

Schedule

8:30 AM: Introduction to Phenix and overview of tools for cryo-EM

8:45 AM: Map tools (density modification, sharpening, map symmetry)

9:30 AM: Break and computer setup

10:00 AM: Model building (docking, ab initio building)

10:30 AM: Atomic model refinement

11:30 AM: Validation (map, model, model to map fit)

12:00: Lunch

1:00 PM: Introduction to the GUI and setup

1:15 PM: Map improvement and model building

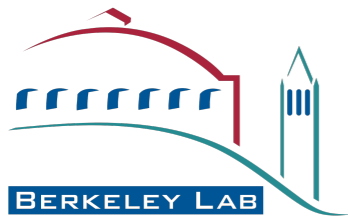
(DM, sharpening, symmetry, segmentation + automated model building)

3:00 PM: Break

3:30 PM: Refinement and validation

4:30 PM: User questions, more select tutorials, discussion, etc

5:30 PM: Finish



U.S. DEPARTMENT OF
ENERGY



**UNIVERSITY OF
CALIFORNIA**

CU Anschutz Medical School, January 2020

Phenix Introduction

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Lawrence Berkeley Laboratory



**UNIVERSITY OF
CAMBRIDGE**

The *Phenix* Project

Lawrence Berkeley Laboratory

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



Los Alamos National Laboratory
New Mexico Consortium
Baylor College of Medicine

Tom Terwilliger,
Li-Wei Hung,
Matt Baker



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Tristan Croll, Rob Oeffner,
Kaushik Hatti, Massimo Sammito,
Duncan Stockwell

Cambridge University



Duke University

Jane & David Richardson,
Vincent Chen, Bradley Hintze,
Michael Prisant, Chris Williams

