

CBMS workbench (virtual), Oct 13 2021



Introduction

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The Project



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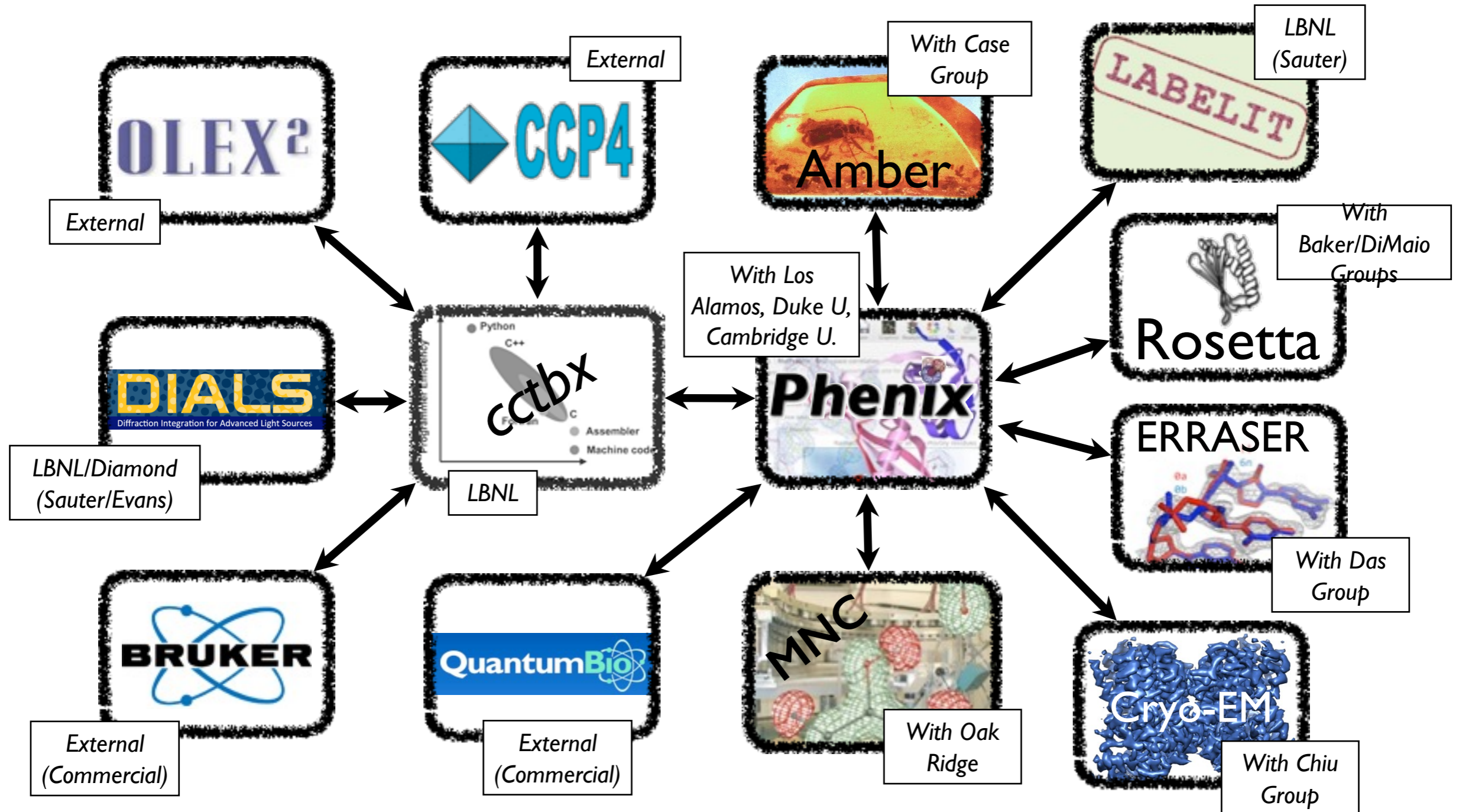


An NIH/NIGMS funded
Program Project

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*?

