Phenix User Workshop, Duke September 2024

Introduction to Phenix

Dorothee Liebschner

Lawrence Berkeley Laboratory

Time	Agenda	Lecturers
8:30	Arrival, coffee/snacks, discussion	
9:00	Welcome/Introduction to Phenix (15 min)	D. Liebschner
9:15	Using AlphaFold predictions for structure determination (30 min)	T. Terwilliger
9:45	MR/Docking (30 min)	R. Read
10:15	15 min break	
10:30	**Tutorial 1** (30 min) ● AlphaFold structure prediction ● Cryo-EM docking with Emplace Local	R. Read, T. Terwilliger
11:00	**Tutorial 2**: MR/MR-SAD with AlphaFold (30 min)	R. Read
11:30	Ligands (30 min)	N. Moriarty
12:00	1 hour lunch break; on-on-one discussions	
13:00	**Tutorial 3**: Ligands (20 min)	N. Moriarty
13:20	Refinement Xray and cryo-EM (60 min)	P. Afonine
14:20	15 min break	
14:35	**Tutorial 4**: Refinement tutorial (30 min)	P. Afonine
15:05	Validation (45 min)	J. Richardson
15:50	**Tutorial 5** Validation (30 min)	C. Williams
16:20	Discussion and questions, survey questionnaire	
17:00	End	

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

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

Los Alamos National Laboratory
New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

