BERKELEY LAB

U.S. DEPARTMENT OF ENERGY

UNIVERSITY OF CALIFORNIA

ACA Meeting 2025
Lombard, July 18th 2025

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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Agenda

Time	Title	Instructor
8:30	Welcome: Introduction to Phenix	DL
8:35	Phenix chatbot	BKP
8:45	**Lecture**: Strategy for X-ray or Cryo-EM structure determination using AlphaFold models	CJW
9:15	Tutorial: Predicting your structure with AlphaFold	BKP
9:30	Tutorial: MR with an AlphaFold model	DL
10:00	Break	
10:15	**Lecture**: refinement (X-ray & cryo-EM) + validation issues cryo-EM	PVA
11:30	Tutorial: X-ray refinement (rnase-s basic tutorial with different options)	DL
12:00	Lunch	
13:00	**Lecture**: Ligands	NWM
13:30	Tutorial: Ligands	NWM
13:50	Tutorial: Douse, cryo-EM docking	DL
14:15	Break	
14:30	Tutorial: Cryo-EM refinement (basic tutorial + Magref)	PVA
15:00	**Lecture**: Model Validation	CJW
15:45	Tutorial: Model Validation	CJW
16:15	PDB deposition	NWM
16:30	Q&A	everyone
16:45	Finish: workshop survey, wrap up	

WiFi:

Westin Meeting Rooms

ACA2025

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

Phenix

The Phenix Project

Lawrence Berkeley Laboratory

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

BERKELEY LAB

University of Cambridge

Randy Read, Airlie McCoy, Alisia Fadini

UNIVERSITY OF CAMBRIDGE

Los Alamos National Laboratory

New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

New Mexico CONSORTIUM

Los Alamos NATIONAL LABORATORY

UTHealth

Matt Baker

UTHealth The University of Texas Health Science Center at Houston

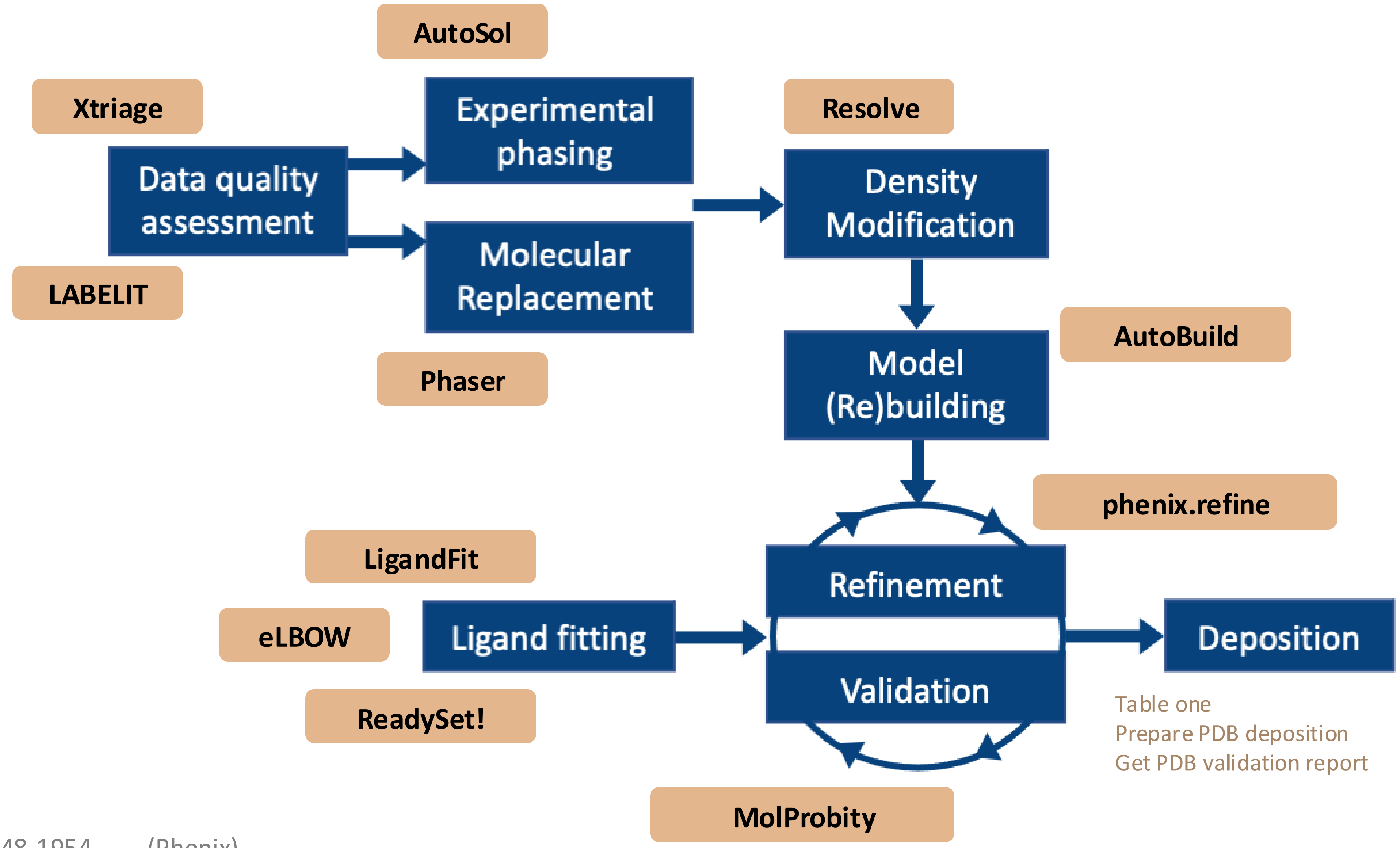
Duke University

Jane 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



AutoSol

Xtriage

Data quality assessment

LABELIT

Experimental phasing

Molecular Replacement

Phaser

Resolve

Density Modification

Model (Re)building

AutoBuild

phenix.refine

Refinement

Validation

MolProbity

LigandFit

eLBOW

Ligand fitting

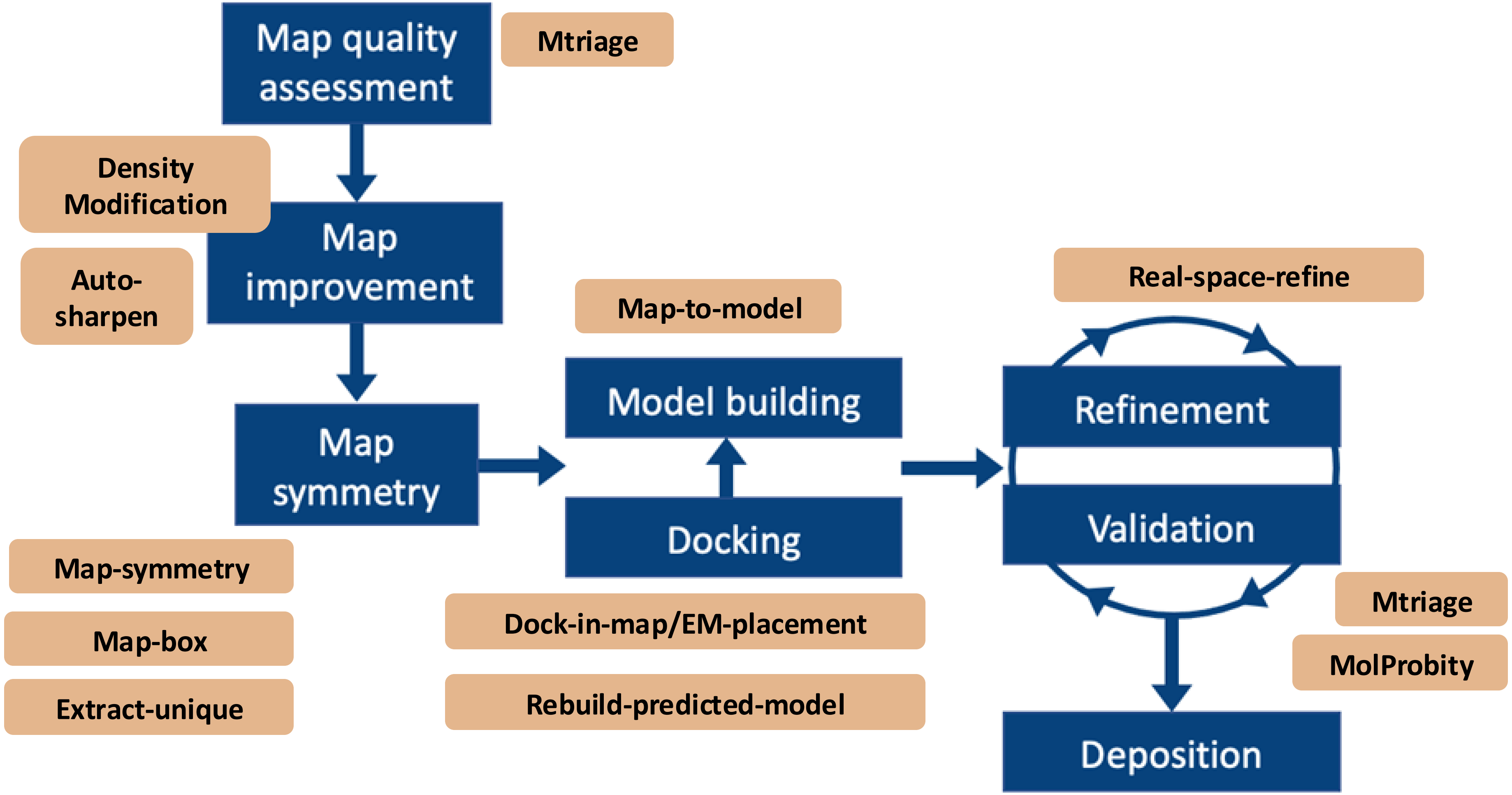
ReadySet!