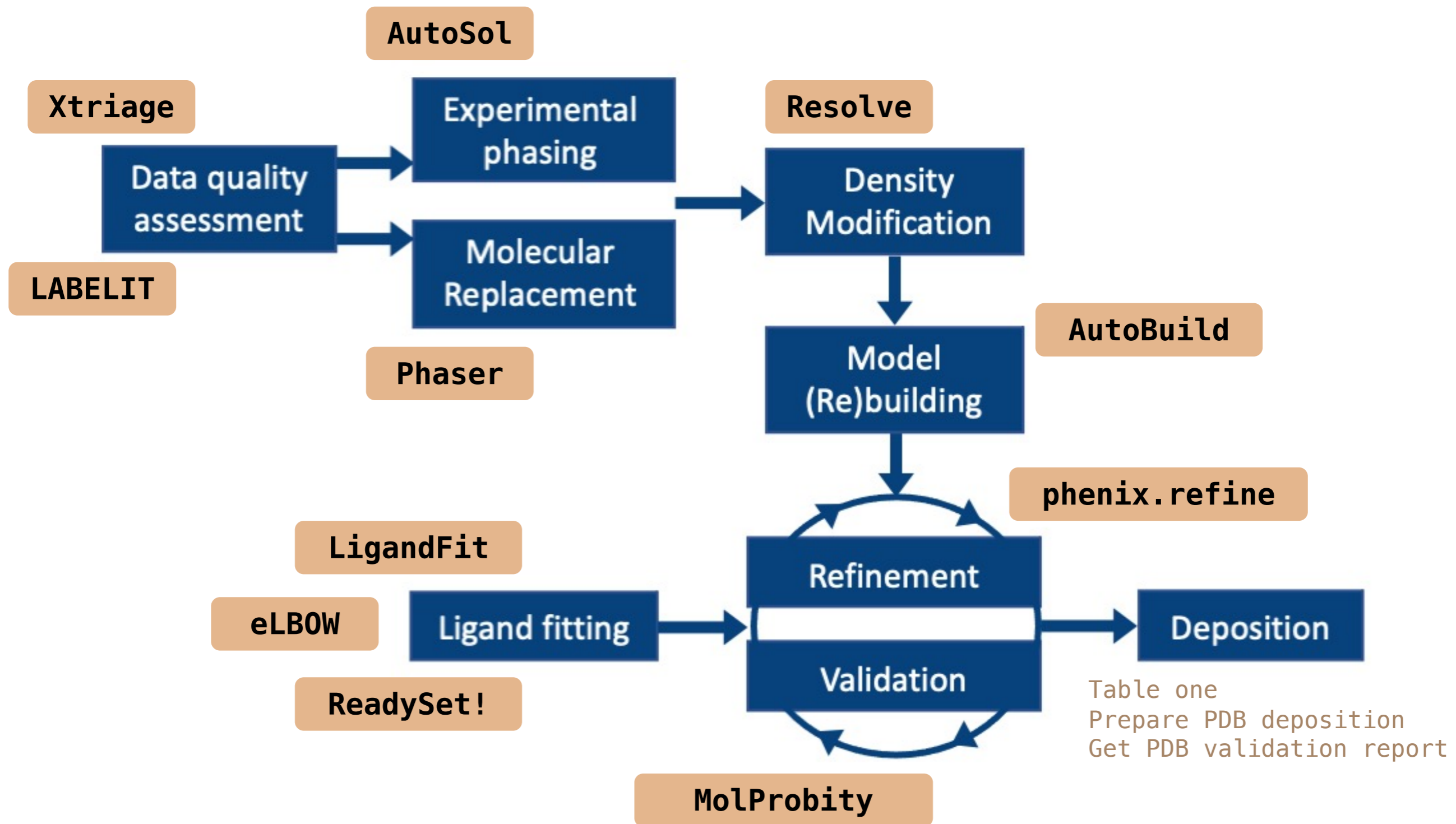
- Package for **automated structure solution**
- Modern programming concepts and new algorithm development
- Designed to be used by **both novices and experienced users**
- Long-term development and **support**
- Why is it called *Phenix*?

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)

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 tabs for 'Actions' and 'Job history'. The main area is divided into two panels: 'Projects' on the left and 'Favorites' on the right. The 'Projects' panel includes a 'Show group' dropdown set to 'All groups', a 'Manage...' button, and buttons for 'Select', 'Delete', 'New project', and 'Settings'. Below these is a table with columns for ID, Last modified, # of jobs, and R-free. The 'Favorites' panel lists various tools and categories such as AlphaFold, Crystals, Cryo-EM, and Models. 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'.

ID	Last modified	# of jobs	R-free
✓ test	Sep 14 2021 02:2...	529	0.0971

Projects

Show group: All groups Manage...

