Phenix User Workshop, ACA 2024

Introduction to Phenix

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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 Hierarchical ENvironment for Integrated Xtallography

The Phenix Project

Lawrence Berkeley Laboratory

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BERKELEY LAB

Los Alamos National Laboratory
New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

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UNIVERSITY OF CAMBRIDGE

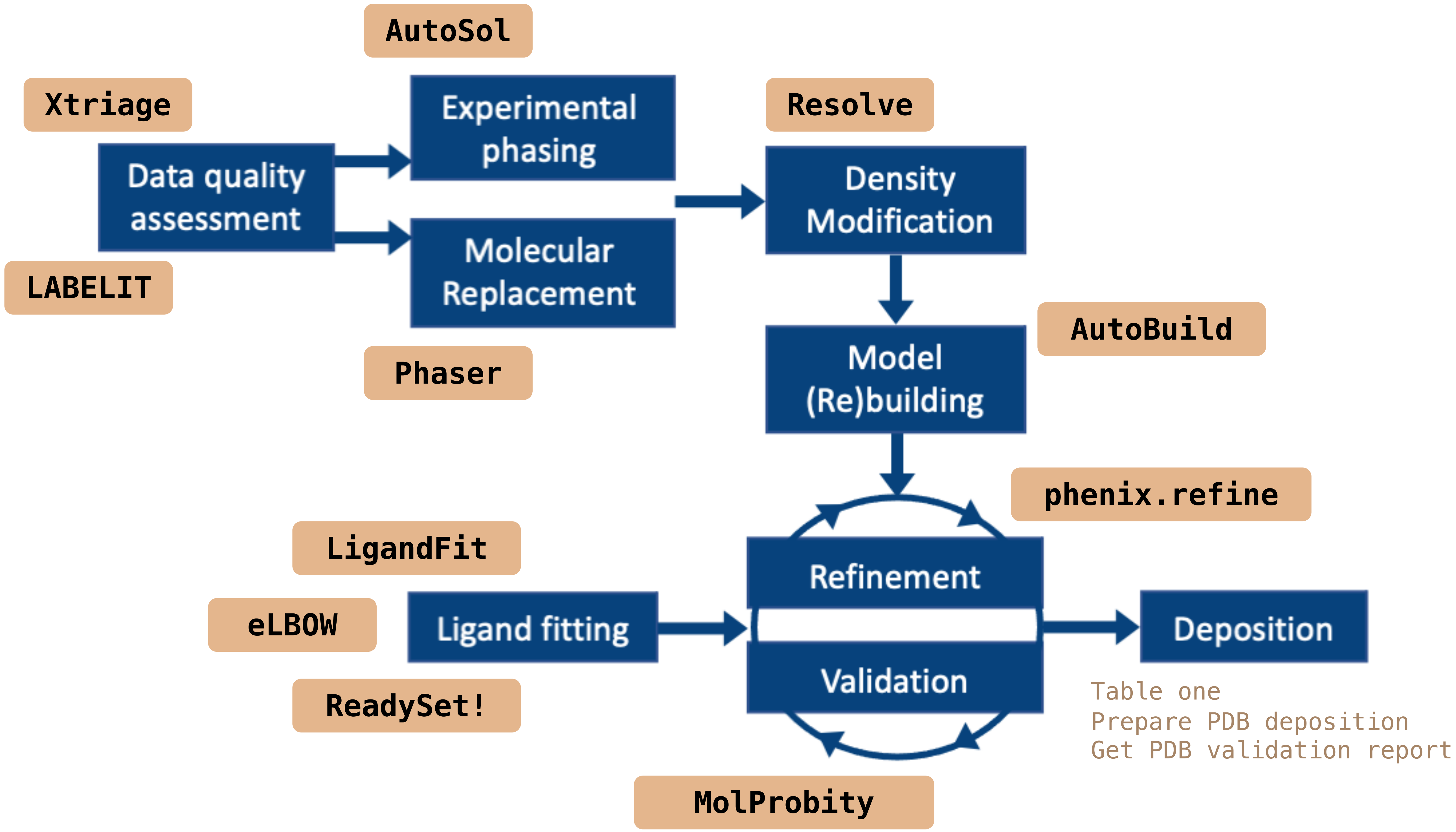
Duke University

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



AutoSol

Xtriage

Data quality assessment

LABELIT

Experimental phasing

Molecular Replacement

Phaser

Resolve

Density Modification

AutoBuild

Model (Re)building

phenix.refine

Refinement

Validation

MolProbity

LigandFit

eLBOW

Ligand fitting

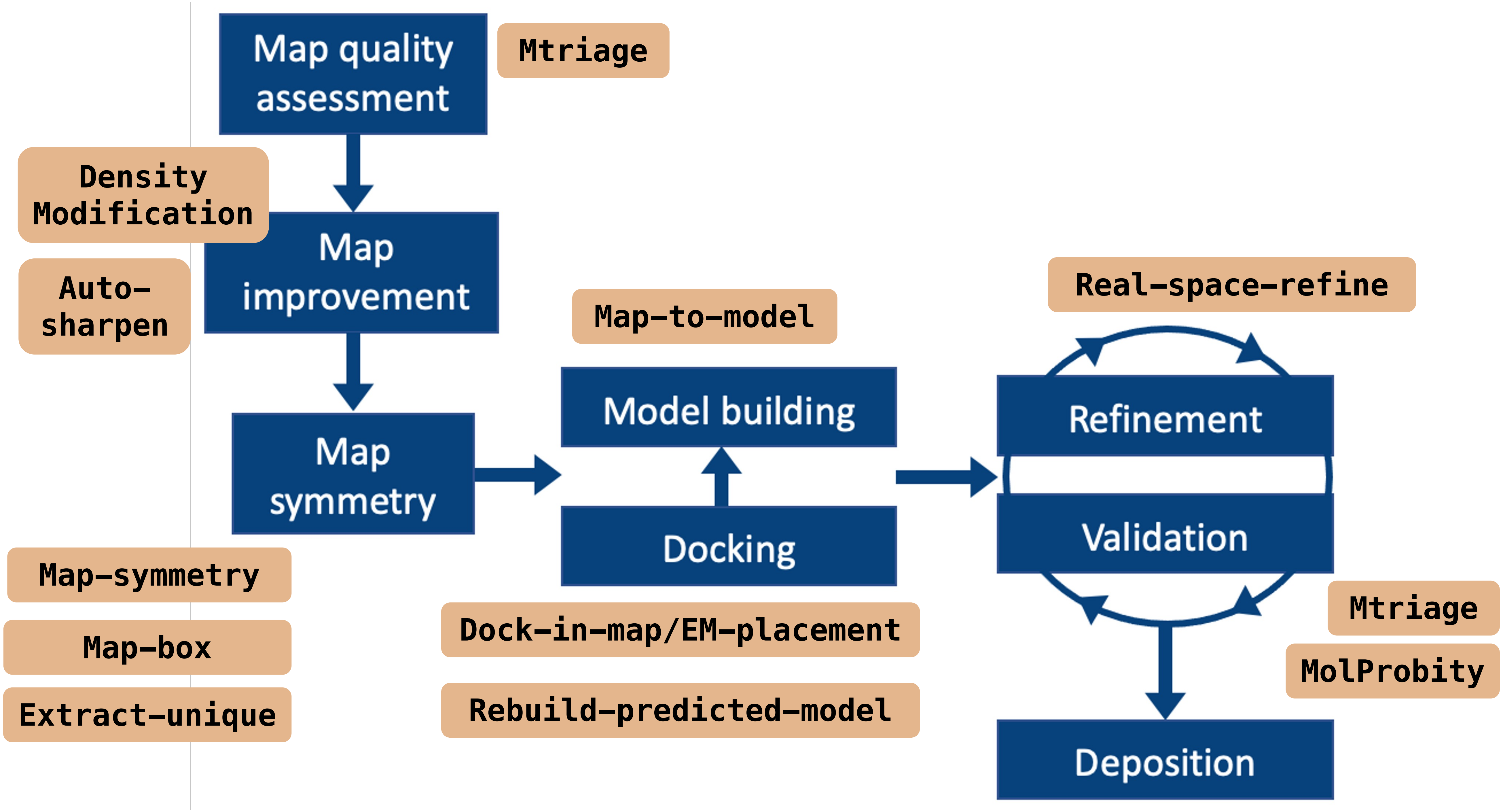
ReadySet!