Deposition

Table one
Prepare PDB deposition
Get PDB validation report

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)

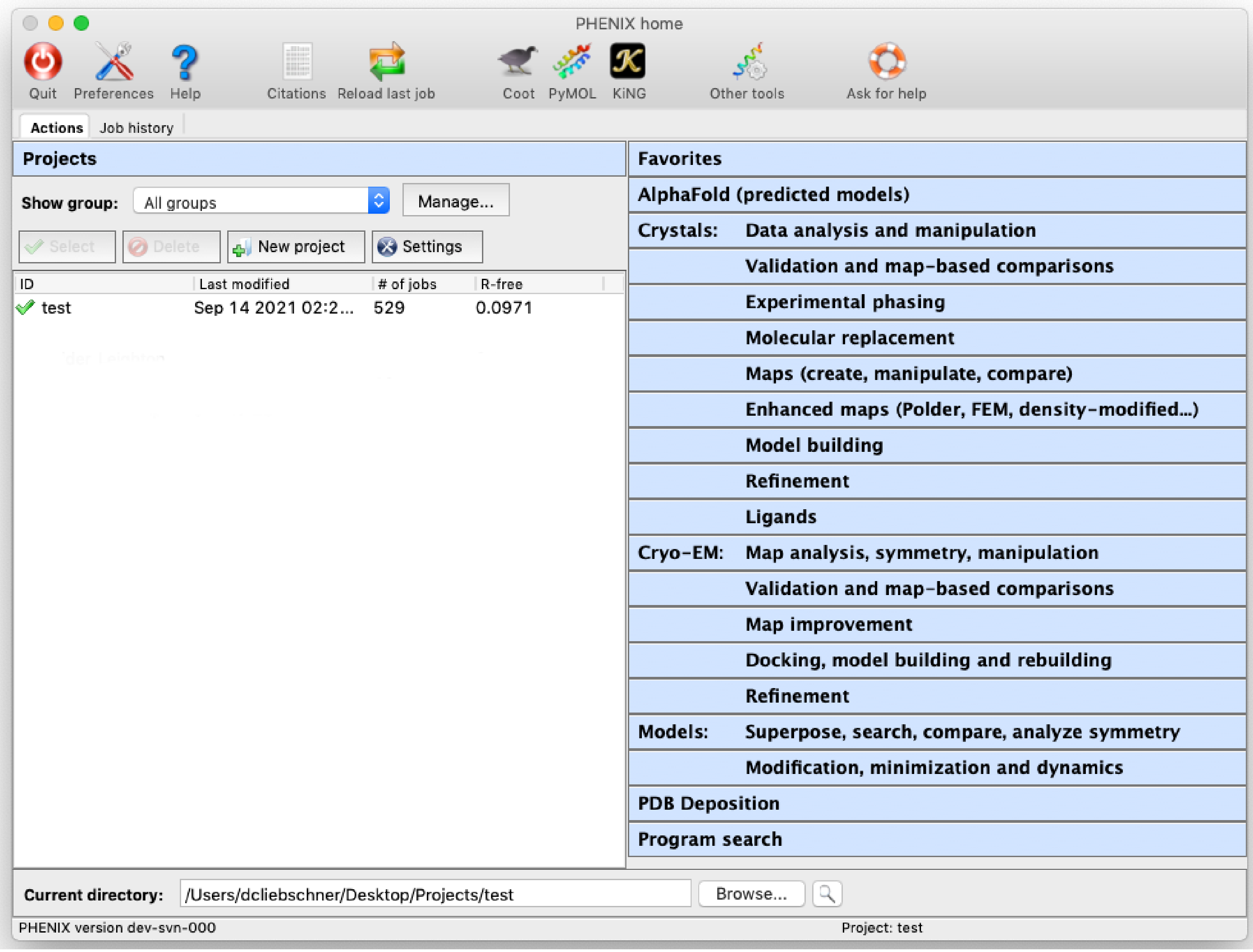
Tool for cryo-EM



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



Show group: All groups

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

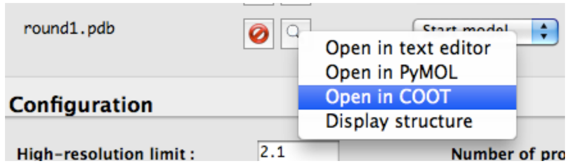
Current directory: /Users/dcliebschner/Desktop/Projects/test