Select Delete New project Settings

Favorites

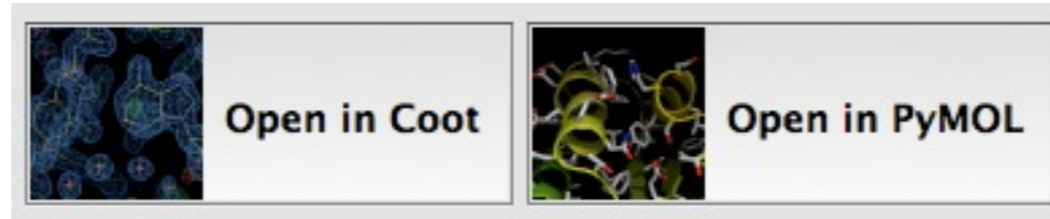
- AlphaFold (predicted models)
- Crystals: Data analysis and manipulation, Validation and map-based comparisons, Experimental phasing, Molecular replacement, Maps (create, manipulate, compare), Enhanced maps (Polder, FEM, density-modified...), Model building, Refinement, Ligands
- Cryo-EM: Map analysis, 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

Current directory: /Users/dcliebschner/Desktop/Projects/test Browse...

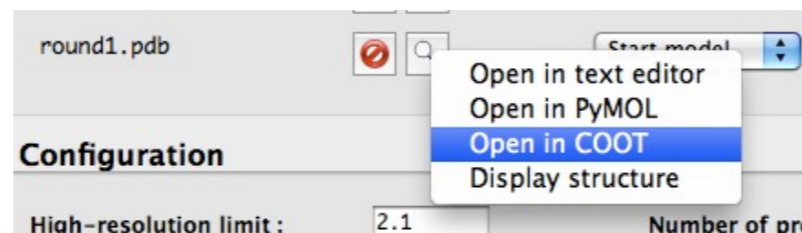
PHENIX version dev-svn-000 Project: test

Coot/PyMOL integration

- Most results can be opened directly in graphics apps



- Any PDB file listed in GUI can also be opened

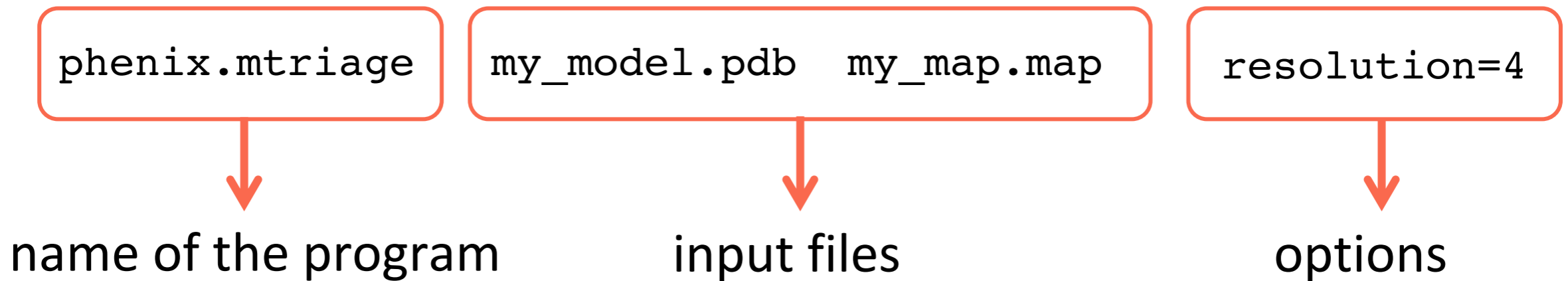


- AutoSol, AutoBuild, and phenix.refine will update Coot continuously while running
- Coot must have Python support (default on Mac)
- Specific paths to executables usually required on Linux