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)

Tools for Cryo-EM



Map quality assessment

Mtriage

Map improvement

Density Modification

Auto-sharpen

Map symmetry

Map-symmetry

Map-box

Extract-unique

Model building

Map-to-model

Docking

Dock-in-map/EM-placement

Rebuild-predicted-model

Refinement

Real-space-refine

Validation

Mtriage

MolProbity

Deposition

Acta Cryst. 2002, D58:1948-1954 (Phenix)
J. Appl. Cryst. 2002, 35:126-136 (cctbx)
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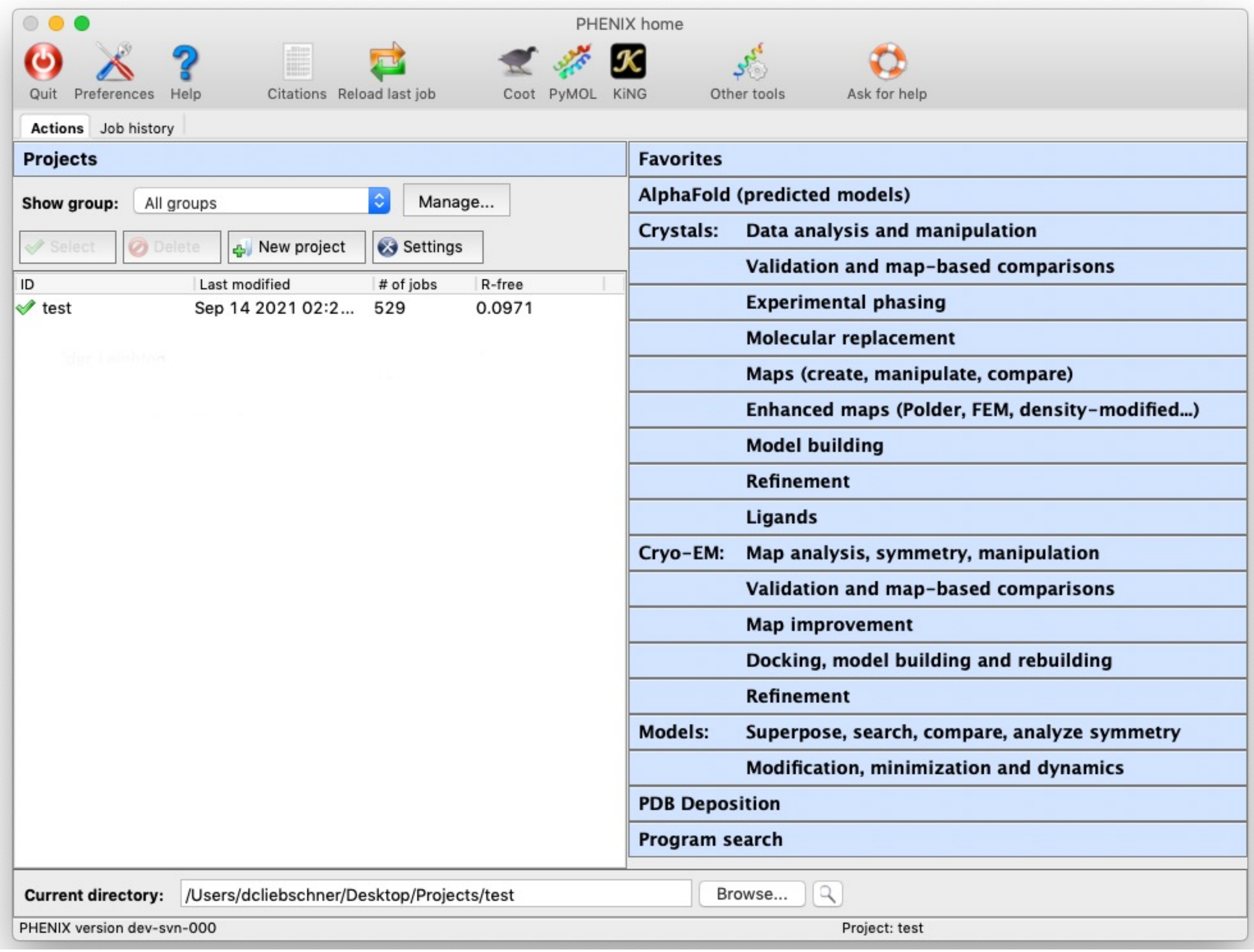
Features

