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COMPUTATIONAL CRYSTALLOGRAPHY INITIATIVE

# Automated Structure Solution and refinement with PHENIX

**Pavel Afonine**

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Physical Biosciences Division  
Lawrence Berkeley National Laboratory, Berkeley CA, USA

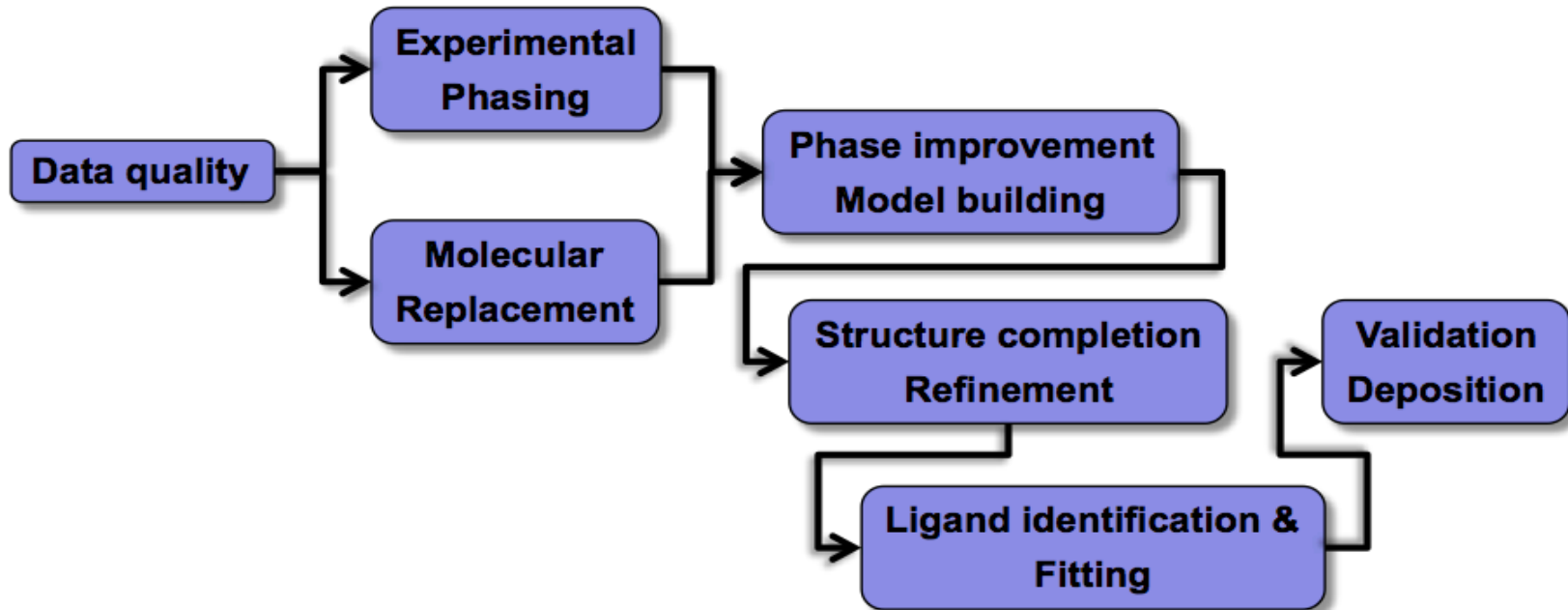
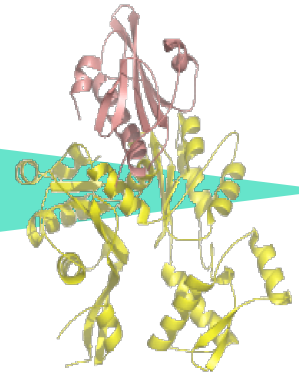
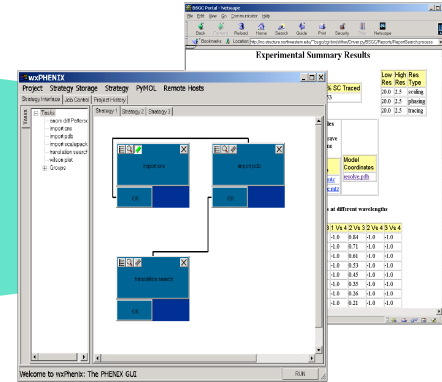
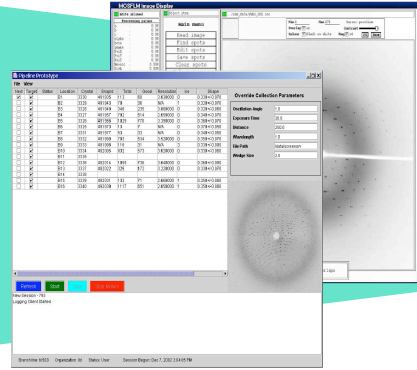
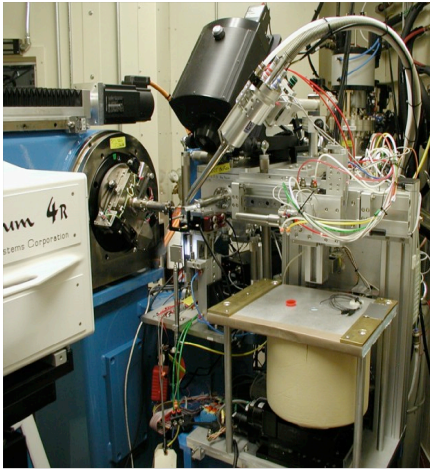
Australasian Crystallography school  
17th-24th July, 2010

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PHYSICAL BIOSCIENCES DIVISION

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# Why Automation ?



- Automation can increase efficiency, and reduce human error

## Why Automation ?

- Can speed up the process and can help reduce errors
- Makes difficult cases more feasible for experts
- Routine structure solution cases are accessible to a wider group of structural biologists
- Software can try more possibilities than we are typically willing to bother with
- Multiple trials or use of different parameters can be used to estimate uncertainties
- If a task is modular and automated, you can run it many times...
  - ... checking different space groups, datasets to use
  - ... checking if your model is biasing the map
  - ... checking if you always get the same model
- What is required:
  - Software carrying out individual steps
  - Seamless connection between steps
  - A way to decide what is good
  - Strategies for structure determination and decision-making

# The PHENIX Project

## Lawrence Berkeley Laboratory

Paul Adams, Ralf Grosse-Kunstleve,  
Pavel Afonine, Nat Echols, Nigel  
Moriarty, Nicholas Sauter, Peter Zwart



## Los Alamos National Laboratory

Tom Terwilliger, Li-Wei Hung



Randy Read, Airlie McCoy,  
Gabor Bunkoczi, Rob Oeffner

## Cambridge University



## Duke University

Jane & David Richardson, Vincent  
Chen, Jeff Headd, Chris Williams,  
Bryan Arendall, Laura Murray



*An NIH/NIGMS funded  
Program Project*



**Phenix**



# PHENIX and Neutron crystallography

## Macromolecular Neutron Crystallography Consortium (MNC)



Los Alamos National Lab

*Paul Langan, Marat Mustyakimov, Benno Schoenborn*



Lawrence Berkeley National Lab (LBNL)