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

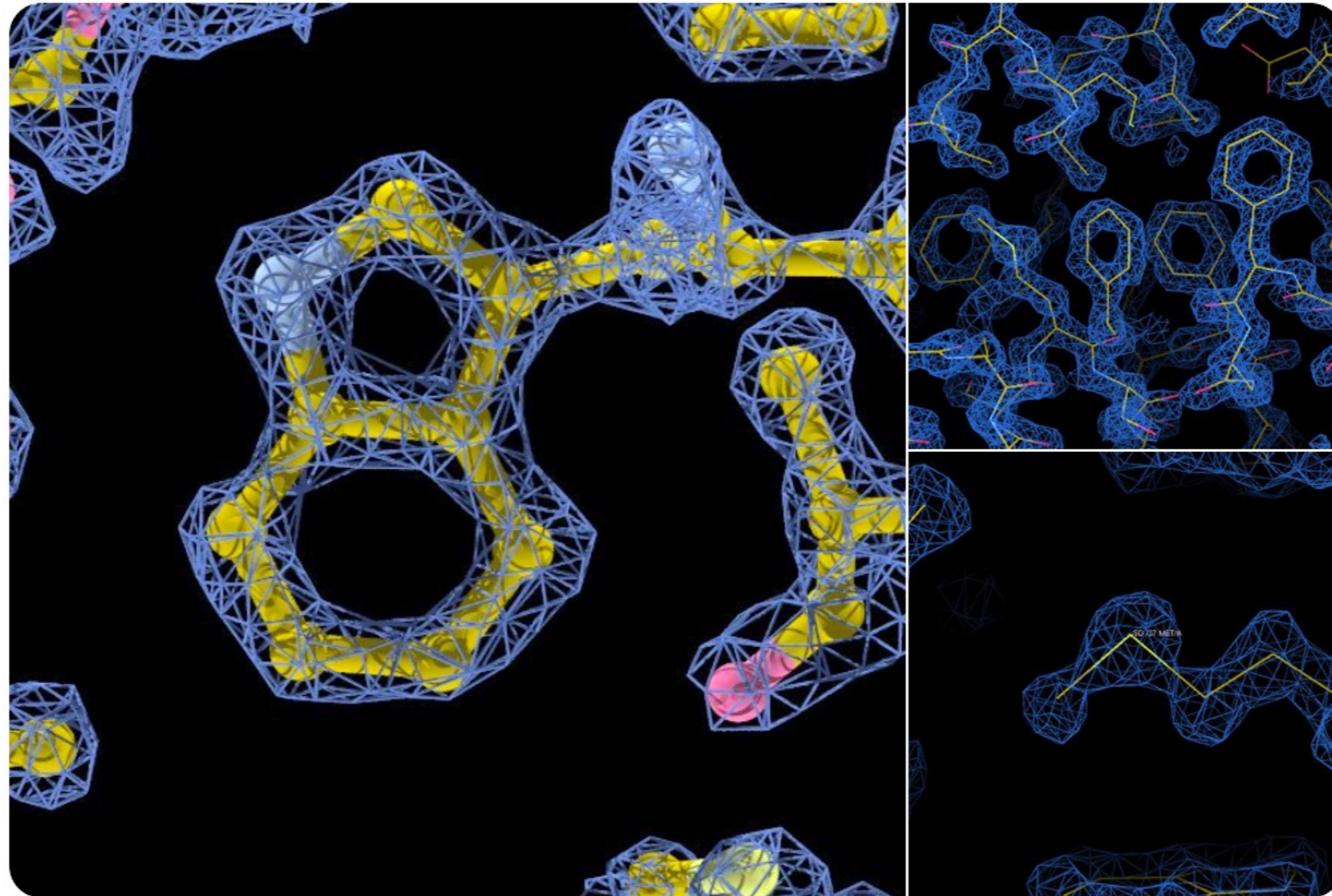
Video Tutorials

The screenshot shows the YouTube channel page for 'Phenix Tutorials'. The channel has 560 subscribers and a red 'SUBSCRIBE 560' button. The video grid includes:

- real_space_refine Tutorial** (5:27): How to run real-space-refine (763 views, 7 months ago)
- Secondary Structure Restraints Tutorial** (6:23): How to use secondary structure restraints (399 views, 8 months ago)
- Multiple refinement strategies Tutorial** (5:46): How to use multiple refinement strategies and... (281 views, 8 months ago)
- Planning a SAD experiment Tutorial** (6:00): Simulate a SAD experiment with... (483 views, 1 year ago)
- Map-to-model Tutorial** (5:33): Automatic map interpretation with map_to_model (1.3K views, 1 year ago)
- Scale-and-merge Tutorial** (7:31): Scaling and merging anomalous data (387 views, 1 year ago)
- Automated map sharpening Tutorial** (6:05): Automated map sharpening
- Ligandfit Tutorial** (5:48): Ligandfit
- Wilson plots and space group identification phenix.xtriage** (8:23): Wilson plots and space group identification
- Twinning phenix.xtriage** (6:08): Twinning
- Translational NCS phenix.xtriage** (4:55): Translational NCS
- Checking data quality with Xtriage** (6:49): Checking data quality with Xtriage

