

Program

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16:30	Q&A
16:50	Finish: workshop survey and wrap up



U.S. DEPARTMENT OF
ENERGY



**UNIVERSITY OF
CALIFORNIA**

Phenix User Workshop, July 29 2022



Introduction

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Lawrence Berkeley Laboratory



**UNIVERSITY OF
CAMBRIDGE**

The Project



Lawrence Berkeley Laboratory

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Moriarty, Billy Poon,
Christopher Schlicksup,
Oleg Sobolev



University of Cambridge

Randy Read, Airlie McCoy,
Tristan Croll, Rob Oeffner



Los Alamos National Laboratory New Mexico Consortium

Tom Terwilliger, Li-Wei Hung



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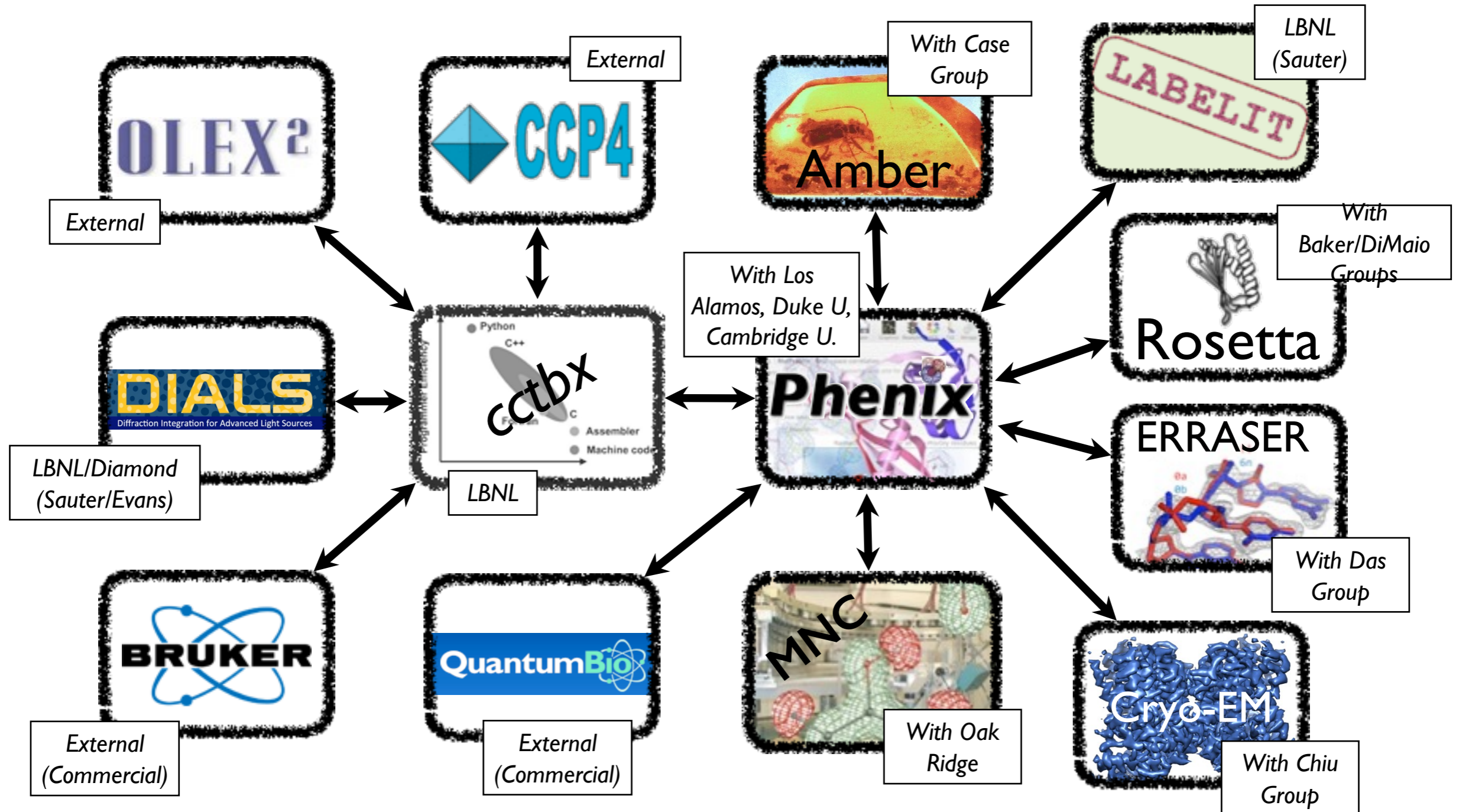