Phenix 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

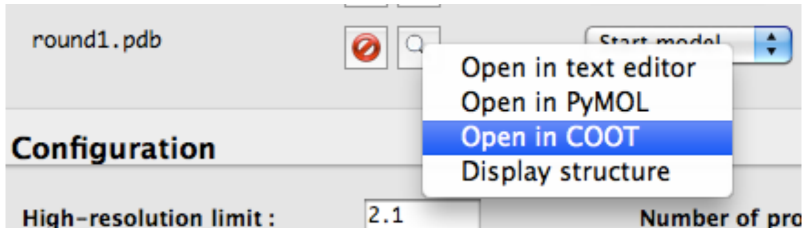
PHENIX version dev-svn-000

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


round1.pdb

Configuration

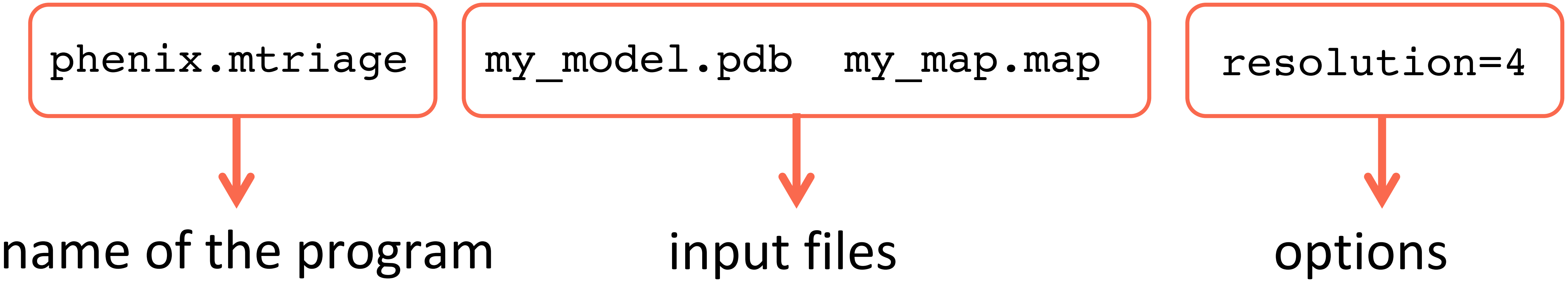
High-resolution limit : 2.1

- 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



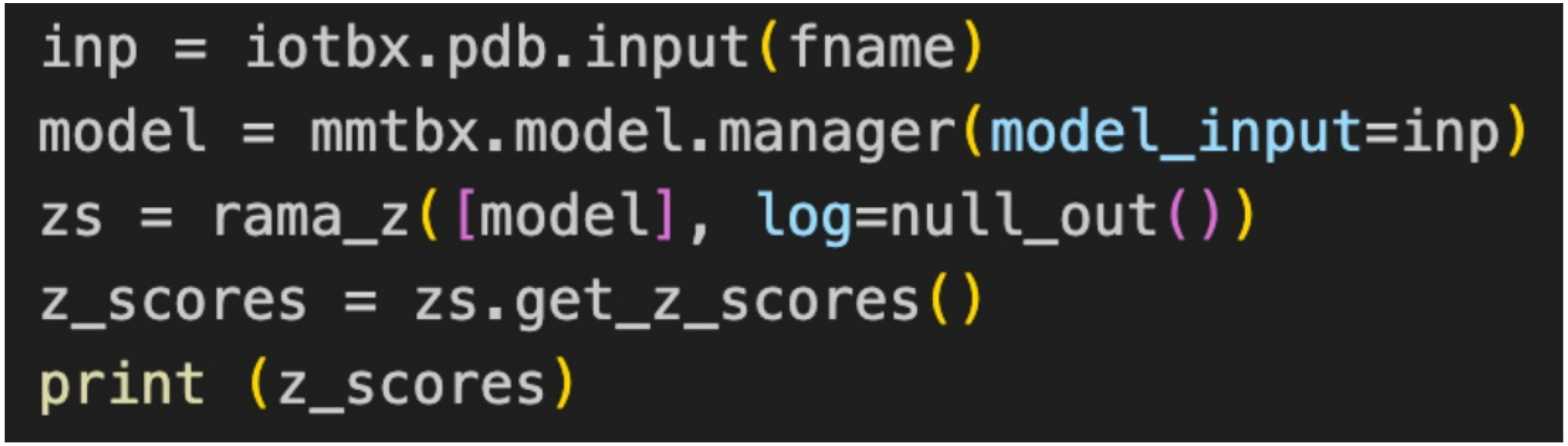
`phenix.mtriage` `my_model.pdb my_map.map` `resolution=4`

