Phenix

Pavel Afonine

Lawrence Berkeley National Laboratory (LBNL)

September 26th, 2024
BNL

LBNL

The Phenix Project

Lawrence Berkeley Laboratory

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

Los Alamos National Laboratory
New Mexico Consortium

Tom Terwilliger, Li-Wei Hung

UTHealth

Matt Baker

University of Cambridge

Randy Read, Airlie McCoy, Alisia Fadini

Duke University

Jane & David Richardson, Christopher Williams, Vincent Chen

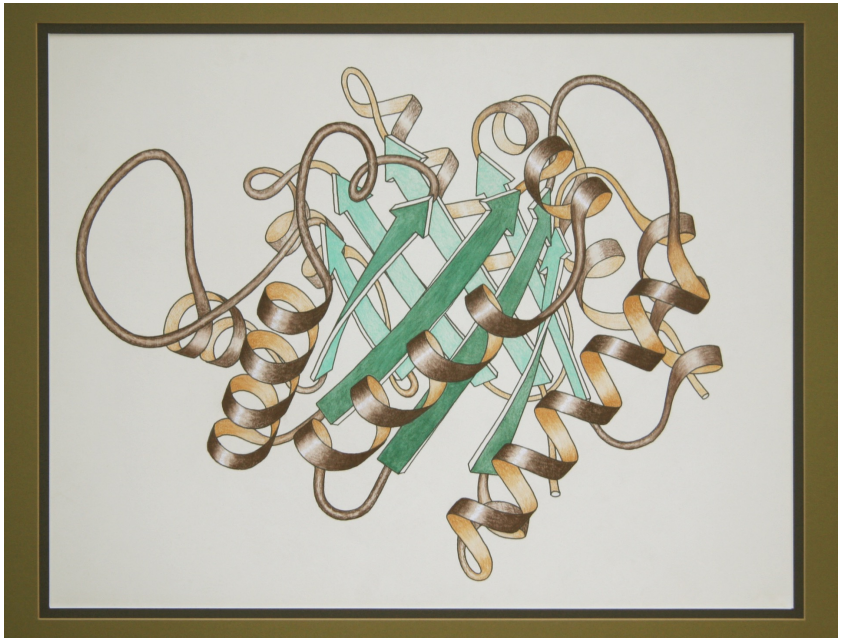
An NIH/NIGMS funded Program Project

Liebschner D, *et al.*, Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in *Phenix*. Acta Cryst. 2019 **D75**:861–877

Who invented ribbon diagram?

Who invented ribbon diagram?

Ribbon schematic of triose P isomerase monomer (PDB: 1TIM)

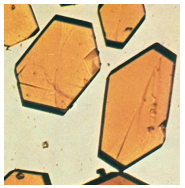


Hand-drawn by J. Richardson, 1981

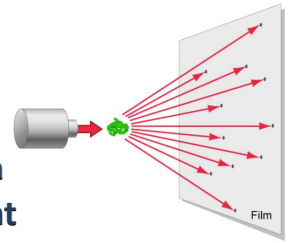
Solving structure by crystallography

Pure sample

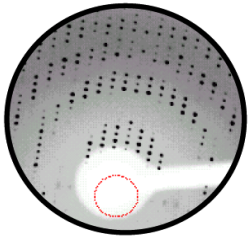
Crystals



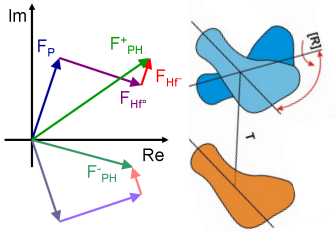
Diffraction experiment



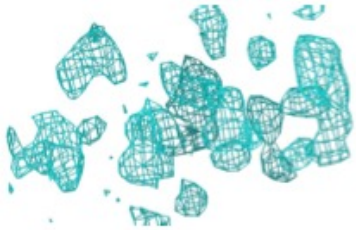
Process & check data



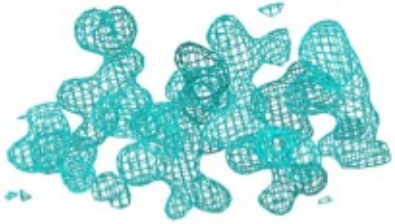
Solve phase problem



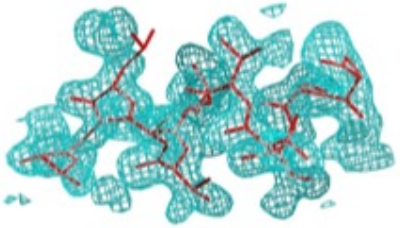
Initial map



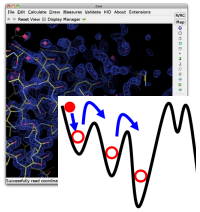
Improved map



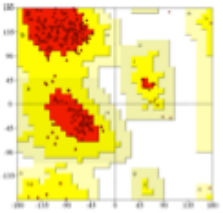
Build model



Refine model



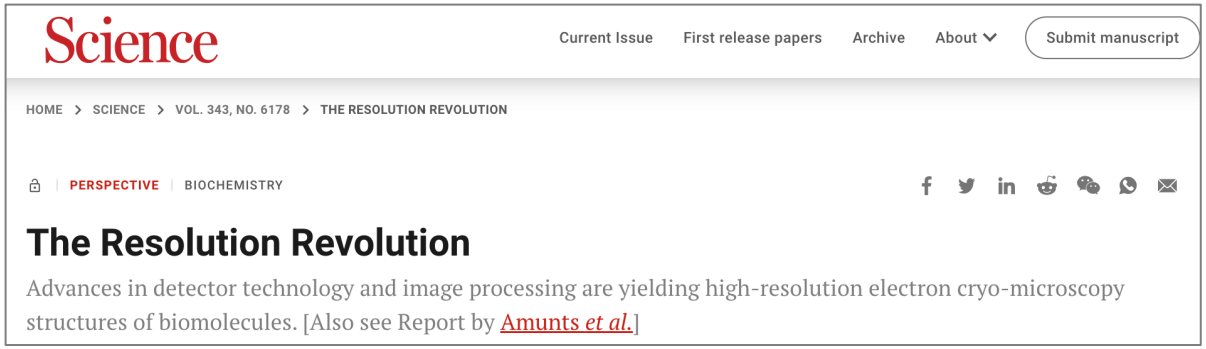
Validate model

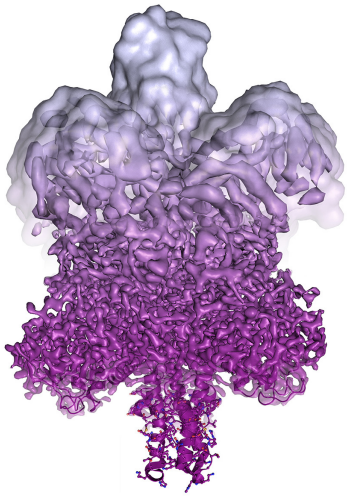


Publish & deposit

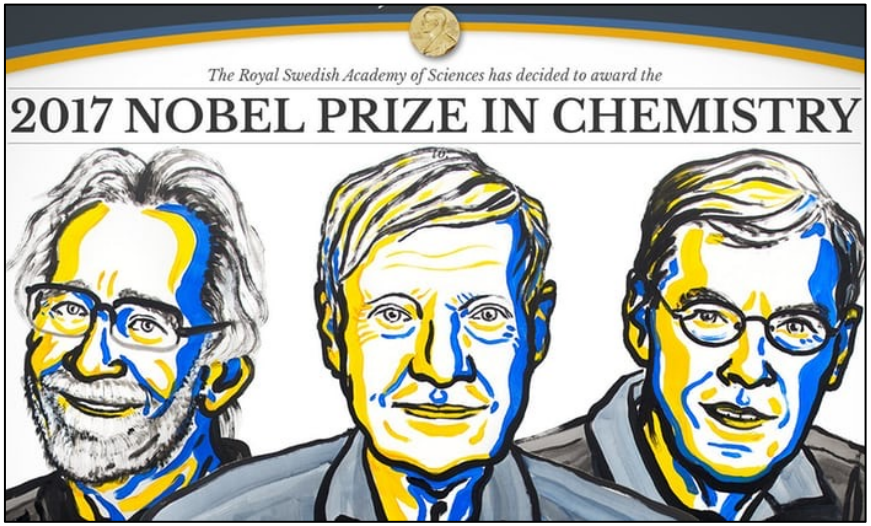
Cryo-EM resolution revolution

Werner Kühlbrandt, 2014





Dubochet, Frank, Henderson

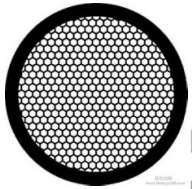


"For developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution"

Solving structure by electron cryo-microscopy

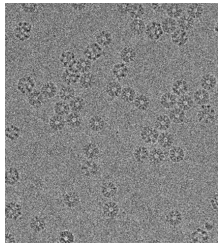
Pure sample

Grid

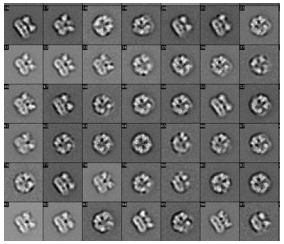


Electron microscope

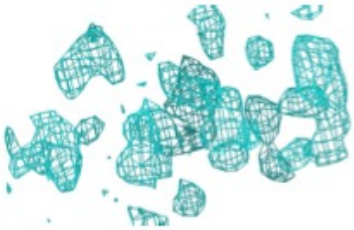
Electron microscope



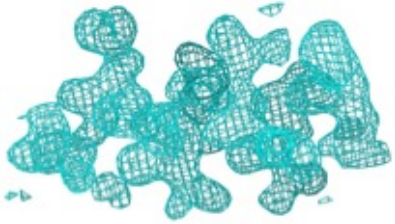
Pick, align & average particles



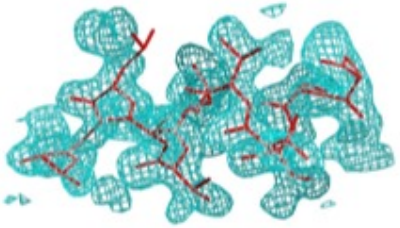
Initial map



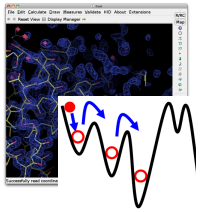
Improved map



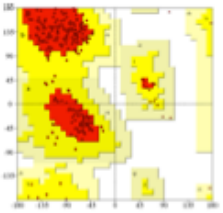
Build model



Refine model



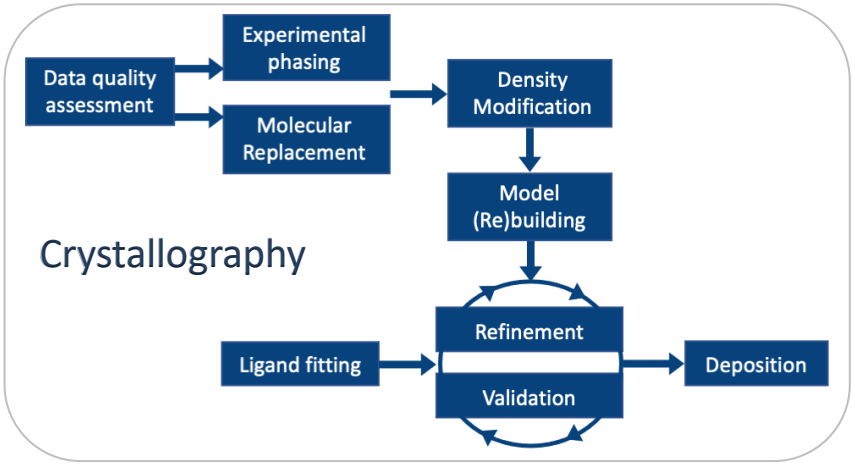
Validate model

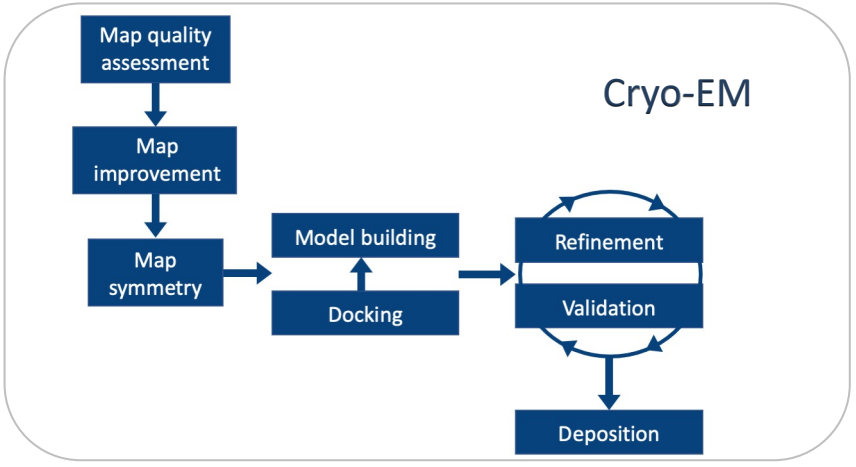


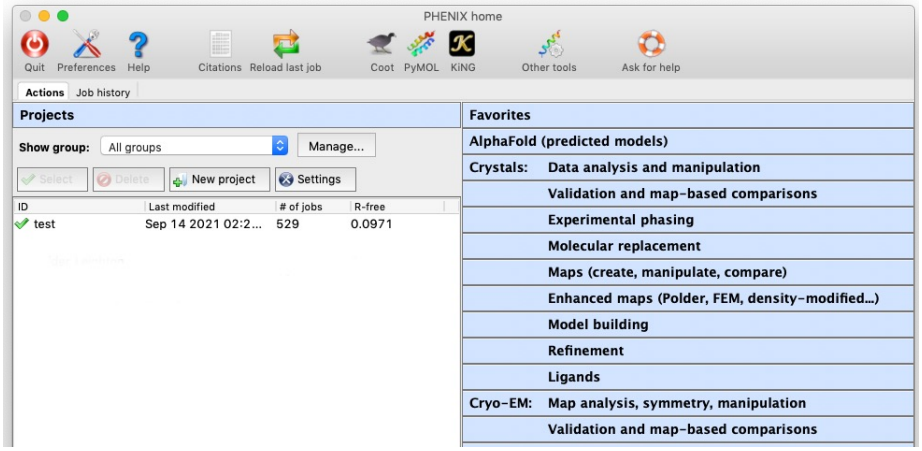
Publish & deposit

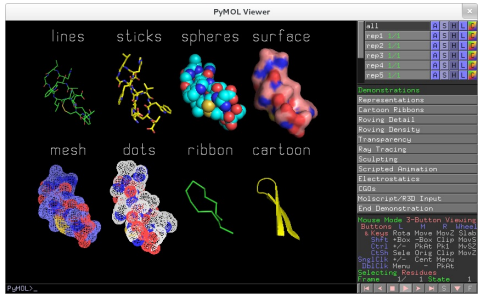
Phenix today

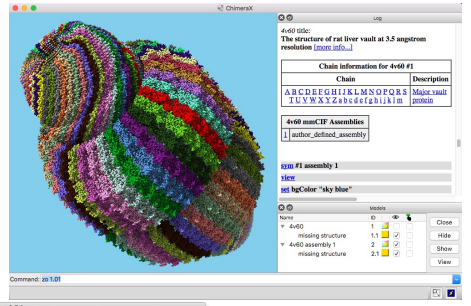
- Complete system for crystallography (X/E/N) and cryo-EM structure solution
- Available at scripting, command line and GUI levels
- Integrated with popular molecular graphics programs: Coot, PyMol and ChimeraX