*Paul Adams, Pavel Afonine*

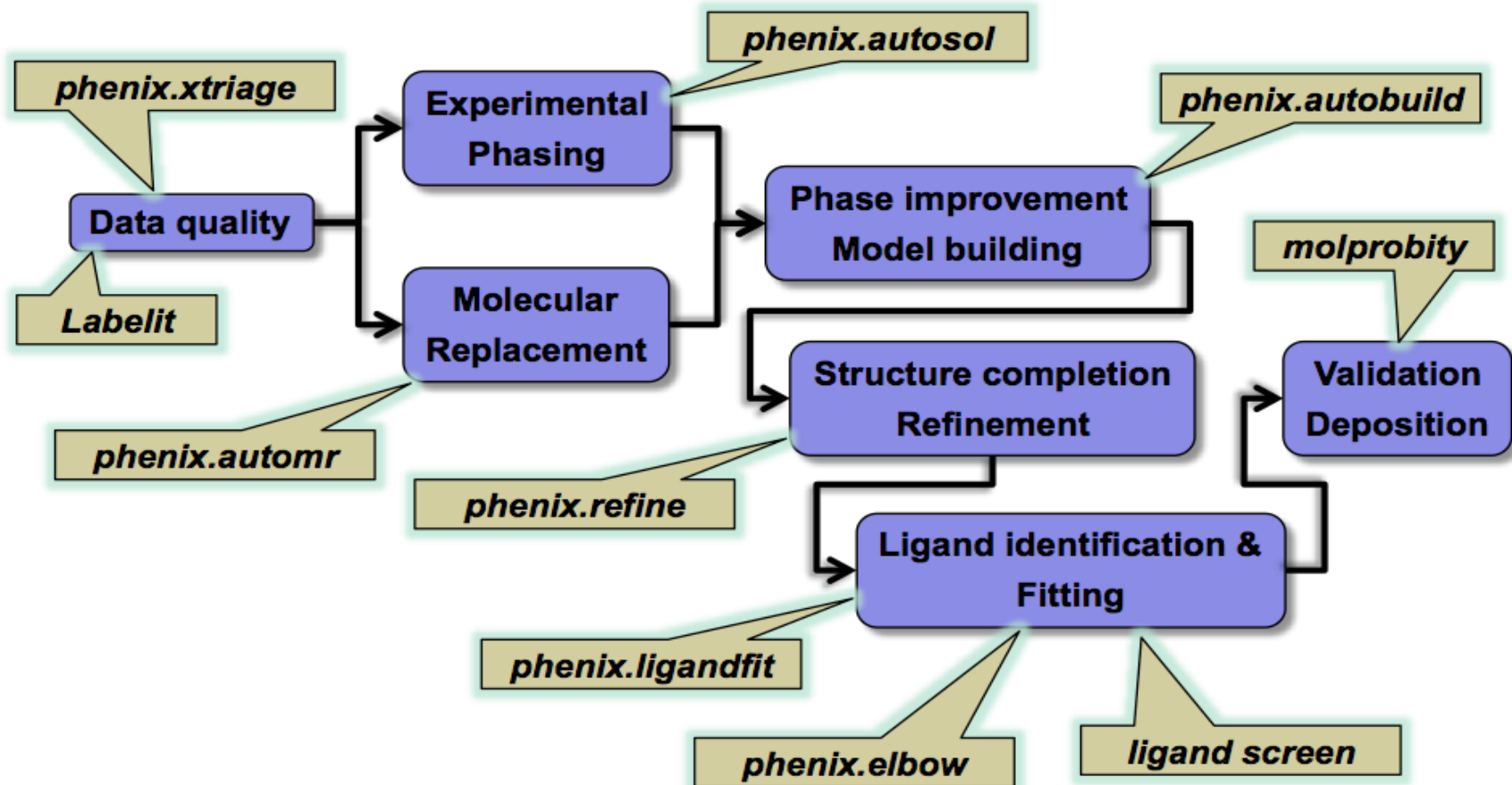
<http://mnc.lanl.gov/>

## The PHENIX project

- PHENIX is a new package for automated structure solution that incorporates handling of both: X-ray and neutron data
- PHENIX is not a pipe-line made of existing programs, but a highly integrated software
- Library based development (Python, C++) and new algorithms
- Designed to be used by both novices and experienced users
- Long-term development and support

## PHENIX: principal tools

Complete set of tools for crystallographic structure determination: from experimental data to PDB deposited structure



## PHENIX: principal tools

- Data quality and pathology analysis (phenix.xtrriage)  
*Completeness, anomalous signal, outliers, tNCS, twinning, missed symmetries.*
- Substructure determination (phenix.hyss)  
*Automated, Patterson/Direct methods dual space recycling.*
- Experimental phasing (PHASER, SOLVE)  
*ML SAD phasing in Phaser, ML SIR/MIR/MAD phasing in SOLVE.  
ML SAD + MR phasing in Phaser*
- Molecular Replacement phasing (PHASER)  
*ML molecular replacement*
- Statistical density modification (RESOLVE)  
*Solvent flattening, histogram matching, automated NCS analysis.*
- Automated model building (RESOLVE, Textal, phenix.refine)  
*Pattern matching methods, loop fitting, NCS, protein and nucleic acids.*
- Structure refinement (phenix.refine)  
*Rigid body, coordinates, simulated annealing, iso/aniso-ADP, TLS, neutron data (joint refinement), twinned refinement, constrained occupancy refinement.*
- Ligand coordinate and restraint generation (phenix.elbow & phenix.reel)  
*Semi-empirical method for coordinate generation, CCP4 monomer library file generation.*
- Model Validation (Molprobit, local electron density analysis, POLYGON)  
*A set of tools for complete, local and global, structure validation.*



## PHENIX: principal tools

- PHENIX programs can be run using:
  - **GUI**: easy for beginners, guided process - less chance of errors
  - **Command line**: convenient for scripting of multiple and large scale tasks
- Command line tools are still easy to run:
  - **Autobuild** (*from starting phases to complete and refined model*):  

```
phenix.autobuild data=scale.mtz model=mr.pdb seq_file=correct.seq
```
  - **Ligandfit** (automatically find and build ligands into density):  

```
phenix.ligandfit data=nsf.mtz model=noligand.pdb ligand=atp.pdb
```
  - **AutoMR** (molecular replacement with Phaser + Autobuild = refined model):  

```
phenix.refine nsf-d2.mtz nsf.pdb
```
  - **phenix.refine** (highly automated structure refinement, X-ray, Neutron):  

```
phenix.refine nsf-d2.mtz nsf.pdb
```
  - **phenix.xtriage** (complete data analysis):  

```
phenix.xtriage porin_fp.mtz
```

# GUI examples

PHENIX home

Quit Preferences Help New project Project settings Job history Citations Coot PyMOL

Click or drag-and-drop files onto a program to launch it. To switch to a project, click the "Choose this project" button.

Projects			
ID	Last modified	# of jobs	R-free
rnase	Jul 12 2010 12:14 PM	0	None
✓ industry_MTP	Jul 12 2010 12:17 PM	0	None

Switch project Delete project

Output directory : /Users/afonine/Desktop/zz/zz1 Browse...

- Reflection tools
- Model tools
- Experimental phasing
- Molecular replacement
- Building and refinement
- Maps
- Ligands
- Validation
- Utilities

PHENIX version 1.6.2-432 Project: industry\_MTP

# GUI examples

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PHENIX version 1.6.2-432 Project: industry\_MTP





**Reflection tools**

**Model tools**

**Experimental phasing**

**Molecular replacement**

**Building and refinement**

-  **AutoBuild**  
*Automated model-building and refinement*
-  **phenix.refine**  
*Automated X-ray and neutron refinement*
-  **Find Helices and Strands**  
*Fast chain tracing*
-  **Fit Loops**  
*Fast placement of missing loops in electron density*

**Maps**

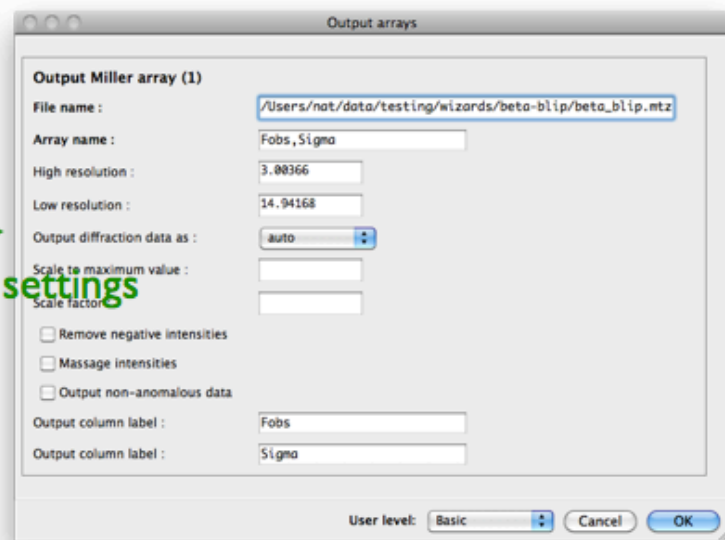
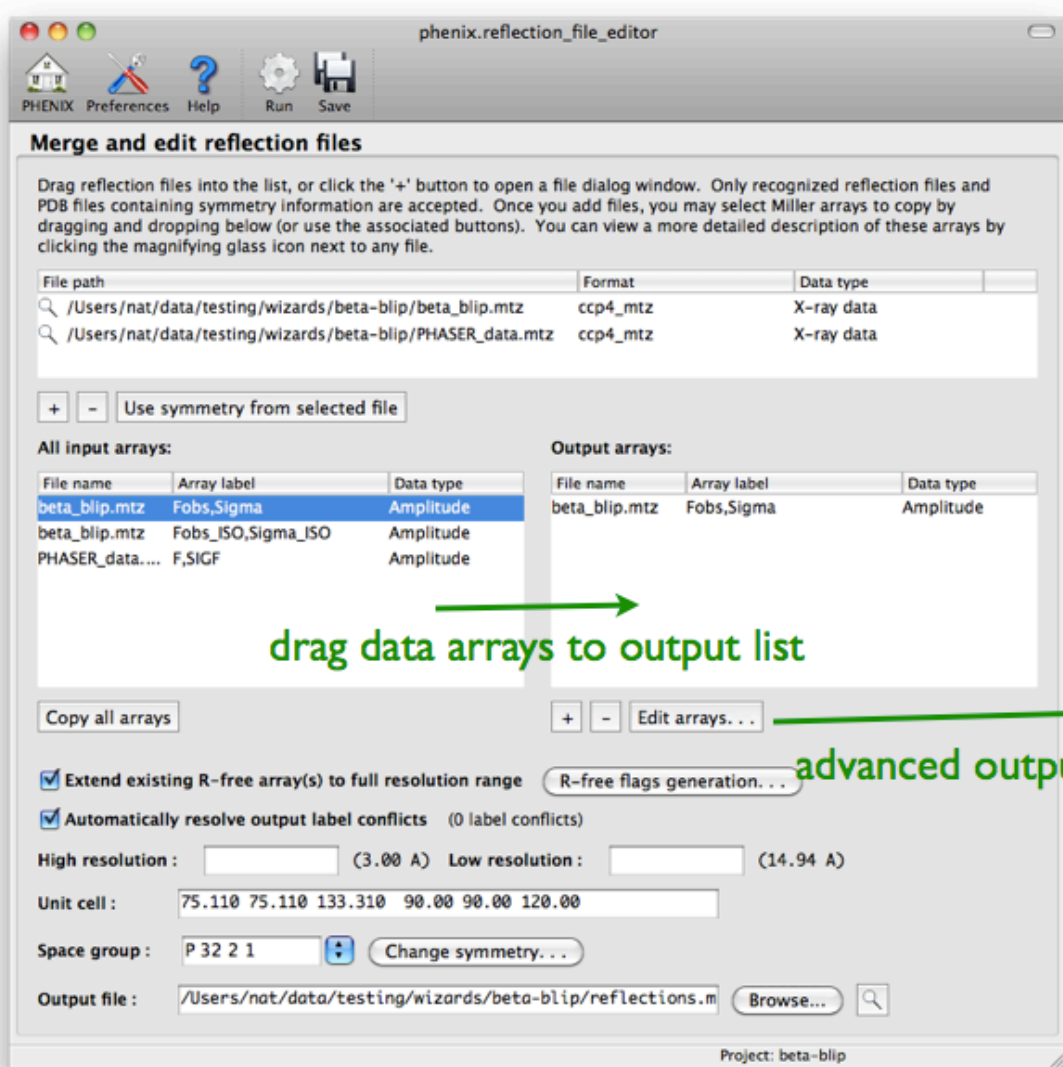
**Ligands**