PHENIX version dev-svn-000 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



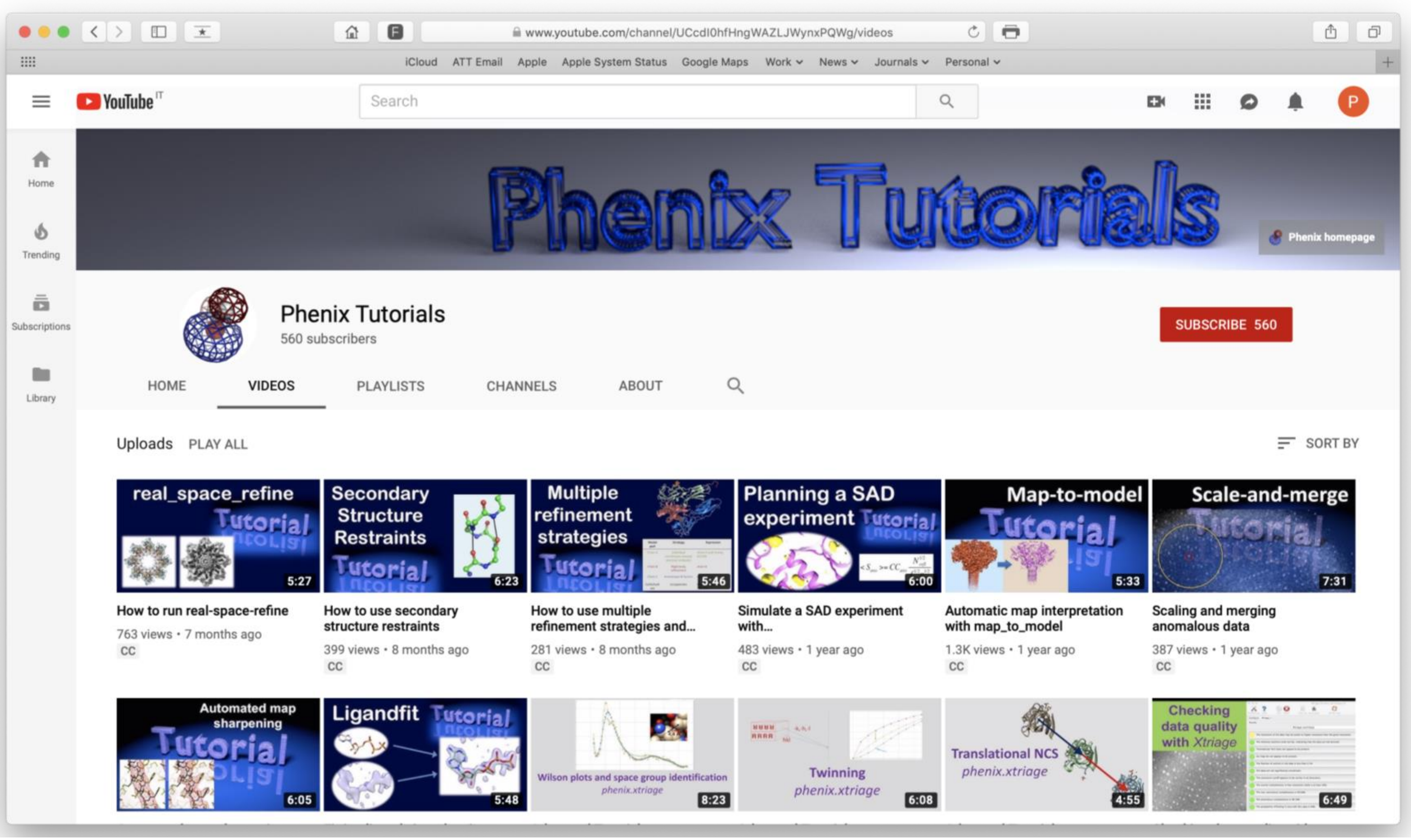
High-resolution limit : 2.1

- Specific paths to executables usually required on Linux

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

Video Tutorials

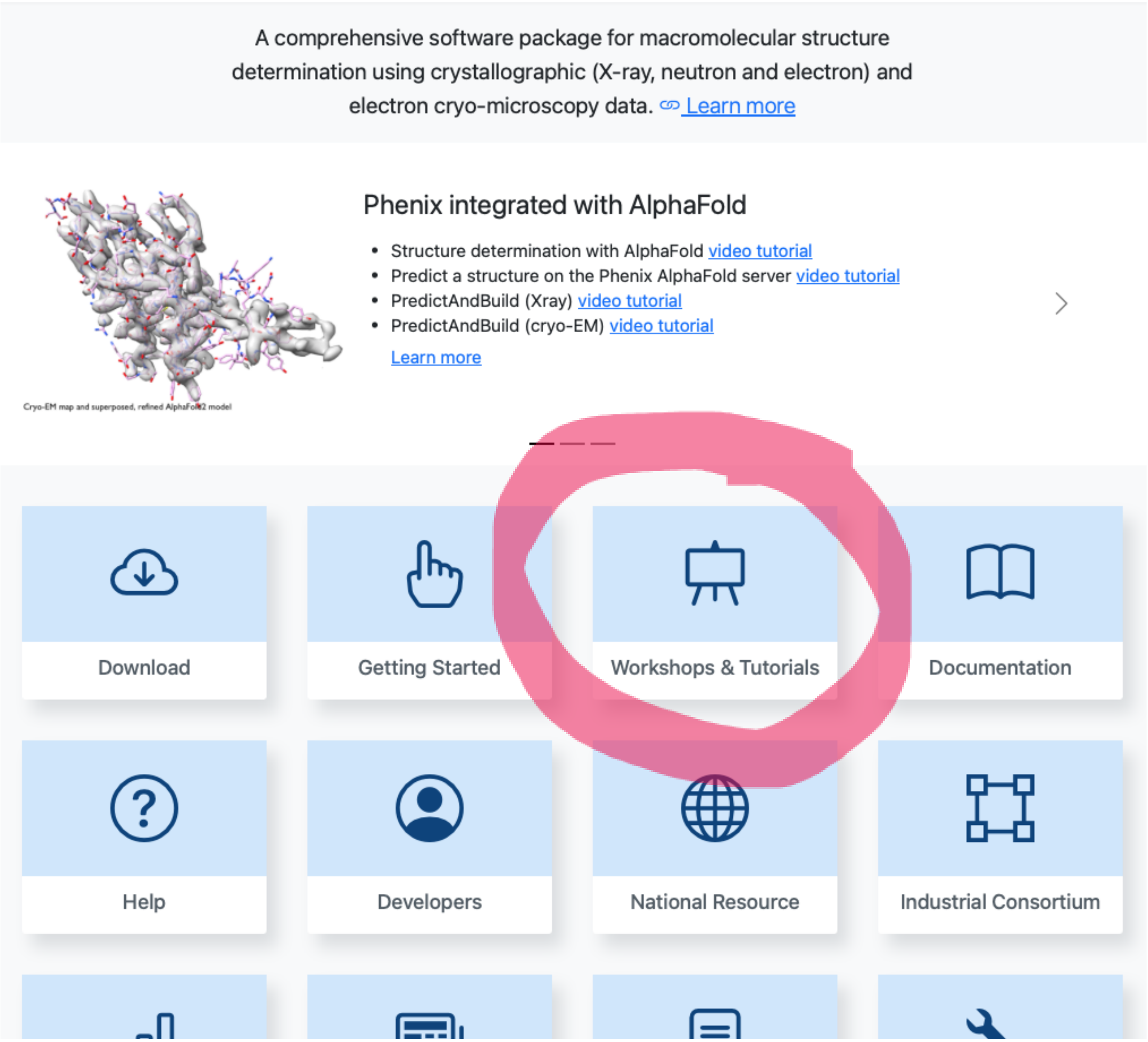
https://www.youtube.com/c/phenixtutorials