UTHealth

Matt Baker

University of Cambridge

Randy Read, Airlie McCoy, Alisia Fadini

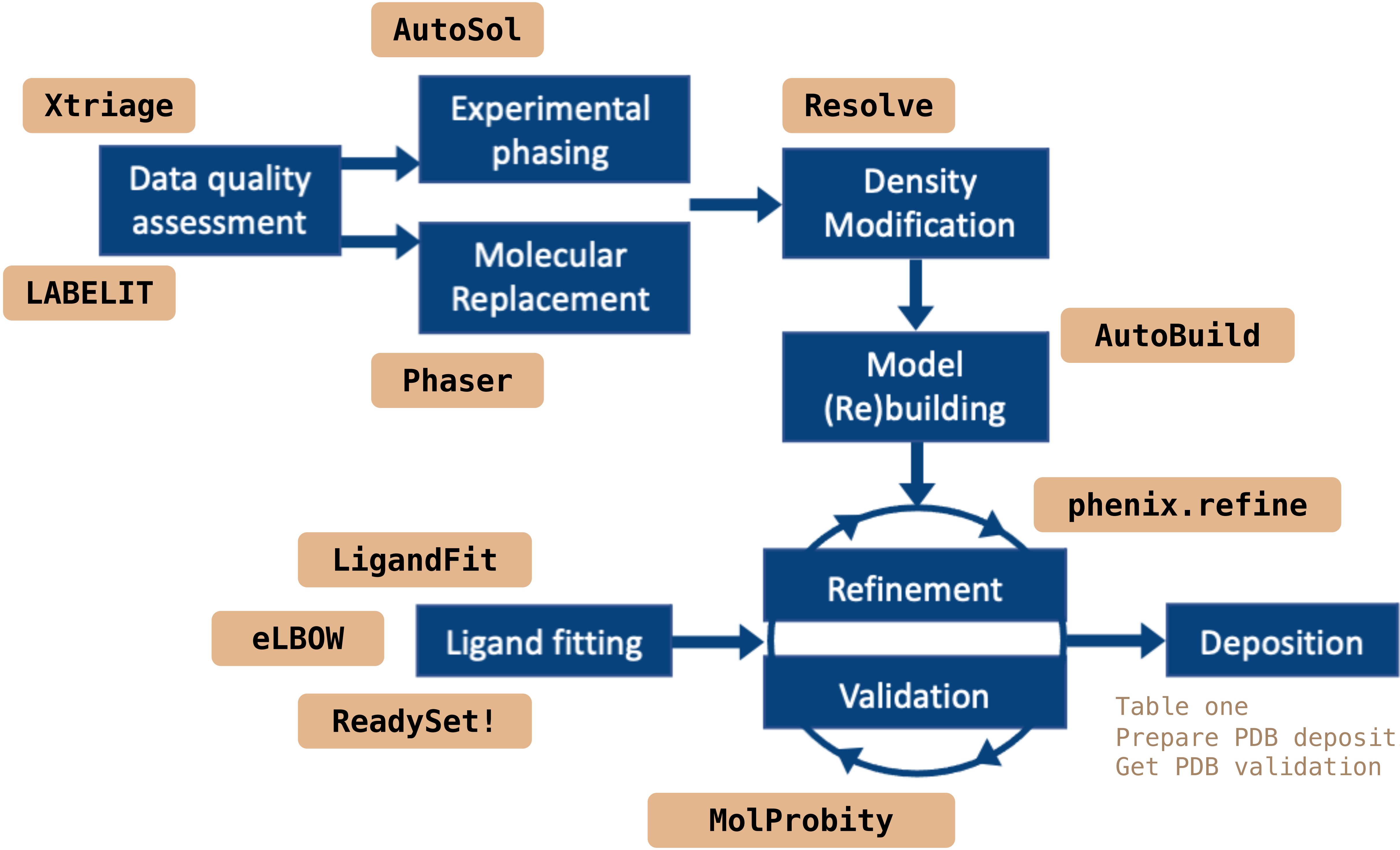
Duke University

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



Xtriage

Data quality assessment

LABELIT

AutoSol

Experimental phasing

Molecular Replacement

Phaser

Resolve

Density Modification

AutoBuild

Model (Re)building

phenix.refine

Refinement

Validation

MolProbity

LigandFit

eLBOW

Ligand fitting

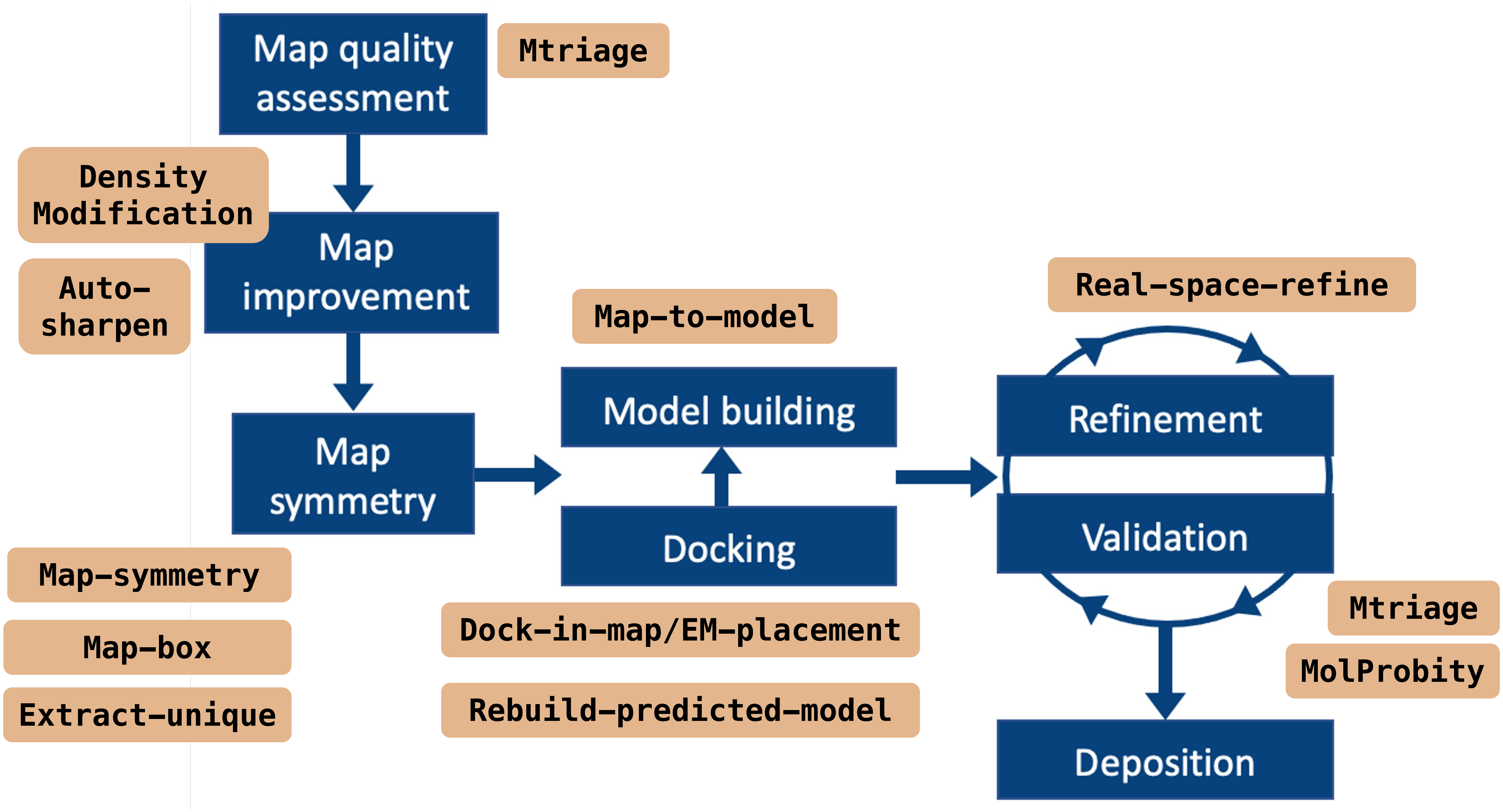
ReadySet!