An NIH/NIGMS funded
Program Project

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

Phenix - a Structural Biology Hub

We have nucleated the development of new computational methods for structural biology



What is *Phenix*?

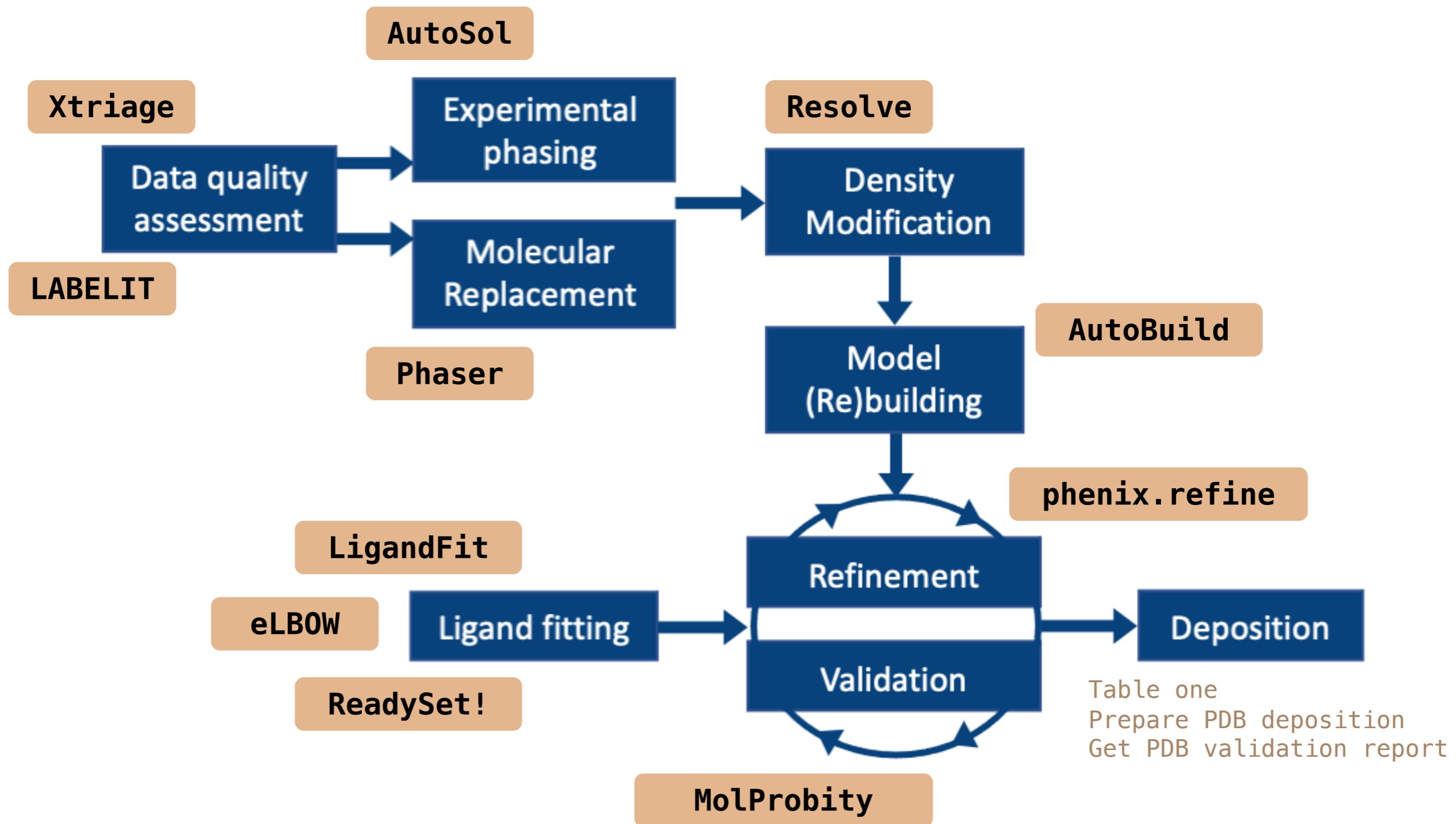
- Package for **automated structure solution**
- Modern programming concepts and new algorithm development
- Designed to be used by **both novices and experienced users**
- Long-term development and **support**
- Why is it called *Phenix*?