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

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

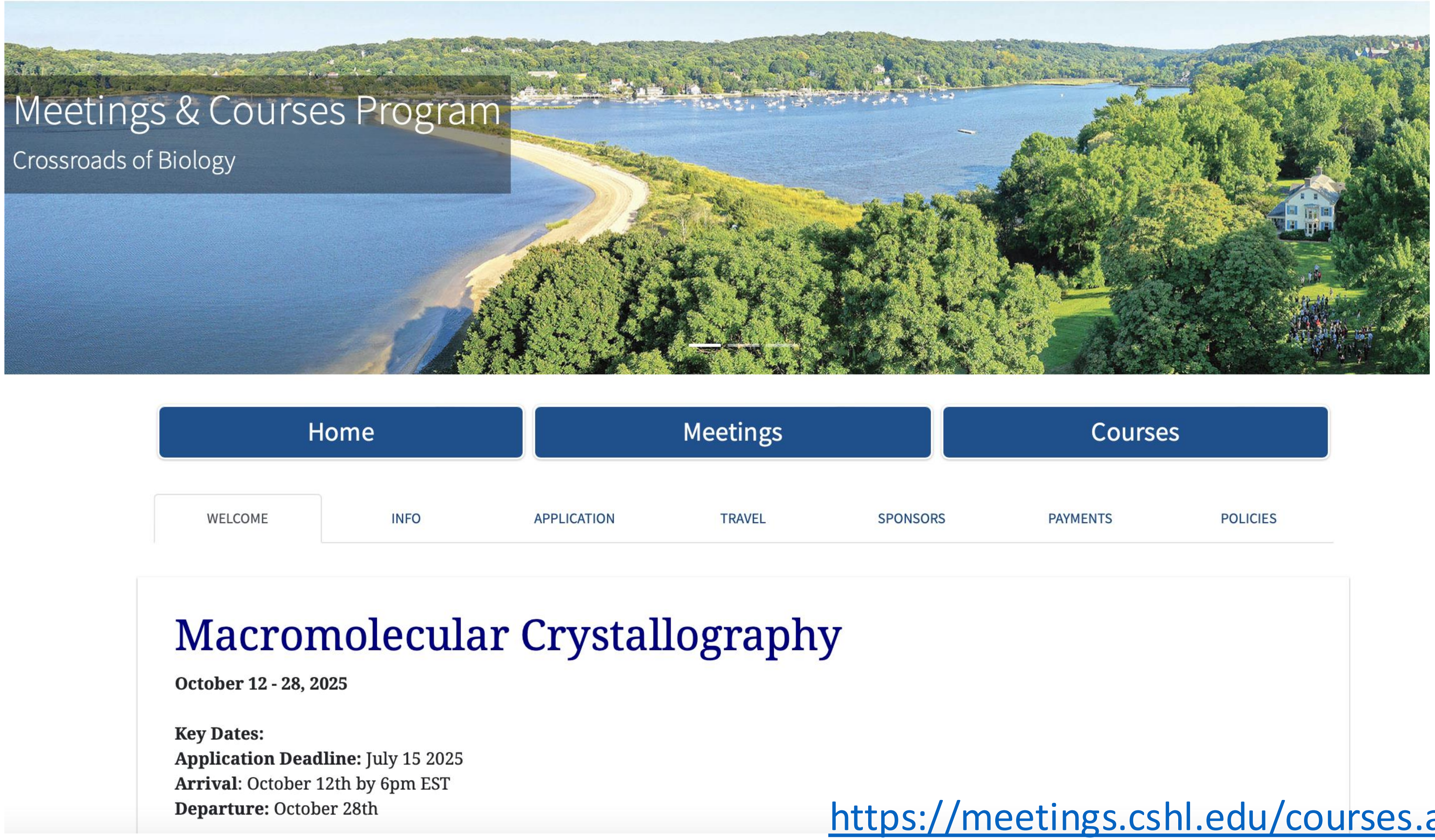
Learn more

Crystallography/cryo-EM courses in the US

CSHL course: Macromolecular Crystallography

CSH Cold Spring Harbor Laboratory

October 12-28, 2025



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)