**Validation**

**Utilities**

# Reflection file editor

Combine and manipulate reflection files in any format, output as MTZ. Capable of extending old R-free sets, and generating new sets as thin shells (for refinement in presence of NCS). *For use with fully processed data only - reflections will be merged and h,k,l indices altered as required.*



(All functionality is also available on the command line as `iotbx.reflection_file_editor`, but we recommend using the GUI for this unless you are scripting an automation pipeline.)

# Automated Molecular Replacement - AutoMR

The screenshot displays the AutoMR software interface. At the top, a menu bar includes PHENIX, Preferences, Help, Run, Abort, Save, Xtrriage, Sculptor, Ensembler, Coot, and PyMOL. The main window is titled 'Configure' and is divided into three sections: 'Input files', 'Configuration', and 'Output'.

**Input files:** The 'Reflections file' is set to `/Users/pdadams/Work/Scratch/phenix/p9-sad/p9.sca`. Below this, there are tabs for 'Search models' and 'Asymmetric unit contents'. The 'Ensemble 1' section is active, showing a list of either percent identities or RMSDs for each coordinate file. The 'EnsembleID' is `p9`, 'Copies to search for' is `1`, 'Identity(s)' is empty, and 'RMSD(s)' is `0.25`. The 'Coordinates' field is `pdadams/Work/Scratch/phenix/p9-sad/AutoSol_run_1/overall_best.pdb`. An 'Add ensemble' button is located below this section.

**Configuration:** The 'High resolution' is `0.0`, 'Data labels' is `i_obs sigma`, and the checkbox for 'Run AutoBuild after MR' is checked. The 'Space group' is `I 4` and the 'Unit cell' parameters are `113.949 113.949 32.474 90.000 90.000 90.000`. An 'All parameters...' button is present.

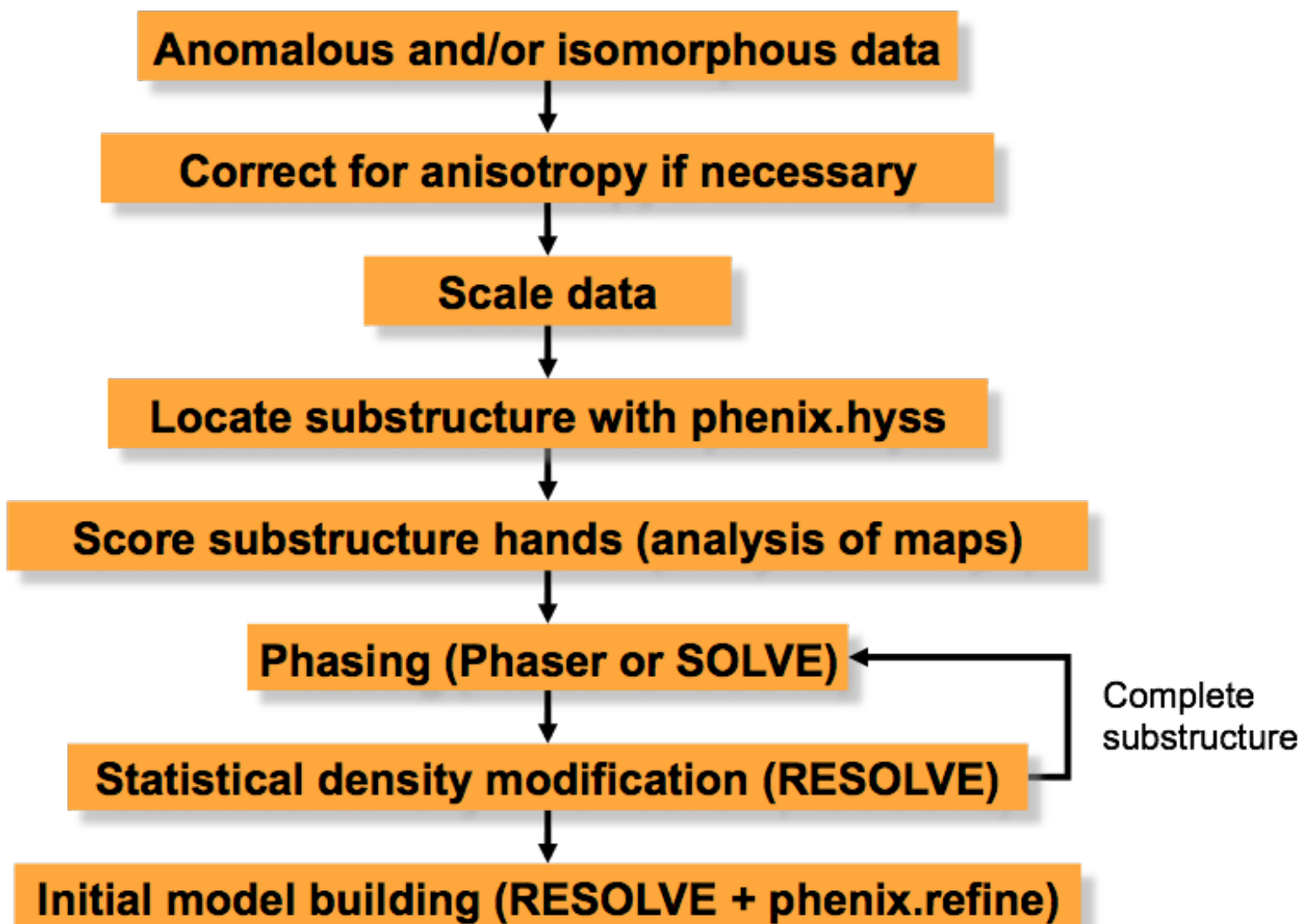
**Output:** The 'Output directory' is `/Users/pdadams/Work/Scratch/phenix/p9-sad`. A note states: 'All output files will be placed in directories named AutoMR\_\*'.

At the bottom left, the Berkeley logo and 'Idle' status are visible. At the bottom right, the project name 'Project: p9-sad\_pdadams' and the University of California, Berkeley seal are shown.

