

Phenix User Workshop, August 22nd 2023



Introduction

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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 **E**Nvironment for **I**ntegrated **X**tallography

The Project



Lawrence Berkeley Laboratory

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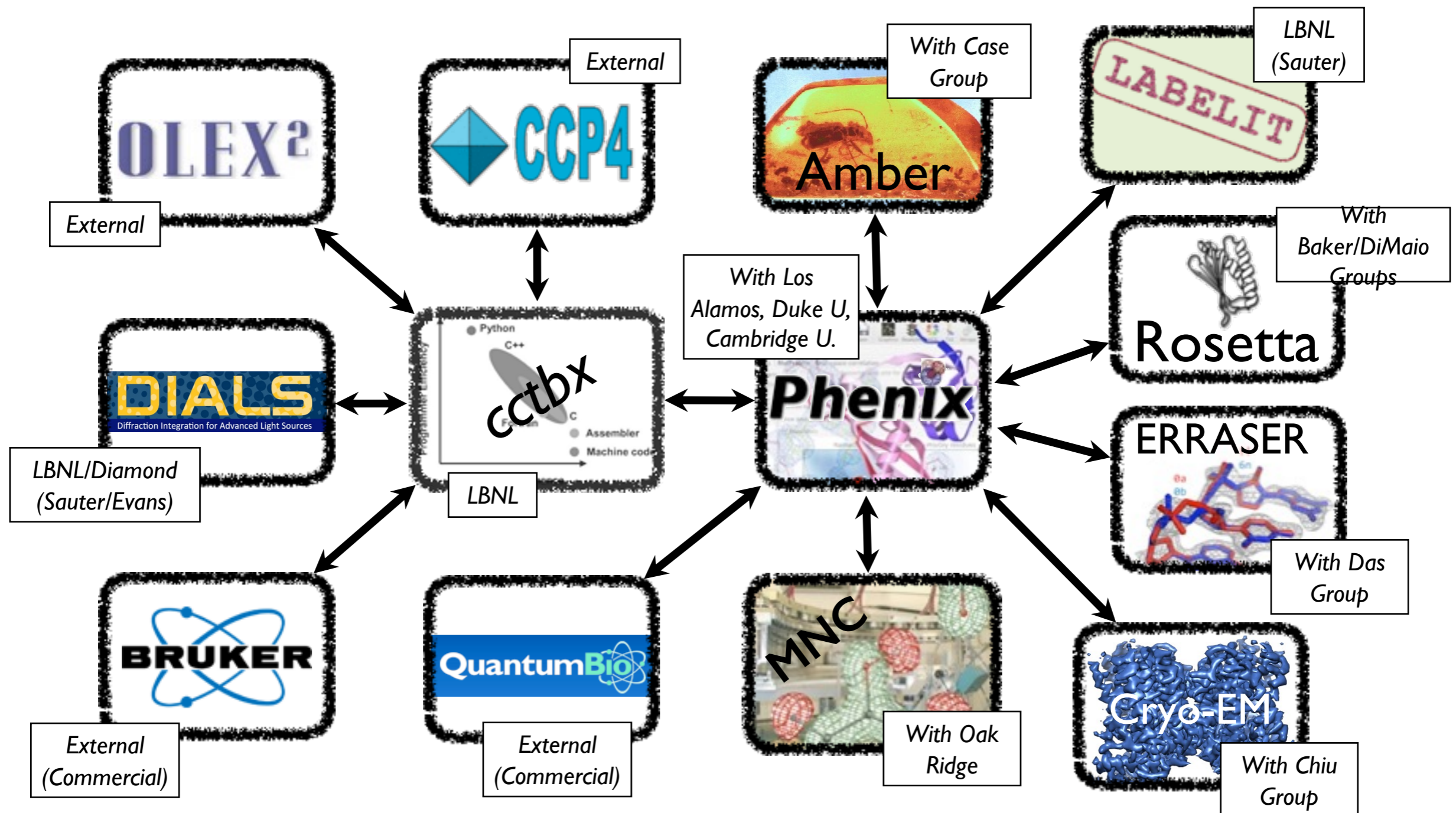


An NIH/NIGMS funded
Program Project

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

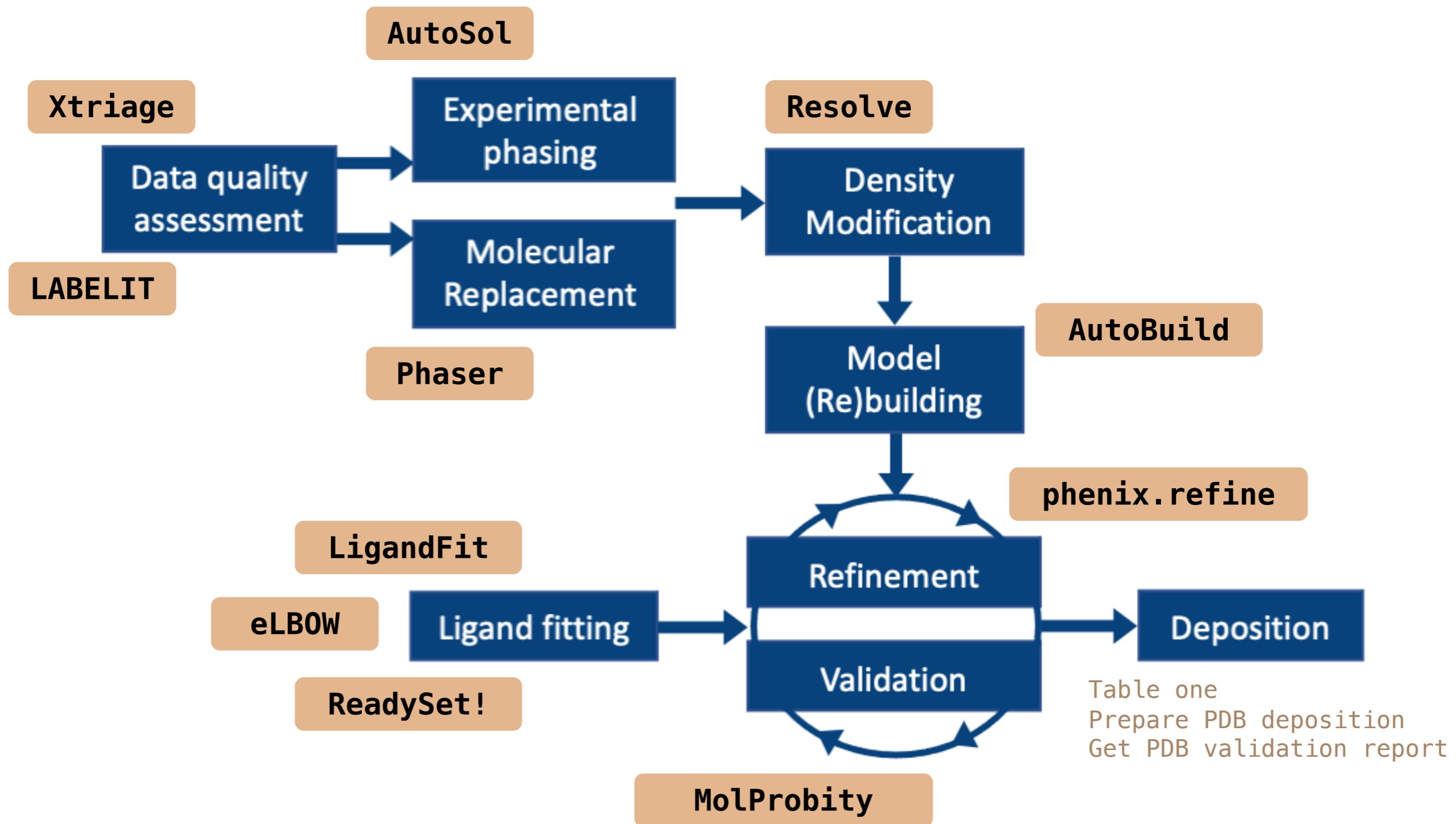
We have nucleated the development of new computational methods for structural biology