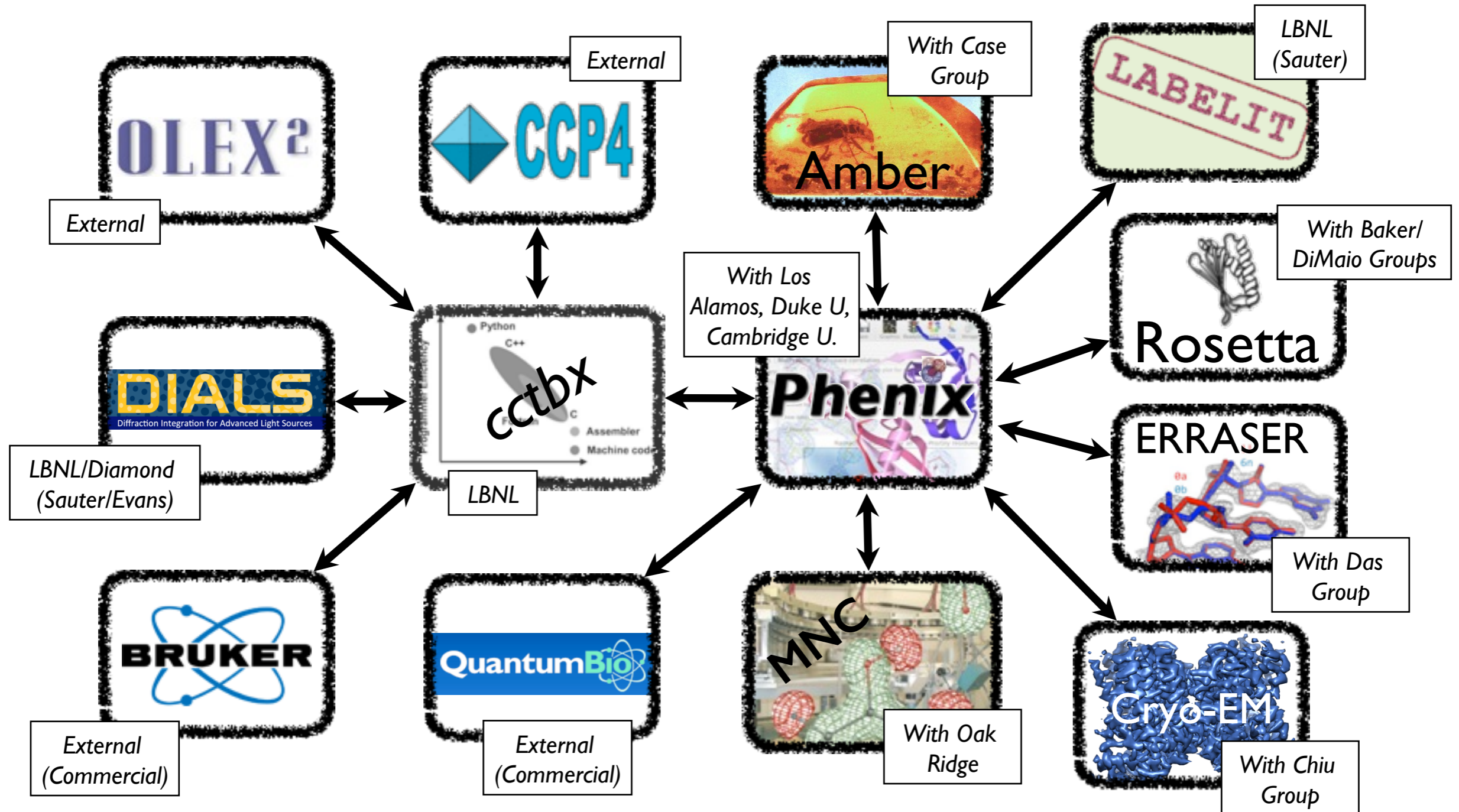


An NIH/NIGMS funded
Program Project

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*?

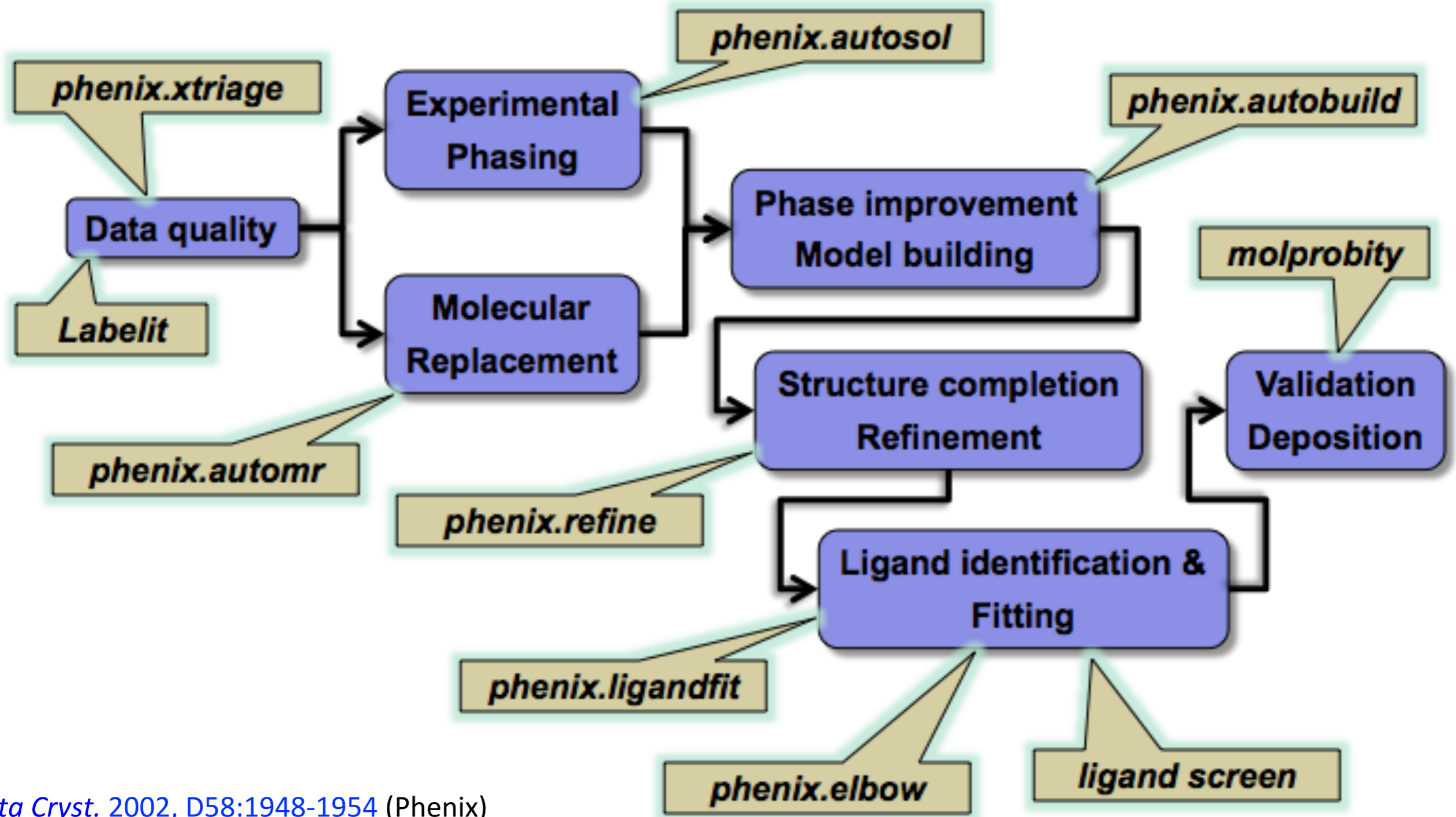
- Package for **automated structure solution**
- Modern programming concepts and new algorithm development
- Designed to be used by **both novices and experienced users**
- Long-term development and **support**
- Why is it called *Phenix*?