Python **H**ierarchical **E**Nvironment for **I**ntegrated **X**tallography

Key Features

- **Python**
 - Easy scripting of repetitive tasks
 - Enables rapid prototyping and development
- **Advanced algorithms**
 - Experimental phasing
 - Molecular replacement
 - Automated model building and rebuilding
 - Structure refinement and validation
 - Ligand coordinate and restraint generation
- **Rapid development and bug fixing**

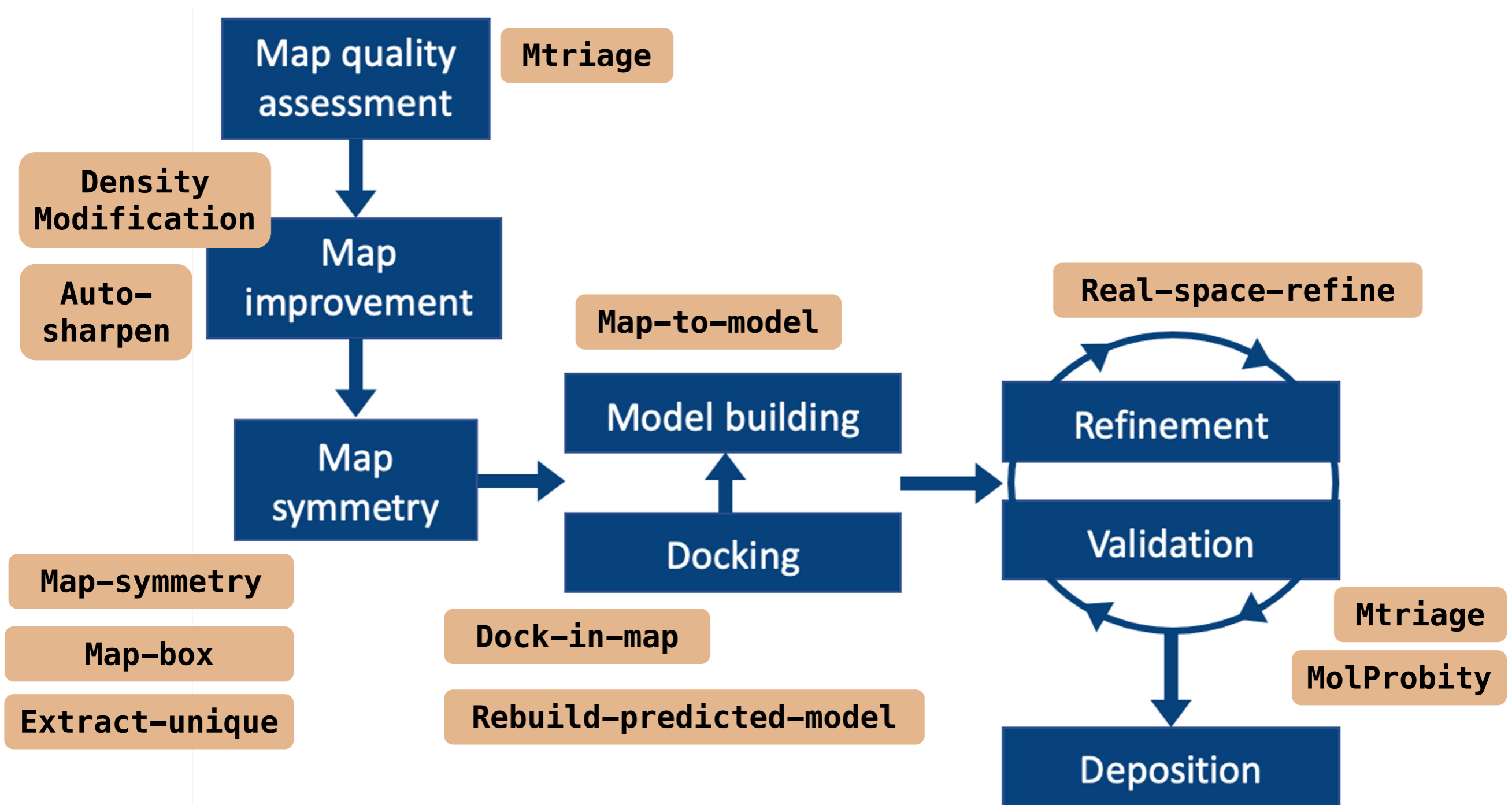
Tools for Crystallography



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)

Tools for Cryo-EM



Phenix GUI

Central GUI to view job control and 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 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 tools and 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