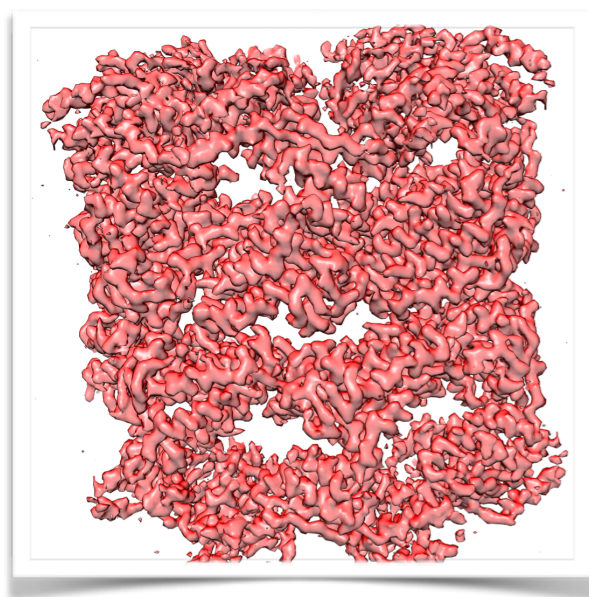
Dorothee Liebschner, Nigel Moriarty,
Miffy Mifsud, Tom Terwilliger