name of the program

input files

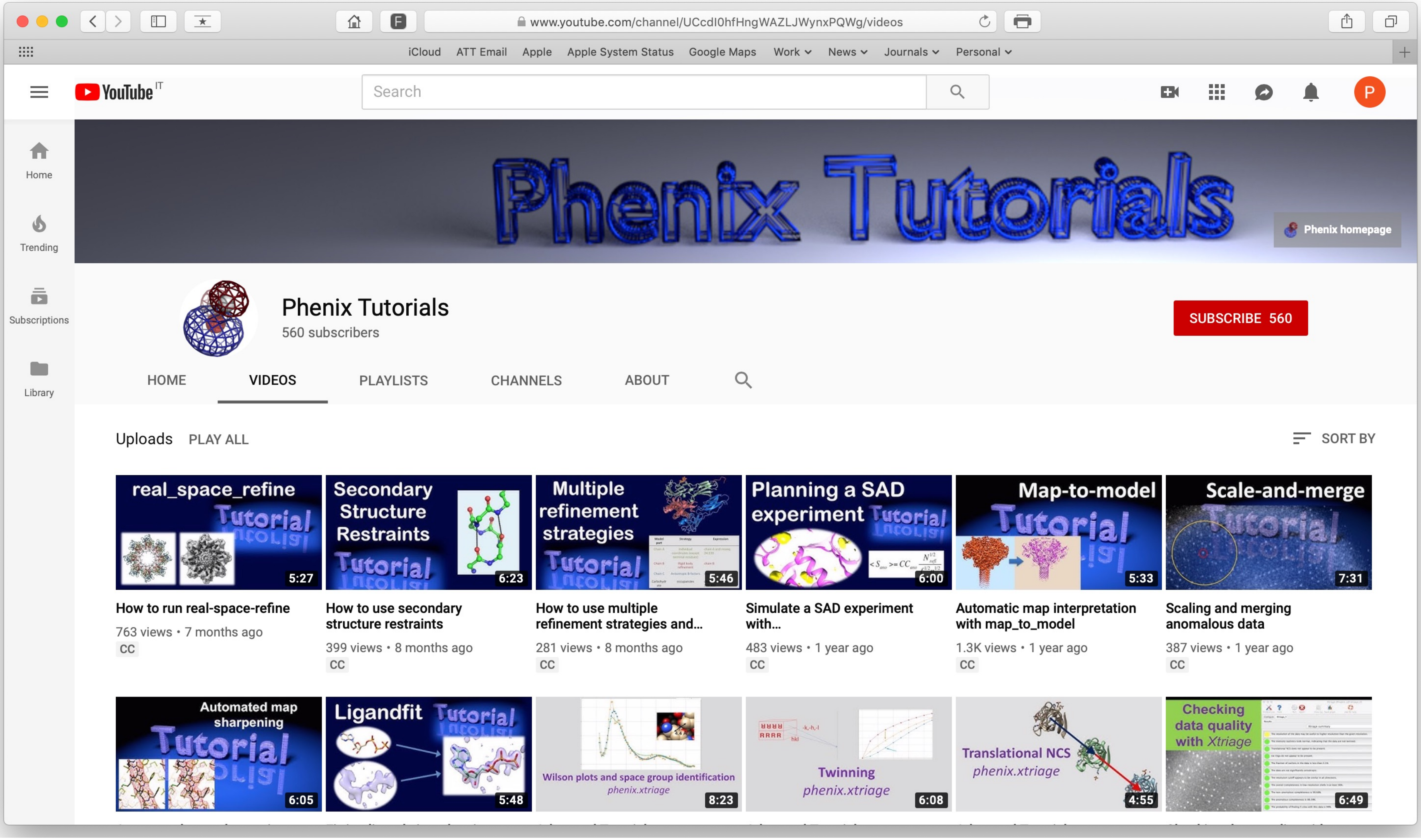
options

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



Phenix Tutorials

560 subscribers