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

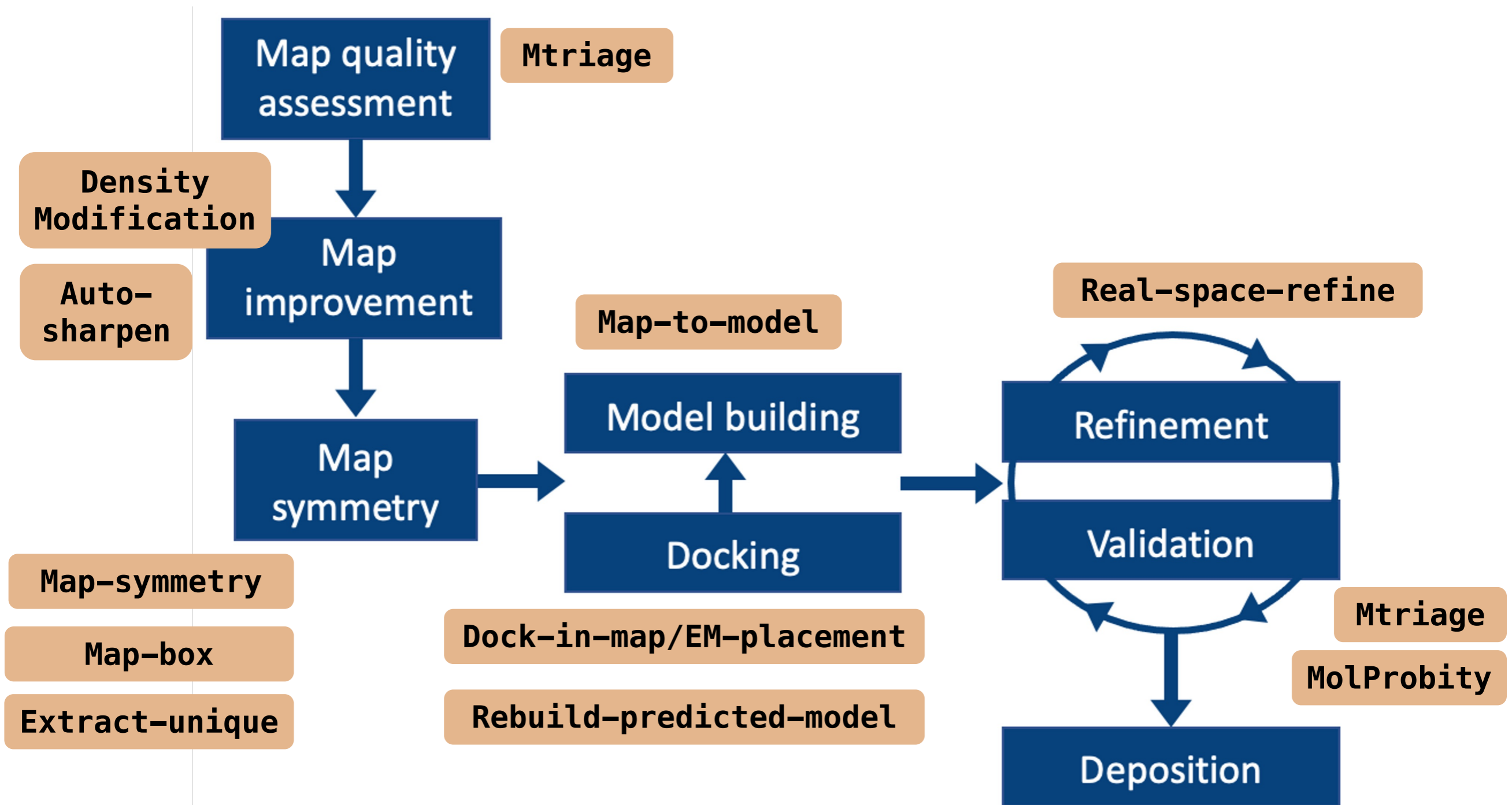


Acta Cryst. 2002, D58:1948-1954
J. Appl. Cryst. 2002, 35:126-136
Acta Cryst. 2010, D66: 213-221
Acta Cryst. 2019 D75:861-877

(Phenix)
(cctbx)
(Phenix)
(Phenix)

Table one
Prepare PDB deposition
Get PDB validation report

Tools for Cryo-EM



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)

Features

Phenix GUI

Central GUI for job control and to 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, ChimeraX, Coot, PyMOL, KiNG, Tools, Help, and Server. Below the menu bar, there are tabs for 'Actions' and 'Job history'. The main area is divided into two panels. The left panel, titled 'Projects', shows a table of projects with columns for ID, Last modified, # of jobs, and R-free. The 'oklahoma' project is selected. The right panel, titled 'Favorites', lists various tool categories such as AlphaFold, Crystals, Validation and map-based comparisons, Experimental phasing, Molecular replacement, Maps, Enhanced maps, Model building, Refinement, Ligands, Cryo-EM, Models, PDB Deposition, and Program search. At the bottom, there is a 'Current directory' field showing the path /Users/oleg/Documents/phenix/testing/GUI/oklahoma, a 'Browse...' button, and a search icon. The status bar at the very bottom indicates 'Phenix version 1.21-5207-000' and 'Project: oklahoma'.

Phenix home

Quit Preferences Help Citations Reload last job ChimeraX Coot PyMOL KiNG Tools Help Server

Actions Job history

Projects

Show group: All groups Manage...

Select Delete New project Import project Settings

ID	Last modified	# of jobs	R-free
✓ oklahoma	Mar 15 2024 09:30 ...	10	0.3380
tutoriaial_adv_re...	Mar 13 2024 04:26 ...	7	0.3391
AF_bromodomai...	Mar 11 2024 05:44 ...	1	---
AF_7mjs_H_Pre...	Mar 07 2024 10:41 ...	3	---
Berkeley_tom_t...	Mar 07 2024 09:01 ...	0	---
UR-6215	Mar 06 2024 02:44...	1	0.0147
1aba-fmodel	Feb 26 2024 11:07 ...	2	---
7rpq_AF_refere...	Feb 26 2024 10:52 ...	10	0.2673
rnase-s_0	Feb 22 2024 09:19 ...	10	0.3028
rnase-s	Aug 21 2023 05:42 ...	2	0.3305
nsf-d2-ligand	Aug 21 2023 06:00 ...	1	---
various_testing	Jun 12 2023 11:23 ...	8	0.1588
phenix-1-12	Mar 10 2023 02:11 ...	2	0.1721
bugathon	Mar 06 2023 04:46...	17	---
3tpj-ensemble-r...	Mar 06 2023 04:05...	1	---

Favorites

- AlphaFold: Predicted models with Crystals or Cryo-EM
- 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

Current directory: /Users/oleg/Documents/phenix/testing/GUI/oklahoma Browse...

Phenix version 1.21-5207-000 Project: oklahoma

Phenix GUI

Central GUI for job history

Phenix home

Quit Preferences Help Citations Reload last job ChimeraX Coot PyMOL KiNG Tools Help Server

Actions **Job history**

Jobs for project **oklahoma**

Show only: All jobs Hide failed or aborted jobs

Sort by: Job ID Show flagged jobs only

ID	Program	Date	Job title or directory	R-free
1	phenix.refine	Mar 14 2024 04:09 PM	default, no restraints	0.3515
2	phenix.refine	Mar 14 2024 04:13 PM	ss default	0.3501
3	phenix.refine	Mar 14 2024 04:27 PM	ss default + NCS torsion default	0.3478
4	phenix.refine	Mar 14 2024 04:47 PM	ss default + NCS constraints	0.3556
5	phenix.refine	Mar 14 2024 04:56 PM	ss default + NCS constraints + reference	0.3466
6	phenix.refine	Mar 15 2024 09:10 AM	ss from hires	0.349
7	phenix.refine	Mar 15 2024 09:16 AM	ss from hires accept outliers	0.3506
8	phenix.refine	Mar 15 2024 09:22 AM	ss from hires accept outliers + torNCS + refmodel	0.3388
⚠ 9	phenix.refine	Mar 15 2024 09:25 AM	ss default + NCS torsion + reference	---
10	phenix.refine	Mar 15 2024 09:30 AM	def SS + tor NCS + refmodel	0.338

Restore job Flag/unflag job ⚠ Toggle failed Delete Show details Auto-run all unique jobs

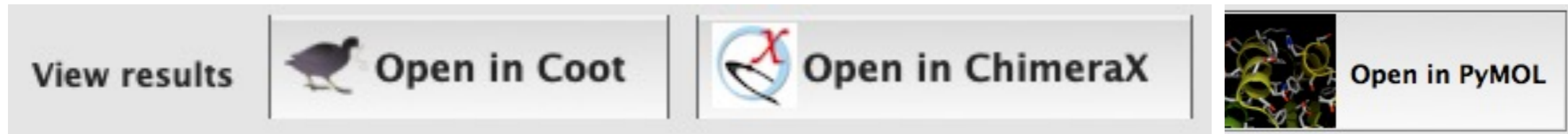
Job history directory: /Users/oleg/Documents/phenix/testing/GUI/oklahoma/.phenix/project_data

Current directory: /Users/oleg/Documents/phenix/testing/GUI/oklahoma Browse...

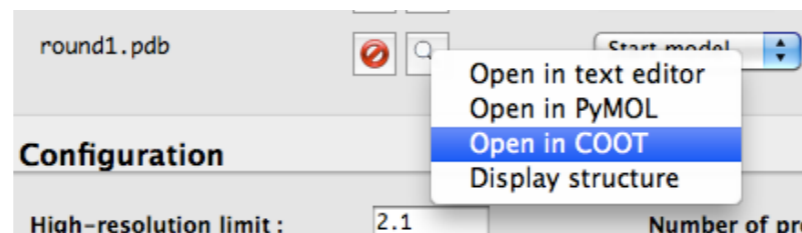
Phenix version 1.21-5207-000 Project: oklahoma

Coot/PyMOL/ChimeraX integration

- Most results can be opened directly in graphics apps



- Any PDB file listed in GUI can also be opened

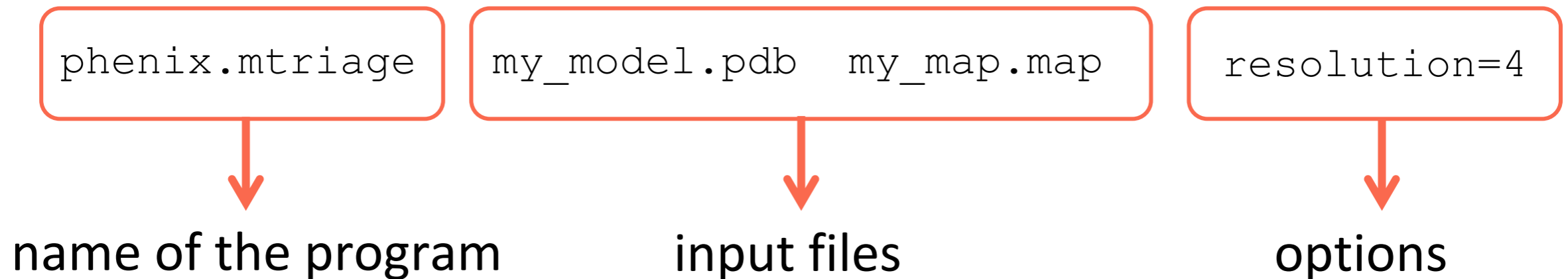


- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running
- Coot must have Python support (default on Mac)
- Specific paths to executables usually required on Linux

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

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

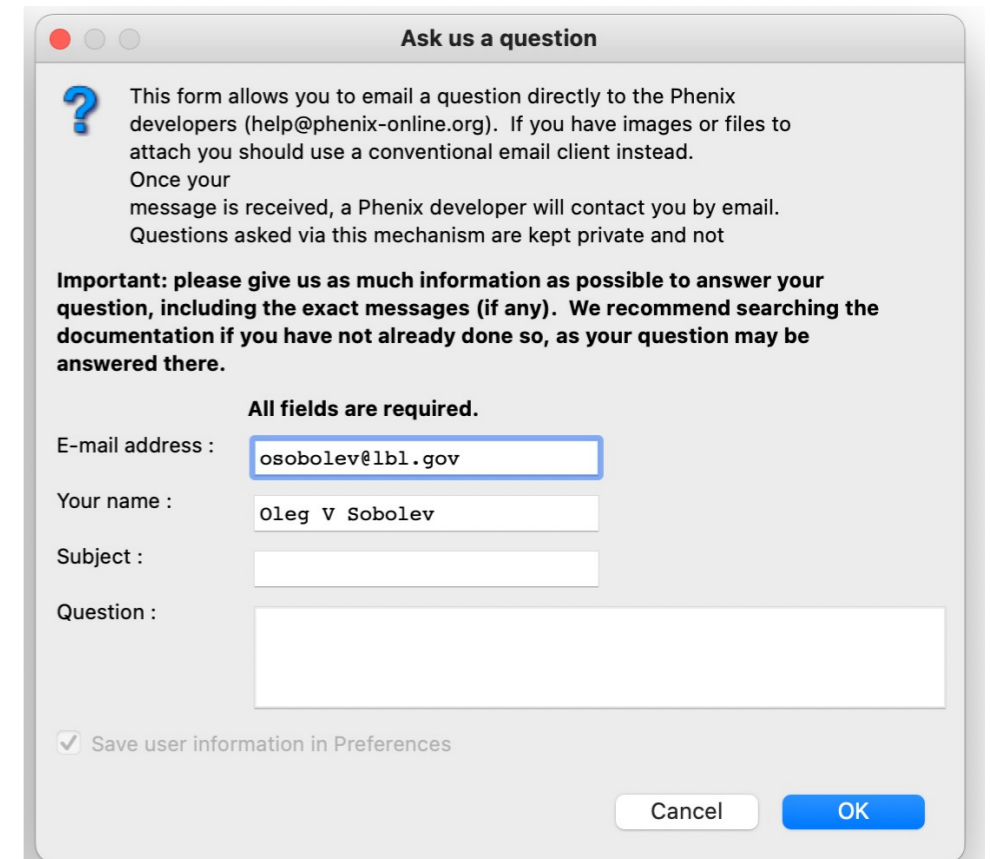
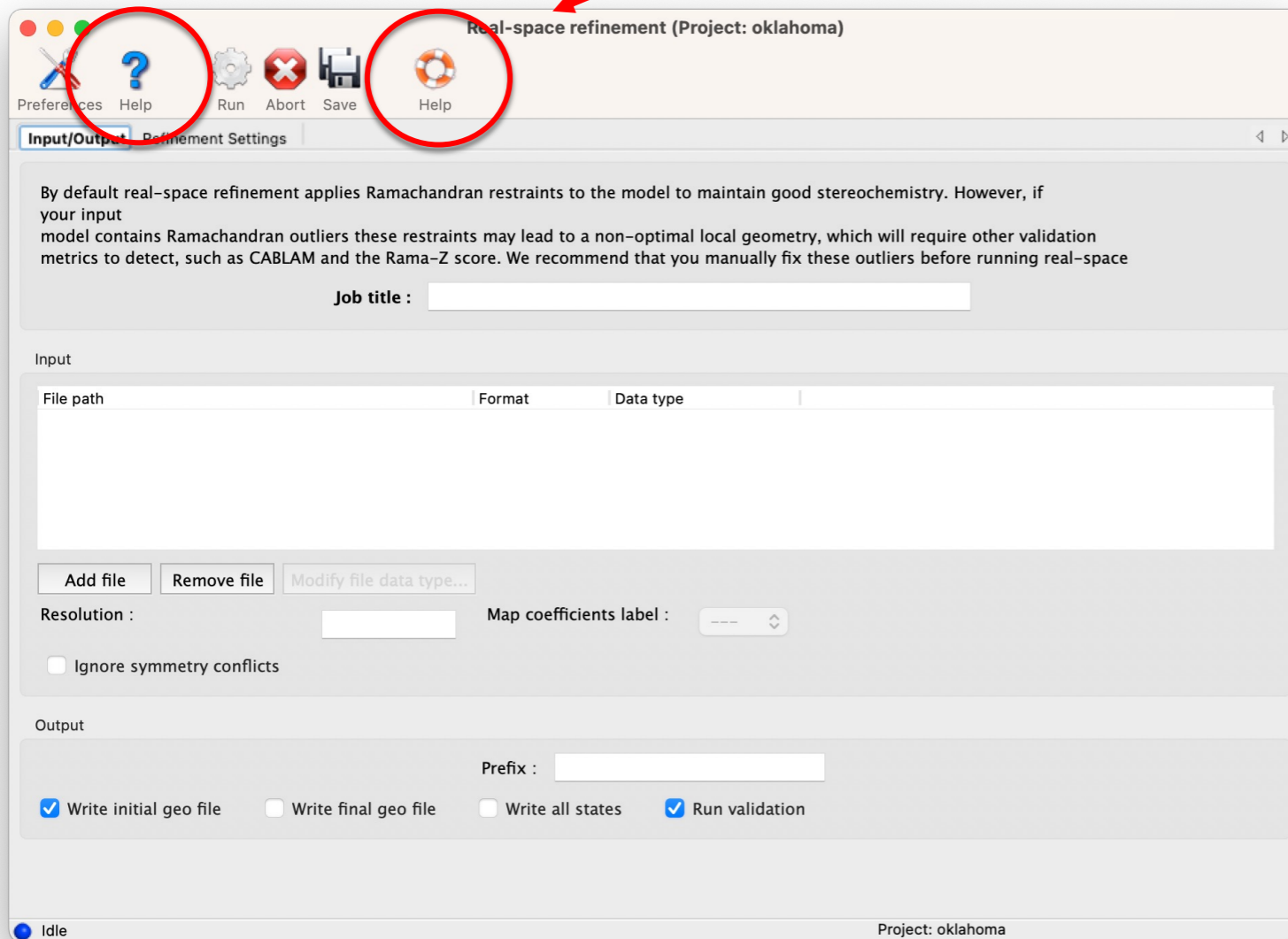
Help | Developers | National Resource | Industrial Consortium

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

How to get help (give feedback)

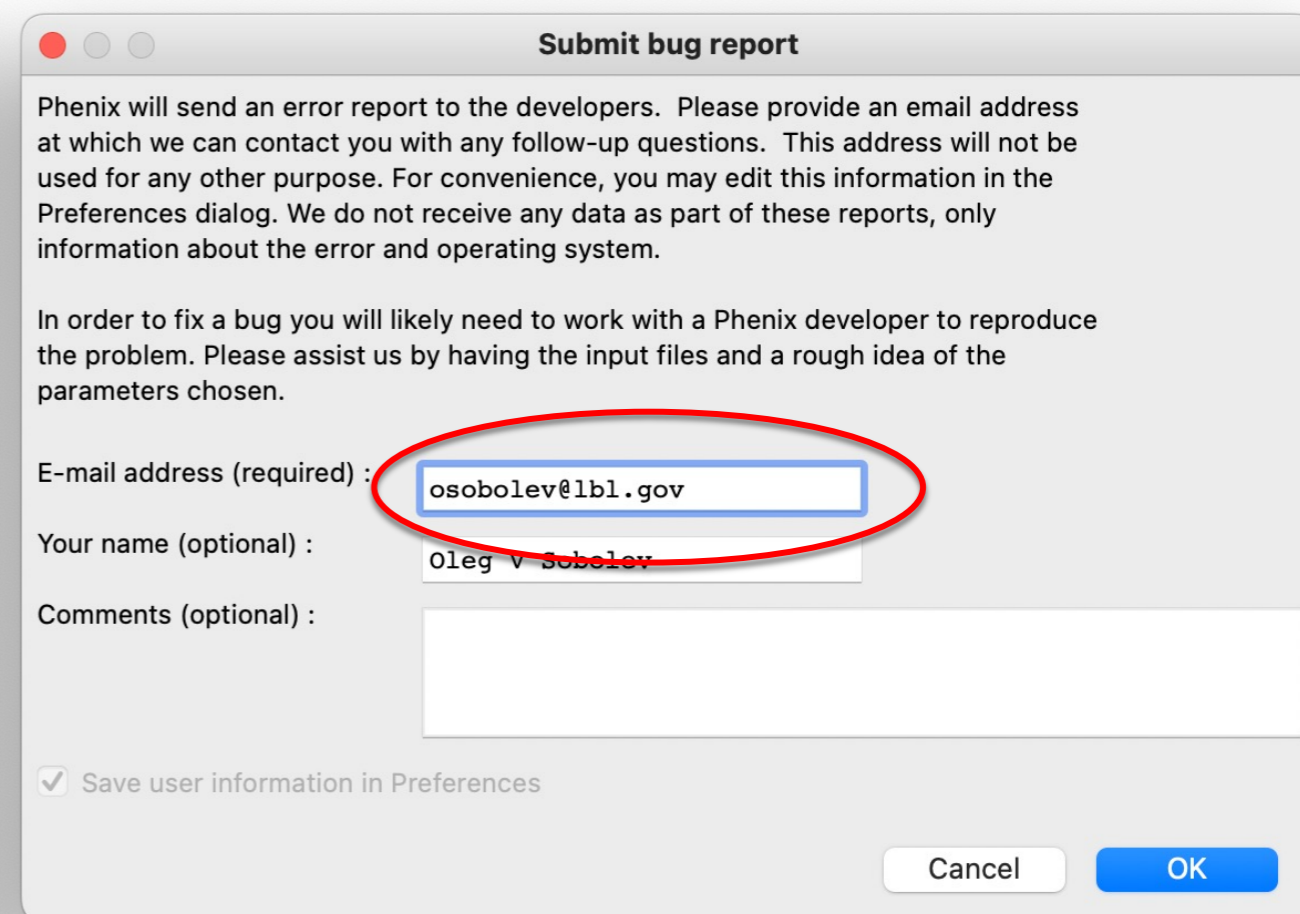
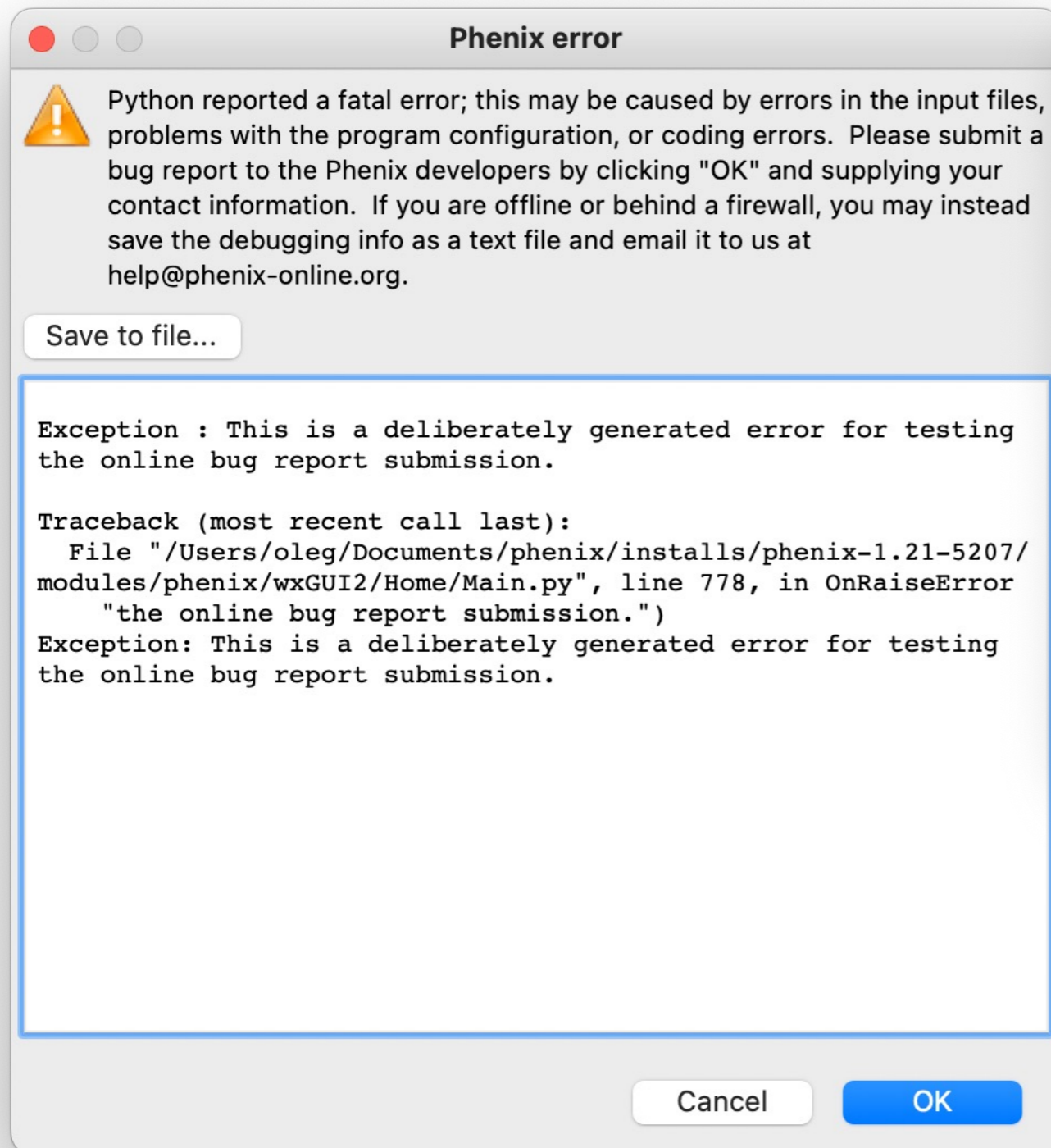
Show documentation

Send question to developers



Reporting crashes (unlikely)

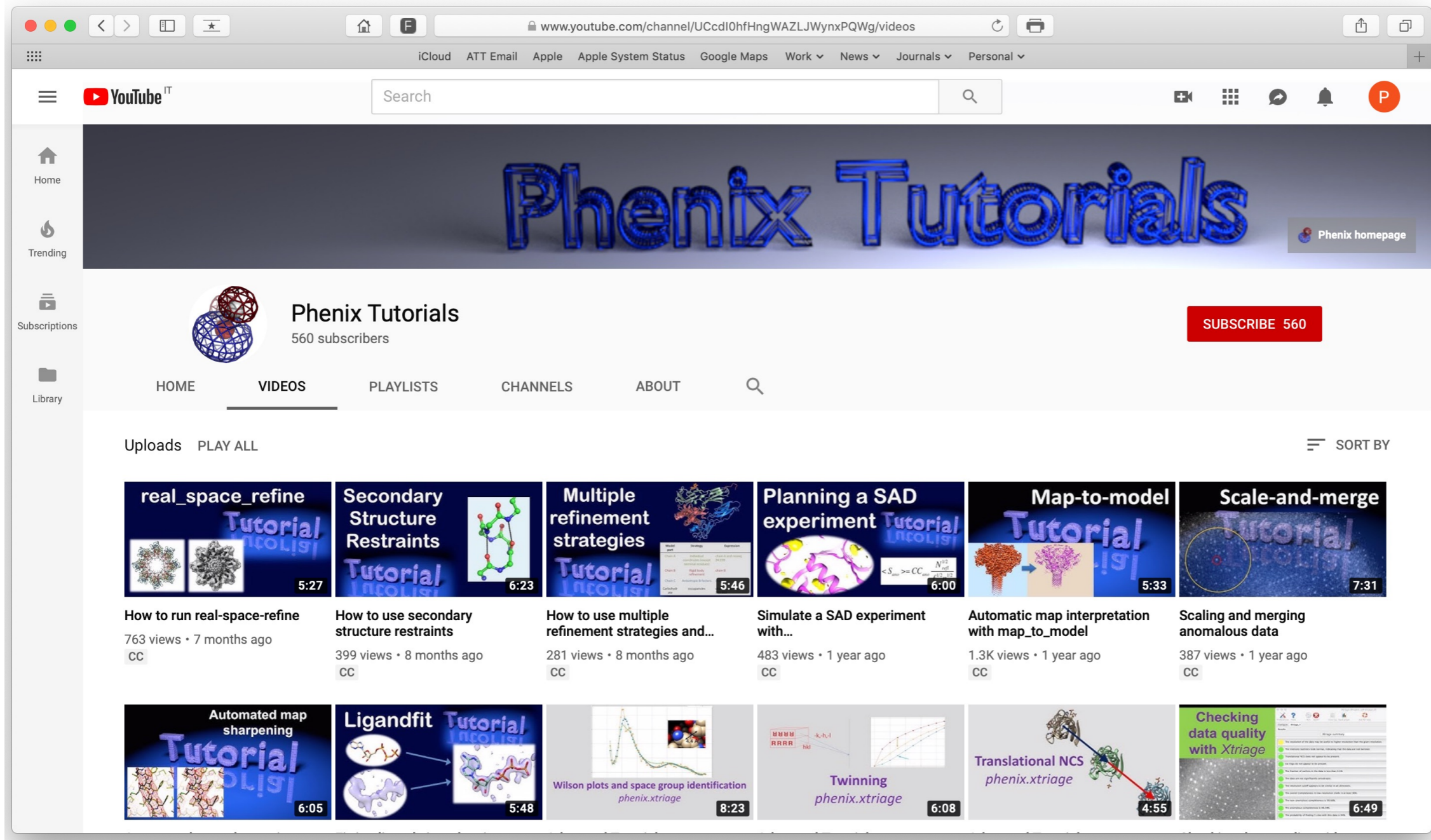
When something unexpected happens – let us know



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

Video Tutorials

-  channel: 62 videos

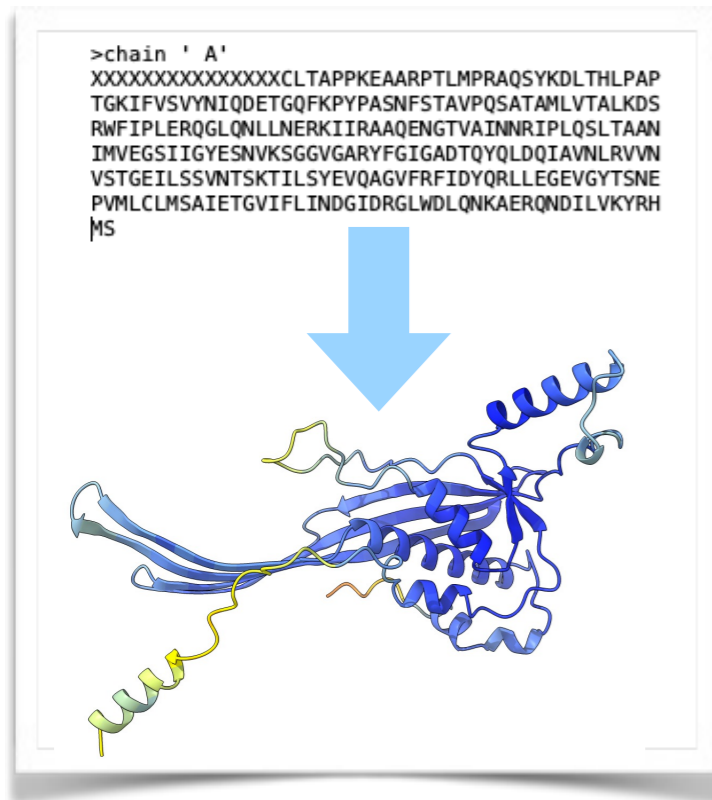


The screenshot shows the YouTube channel page for 'Phenix Tutorials'. The channel has 560 subscribers and a 'SUBSCRIBE 560' button. The page displays a grid of 12 video tutorials. The first row includes: 'real_space_refine Tutorial' (5:27), 'Secondary Structure Restraints Tutorial' (6:23), 'Multiple refinement strategies Tutorial' (5:46), 'Planning a SAD experiment Tutorial' (6:00), 'Map-to-model Tutorial' (5:33), and 'Scale-and-merge Tutorial' (7:31). The second row includes: '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), and 'Checking data quality with Xtriage' (6:49). The page also features a search bar, navigation tabs (HOME, VIDEOS, PLAYLISTS, CHANNELS, ABOUT), and a sidebar with options like Home, Trending, Subscriptions, and Library.

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

Some highlights

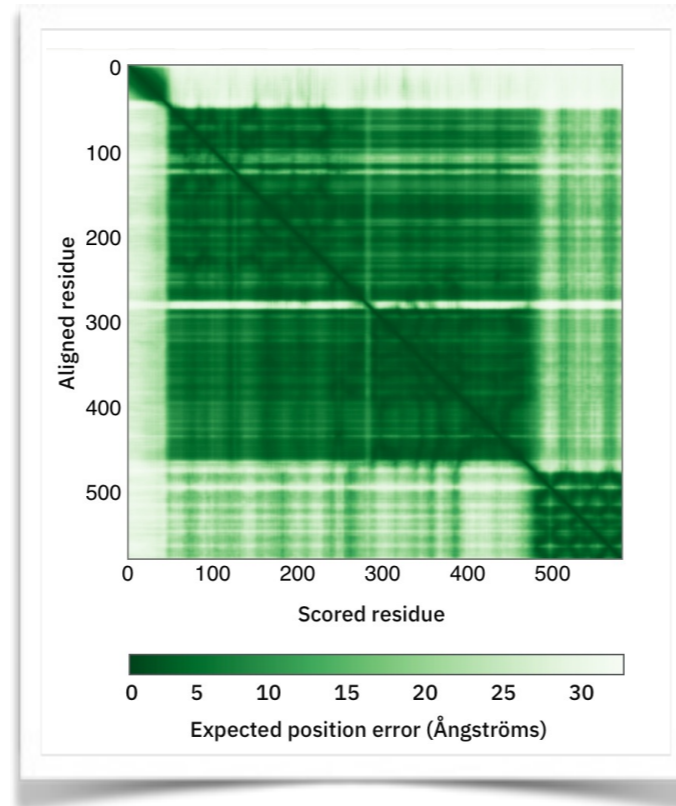
New tools for predicted models in Phenix



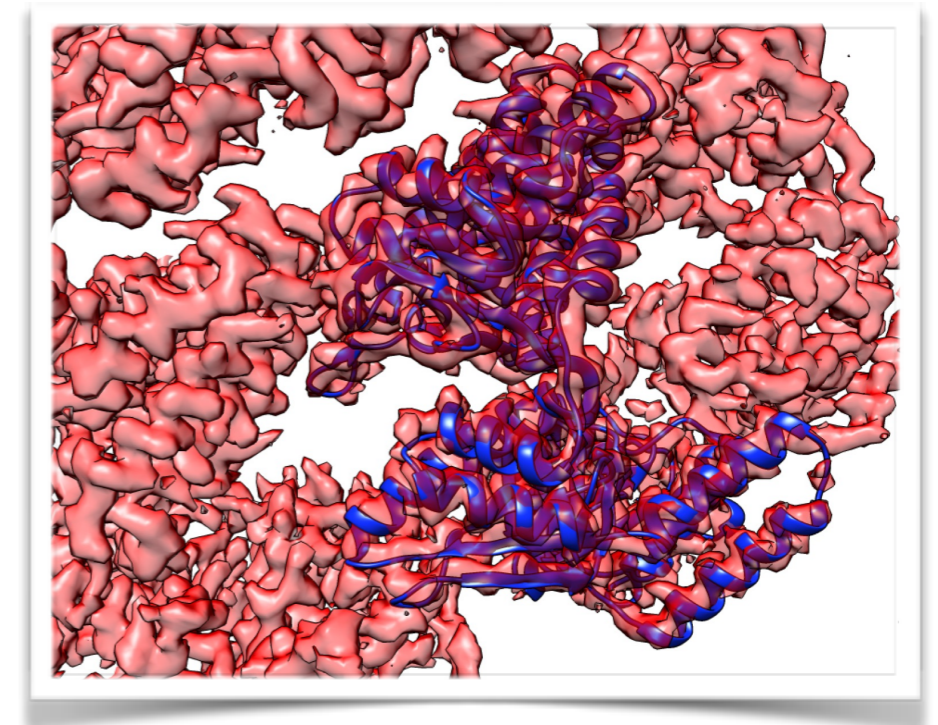
AlphaFold model prediction

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

Later today



Process predicted model

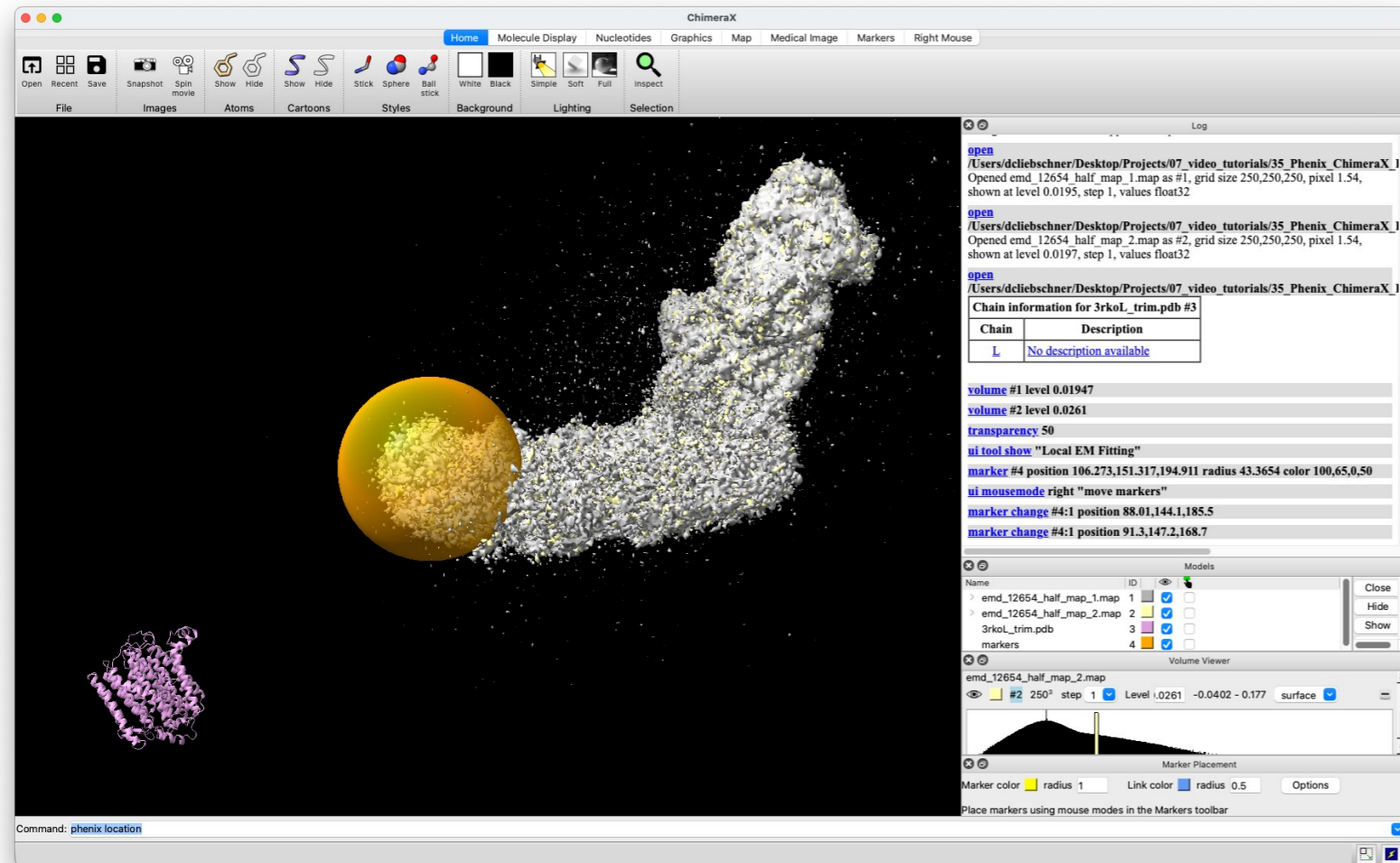


Predict and Build

(Iterative AlphaFold prediction, docking, and rebuilding)

Fully automatic!

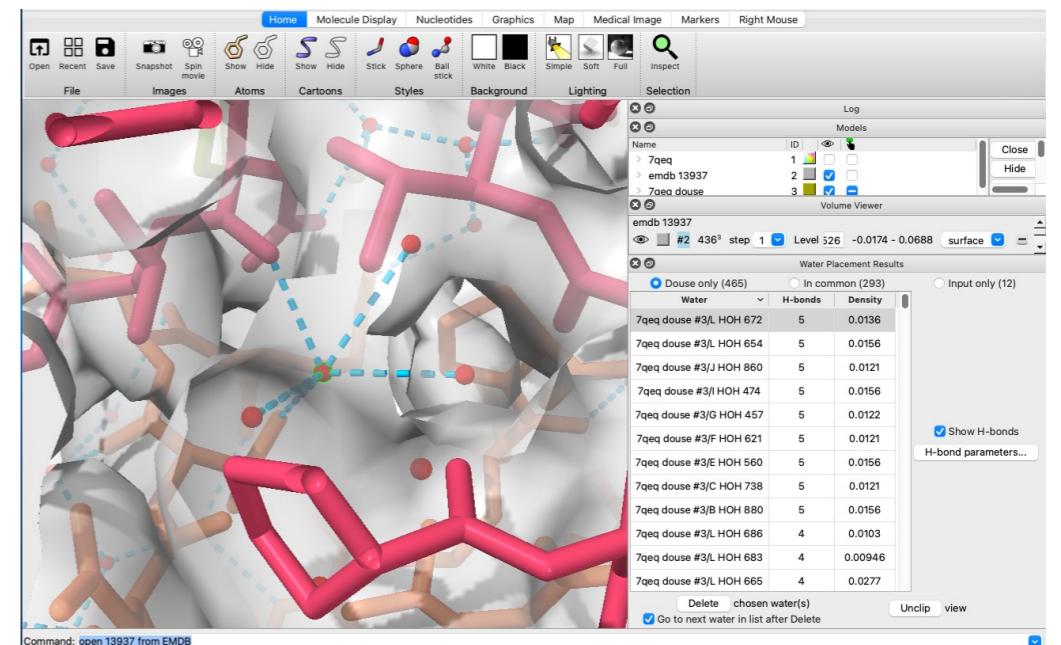
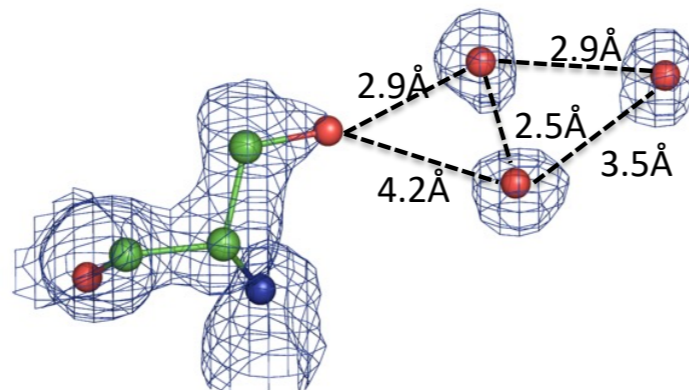
Run Phenix tools through ChimeraX



Local EM fitting
(EM placement)

Tomorrow

Automated water building
(phenix.douse)



Acknowledgements

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Phenix Testers & Users

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