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**

Automation of Structure Solution



[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)

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. The left panel, titled 'Projects', shows a table of project entries with columns for ID, Last modified, # of jobs, and R-free. The right panel, titled 'Favorites', lists various tool categories such as Data analysis, Experimental phasing, Molecular replacement, Model building, Refinement, Cryo-EM, Mtriage, Map to Model, Real-space refinement, Comprehensive validation (cryo-EM), EMRinger, ResolveCryoEM, Autosharpen Map, Dock in map, and Sequence From Map. At the bottom, there is a 'Current directory' field showing the path /Users/dcliebschner/Documents/rotavirus-model-building and a 'Project: rotavirus-model-building' label.

PHENIX home

Quit Preferences Help Citations Reload last job Coot PyMOL KiNG Other tools Ask for help

Actions Job history

Projects

Show group: All groups Manage...

Select Delete New project Settings

ID	Last modified	# of jobs	R-free
test	Jan 25 2020 07:12...	468	0.0971
poler_survey	Oct 09 2019 04:52...	52	---
polder_Leighton	Sep 17 2019 04:4...	5	0.1554
review_neutron	Aug 27 2018 10:44...	16	0.1595
structure_compa...	Jun 07 2017 02:52...	33	---
groel_map_sym...	Jan 27 2020 01:59...	4	---
groel_dock_refine	Jan 27 2020 07:49...	1	---
✓ rotavirus-model...	Jan 28 2020 11:32...	2	---

Favorites

Data analysis

Experimental phasing

Molecular replacement

Model building

Refinement

Cryo-EM

Mtriage
Analyze quality of maps in CCP4 format

Map to Model
Model-building into cryo-EM and low-resolution maps

Real-space refinement
Automated refinement using real-space maps (Cryo-EM, X-ray, ...)

Comprehensive validation (cryo-EM)
Model quality assessment, including real-space correlation, for cryo-EM structures

EMRinger
Model validation for de novo electron microscopy structures

ResolveCryoEM
Density modify cryo EM maps

Autosharpen Map
Tool for sharpening a map

Dock in map
Tool for docking a model in to map

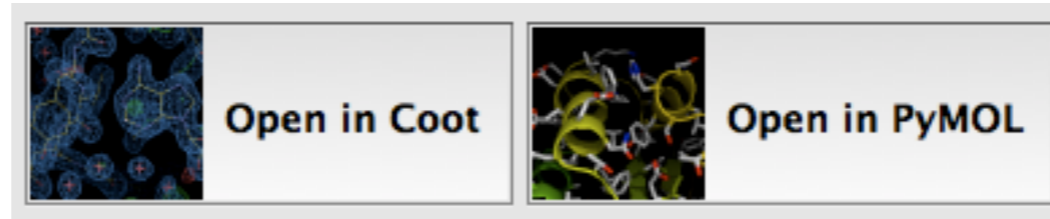
Sequence From Map

Current directory: /Users/dcliebschner/Documents/rotavirus-model-building Browse...

