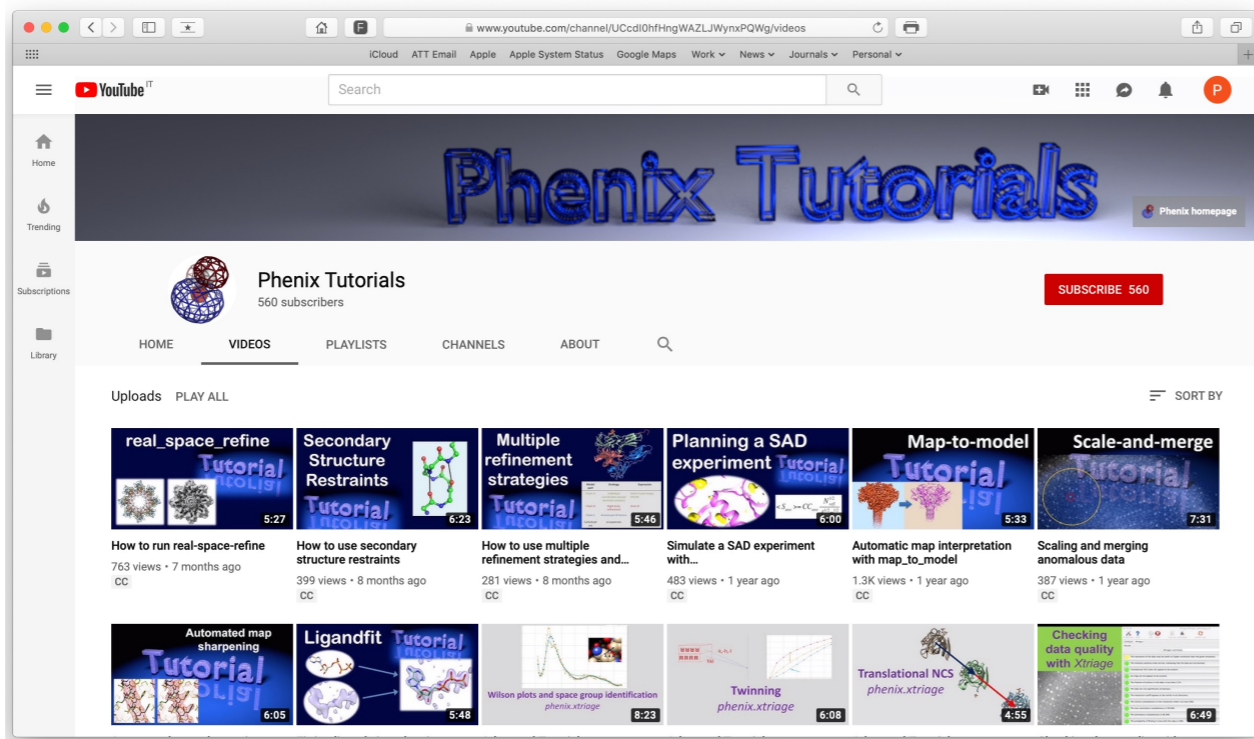
## Phenix integrated with AlphaFold

- 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](#)



# Troubleshooting

- Phenix team members will be in the room
- YouTube video tutorials  
<https://www.youtube.com/c/phenixtutorials>



The image shows a screenshot of a web browser displaying the YouTube channel page for "Phenix Tutorials". The browser's address bar shows the URL [www.youtube.com/channel/UCcdl0hFngWAZLjWynxPQWg/videos](https://www.youtube.com/channel/UCcdl0hFngWAZLjWynxPQWg/videos). The YouTube interface includes a search bar, navigation icons (Home, Trending, Subscriptions, Library), and a channel banner for "Phenix Tutorials" with 560 subscribers. Below the banner, there are tabs for HOME, VIDEOS, PLAYLISTS, CHANNELS, and ABOUT. The "VIDEOS" tab is selected, showing a grid of video thumbnails. The thumbnails include titles such as "real\_space\_refine Tutorial", "Secondary Structure Restraints Tutorial", "Multiple refinement strategies Tutorial", "Planning a SAD experiment Tutorial", "Map-to-model Tutorial", "Scale-and-merge Tutorial", "Automated map sharpening Tutorial", "Ligandfit Tutorial", "Wilson plots and space group identification", "Twinning", "Translational NCS", and "Checking data quality with Xtriage". Each thumbnail also displays the video's duration and view count.

# CSHL course: Macromolecular Crystallography



Cold Spring Harbor Laboratory



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Crossroads of Biology

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## Macromolecular Crystallography

October 13 - 29, 2024

**Key Dates:**

**Application Deadline:** July 15 2024

**Arrival:** October 13th by 6pm EST

**Departure:** October 29th

# Rapidata



## RapiData 2024 at SSRL

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

#### April 29 - May 4, 2024

[Home](#)

[Announcement](#)

[Application and Registration](#)

[Schedule](#)

[Participant Information](#)

[Sponsor Information](#)

[Transportation](#)

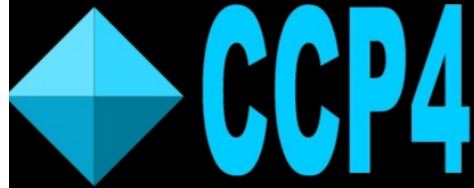


**Stanford Synchrotron  
Radiation Lightsource**

### Event Information

Course dates: April 29 - May 4, 2024

# CCP4 school Argonne



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



[Home](#) [2023 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 15th 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 2023 school will take place at the Advanced Photon Source (APS) synchrotron site at Argonne National Laboratory, near Chicago.

# Acknowledgements

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## **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

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## **University of Washington**

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## **Oak Ridge National Laboratory**

Marat Mustyakimov, Paul Langan

## **Other Collaborators**

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Alexandre Urzhumtsev & Vladimir Lunin  
Garib Murshudov & Alexi Vagin  
Paul Emsley, Bernhard Lohkamp, Kevin Cowtan  
David Abrahams  
Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory