An NIH/NIGMS funded Program Project

The Phenix Project

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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 Hierarchical ENvironment for Integrated Xtallography**
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. 2010, D66: 213-221 (Phenix)
ACTA Cryst. 2019 D75:861–877 (Phenix)
Phenix GUI

Central GUI to view job control and launch new jobs
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**

- **name of the program**: `phenix.mtriage`
- **input files**: `my_model.pdb` `my_map.map`
- **options**: `resolution=4`

**Run in a python script**

```python
try:
    easy_run.call("phenix.mtriage\ my_model.pdb\ my_map.map")
except Exception as e:
    msg = traceback.format_exc()
    print(msg)
```
Phenix Availability

Supported on:
- Linux (RedHat, Fedora)
- Mac OSX
- Windows

Extensive documentation (online and via GUI)

Nightly builds

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<th>Status</th>
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Video Tutorials

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
- Model and map validation
## Acknowledgements

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Outline

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