RapiData 2025 at SSRL
Data Collection and Structure Solving: A Practical Course in Macromolecular X-Ray Diffraction Measurement
May 5 - May 10, 2025

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)

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

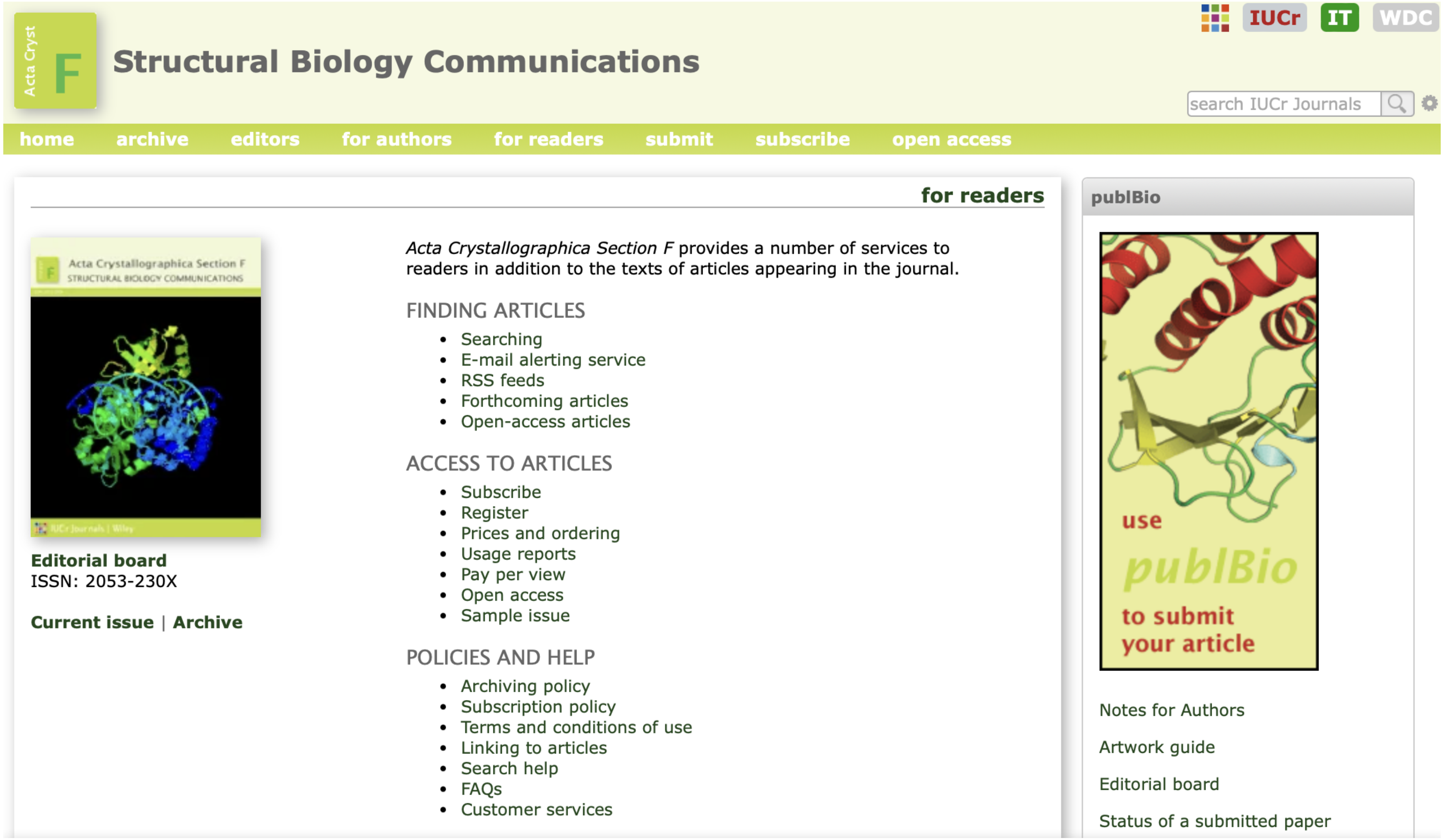
CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond

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.



Structural Biology Communications

for readers

Editorial board
ISSN: 2053-230X

Current issue | **Archive**

Acta Crystallographica Section F provides a number of services to readers in addition to the texts of articles appearing in the journal.