Impressive Cryo-EM Achievements

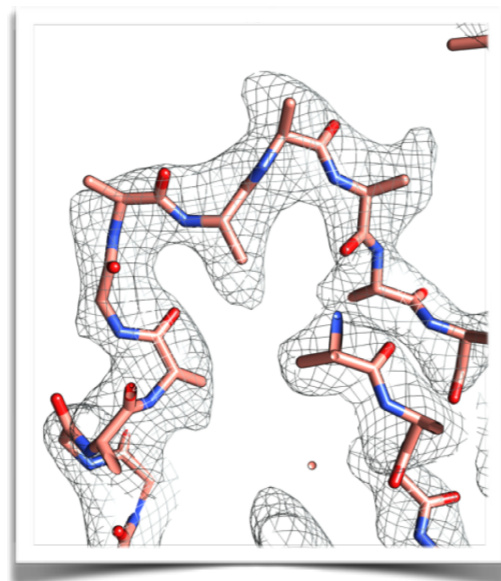


Namba Lab, Osaka

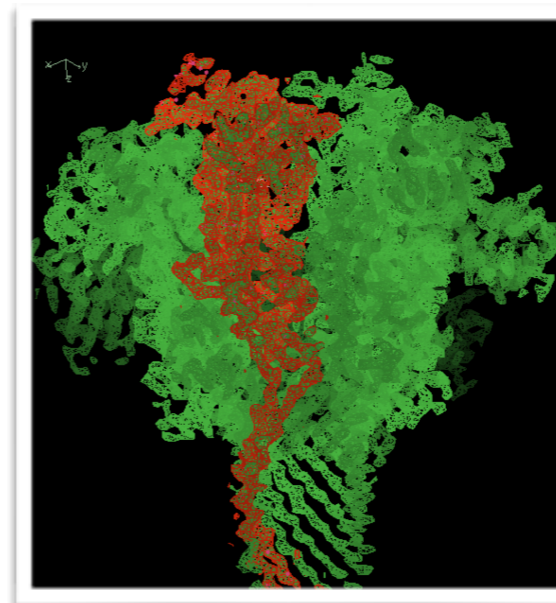
New Tools for cryo-EM in *Phenix*



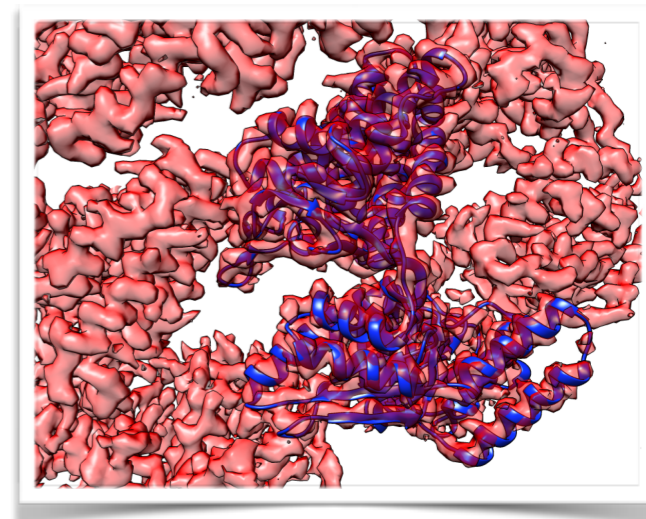
Symmetry from a map



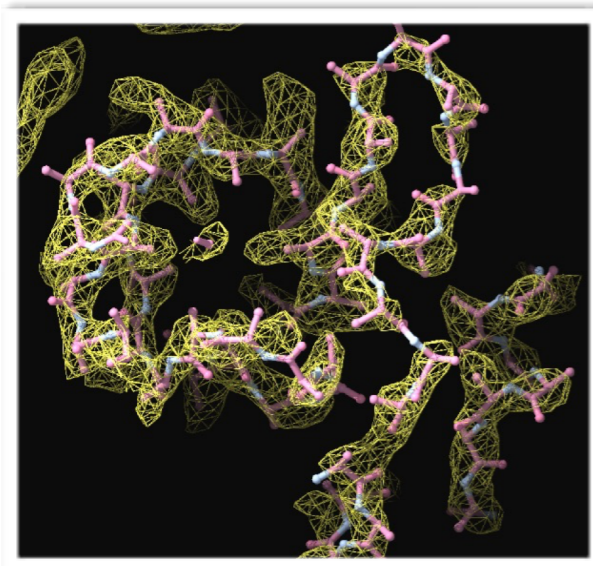
Automated map sharpening



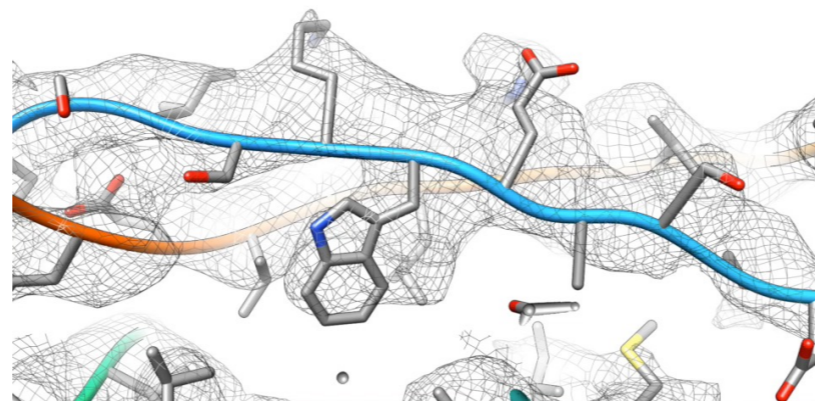
Map segmentation



Rigid model docking



Automated model building



Real space refinement

Comprehensive validation (CryoEM) (Project: rea-space-refine-6crz)

Input/Output ValidationCryoEM_7

Summary Model Model vs. Data Data

Files

Model: /Users/PDAdams/Documents/rea-space-refine-6crz/model.pdb
Map: /Users/PDAdams/Documents/rea-space-refine-6crz/map.ccp4

Open in Coot Export Table 1

White cells are mostly informational.
Green cells imply that the values are in an acceptable range.
Yellow cells imply that the values need to be checked carefully.
Red cells imply that the values are concerning and that the model should be checked very thoroughly.
Clicking on a row will bring up a panel with more detailed information.

Model		Ramachandran	
MolProbity		Outliers (%)	0.00 (Goal: < 0.2%)
MolProbity score	1.72	Allowed (%)	6.45
Clash score	5.44	Favored (%)	93.55 (Goal: > 98%)
Rotamer outliers (%)	0.00 (Goal: < 1%)		
CP outliers	0 (Goal: 0)		

CaBLAM		Peptide Plane	
Outliers (%)	3.88 (Goal: <= 1%)	cis-proline (%)	0.00
Disfavored (%)	8.96 (Goal: <= 5%)	twisted proline (%)	0.00
Ca outliers (%)	1.19 (Goal: <= 0.5%)	cis-general (%)	0.00
		twisted general (%)	0.00

Geometry Restraints

Bond	Angle	Dihedral
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Model and map validation

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Phenix Testers & Users

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- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

Outline

- Phenix introduction
- Tools for crystallography in Phenix
- NEW: Phenix with AlphaFold models
- Demo: MR + AlphaFold
- (Demo: Refinement)