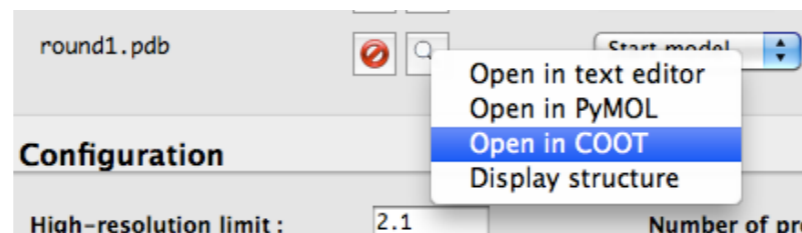
PHENIX version dev-svn-000 Project: rotavirus-model-building

Coot/PyMOL integration

- Most results can be opened directly in graphics apps



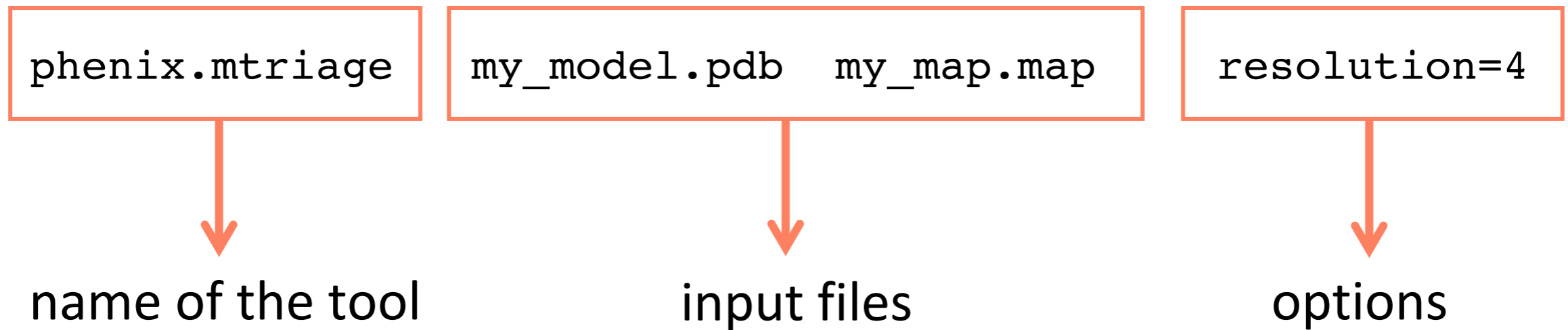
- Any PDB file listed in GUI can also be opened



- 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 via a 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