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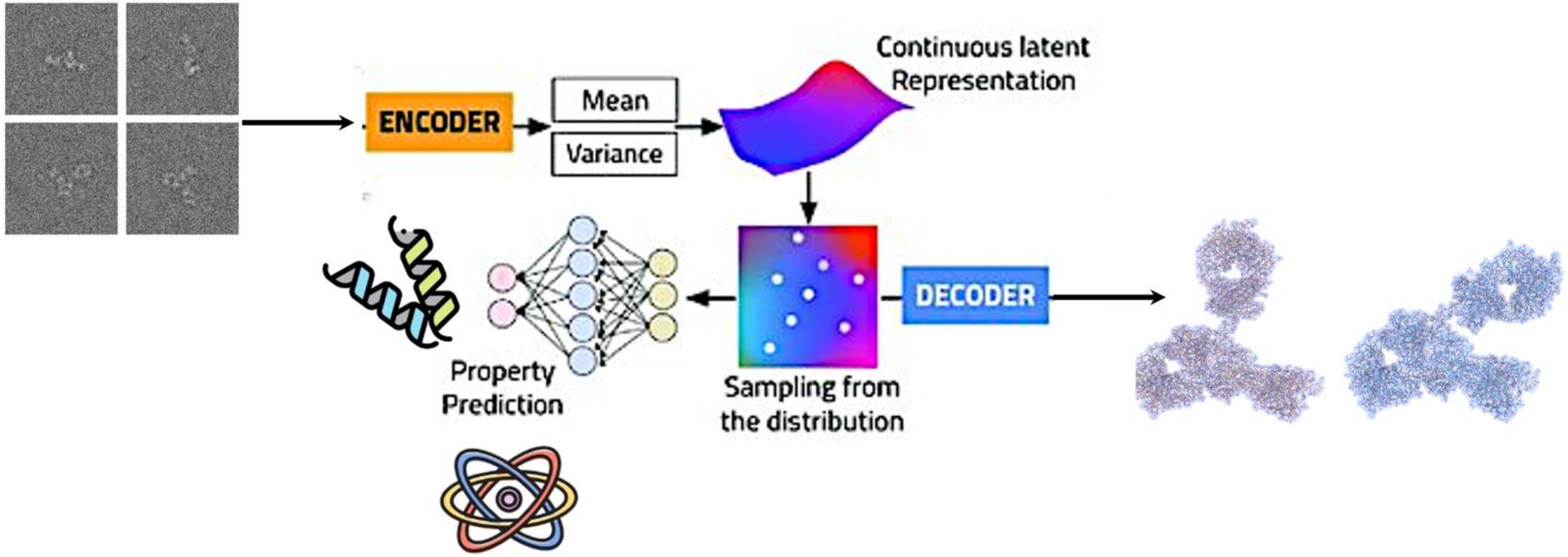
Artwork guide

Editorial board

Status of a submitted paper

Computational Postdoctoral Fellow (Cryo-EM)



JOB DESCRIPTION

In this exciting role, you will develop new mathematical approaches and computational algorithms to investigate protein conformational states from cryo-electron microscopy (Cryo-EM) experiments, including single-particle imaging and cellular tomography. This work will involve research and development of new hybrid methods that combine deep generative modeling, traditional optimization-based methods, numerical linear algebra, and Fourier analysis.

You can see the full position description by going to the job posting #104578 at [jobs.lbl.gov.](https://jobs.lbl.gov)

APPLY TODAY

Scan QR Code to see full job listing

Acknowledgements

Berkeley Laboratory
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Los Alamos Laboratory/New Mexico Consortium
Tom Terwilliger, Li-Wei Hung

Baylor College of Medicine
Matt Baker

Cambridge University
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University of Washington
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Oak Ridge National Laboratory
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David Abrahams
Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

The Phenix Project

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Please fill out the survey!

Sunday, July 20th

2.1.6 Combining experimental data with predicted models for structure determination

(chair: **Christopher Williams**)

2.1.3 Innovations in Algorithms and Computational Methods

10:30am **Pavel Afonine**: Analytical Differentiable Finite-Resolution Density Map Calculation
11:10 am **Alisia Fadini**: AlphaFold as a Prior: Guiding Protein Structure Prediction with Rocket

2.2.4 General Interest II

2:00 pm **Billy Poon**: New and Updated Features in Phenix

2.2.1 Emerging Modalities in Pharma Part 2

3:30 pm **Dorothee Liebschner:** Validating Ligands with Phenix

Survey