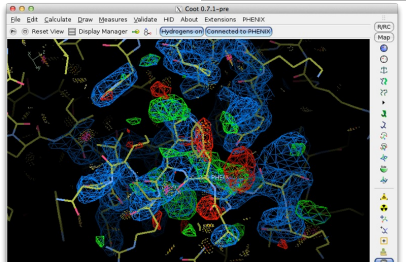










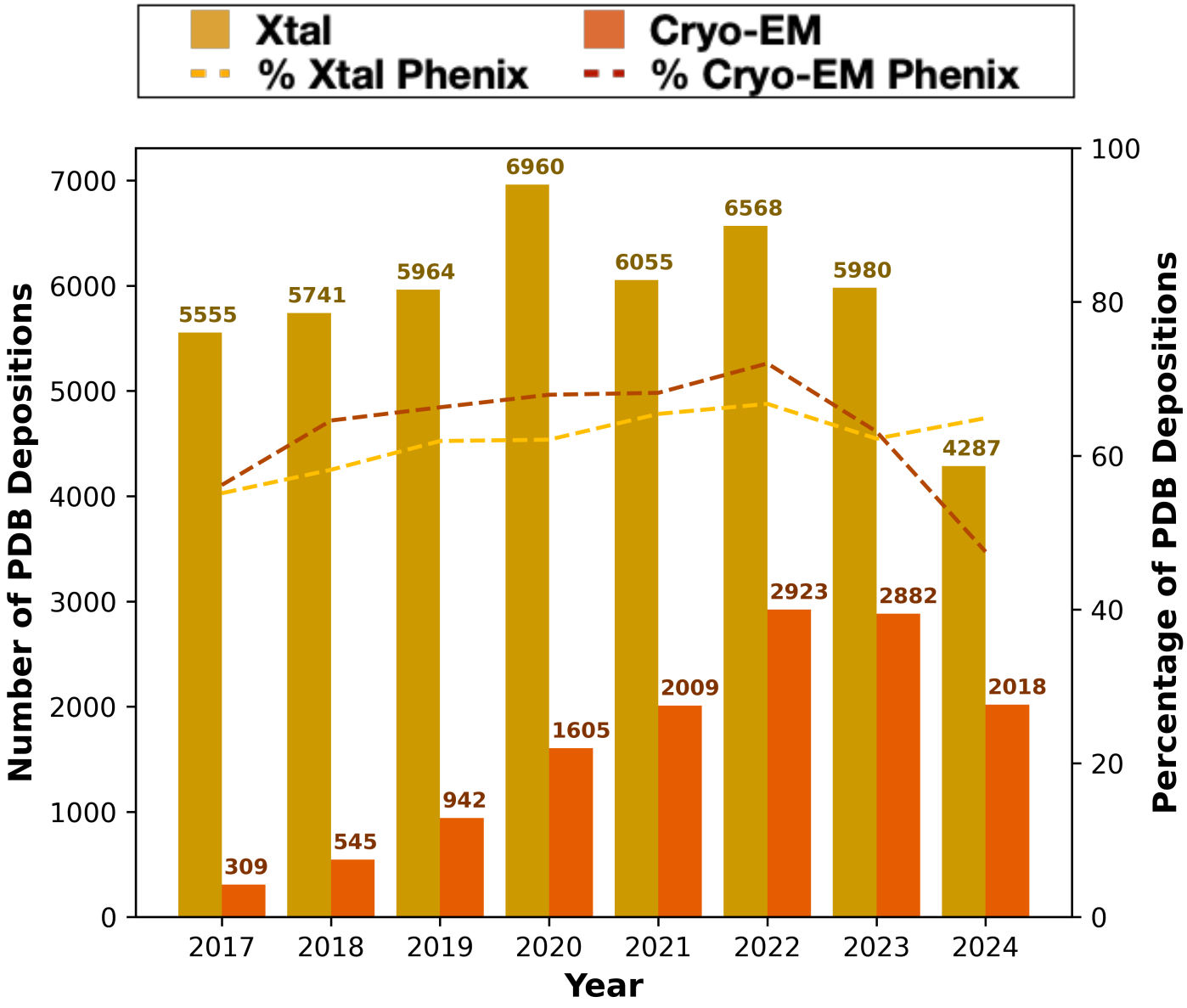


Phenix metrics

220 publications | **18447** citations | **82101** models in PDB | **35000** users | **33** countries

