Phenix User Workshop, August 22nd 2023

Introduction

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Lawrence Berkeley Laboratory

What is Phenix?

What is *Phenix*?

- Package for **automated structure solution** (crystallography, cryo-EM)
- 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 **EN**vironment for **I**ntegrated **X**tallography

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

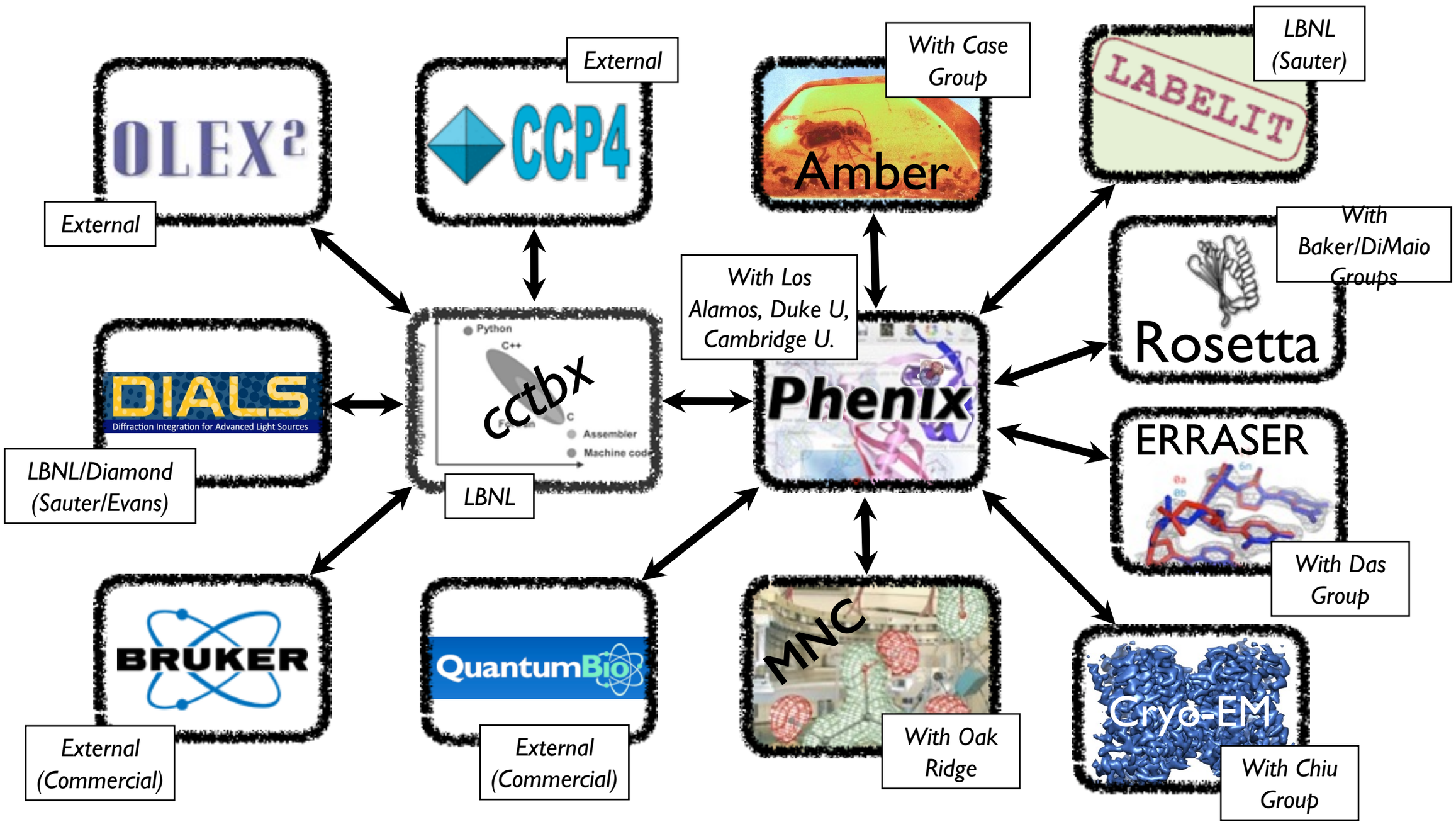
Jane & David Richardson, Christopher Williams, Vincent Chen

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

Phenix - a Structural Biology Hub

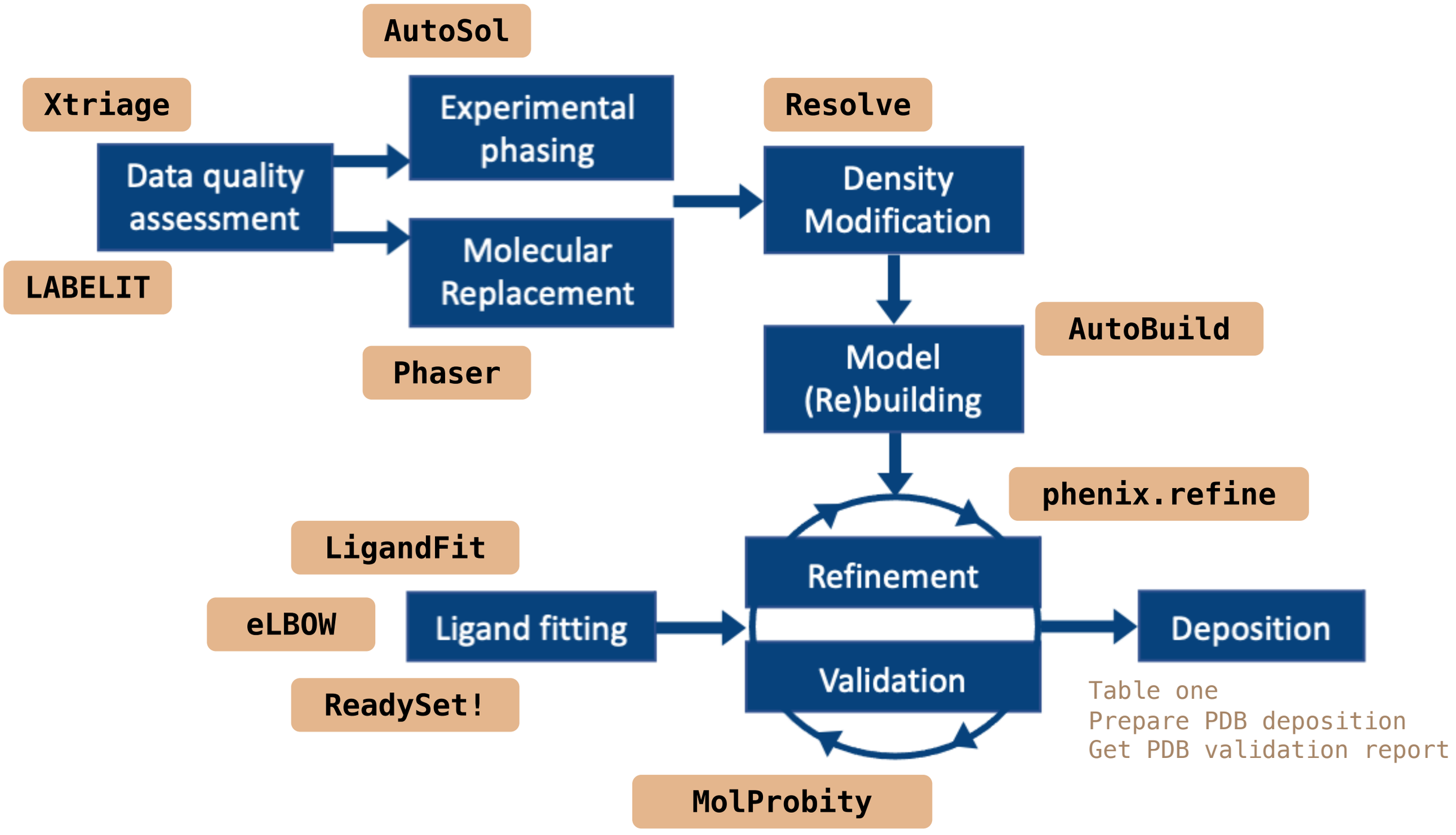
We have nucleated the development of new computational methods for structural biology



Key Features

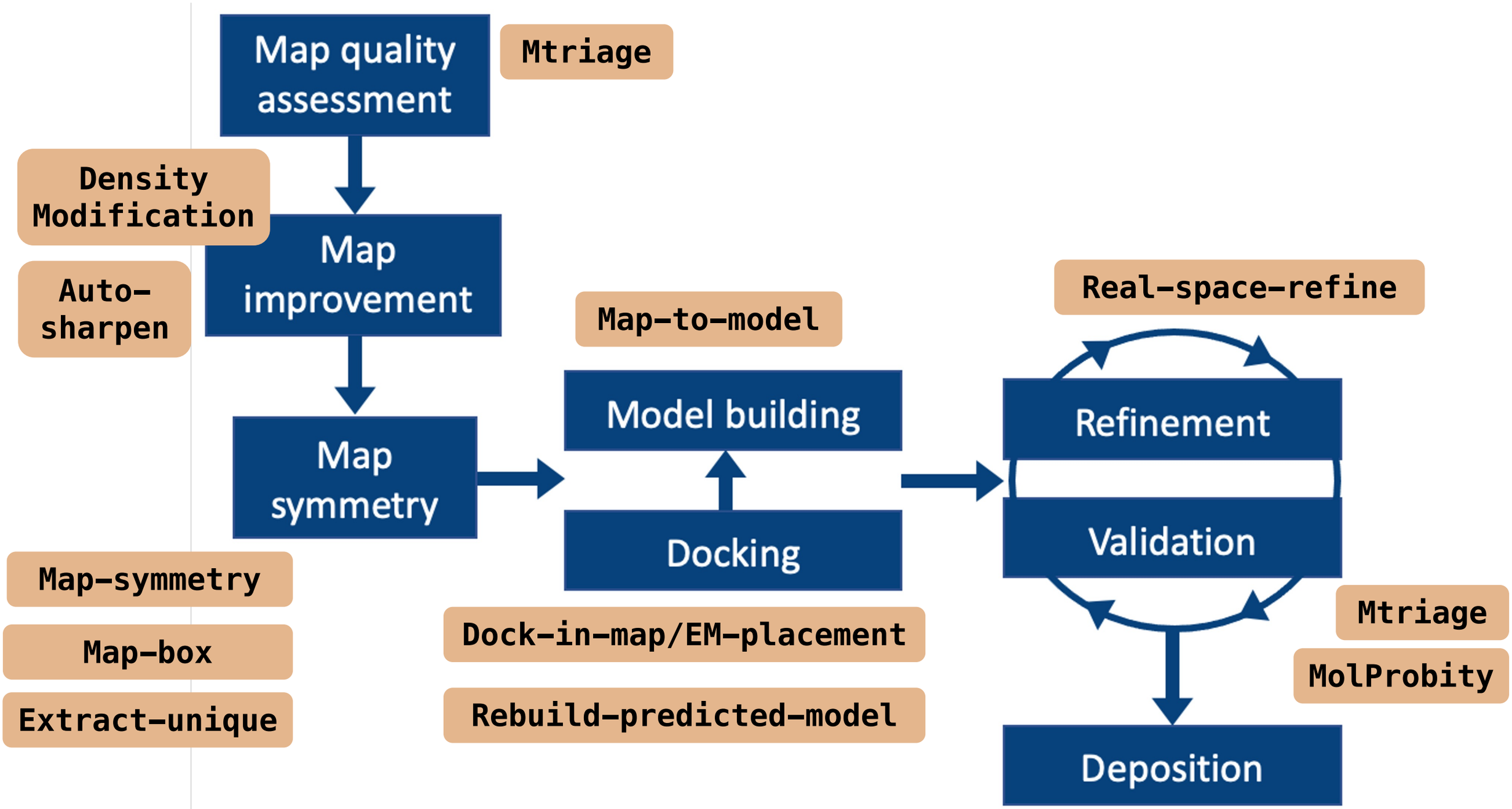
- **Python**
  - Easy scripting of repetitive tasks
  - Enables rapid prototyping and development
- **Advanced algorithms**
  - Experimental phasing
  - Molecular replacement
  - Automated model building and rebuilding
  - Structure refinement and validation
  - Ligand coordinate and restraint generation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

Tools for Crystallography



Acta Cryst. 2002, D58:1948-1954 (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



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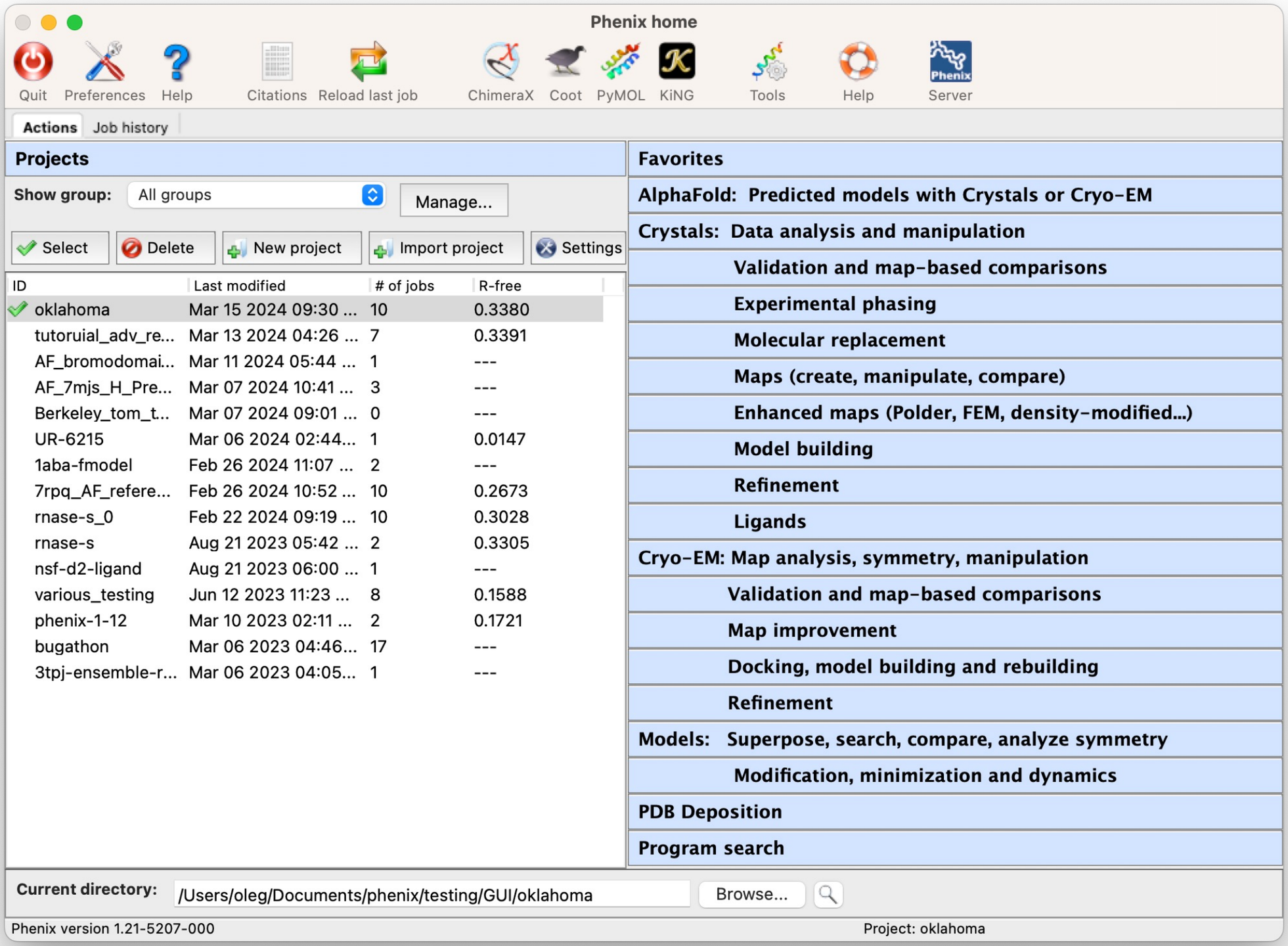
Features

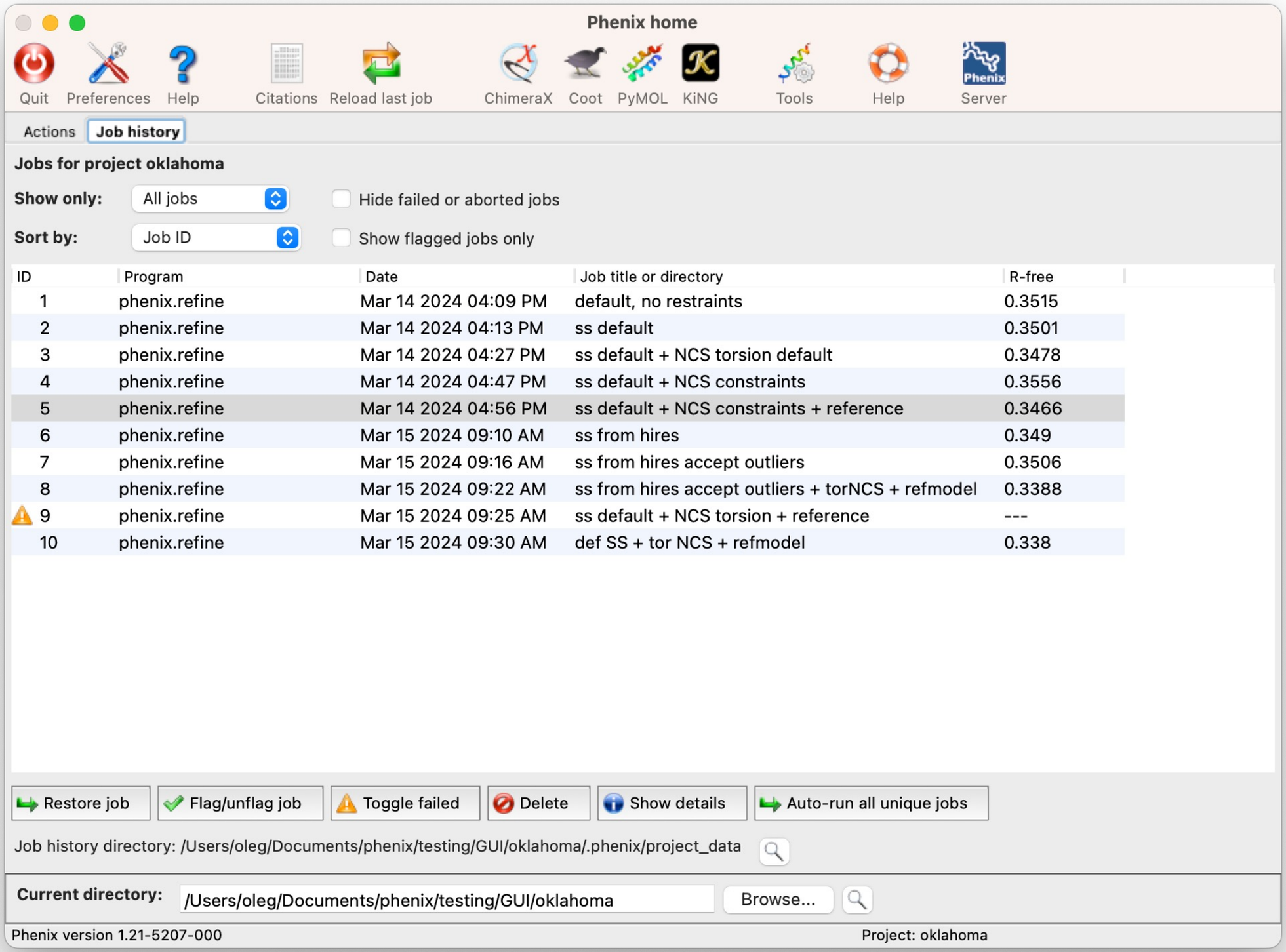
Phenix GUI

Central GUI for job control and to launch new jobs



Phenix GUI

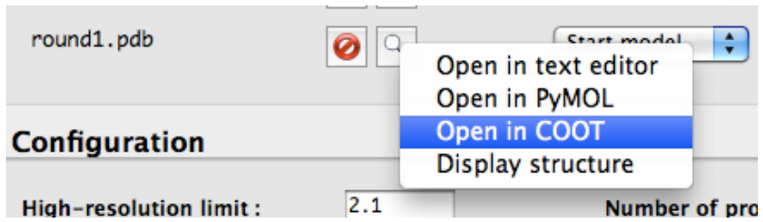
Central GUI for job history



Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps

- Any PDB file listed in GUI can also be opened

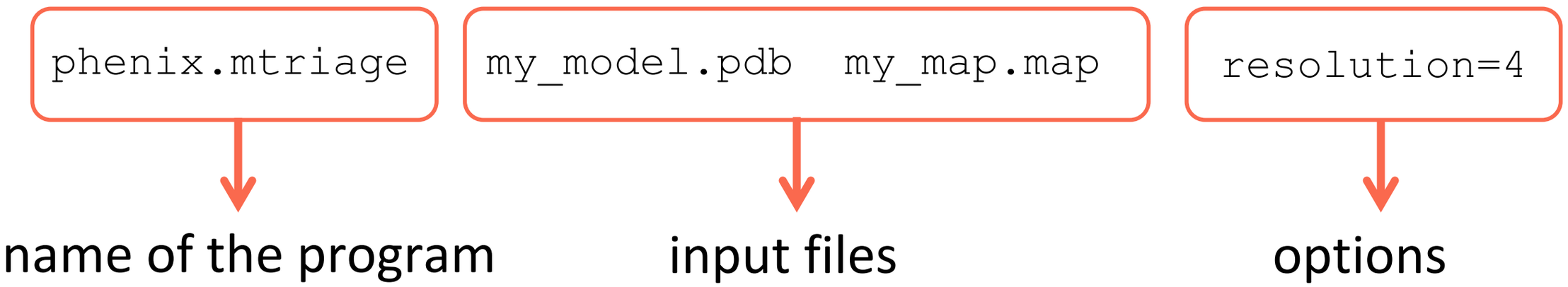


- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running
- Coot must have Python support (default on Mac)
- Specific paths to executables usually required on Linux

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

Command Line Tools

Run on the terminal



Run in a python script

```
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)
```

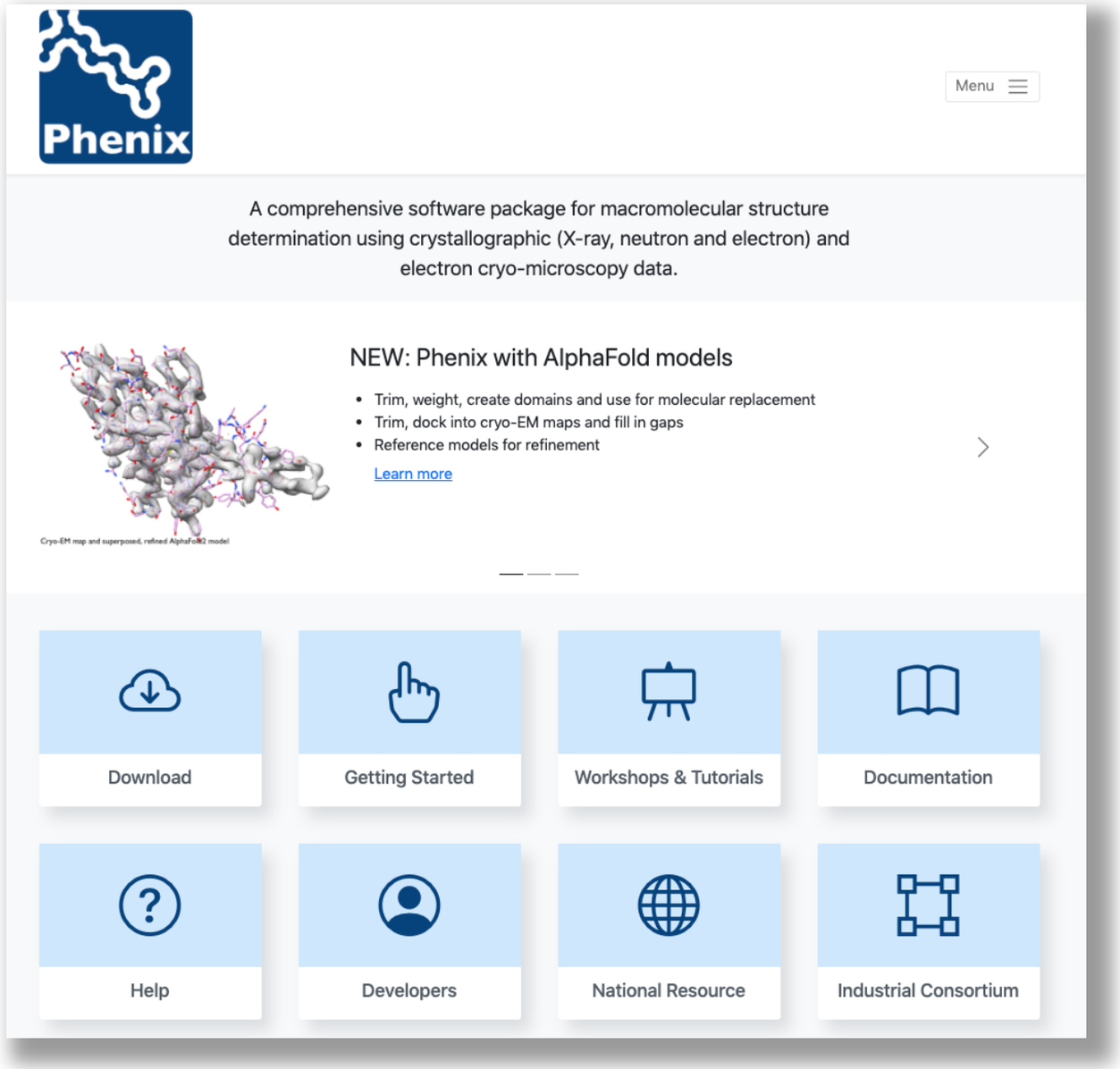
Phenix Availability

phenix-online.org

Supported on:

- Linux
- macOS
- Windows

Extensive documentation (online and via GUI)



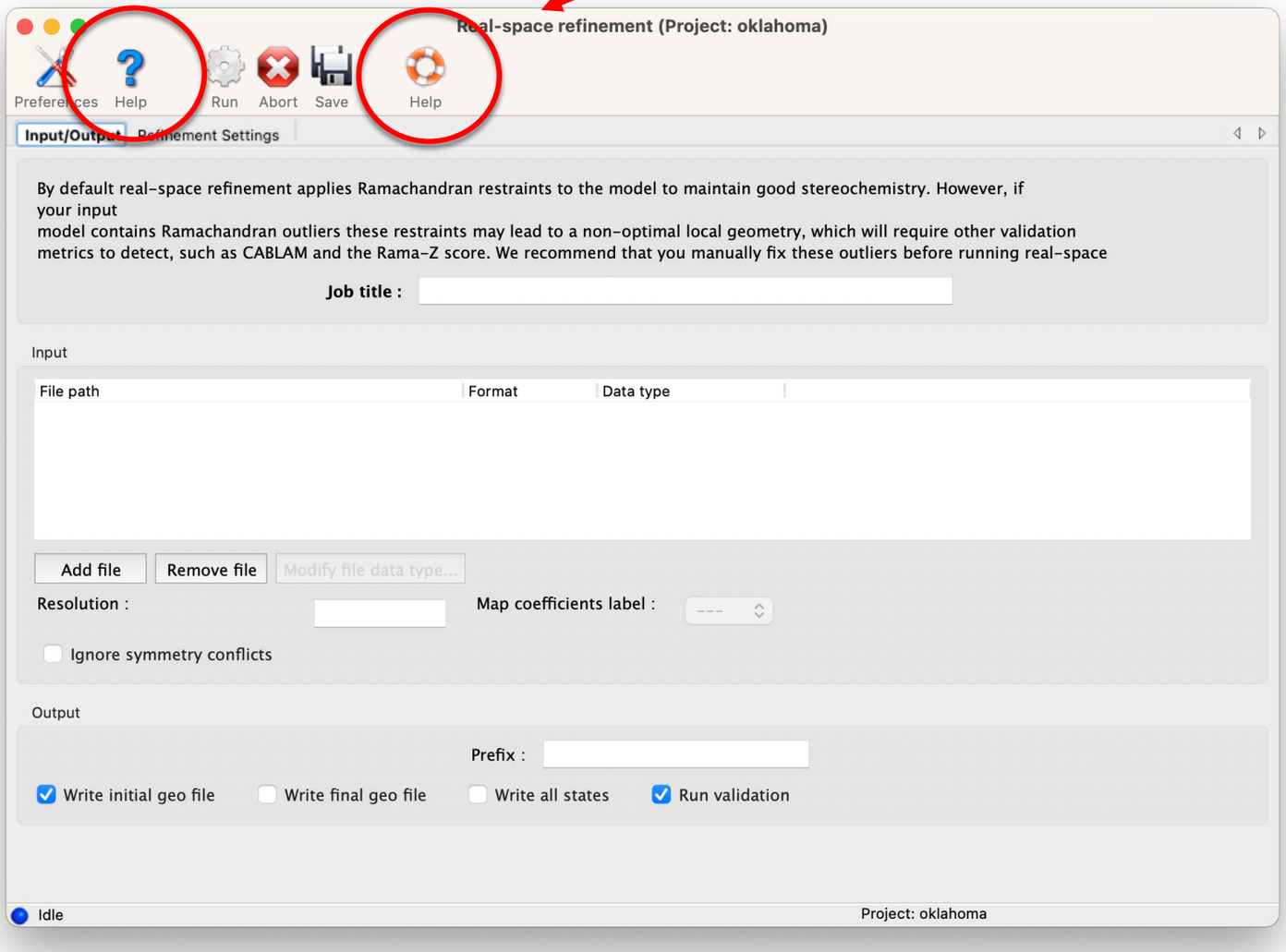
Nightly builds

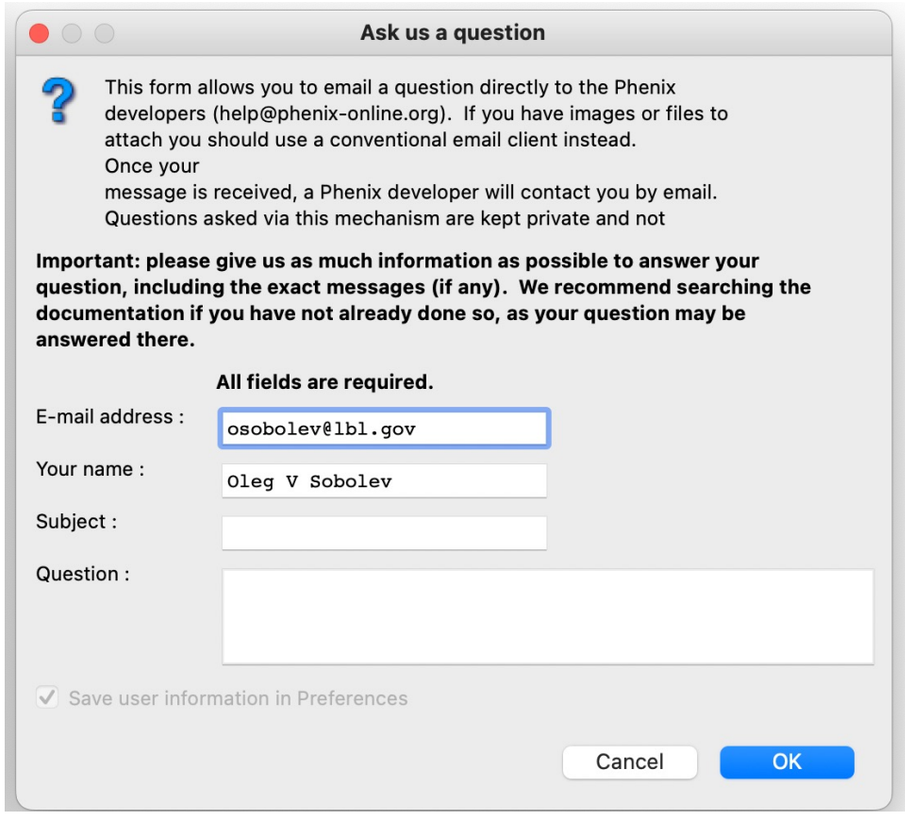
Version	Date	Status	Logs	Info
dev-3758	2020-01-22	successful	ci, intel-linux-2.6-x86_64-centos6, mac-intel-osx-x86_64, intel-windows-x86_64	docs; changelog
dev-3753	2020-01-17	successful	ci, intel-linux-2.6-x86_64-centos6, mac-intel-osx-x86_64, intel-windows-x86_64	docs; changelog
dev-3751	2020-01-15	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**

How to get help (give feedback)

Show documentation

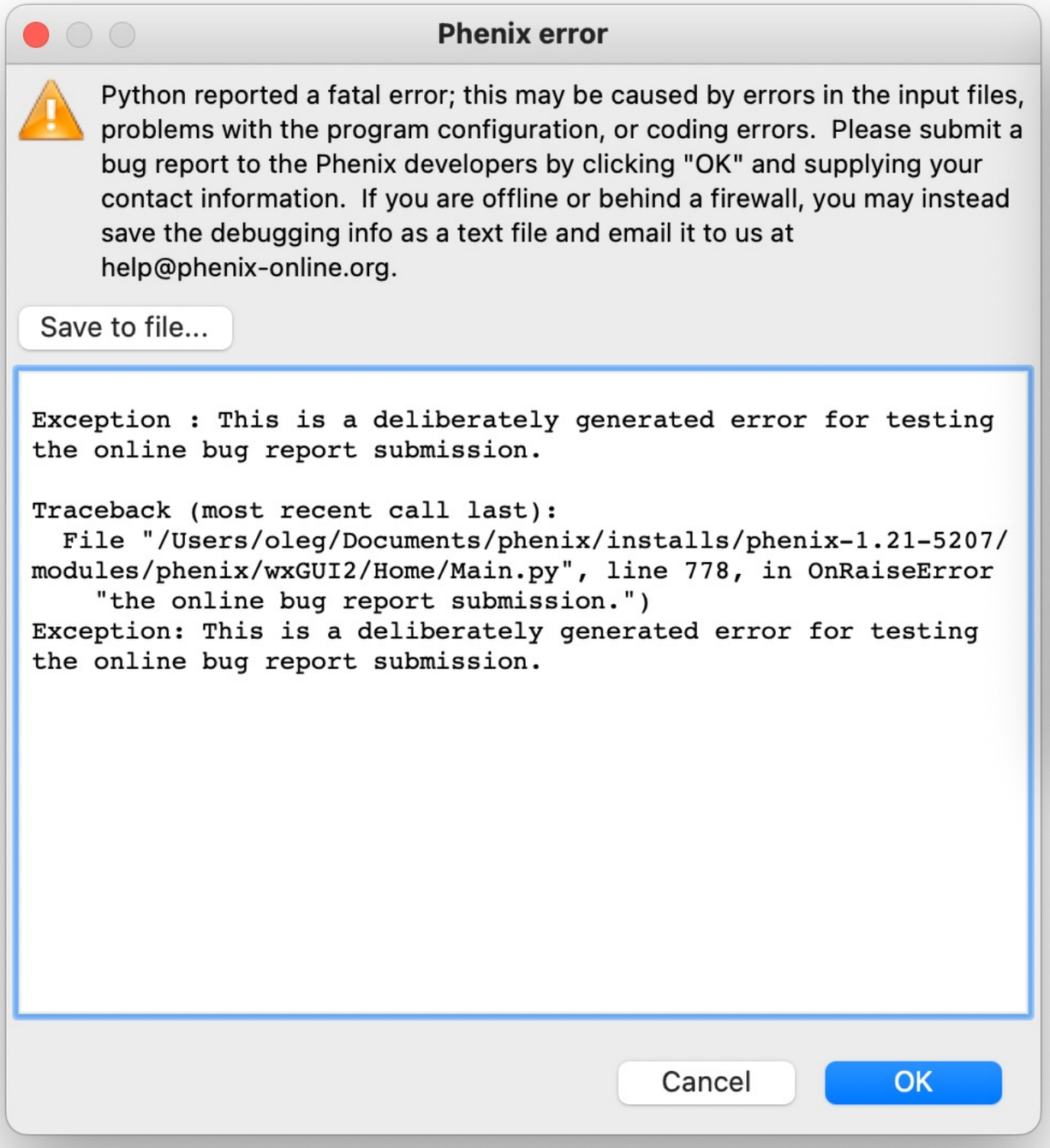
Send question to developers

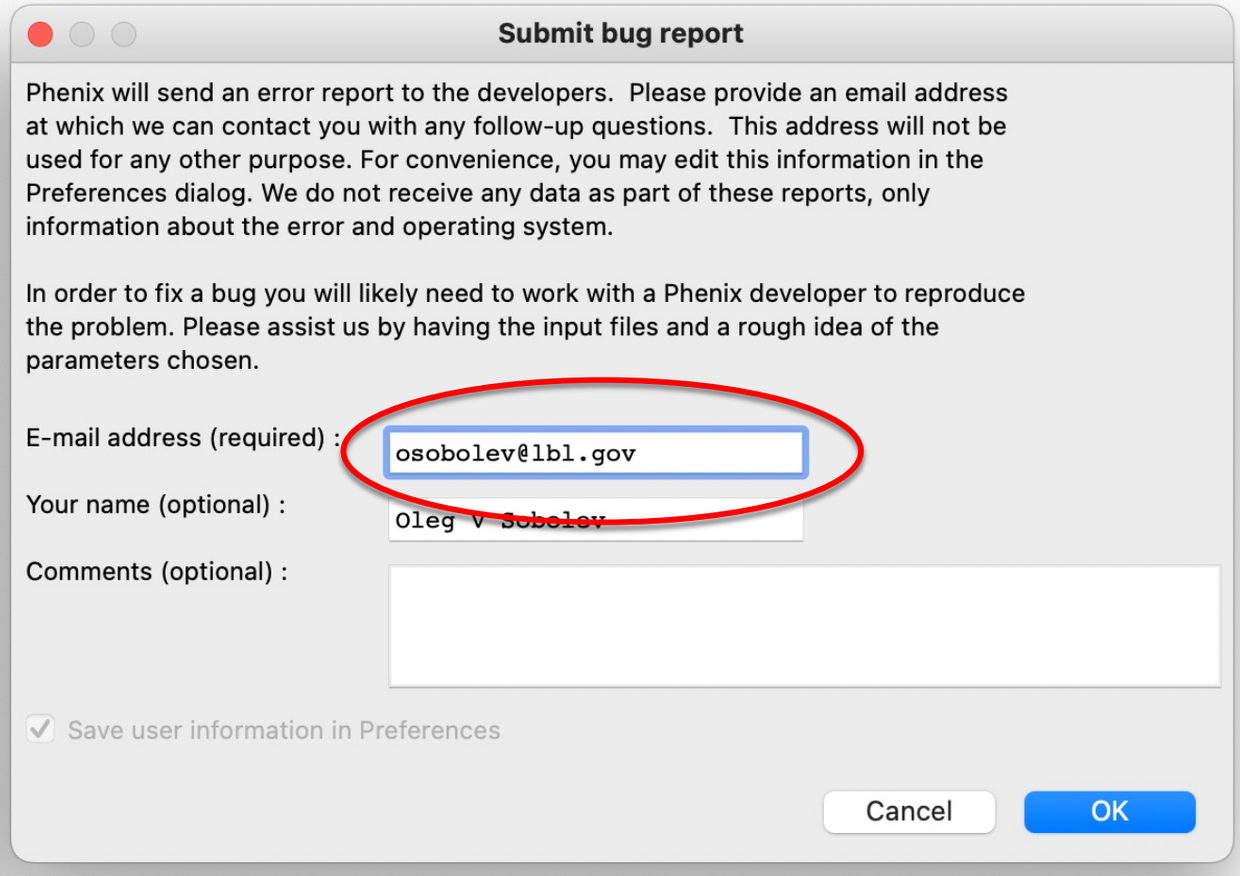




Reporting crashes (unlikely)

When something unexpected happens – let us know

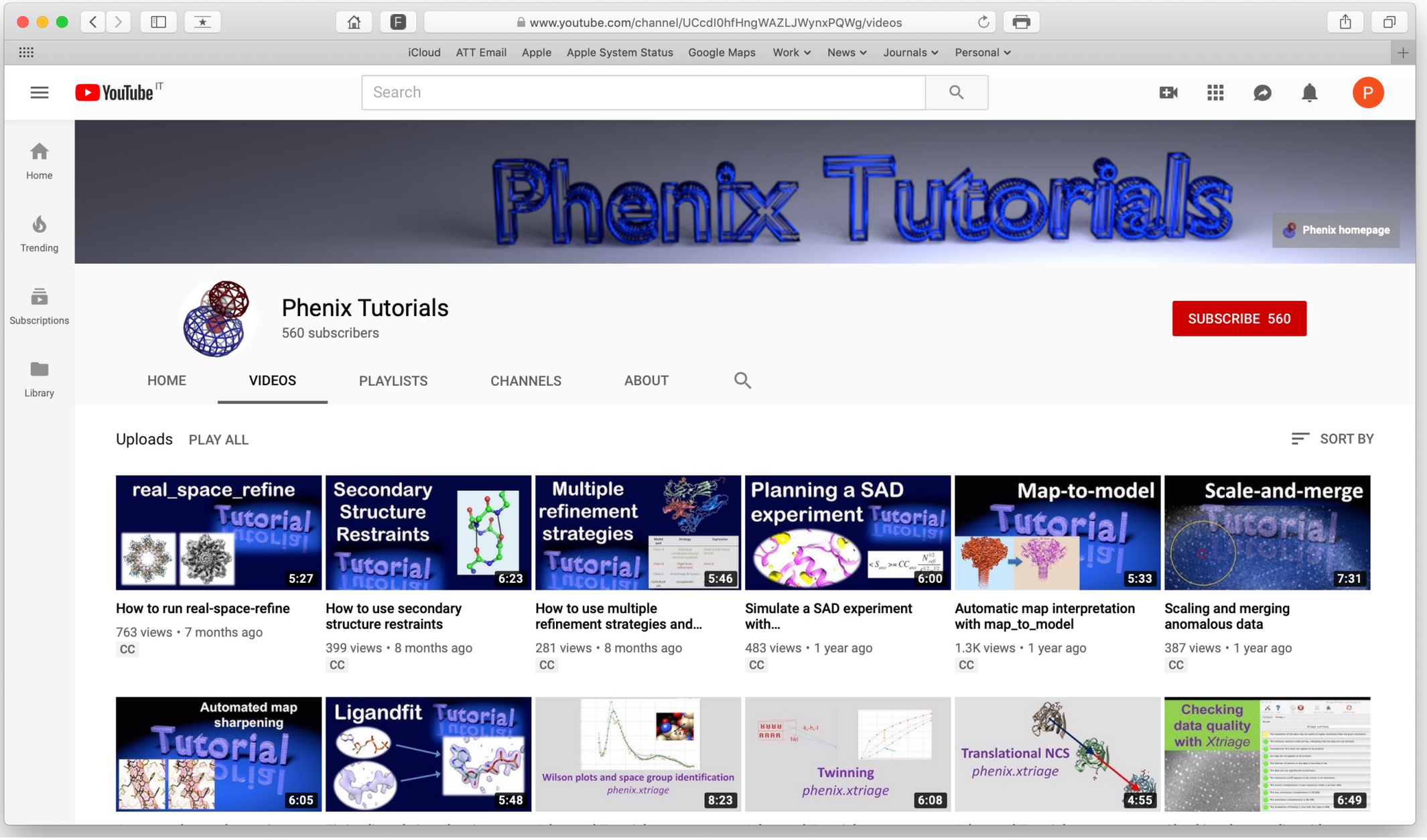




Valid e-mail so we can get back to you for more info or with solution

Video Tutorials

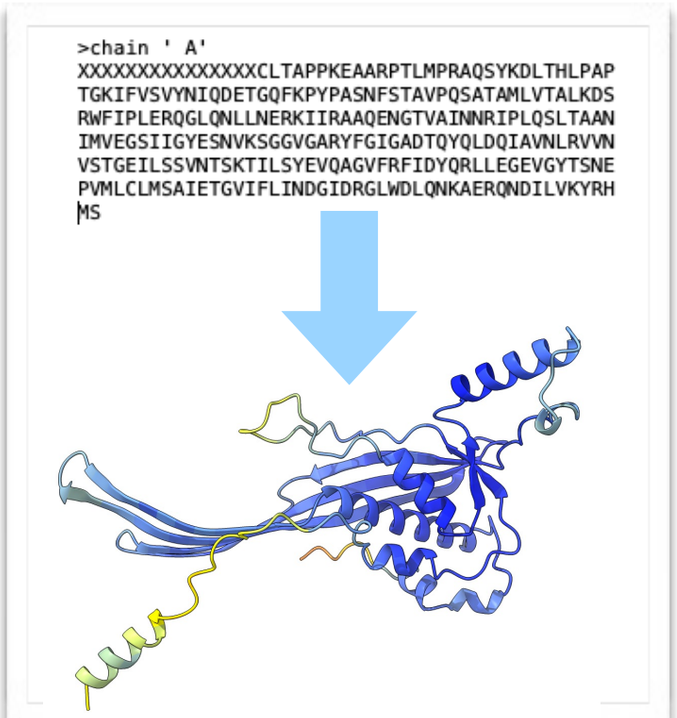
- YouTube channel: 62 videos



Dorothee Liebschner, Nigel Moriarty,
Tom Terwilliger, Christopher Schlicksup, Vincent Chen

Some highlights

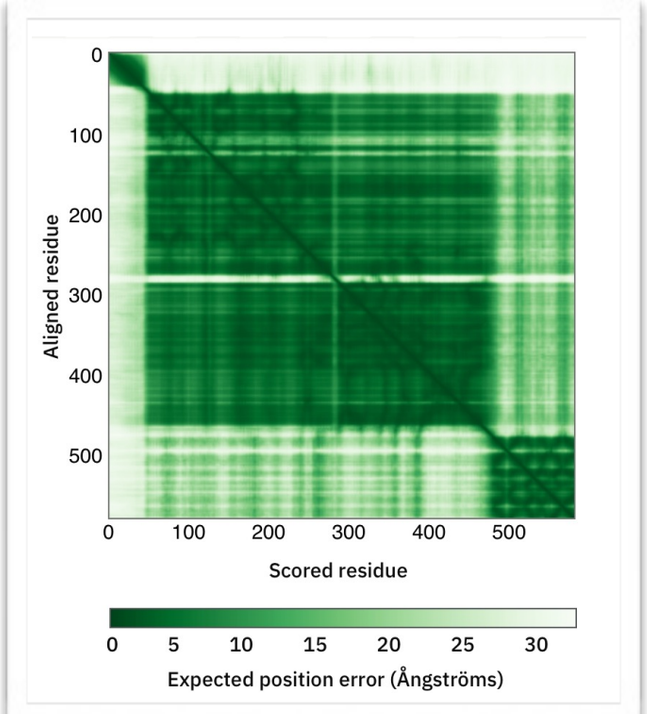
New tools for predicted models in Phenix



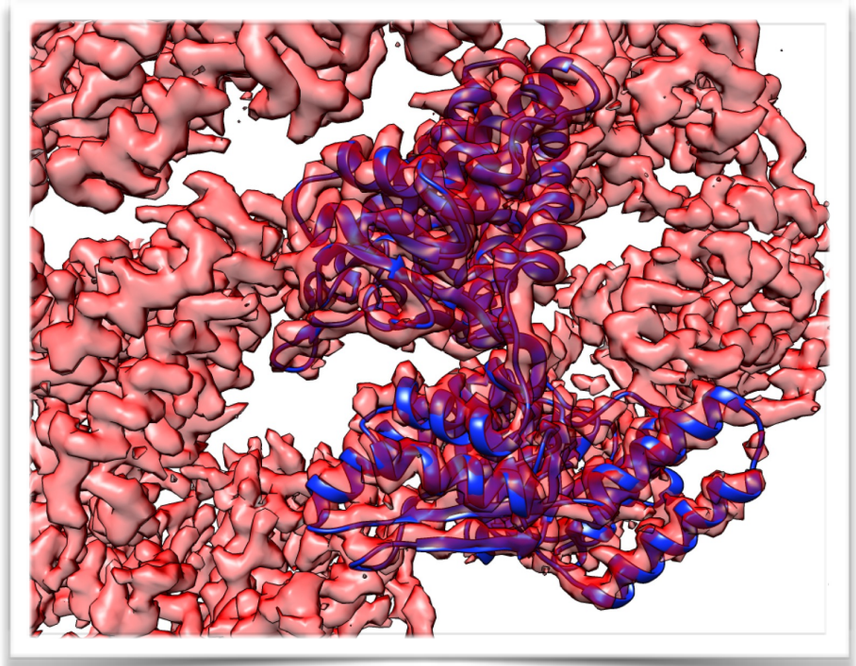
AlphaFold model prediction

(Phenix server, no need to have AF installed locally)

Later today



Process predicted model

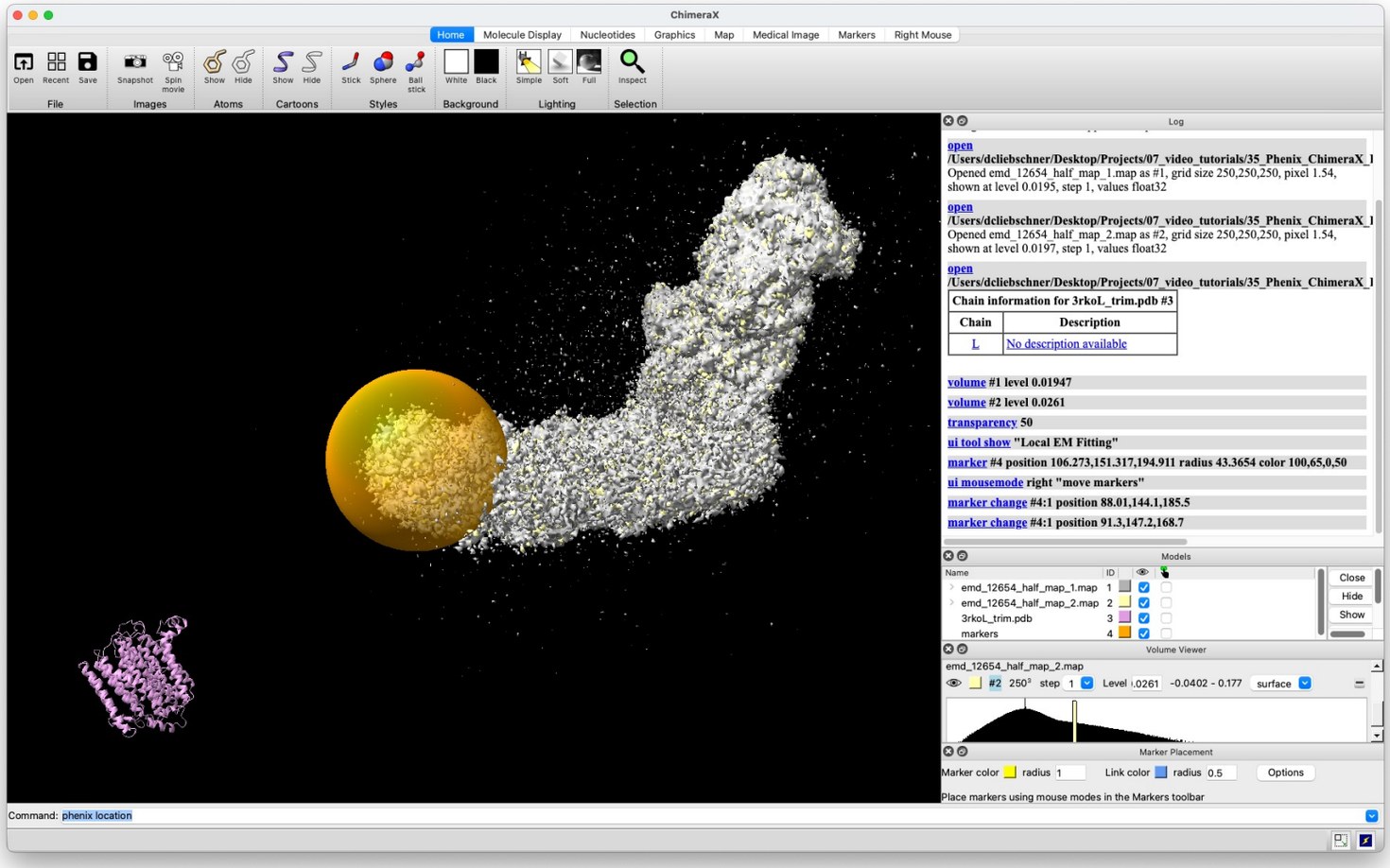


Predict and Build

(Iterative AlphaFold prediction, docking, and rebuilding)

Fully automatic!

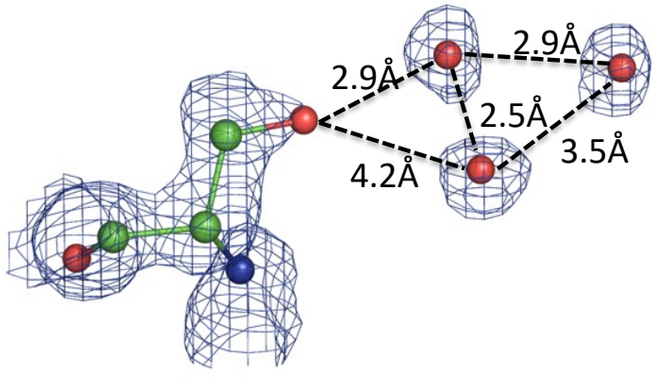
Run Phenix tools through ChimeraX

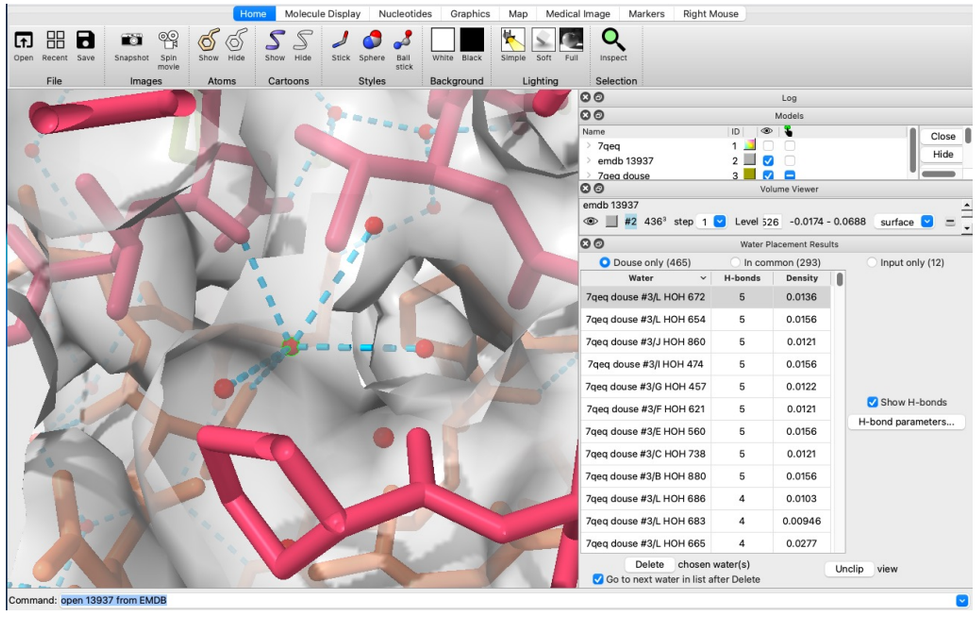


Local EM fitting (EM placement)

Tomorrow

Automated water building (phenix.douse)





Acknowledgements

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Phenix Testers & Users

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