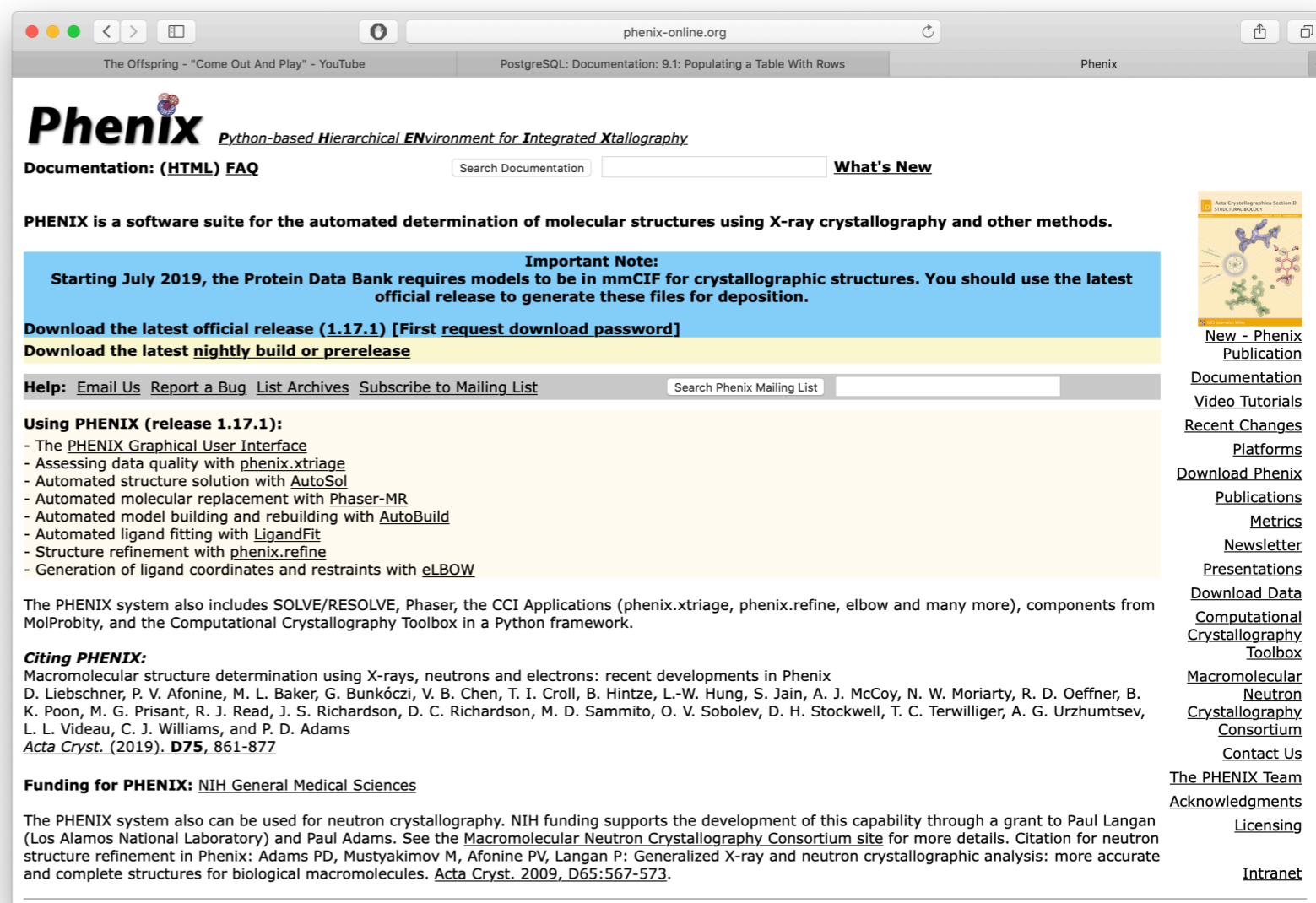
phenix-online.org

Supported on:

- Linux (RedHat, Fedora)
- Mac OSX
- Windows

Extensive documentation

Nightly builds:



The screenshot shows the Phenix website homepage. At the top, there is a navigation bar with links for "Documentation: (HTML) FAQ", "Search Documentation", and "What's New". Below this, a blue banner contains an "Important Note" about the Protein Data Bank requirements starting in July 2019. A yellow banner below that provides links to "Download the latest official release (1.17.1)" and "Download the latest nightly build or prerelease". The main content area lists "Using PHENIX (release 1.17.1)" with a bulleted list of features and tools. A sidebar on the right contains a vertical list of links including "New - Phenix Publication", "Documentation", "Video Tutorials", "Recent Changes", "Platforms", "Download Phenix Publications", "Metrics", "Newsletter", "Presentations", "Download Data", "Computational Crystallography Toolbox", "Macromolecular Neutron Crystallography Consortium", "Contact Us", "The PHENIX Team", "Acknowledgments", "Licensing", and "Intranet".