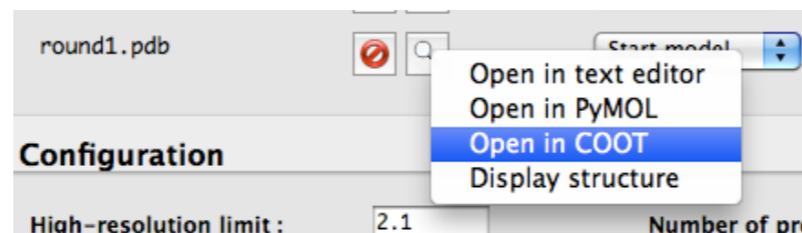
At the bottom, there is a 'Current directory' field showing '/Users/dcliebschner/Desktop/Projects/test' and a 'Browse...' button. The status bar at the very bottom indicates 'PHENIX version dev-svn-000' and 'Project: test'.

Coot/PyMOL integration

- Most results can be opened directly in graphics apps



- Any PDB file listed in GUI can also be opened

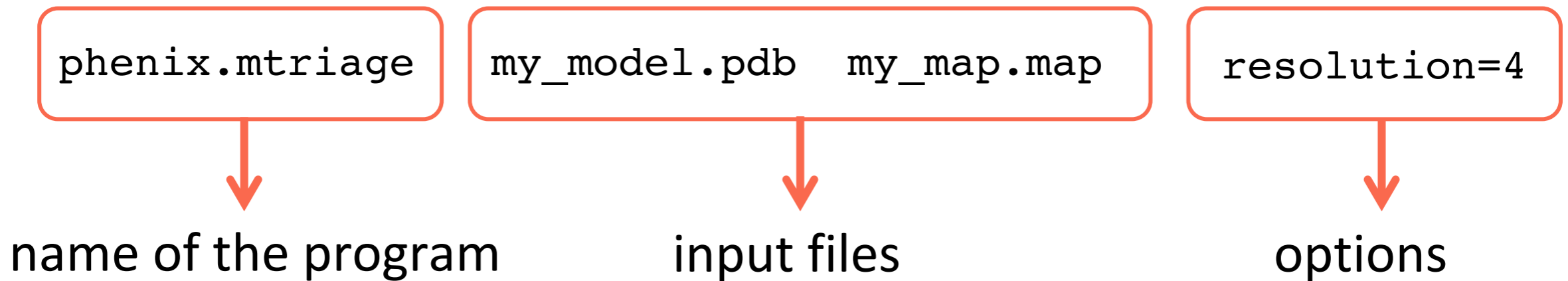


- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running
- Coot must have Python support (default on Mac)
- Specific paths to executables usually required on Linux