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How to use secondary structure restraints
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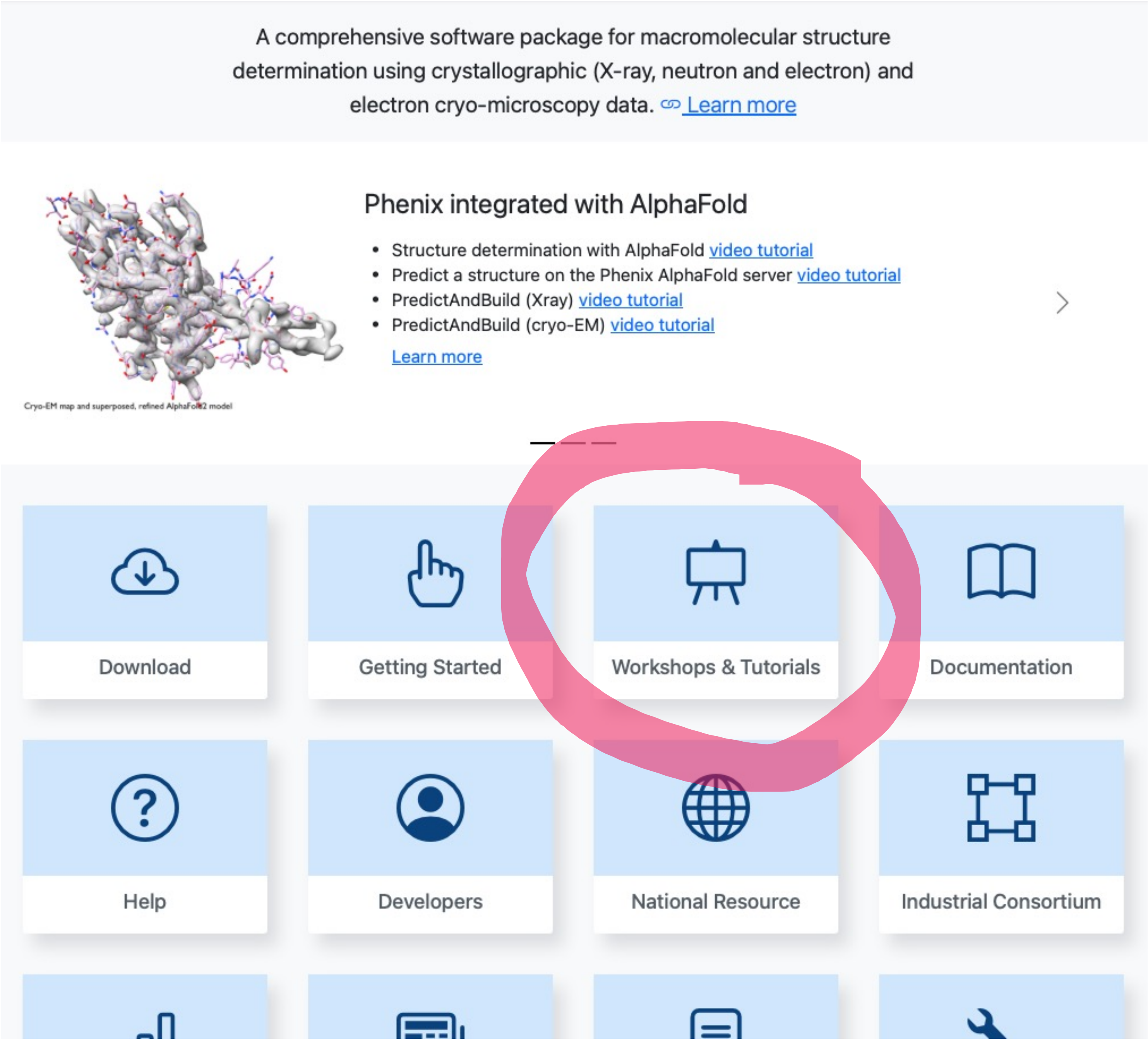
1.3K views • 1 year ago