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

www.youtube.com/channel/UCcdI0hfHngWAZLJWynxPQWg/videos

YouTube IT Search

Phenix Tutorials

560 subscribers

SUBSCRIBE 560

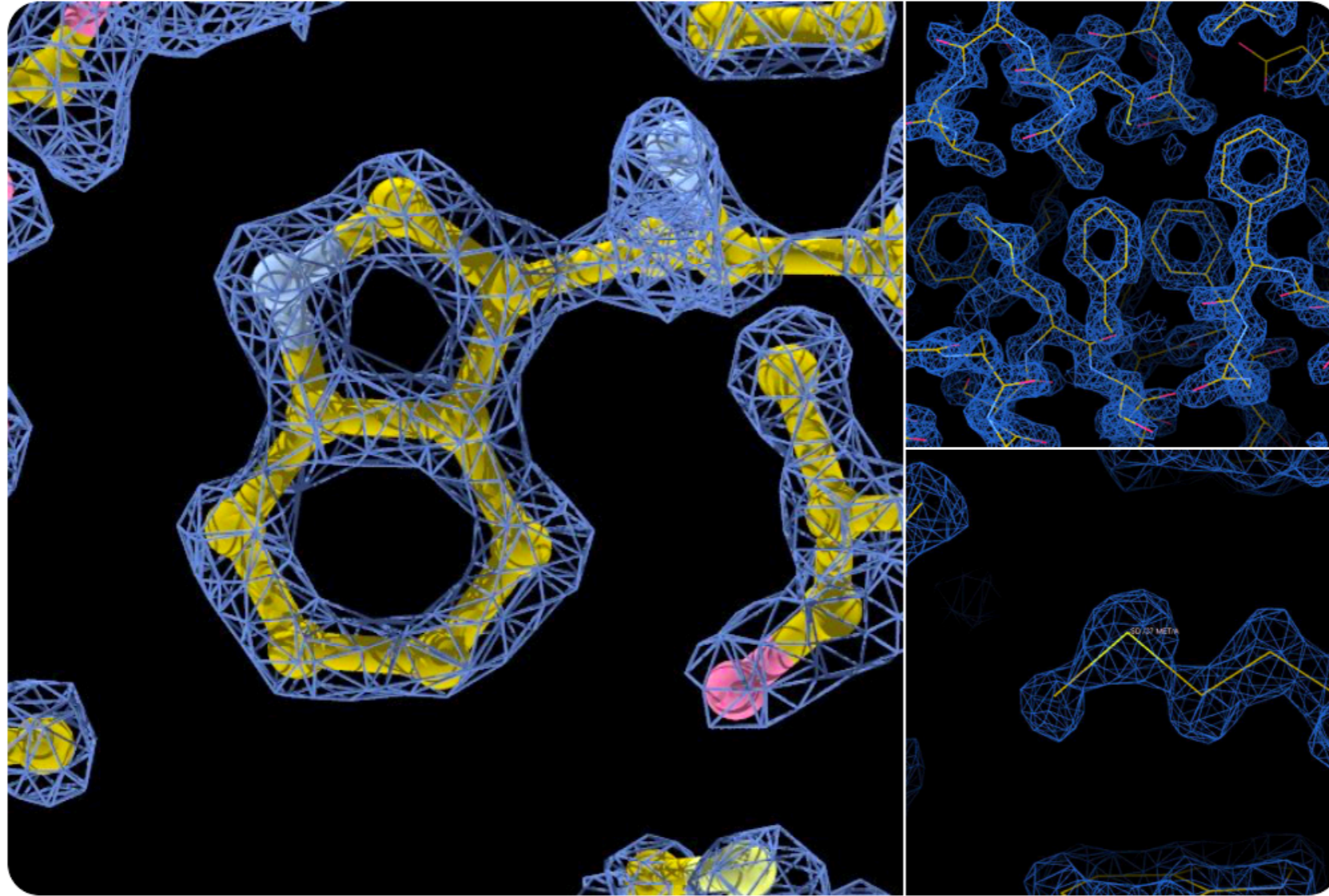
HOME VIDEOS PLAYLISTS CHANNELS ABOUT

Uploads PLAY ALL SORT BY

Thumbnail	Title	Views	Upload Date	License
real_space_refine Tutorial	How to run real-space-refine	763 views	7 months ago	CC
Secondary Structure Restraints Tutorial	How to use secondary structure restraints	399 views	8 months ago	CC
Multiple refinement strategies Tutorial	How to use multiple refinement strategies and...	281 views	8 months ago	CC
Planning a SAD experiment Tutorial	Simulate a SAD experiment with...	483 views	1 year ago	CC
Map-to-model Tutorial	Automatic map interpretation with map_to_model	1.3K views	1 year ago	CC
Scale-and-merge Tutorial	Scaling and merging anomalous data	387 views	1 year ago	CC
Automated map sharpening Tutorial	Automated map sharpening			
Ligandfit Tutorial	Ligandfit			
Wilson plots and space group identification phenix.xtriage	Wilson plots and space group identification phenix.xtriage			
Twinning phenix.xtriage	Twinning phenix.xtriage			
Translational NCS phenix.xtriage	Translational NCS phenix.xtriage			
Checking data quality with Xtriage	Checking data quality with Xtriage			