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

Command Line Tools

Run on the terminal



Run in a python script

```
try:  
    easy_run.call("phenix.mtriage my_model.pdb my_map.map")  
except Exception as e:  
    msg = traceback.format_exc()  
    print(msg)
```

Phenix Availability

phenix-online.org

Supported on:

- Linux (RedHat, Fedora)
- Mac OSX
- Windows

Extensive documentation
(online and via GUI)

Nightly builds

Phenix

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

NEW: Phenix with AlphaFold models

- Trim, weight, create domains and use for molecular replacement
- Trim, dock into cryo-EM maps and fill in gaps
- Reference models for refinement

[Learn more](#)

Cryo-EM map and superposed, refined AlphaFold model

Download | Getting Started | Workshops & Tutorials | Documentation | Help | Developers | National Resource | Industrial Consortium

Version	Date	Status	Logs	Info
dev-3758	2020-01-22	successful	ci , intel-linux-2.6-x86_64-centos6 , mac-intel-osx-x86_64 , intel-windows-x86_64	docs ; changelog
dev-3753	2020-01-17	successful	ci , intel-linux-2.6-x86_64-centos6 , mac-intel-osx-x86_64 , intel-windows-x86_64	docs ; changelog
dev-3751	2020-01-15	successful	ci , intel-windows-x86_64 , intel-linux-2.6-x86_64-centos6 , mac-intel-osx-x86_64	docs ; changelog
1.17.1-3660	2019-10-16	successful	ci , intel-windows-x86_64 , intel-linux-2.6-x86_64-centos6 , mac-intel-osx-x86_64	Official 1.17.1 release; docs ; changelog

Video Tutorials

www.youtube.com/channel/UCcdl0hfHngWAZLJWynxPQWg/videos

YouTube IT Search

Phenix Tutorials

560 subscribers

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Video Title	Duration	Views	Time Ago
real_space_refine Tutorial	5:27	763	7 months ago
Secondary Structure Restraints Tutorial	6:23	399	8 months ago
Multiple refinement strategies and...	5:46	281	8 months ago
Planning a SAD experiment Tutorial	6:00	483	1 year ago
Map-to-model Tutorial	5:33	1.3K	1 year ago
Scale-and-merge Tutorial	7:31	387	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, Nigel Moriarty, Miffy Mifsud, Tom Terwilliger

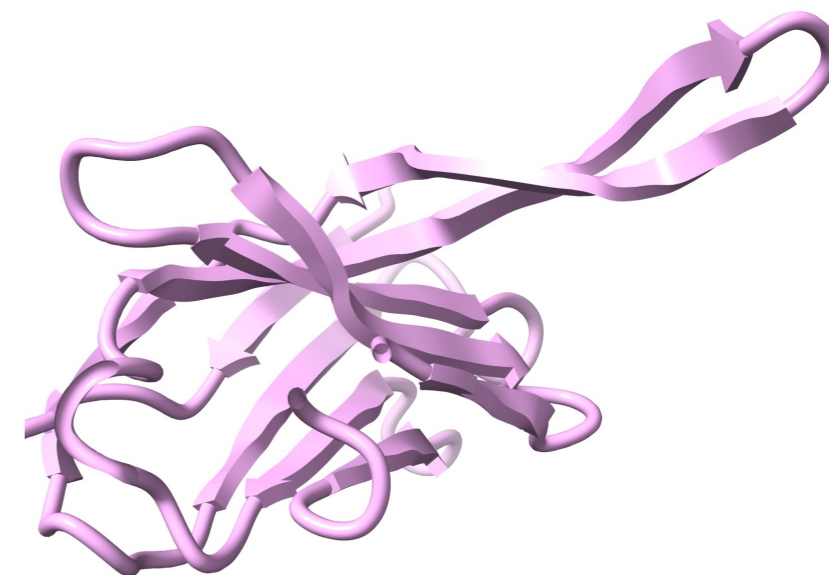
Accurate predicted models



EVQLVESGGGLVQPGGSLRLSCAASGFN**I**YSS**S**IHWVRQAPGKGLEWVAYI
.....**F**.....**M**.....Q.....
.....K.....**Y**.....**L**.....A.....
.....A.....V.....
.....A.....
.....**L**.....**V**.....E.....
.....A.....Q.....