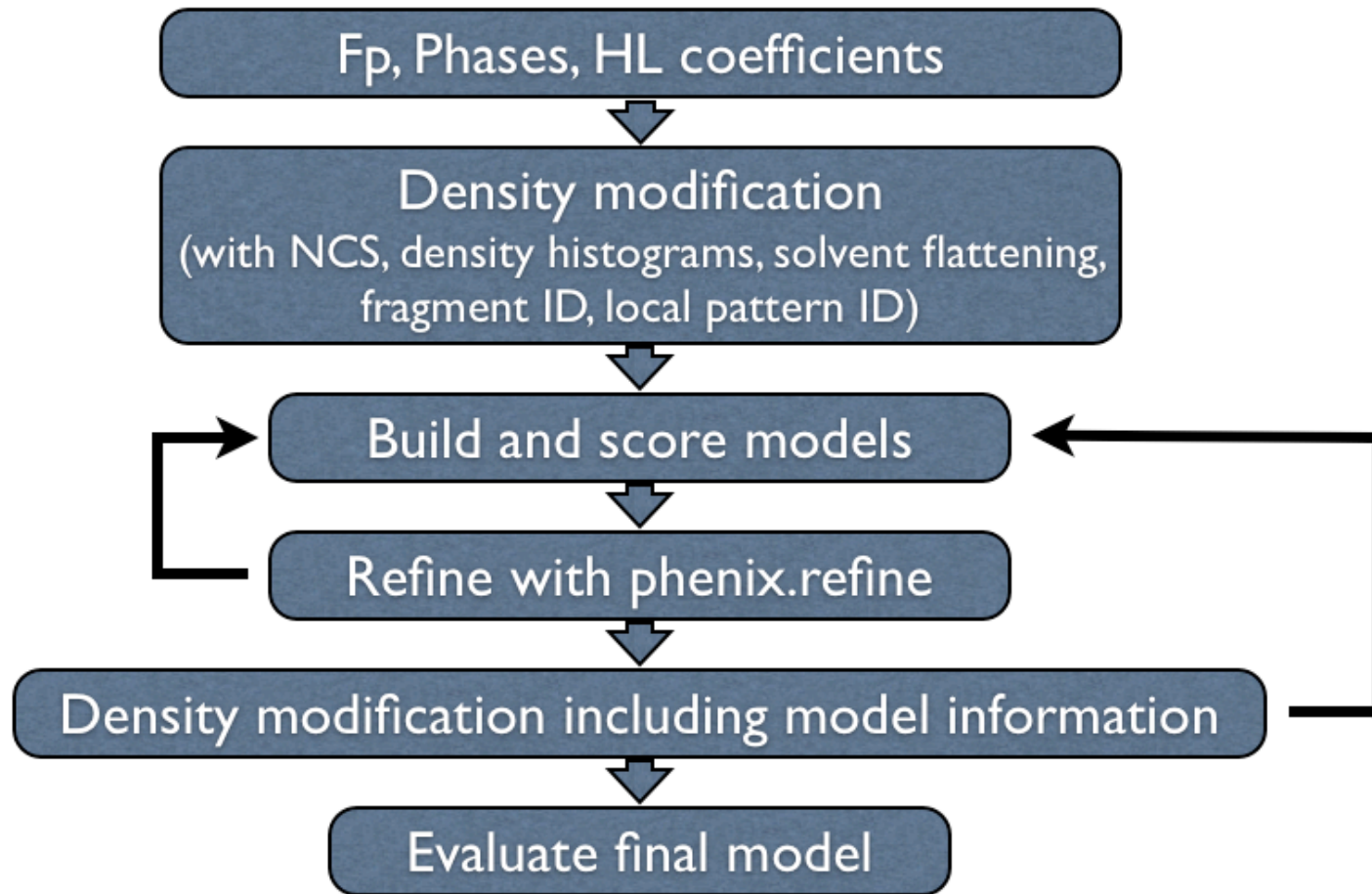
## Automated structure solution

- The steps of substructure location, experimental phasing, density modification, and initial model building can be linked together and run automatically
- One of the biggest challenges is automatically deciding which results are best at each step and should be carried forward in the process
  - Choice between different substructure solutions
  - Choice of substructure hand
  - Has completing the substructure made the map better or worse?
  - Choice of phase improvement parameters

## Automated structure solution: AutoSol Procedure



# Automated Model Building/Rebuilding



*Acta Cryst.* 2007, **D63**:597-610.

*Acta Cryst.* 2008, **D64**:61-69.

*Acta Cryst.* 2008, **D64**:515-524.

Tom Terwilliger, Pavel Afonine, Ralf Grosse-Kunstleve

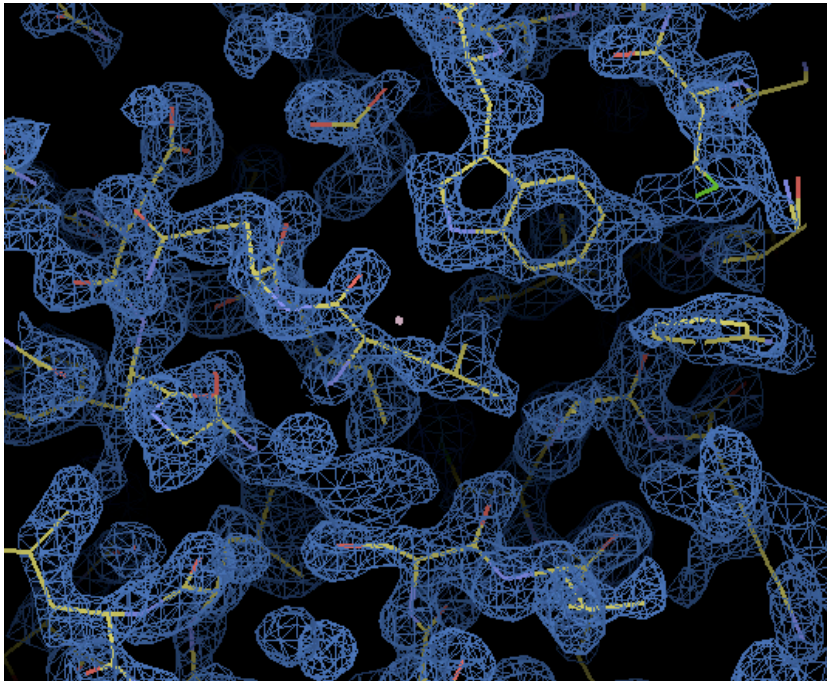
**Phenix**



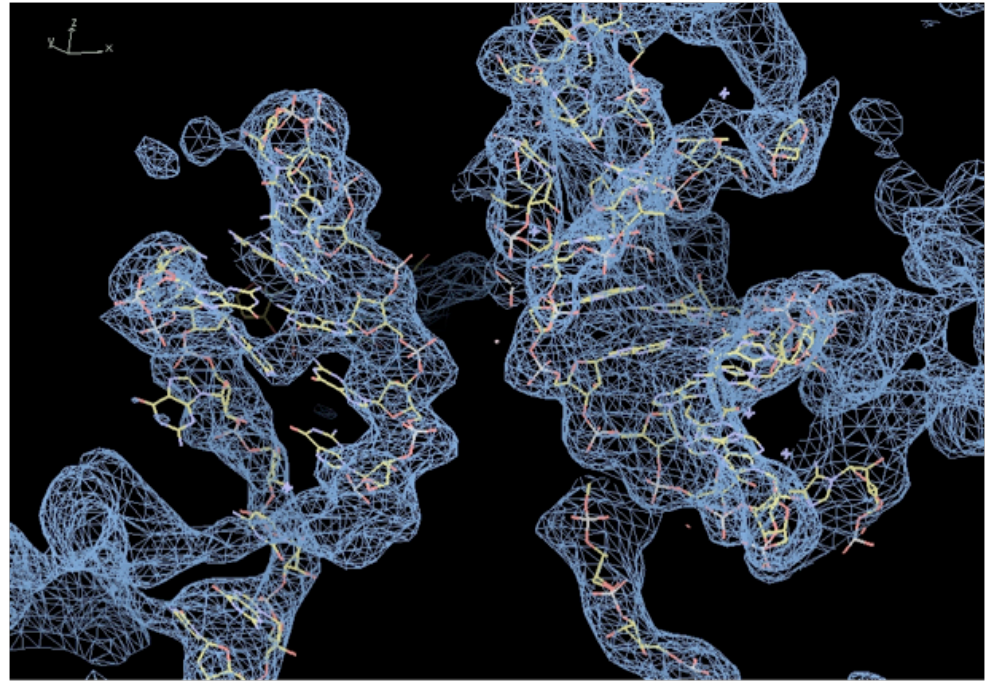


## Automated Model Building/Rebuilding

- Proteins and nucleic acids
- Low to high resolution (3.5Å or better)
- Location of secondary structure elements followed by extension, loop building and side chain docking



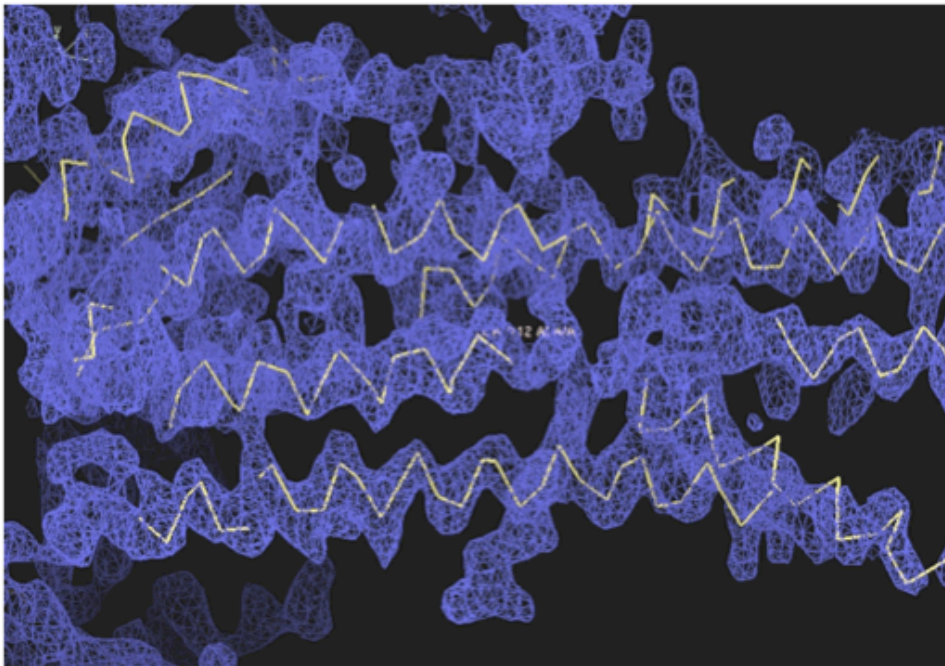
*Gold Lysozyme at 1.5 Å*



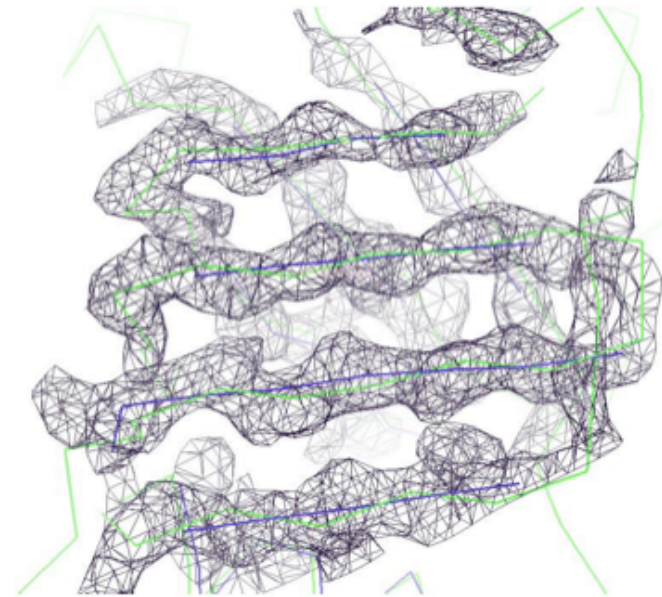
*Group II intron at 3.5 Å. Data courtesy of J. Doudna*

# Rapid Secondary Structure Fitting

- `phenix.find_helices_strands <map-file> <seq-file>`
  - Rapid location of helices and strands - followed by sequence fitting
  - Fast - seconds to minutes depending on resolution and cell dimensions
  - Works at low resolution (tested at 4Å or better)



*Ca<sup>2+</sup> ATPase SAD map at 3.1 Å. Data courtesy of P. Nissen*

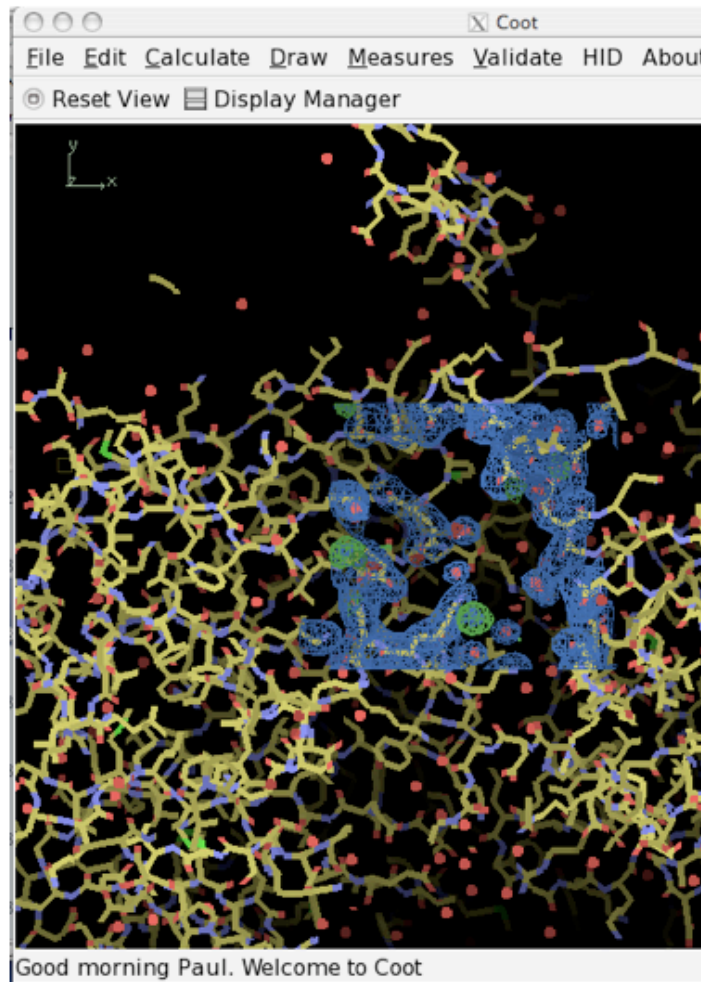


*GroEL SIR averaged map at 2.7 Å*

Tom Terwilliger, Los Alamos National Laboratory



# Results - Rebuilding and Validation



Validation results for /Users/pdams/Work/Scratch/phenix-test/refine/bad/Refine\_0/refine\_001.pdb

The validation performed by PHENIX is currently a subset of the full Molprobit analysis available on the web server. We recommend that academic groups use the server version to obtain more detailed information on structure quality, as well as files necessary to show validation results in Coot. You can start this process by clicking the Molprobit button on the left.

**Ramachandran outliers:**

Chain	Residue	Residue type	Score	Phi	Psi
A	LEU 45	General	0.02	68.0	106.1
A	SER 49	General	0.02	-79.0	-110.8
A	SER 76	General	0.02	-70.5	-97.4
A	LYS 78	General	0.04	-61.4	56.4
A	GLY 79	Glycine	0.04	-46.3	3.8
A	ASN 81	General	0.02	62.4	122.9
A	LYS 203	General	0.00	42.7	-77.8
A	GLU 204	General	0.00	134.3	152.6
A	LEU 207	Prepro	0.00	76.2	118.6
A	PHE 210	General	0.00	43.6	166.6
A	LEU 292	General	0.00	4.2	174.2
A	ARG 293	General	0.04	72.9	137.8
A	TYR 424	General	0.00	-68.5	-122.0
A	SER 425	General	0.02	-171.3	-47.3
A	THR 426	General	0.02	48.0	96.9

**Rotamer outliers:**

Chain	Residue	Score	Chi1	Chi2	Chi3	Chi4
A	ILE 6	0.39	163.3	97.6	-	-
A	THR 8	0.00	154.8	-	-	-

Refinement complete Project: None



Phenix



# Parallel validation of multiple structures

- Identifies points of difference between structures of the same protein, with optional map superpositioning

The screenshot displays the Coot software interface for parallel structure comparison. The main window is titled "Parallel structure comparison" and contains a table with the following data:

Rotamers	Ramachandran	Missing atoms	Secondary structure	19 LEU	21 LYS	23 LYS	24 GLU	25 ASP	27 LEU	28 LYS	29 LYS	31 GLU
3fhi.pdb:A	---	OUTLIER	tt0	m-20	mt	---	mtmm	---	---	---	---	m
3dnd.pdb:A	TLIER	OUTLIER	tttt	tt0	m-20	OUTLIER	mtmm	mttt	mm-40	---	---	OK
113r.pdb:E	---	---	tttp	---	m-20	mt	---	mttt	mm-40	---	---	m
3fjq.pdb:E	---	tmim?	tttt	mt-10	m-20	mt	---	mttt	mm-40	---	---	m
1syk.pdb:A	n?	mttt	tptm	tp10	t70	OUTLIER	mpet	mttt	tp10	---	---	m
1syk.pdb:B	n?	mttt	tptm	tp10	t70	OUTLIER	mpet	mttt	mt-10	---	---	m
3dne.pdb:A	TLIER	mppt	ttpt	mt-10	m-20	OUTLIER	mtmm	mttt	mm-40	---	---	OK

The interface also includes a "Coot controls" dialog box with a list of models to be compared:

- 3fhi.pdb:chain A
- 3dnd.pdb:chain A
- 113r.pdb:chain E
- 3fjq.pdb:chain E
- 1syk.pdb:chain A
- 1syk.pdb:chain B
- 3dne.pdb:chain A

The main 3D view shows a protein structure with multiple chains superimposed in different colors (blue, red, green, yellow). A status bar at the bottom indicates "Structure comparison" and provides a brief description: "Identify differences between multiple structures of the same protein, using multiple criteria".

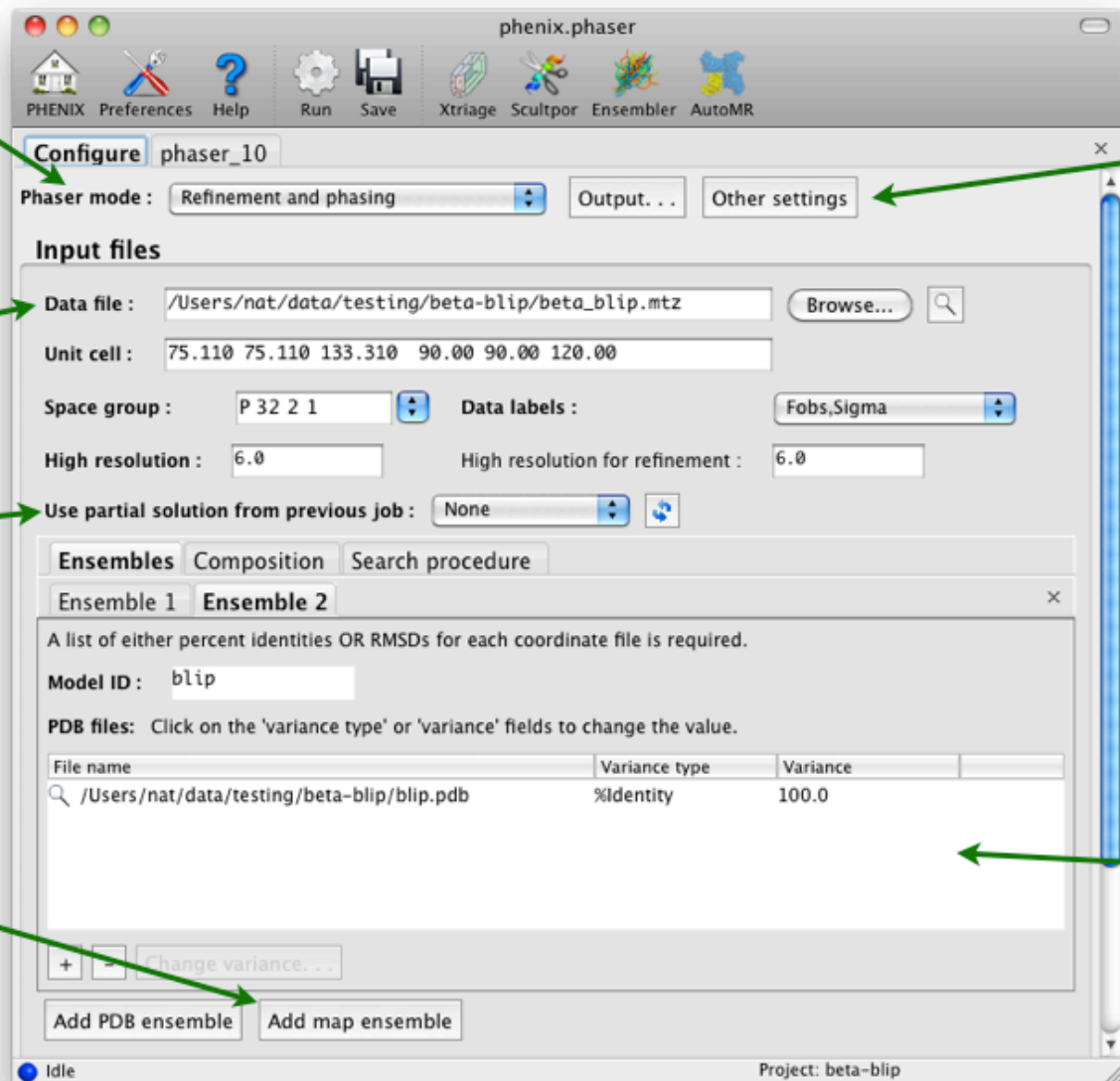
# Phaser GUI

Supports modes  
MR\_AUTO, MR\_FRF,  
MR\_BRF, MR\_FTF,  
MR\_BTF, MR\_PAK,  
MR\_RNP

Any reflection file  
format permitted

One-click re-use of  
partial solutions  
from past runs

Can use a low-  
resolution map as  
a search model



Most keywords  
found here

Drag-and-drop  
supported

Nearly all of the features present in the CCP4i Phaser GUI should be available here, including the complete keywords. The known exceptions are a few of the less-used modes such as normal mode analysis; these may be added to a future version.

# Phaser GUI

Phaser parameters

**Reflection binning**

Minimum number of bins : 6

Maximum number of bins : 50

Width of bins (number of reflections) : 500

Coefficients for binning function : 0 1 0

Box scale for ensemble F(calc) : 4.0

**Patterson decomposition**

Fix the radius for decomposition of the Patterson : 0.0

Minimum L value for the decomposition of the Patterson : 4

Maximum L value for the decomposition of the Patterson : 100

**Anisotropy correction**

Protocol : default

**SigmaN refinement macrocycle (1)**

Refine anisotropy

All "keywords" not shown on the main page are collected in a single dialog window, the content of which depends on the mode currently selected.

Built-in graphs.

Configure phaser\_10

Run status | Graphs | Results

Status

Restored job

Current best solution:	RF	Z-score	TF	Z-score	Packing clashes	Log-likelihood gain
	4.4	11.6	0	100.0		
	3.9	12.4	0	257.0		

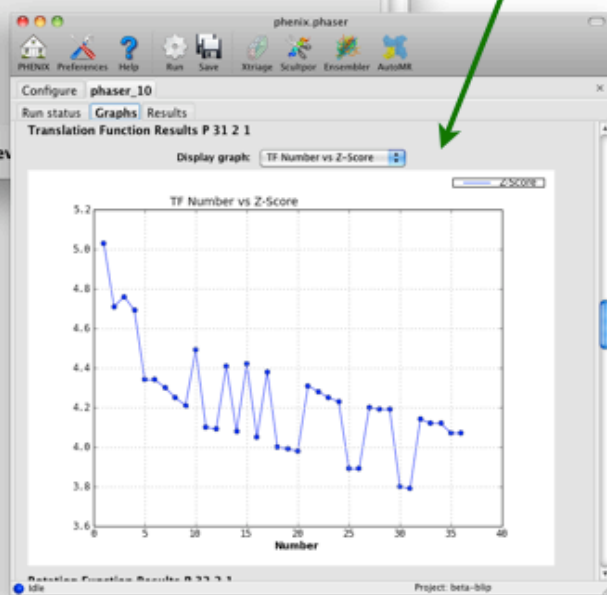
Display log file

Warnings

[no warnings]

Summary

```
Corrected structure factors (Fobs/Fcalc)
beta-blip_phaser.1.pdb
beta-blip_phaser.1.mtz
-----
*** Phaser Module: AUTOMATED MOLECULAR REPLACEMENT 2.2.4 ***
-----
SpaceGroup of Solution: P 32 2 1
SINGLE solution
Solution written to PDB file: beta-blip_phaser.1.pdb
Solution written to MTZ file: beta-blip_phaser.1.mtz
```



Configure phaser\_10

Run status | Graphs | Results

Summary

Phaser has found 1 MR solution(s).

Top LLG : 256.537

Spacegroup : P 32 2 1

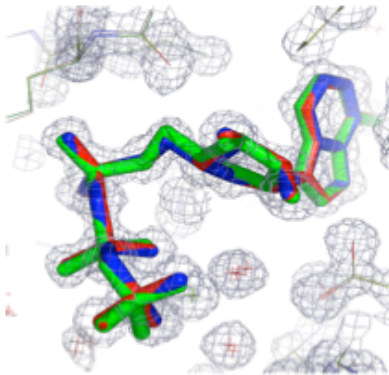
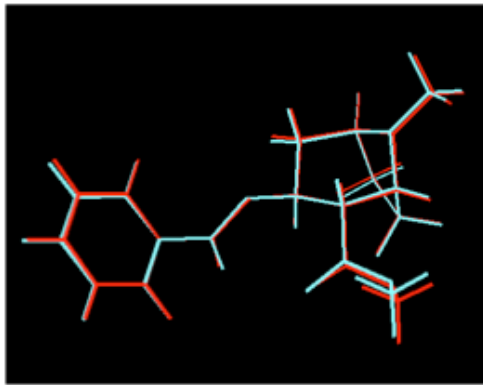
Output files

File path	Format	Data type
beta-blip_phaser.1.mtz	ccp4_mtz	Solution #1 phases and maps
beta-blip_phaser.1.pdb	PDB	Solution #1 model
beta-blip_phaser.log	text	Phaser console output
beta-blip_phaser_data.mtz	ccp4_mtz	Final input data

Open in Coot | Open in PyMOL | Display model and maps

# Ligands handling

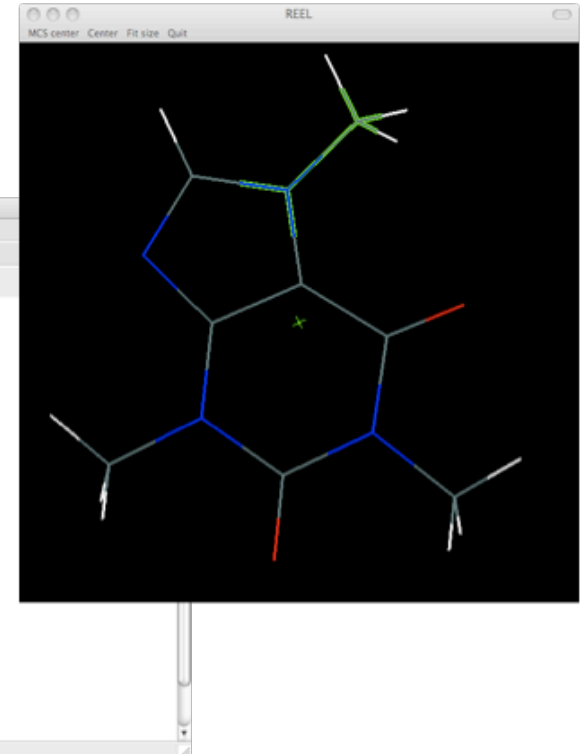
- Creation of ligand coordinates and restraints is typically a time consuming process
- phenix.elbow uses a semi-empirical method to generate atomic coordinates from a chemical topology, then calculates restraint values
- phenix.reel provides a graphical interface to manipulate restraints



Restraints Editor Especially Ligands (REEL)

Atoms	Bonds	Angles	Dihedrals	Planes	Chirals						
?	comp_id	atom_id_1	atom_id_2	type	value_dist	value_dist_esd					
<input checked="" type="checkbox"/>	LIG	N02	C01	single	1.470320	0.020000					
<input checked="" type="checkbox"/>	LIG	C03	N02	single	1.418530	0.020000					
<input checked="" type="checkbox"/>	LIG	O04	C03	double	1.226510	0.020000					
<input checked="" type="checkbox"/>	LIG	N05	C03	single	1.420730	0.020000					
<input checked="" type="checkbox"/>	LIG	C06	N05	single	1.477410	0.020000					
<input checked="" type="checkbox"/>	LIG	C07	N05	single	1.421460	0.020000					
<input checked="" type="checkbox"/>	LIG	O08	C07	double	1.220250	0.020000					
<input checked="" type="checkbox"/>	LIG	C09	C07	single	1.441100	0.020000					
<input checked="" type="checkbox"/>	LIG	C11	N10	single	1.459450	0.020000					
<input checked="" type="checkbox"/>	LIG	C12	N10	aromatic	1.388260	0.020000					
<input checked="" type="checkbox"/>	LIG	N13	C12	aromatic	1.371300	0.020000					
<input checked="" type="checkbox"/>	LIG	N10	C09	aromatic	1.398300	0.020000					
<input checked="" type="checkbox"/>	LIG	C14	C09	aromatic	1.407100	0.020000					
<input checked="" type="checkbox"/>	LIG	N02	C14	single	1.385300	0.020000					
<input checked="" type="checkbox"/>	LIG	N13	C14	aromatic	1.397370	0.020000					
<input checked="" type="checkbox"/>	LIG	H011	C01	single	1.104640	0.020000					
<input checked="" type="checkbox"/>	LIG	H012	C01	single	1.099230	0.020000					
<input checked="" type="checkbox"/>	LIG	H013	C01	single	1.104490	0.020000					
<input checked="" type="checkbox"/>	LIG	H061	C06	single	1.101020	0.020000					
<input checked="" type="checkbox"/>	LIG	H062	C06	single	1.103610	0.020000					
<input checked="" type="checkbox"/>	LIG	H063	C06	single	1.102460	0.020000					
<input checked="" type="checkbox"/>	LIG	H111	C11	single	1.102950	0.020000					
<input checked="" type="checkbox"/>	LIG	H112	C11	single	1.103060	0.020000					
<input checked="" type="checkbox"/>	LIG	H113	C11	single	1.102850	0.020000					

Finished loading molecule from caffeine.cif



## Challenges for Automation

- Structure completion
  - Automated identification, fitting and refinement of ligands, metals, ions
  - Identification, fitting and refinement of discrete disorder (multiple conformations)
  - Representing other forms of disorder
  - Building poorly-defined regions
- Building complexes of protein and nucleic acid
- Identification of the best combination of datasets or fractions of datasets to use
- Handling different kinds of twinning and integrating it into the whole structure solution process
- Representations of uncertainty
- Automatic analysis of radiation damage
- Automated understanding of chemistry
- Optimal structure solution in the presence of twinning
- ... and many more



Phenix  
http://www.phenix-online.org/

NEW Development release of PHENIX version 1.4 now available

# Phenix

Python-based Hierarchical Environment for Integrated Xtallography

PHENIX is a new software suite for the automated determination of macromolecular structures using X-ray crystallography and other methods.

**Citing PHENIX:**  
PHENIX: building new software for automated crystallographic structure determination P.D. Adams, R.W. Grosse-Kunstleve, L.-W. Hung, T.R. Ioerger, A.J. McCoy, N.W. Moriarty, R.J. Read, J.C. Sacchettini, N.K. Sauter and T.C. Terwilliger. *Acta Cryst.* D58, 1948-1954 (2002)

**Download the latest development release (1.4-3) [First request download password]**

Help: [FAQ](#) [Mailing List Subscription](#) [List Archives](#) [Report a Bug](#) [Email for Help](#)

**Using PHENIX (release 1.4-3):** [Full Documentation](#) [PDF](#)

- Assessing data quality with [phenix.xtriage](#)
- Automated structure solution with [AutoSol](#)
- Automated molecular replacement with [AutoMR](#)
- Automated model building and rebuilding with [AutoBuild](#)
- Automated ligand fitting with [LigandFit](#)
- Structure refinement with [phenix.refine](#)
- Generation of ligand coordinates and restraints with [elbow](#)
- The [PHENIX Graphical User Interface](#)

[Documentation for 1.3-final](#)

The PHENIX system also includes SOLVE/RESOLVE, Phaser, Textal, the CCI Applications (phenix.xtriage, phenix.refine, elbow and many more), components from Molprobit, and the Computational Crystallography Toolbox in a Python framework.

**Funding for PHENIX:** [Protein Structure Initiative \(NIH General Medical Sciences\)](#)







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**The PHENIX Industrial Consortium** [Information](#)

For-profit groups can obtain access to PHENIX through a Consortium agreement. This provides a license to use PHENIX and research funds to develop new features in PHENIX tailored to the needs of commercial users. [Members](#)  
[Download](#)  
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**Groups developing PHENIX:**

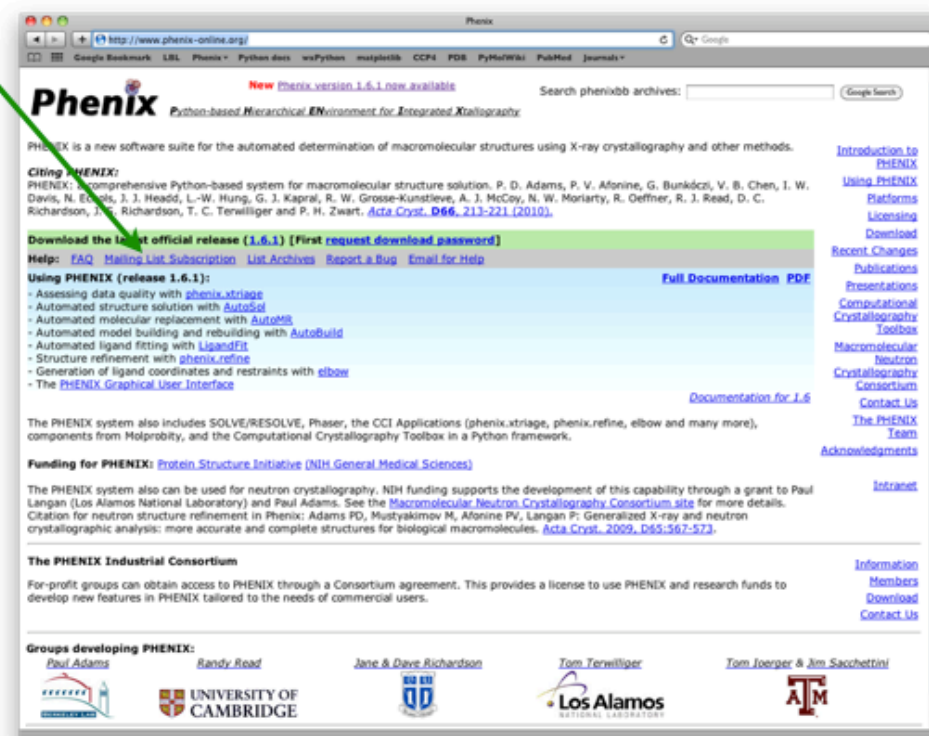
<a href="#">Paul Adams</a>	<a href="#">Randy Read</a>	<a href="#">Jane &amp; Dave Richardson</a>	<a href="#">Tom Terwilliger</a>	<a href="#">Tom Ioerger &amp; Jim Sacchettini</a>	
					

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www.phenix-online.org

# PHENIX resources online

- [help@phenix-online.org](mailto:help@phenix-online.org): user support
- [bugs@phenix-online.org](mailto:bugs@phenix-online.org): bug reports
- [phenixbb@phenix-online.org](mailto:phenixbb@phenix-online.org): message board (subscribers only)



# Obtaining PHENIX

- Free to academic users; simple online registration required (*please use your academic email address!*)
- Regular official releases (typically 2-8 months)
- Nightly builds

**Phenix** Python-based Hierarchical Environment for Integrated Xtallography

### PHENIX nightly build distribution

These installers are built automatically using the current source code. Although some automated testing occurs as part of the build system, and we do not release installers that have known major problems, they have not been checked as thoroughly as the official distributions, and individual programs may be broken. **Use at your own risk!** Each installer directory should contain reports about any errors that occurred during building/testing. In most cases, if you do not see any errors, the installer can be considered functional enough for daily use. Official releases and builds deemed to be "stable" are noted as such and highlighted in bold type.

If you do choose to use the nightly builds, we recommend updating frequently; once a build disappears from the list here, it can be assumed to be obsolete.

If you encounter errors when using any of these builds, please update to the most recent version before sending a bug report. (It is generally a good idea to update frequently anyway, since the code changes rapidly.) We recommend keeping the most recent official distribution (version 1.6) installed as well, since it is more stable.

**You will need proper authentication to download the installer; see the [main download page](#) for details.**

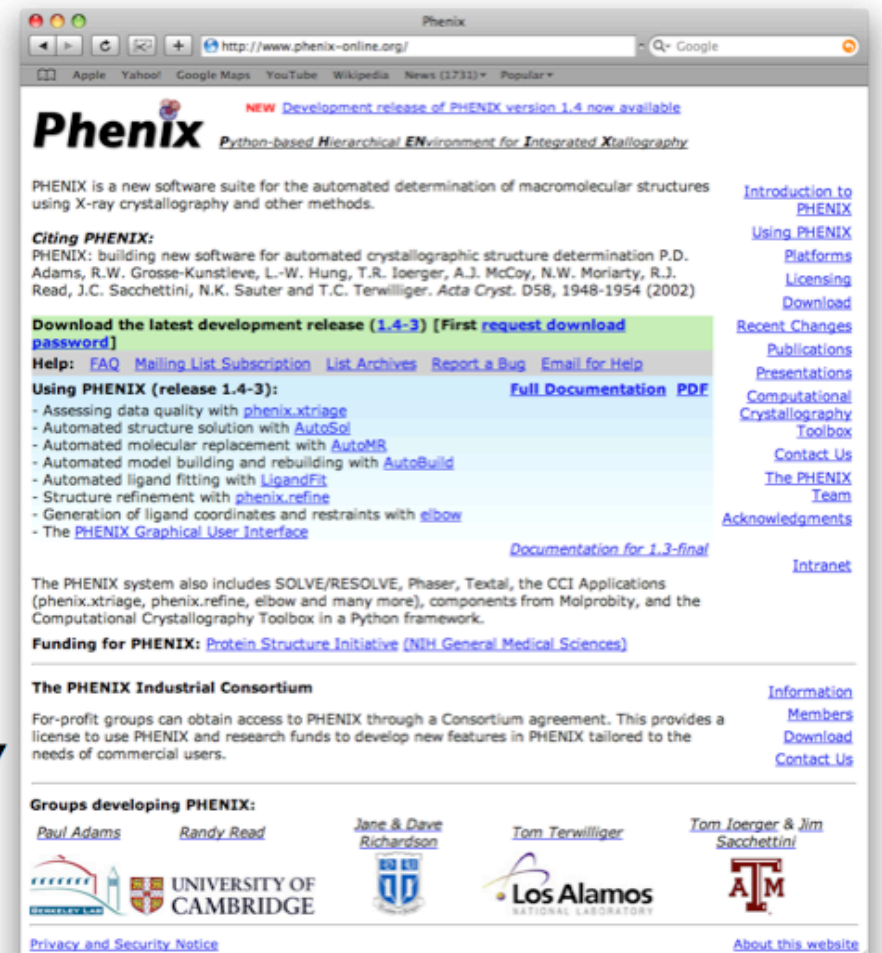
Version	Date	Status	Logs	Info
<b>1.6-1-357</b>	<b>2010-03-29</b>	<b>successful</b>	<a href="#">s03s_01_000s_0300s_0300s_m00s</a>	<b>Official 1.6.1 release; <a href="#">docs</a></b>
<b>1.6-249</b>	<b>2010-01-20</b>	<b>successful</b>	<a href="#">s03s_01_000s_0300s_0300s_m00s</a>	<b>Official 1.6 release; <a href="#">docs</a></b>
<b>1.5-2</b>	<b>2009-09-28</b>	<b>successful</b>	<a href="#">s03s_01_000s_0300s_0300s_m00s</a>	<b>Official release for version 1.5; <a href="#">docs</a></b>

Questions/comments to [help@phenix-online.org](mailto:help@phenix-online.org)  
[Administrative interface](#)

[http://www.phenix-online.org/download/nightly\\_builds.cgi](http://www.phenix-online.org/download/nightly_builds.cgi)

# PHENIX Distribution

- Regular releases
- Supported on:
  - Linux (RedHat, Fedora)
  - Mac OSX
- Regular development releases:
  - Nightly builds
  - <http://www.phenix-online.org/>
- Extensive documentation



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## ● Duke University

- Jane Richardson & David Richardson, Ian Davis, Vincent Chen, Jeff Headd, Chris Williams, Bryan Arendall, Laura Murray

## ● Texas A&M University

- Tom Ioerger, Eric McKee, James Sacchettini

## ● Others

- Garib Murshudov & Alexi Vagin
- Kevin Cowtan, Paul Emsley, Bernhard Lohkamp
- CCP4 developers
- Alexandre Urzhumtsev & Vladimir Lunin
- David Abrahams
- PHENIX Testers & Users: James Fraser, Herb Klei, Warren Delano, Paul Emsley, Bernhard Lokhamp, William Scott, Joel Bard, Bob Nolte, Frank von Delft, Scott Classen, Ben Eisenbraun, Phil Evans, Felix Frolow, Christine Gee, Miguel Ortiz-Lombardia, Blaine Mooers, Daniil Prigozhin, Miles Pufall, Edward Snell, Eugene Valkov, Erik Vogan, Andre White, and many more

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- Lawrence Berkeley Laboratory
- PHENIX Industrial Consortium

**Paul Adams – project director**



## Reporting bugs, problems, asking questions

- **Something didn't work as expected?... program crashed?... missing feature?...**

**Not Good:** silently give up and run away looking for alternative software.

**Good:** report us a problem, ask a question, request a feature (explain why it's good to have), ask for help.

- **Reporting a bug:**

**Not good:** "Hi! PHENIX crashed, I don't know what to do."

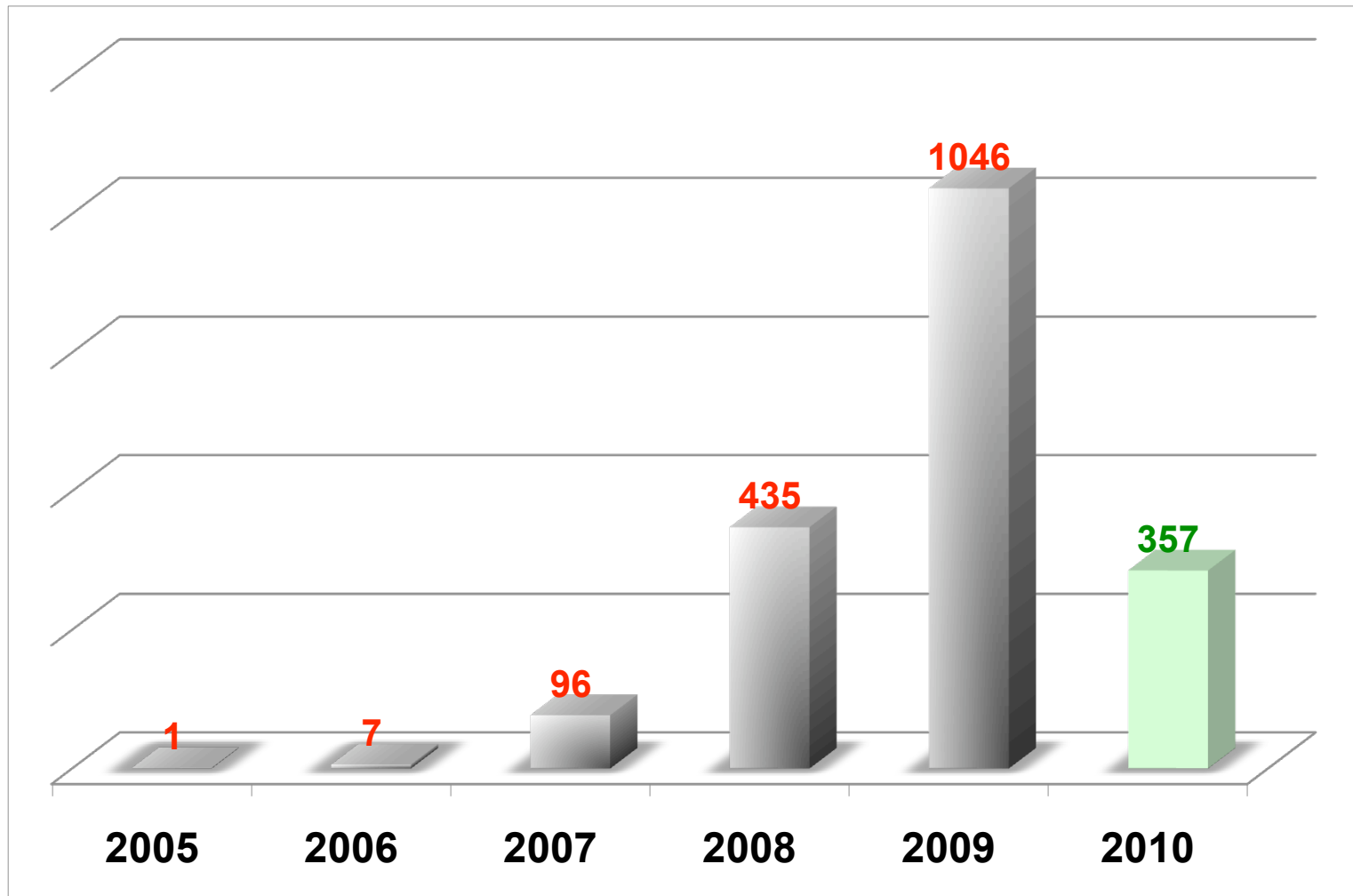
**Good:** "Hi! PHENIX crashed. Here are:

- 1) PHENIX version;
- 2) Command and parameters I used;
- 3) Input and output files (at least logs)."

**Subscribe to PHENIX bulletin board: [www.phenix-online.org](http://www.phenix-online.org)**

## PHENIX use (July 12, 2010)

Number of structures in PDB with “REMARK 3 PROGRAM PHENIX”



**User tested !**