Scaling and merging anomalous data
387 views • 1 year ago

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

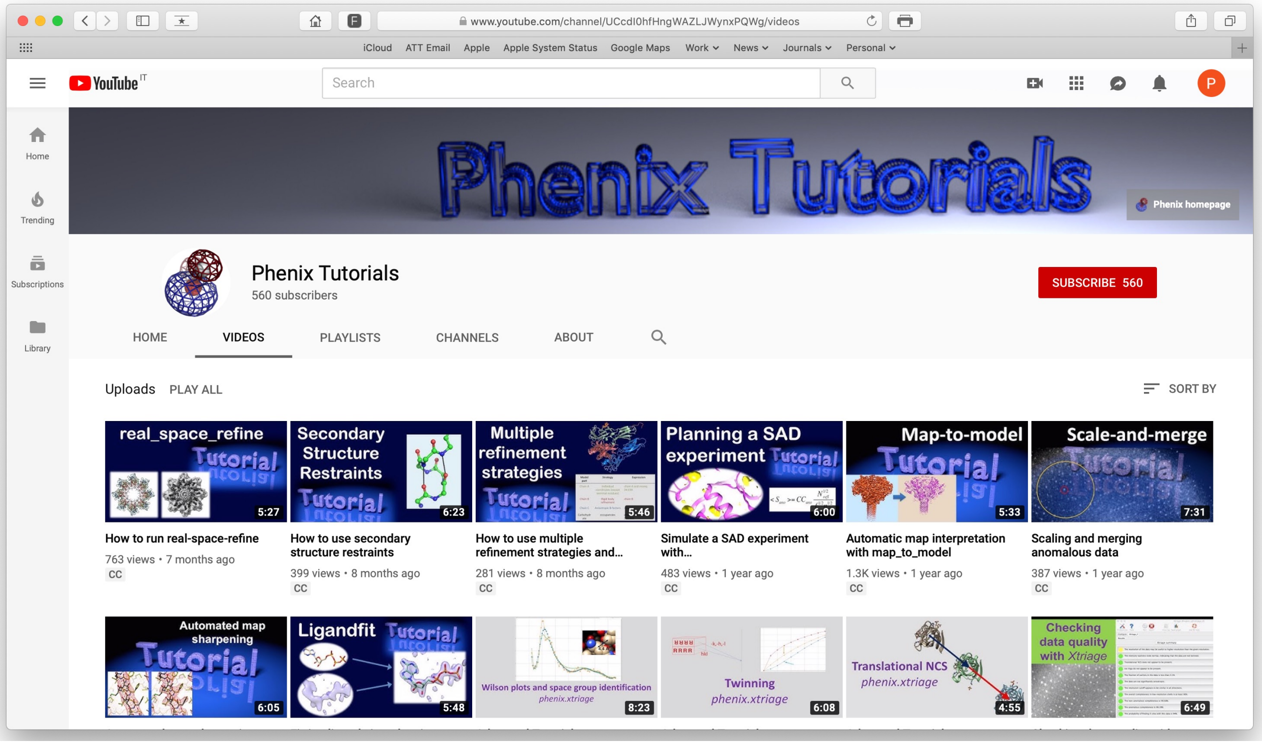
Phenix integrated with AlphaFold

- 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



Phenix Tutorials
560 subscribers

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Automatic map interpretation with map_to_model
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5:33

Scaling and merging anomalous data
387 views • 1 year ago
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7:31

6:05

5:48

8:23

6:08

4:55

6:49

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Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

Practical information

- Morning break: 10am (15 min)
- Afternoon break: 2:45 pm (15 min)
- Lunch break: 11:45 – 12:45
- We do not provide lunch!
  - Pint Brothers Alehouse
  - Wendy’s (< 10min walk)