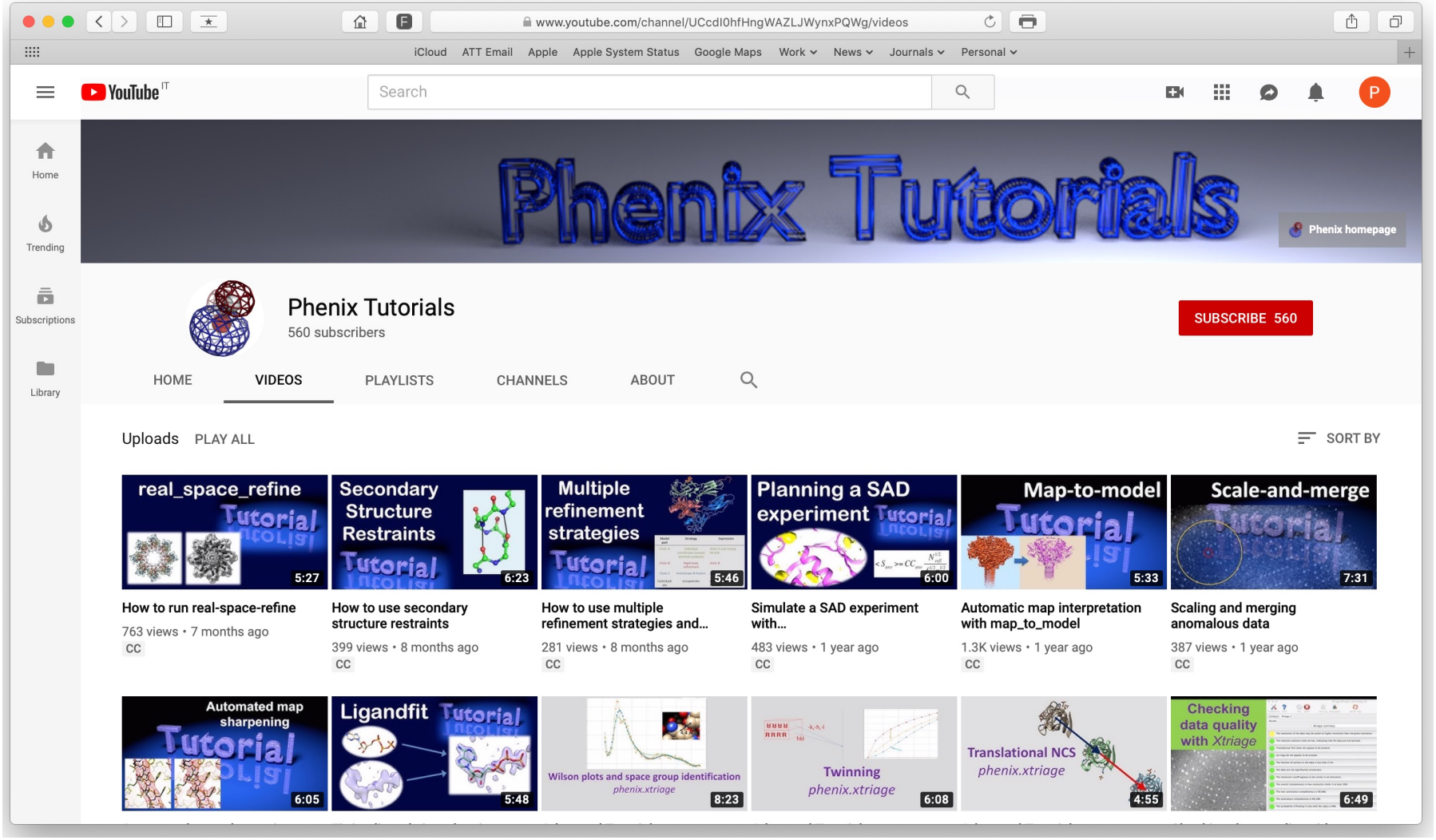
About 70 industry users

Phenix metrics

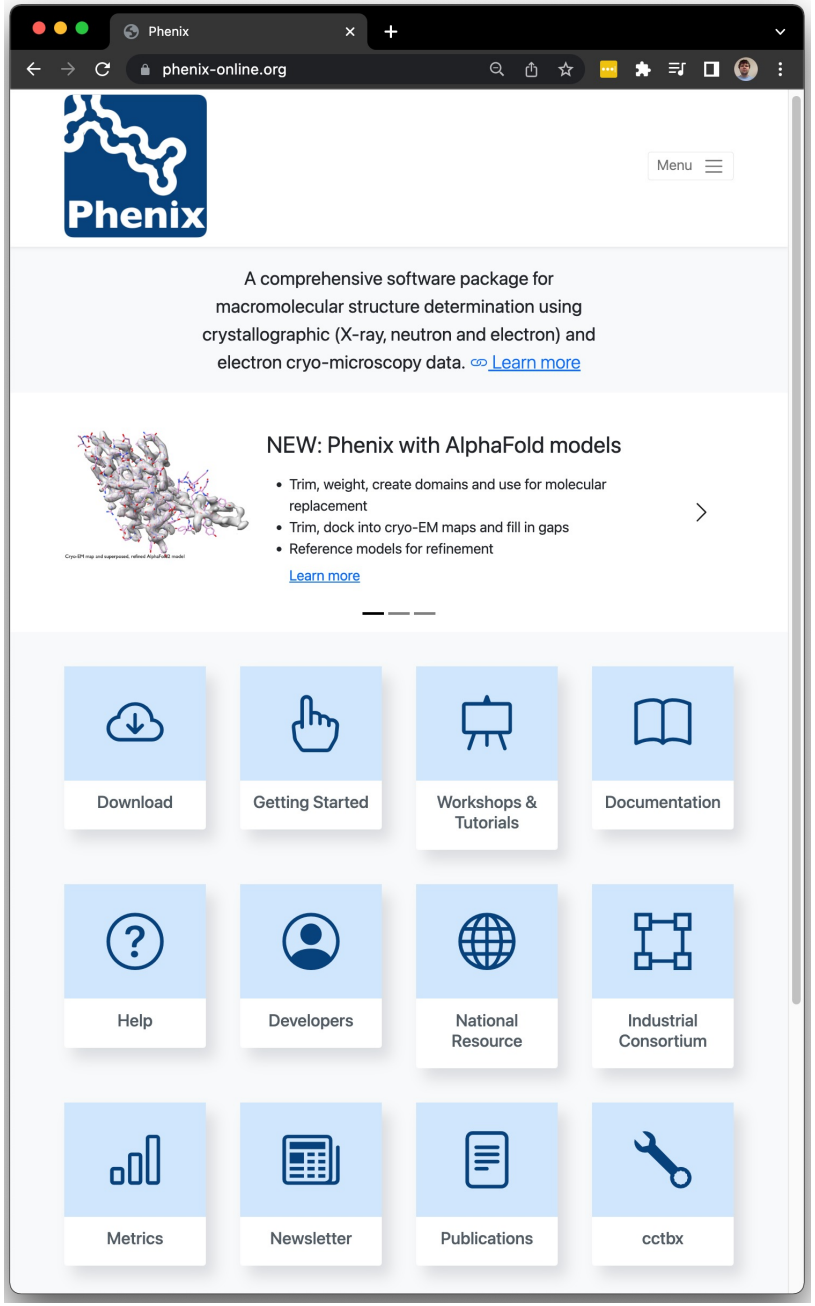


Keep up with trends: video tutorials

- YouTube channel: 67 videos



Phenix resources



Phenix paper

Video tutorials

Documentation

Relevant papers

Bi-annual newsletters

Slides from workshops

User support

- **Feedback, questions, help**

  Mailing list (anyone signed up): phenixbb@phenix-online.org
  Bug reports (developers only): bugs@phenix-online.org
  Ask for help (developers only): help@phenix-online.org

- **Reporting a bug or asking for help:**
  - We can't help you if you don't help us to understand your problem
  - Make sure the problem still exist using the latest *Phenix* version
  - Send us all inputs (files, non-default parameters) and tell us steps that lead to the problem
  - All data sent to us is kept confidentially