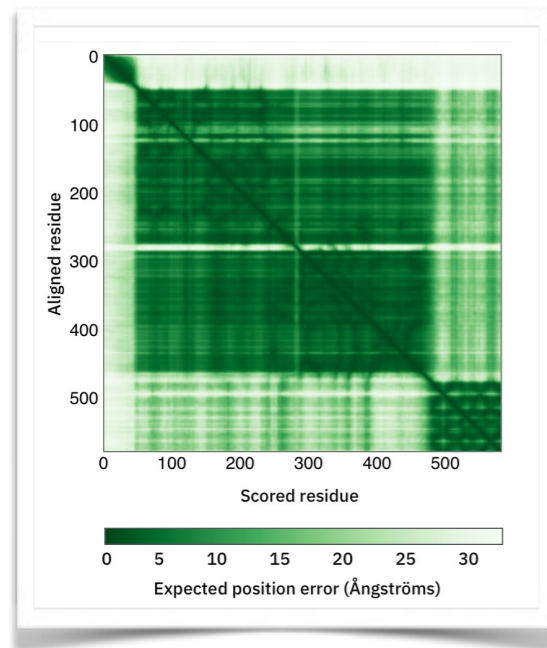
Sequence

Multiple sequence alignment

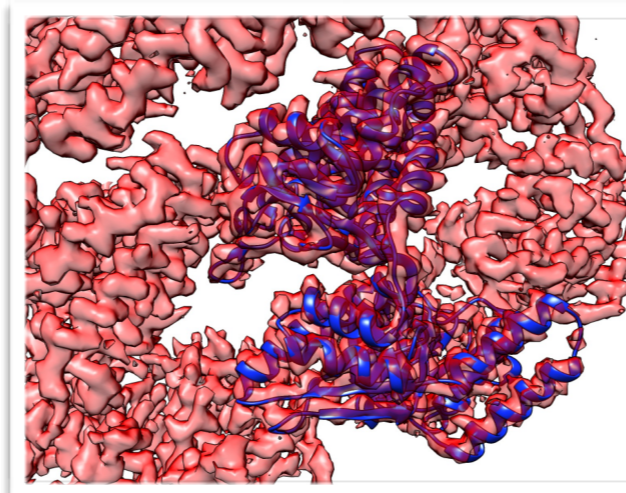


3D prediction

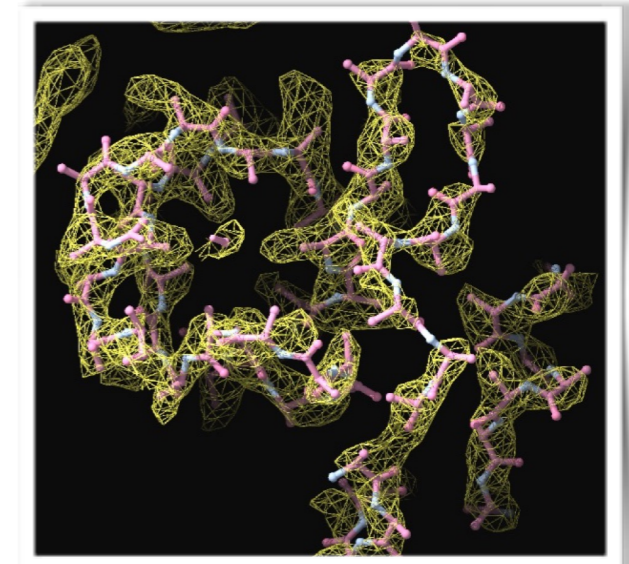
New tools for predicted models in Phenix



Process predicted model



Dock_predicted_model



Rebuild predicted model



Phenix Tutorials



Phenix Tutorials
1.45K subscribers



Tom Terwilliger: AlphaFold changes everything

Acknowledgements

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Baylor College of Medicine

Matt Baker

Cambridge University

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David Abrahams
Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

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