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

Density Modification

Auto-sharpen

Map improvement

Map symmetry

Map-symmetry

Map-box

Extract-unique

Map-to-model

Model building

Docking

Dock-in-map/EM-placement

Rebuild-predicted-model

Real-space-refine

Refinement

Validation

Mtriage

MolProbity

Deposition

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J. Appl. Cryst. 2002, 35:126-136	(cctbx)
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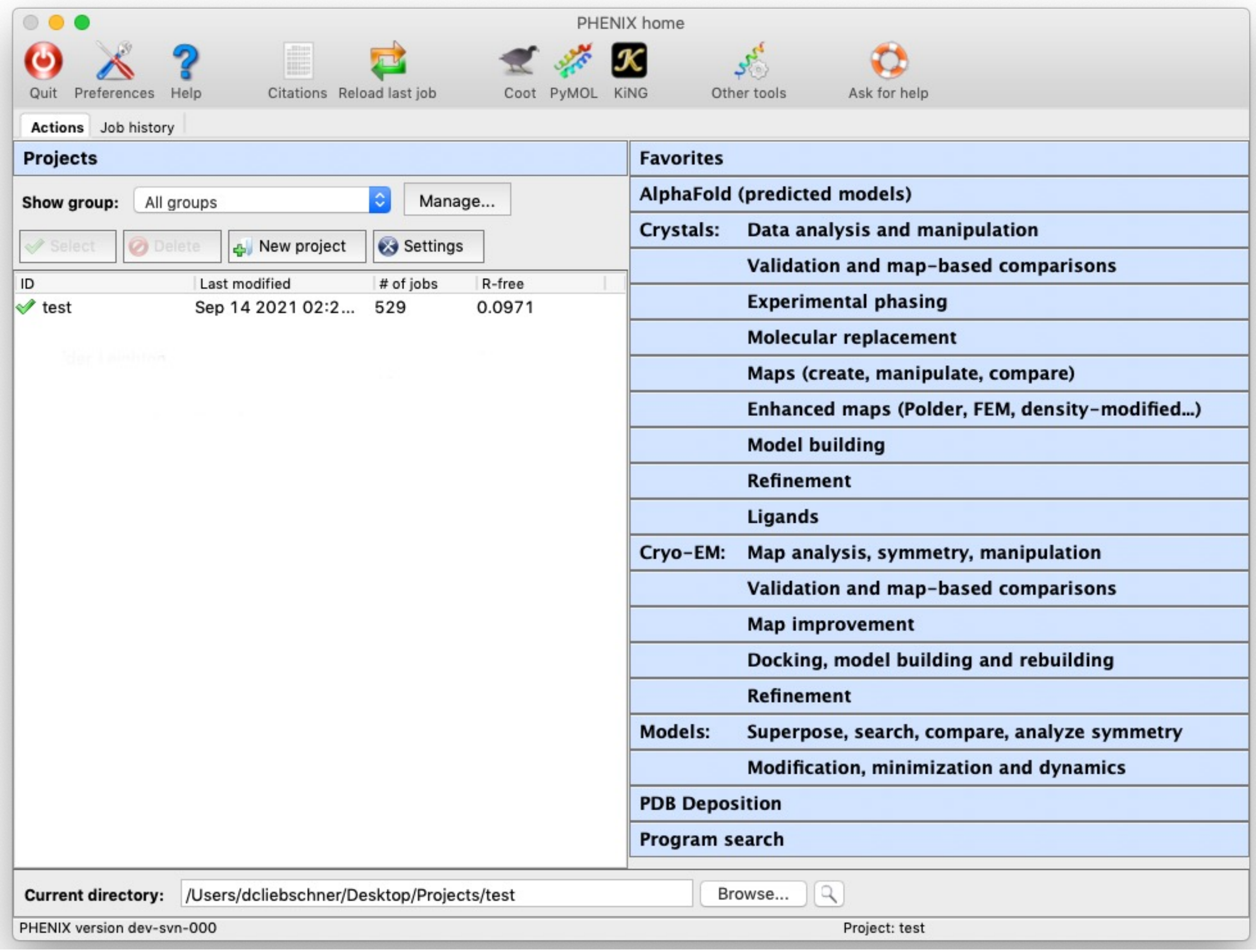
Acta Cryst. 2019 D75:861–877	(Phenix)

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

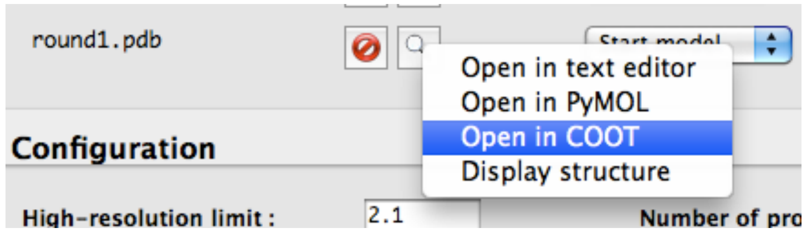
PHENIX version dev-svn-000

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



High-resolution limit : 2.1

- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running

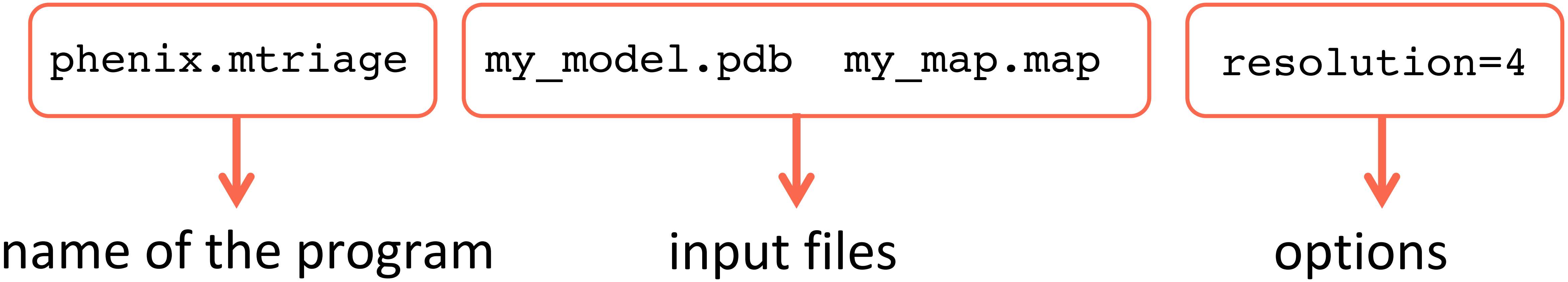
- Coot must have Python support (default on Mac)

- Specific paths to executables usually required on Linux

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

Command Line Tools

Run on the terminal



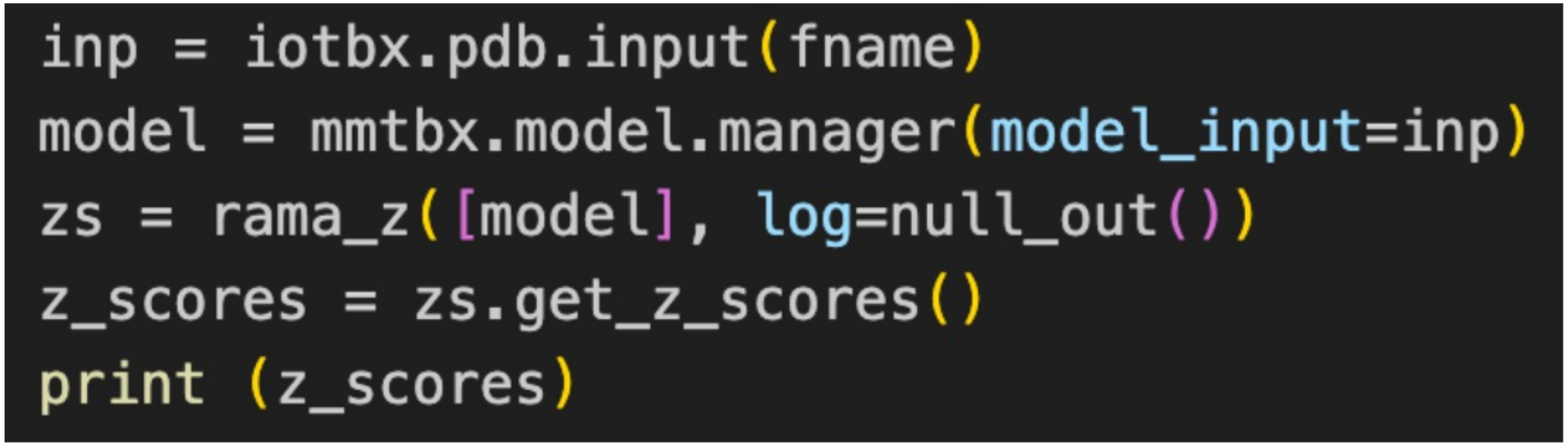
```
phenix.mtriage   my_model.pdb   my_map.map   resolution=4
```

name of the program

input files

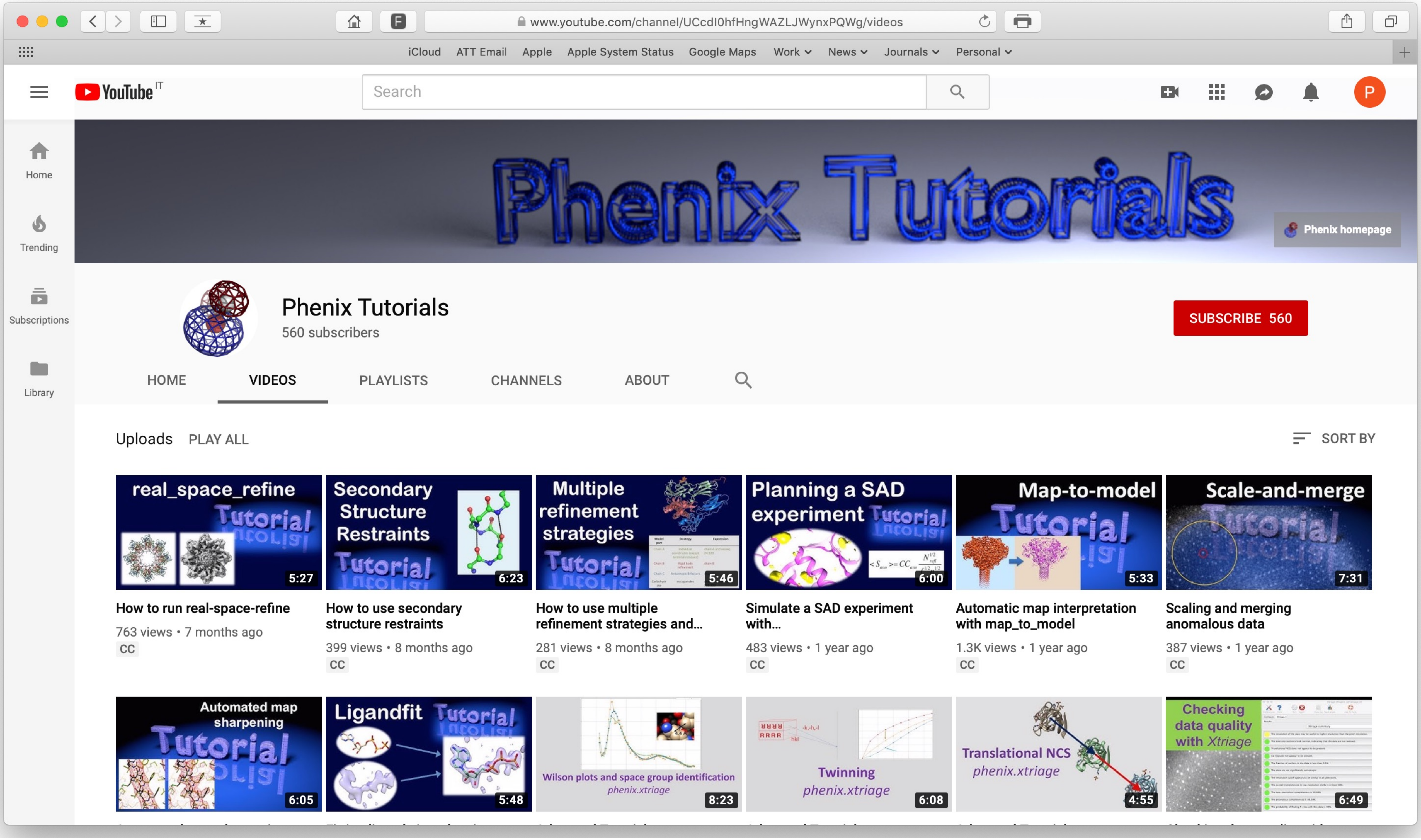
options

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



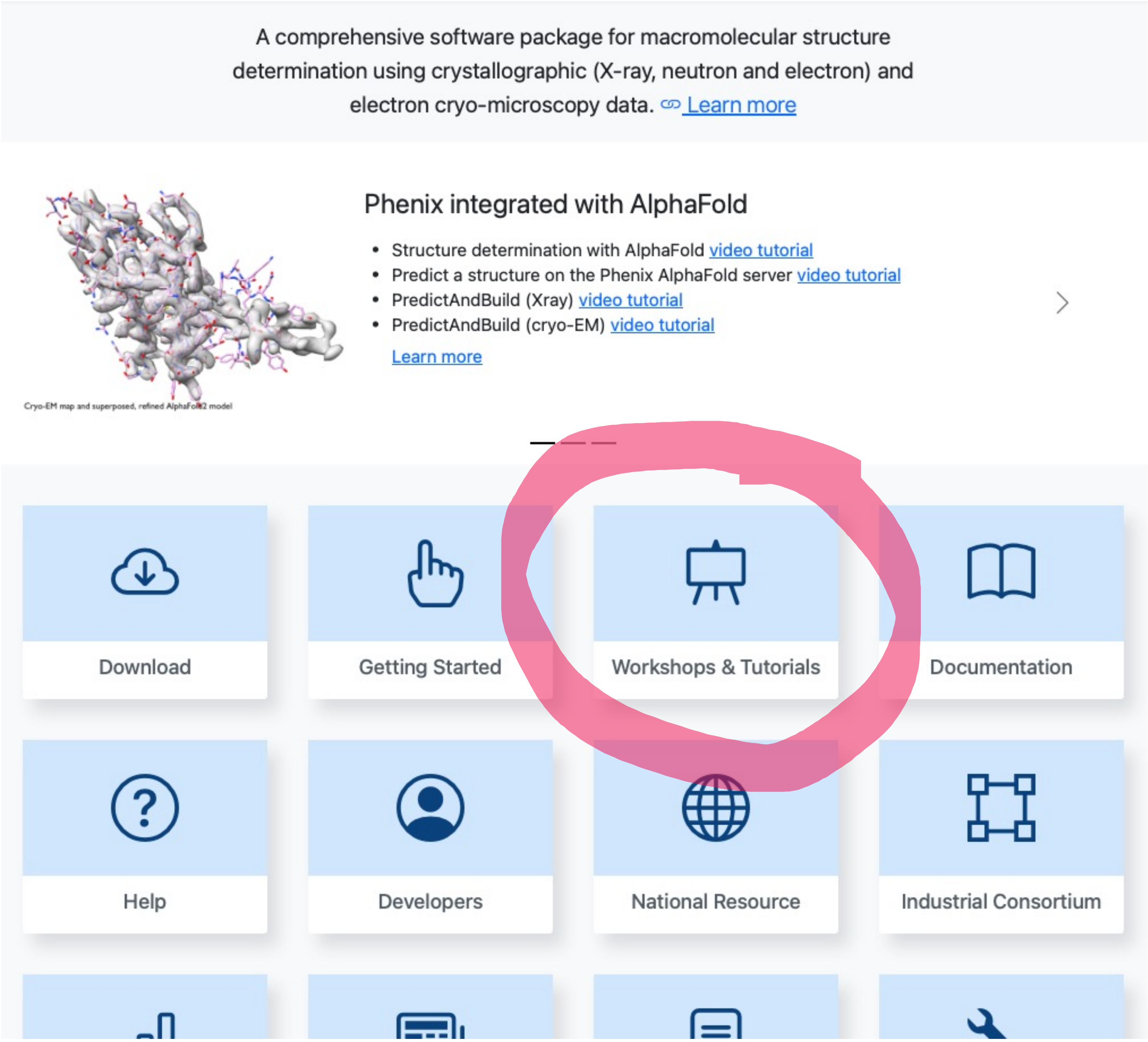
Phenix Tutorials
560 subscribers

- How to run real-space-refine — 5:27 — 763 views • 7 months ago — CC
- How to use secondary structure restraints — 6:23 — 399 views • 8 months ago — CC
- How to use multiple refinement strategies and... — 5:46 — 281 views • 8 months ago — CC
- Simulate a SAD experiment with... — 6:00 — 483 views • 1 year ago — CC
- Automatic map interpretation with map_to_model — 5:33 — 1.3K views • 1 year ago — CC