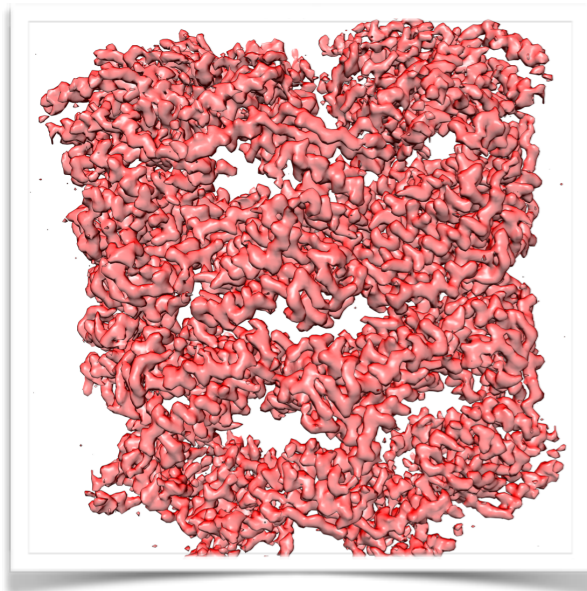
*Dorothee Liebschner, Nigel Moriarty,
Miffy Mifsud, Tom Terwilliger*

Impressive Cryo-EM Achievements

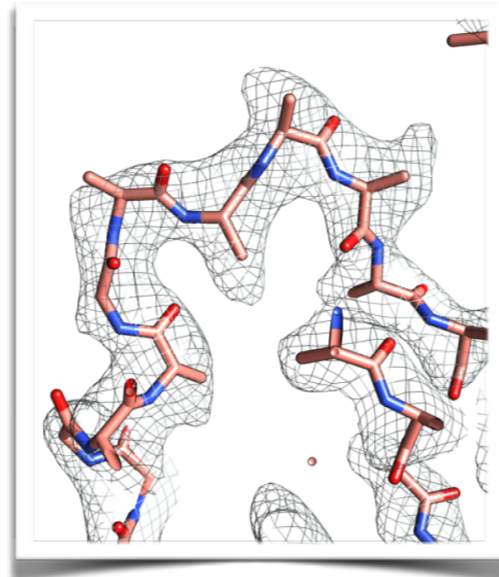


Namba Lab, Osaka

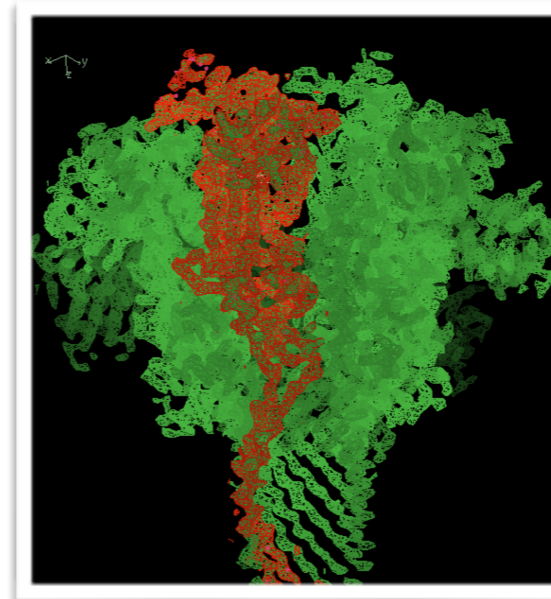
New Tools for Cryo-EM in *Phenix*



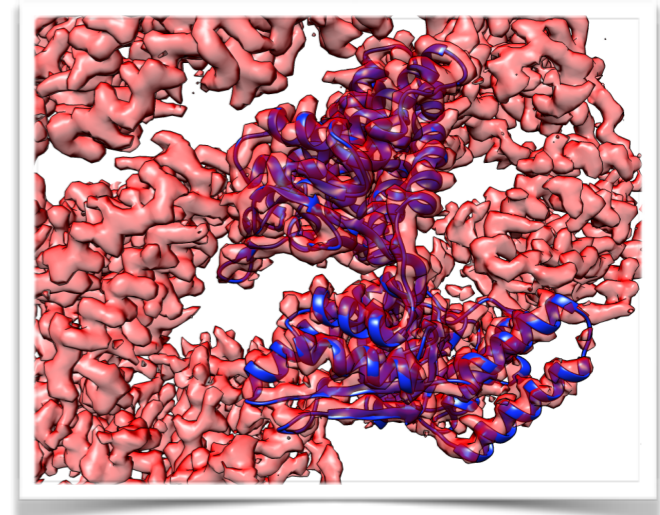
Symmetry from a map



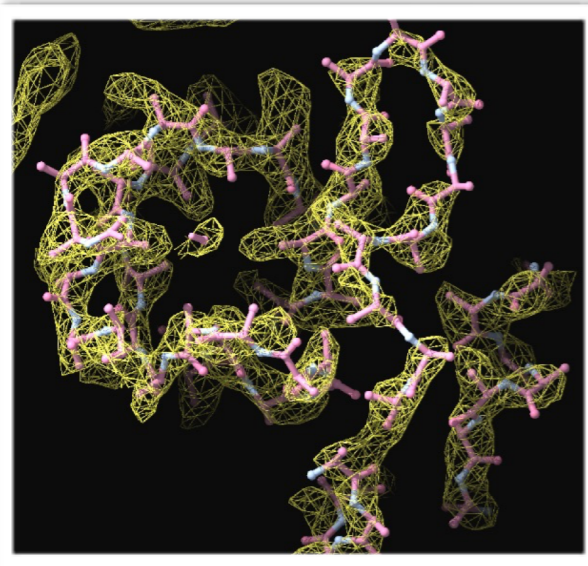
Automated map sharpening



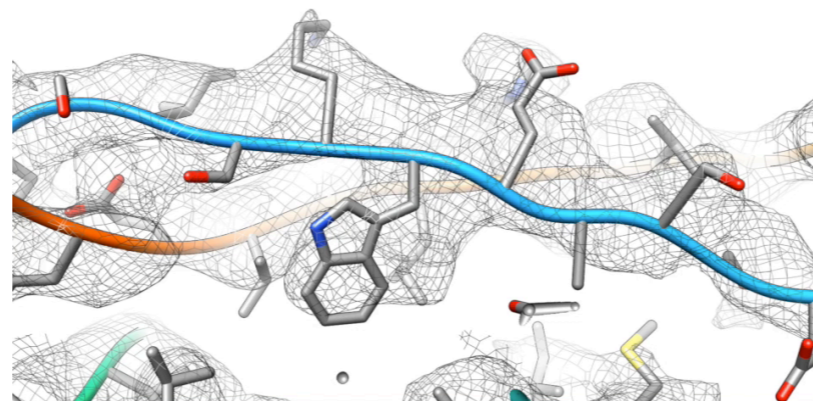
Map segmentation



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

Acknowledgements

Berkeley Laboratory

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Los Alamos Laboratory/New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

Baylor College of Medicine

Matt Baker

Cambridge University

Randy Read, Airlie McCoy, Gabor Bunckozi, Tristan Croll, Rob Oeffner, Kaushik Hatti, Massimo Sammito, Duncan Stockwell, Laurent Storoni

Duke University

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Ben Barad, Yifan Cheng, Jaime Fraser

University of Washington

Frank DiMaio, Ray Wang, David Baker

Oak Ridge National Laboratory

Marat Mustyakimov, Paul Langan

Other Collaborators

Corey Hryc, Zhao Wang, Wah Chiu
Pawel Janowski, David Case
Dale Tronrud, Donnie Berholz, Andy Karplus
Alexandre Urzhumtsev & Vladimir Lunin
Garib Murshudov & Alexi Vagin
Paul Emsley, Bernhard Lohkamp, Kevin Cowtan
David Abrahams
PHENIX Testers & Users

Funding

- NIH/NIGMS: P01GM063210, P50GM062412, P01GM064692, R01GM071939
- PHENIX Industrial Consortium
- Lawrence Berkeley Laboratory

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