- Scaling and merging anomalous data — 7:31 — 387 views • 1 year ago — CC
- 6:05
- 5:48
- 8:23
- 6:08
- 4:55
- 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

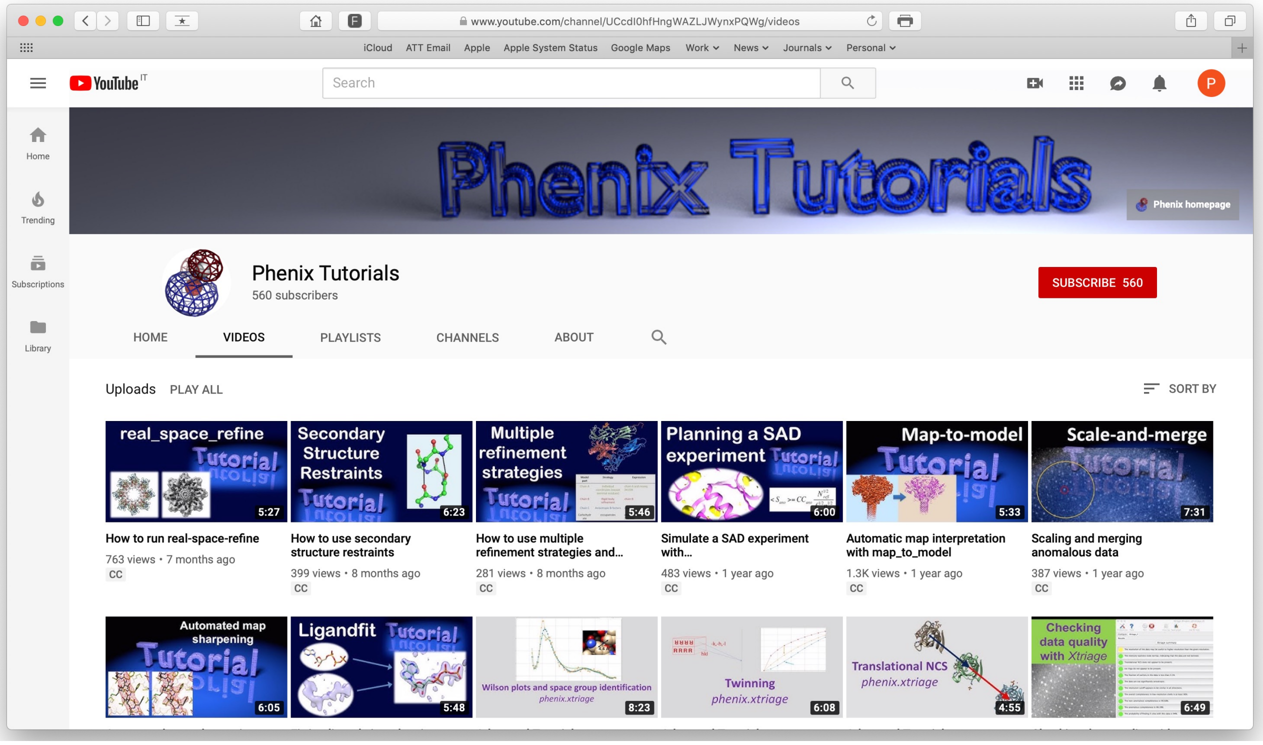
Phenix integrated with AlphaFold

- 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



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Uploads PLAY ALL

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763 views • 7 months ago

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Acknowledgements

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David Abrahams
Phenix Testers & Users

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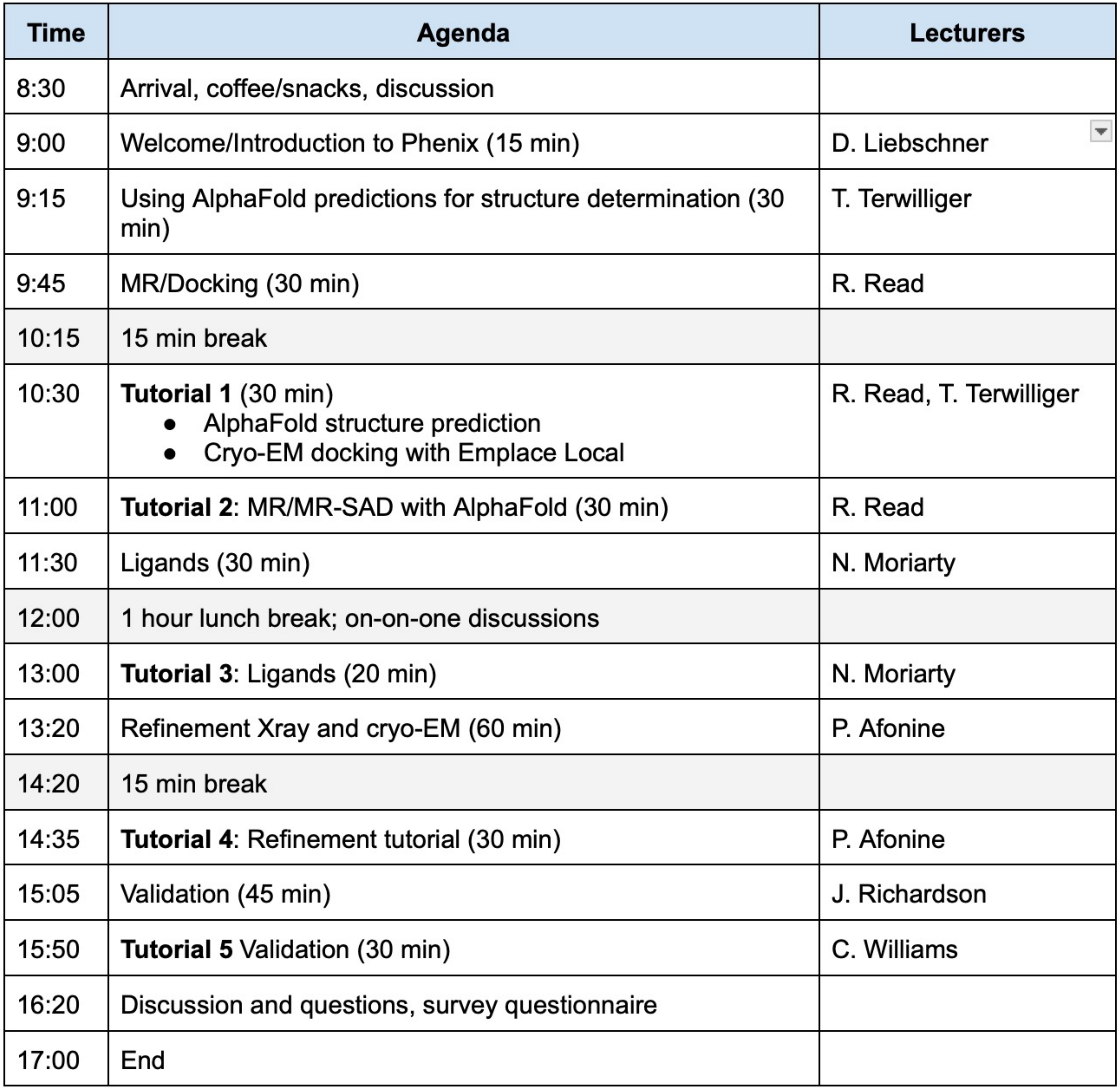
- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

Practical information

- Morning break: 10:15 am (15 min)
- Afternoon break: 2:20 pm (15 min)
- Lunch break: 12pm – 1pm
- We do not provide lunch (lots of options in walking distance)



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