CBMS workbench (virtual), Oct 13 2021

AlphaFold for MR

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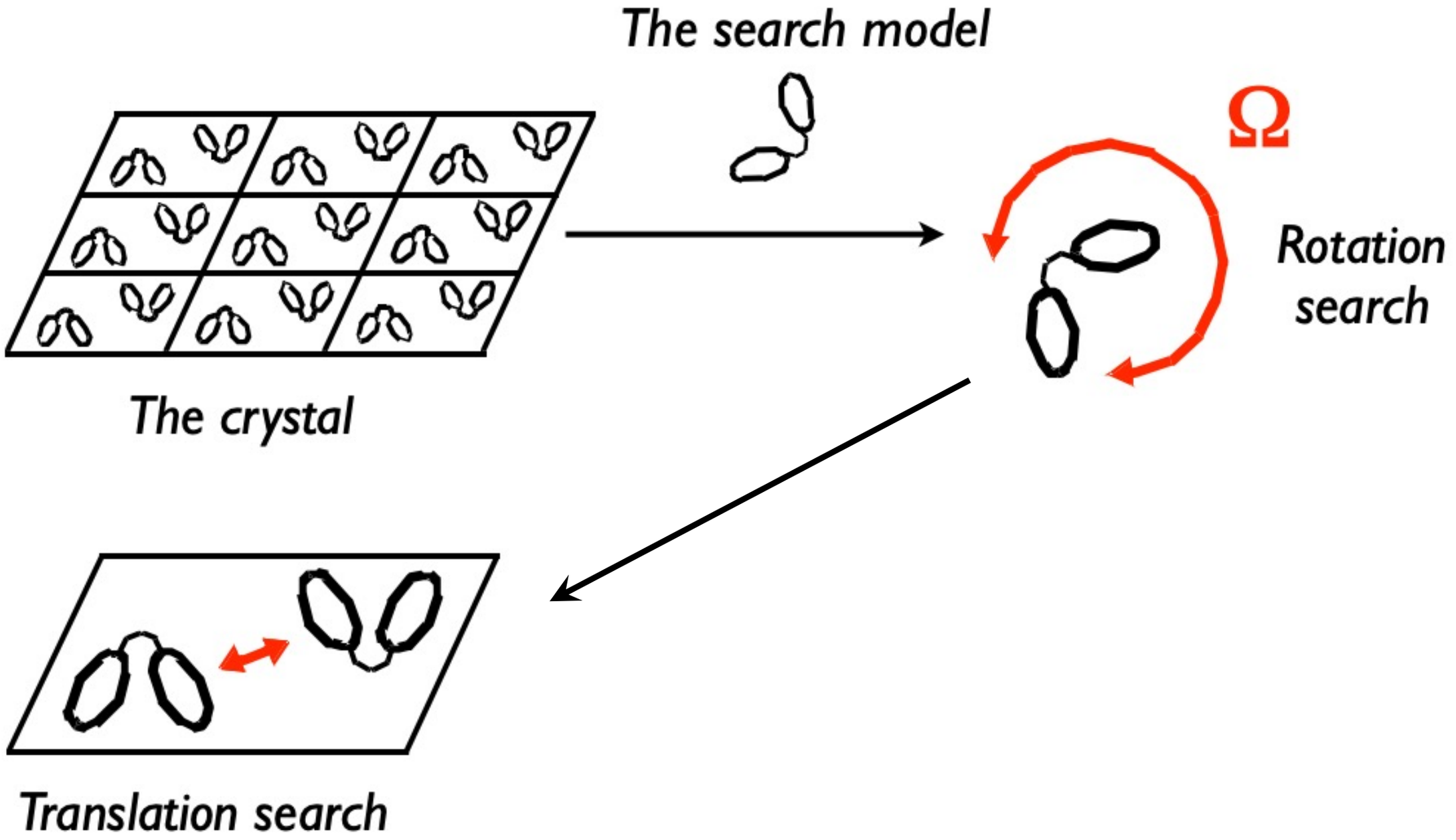
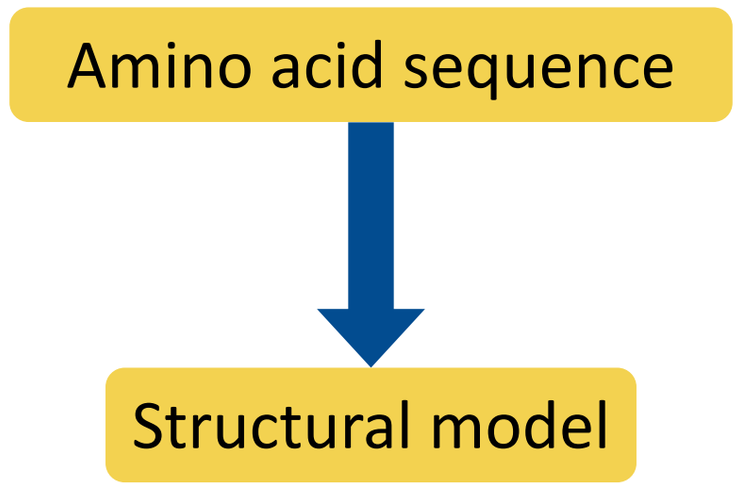
Molecular replacement (MR)

Use a previously known structure to get phase estimates



AlphaFold

AI scientists from Google DeepMind won CASP14 (Critical Assessment of Structural Prediction competition)



The average rmsd is ~1.6 Å!

The code is available on GitHub and can be run on google Colab:

- https://github.com/deepmind/alphafold
- https://colab.research.google.com/github/deepmind/alphafold/blob/main/notebooks/AlphaFold.ipynb

AlphaFold

Amino acid sequence

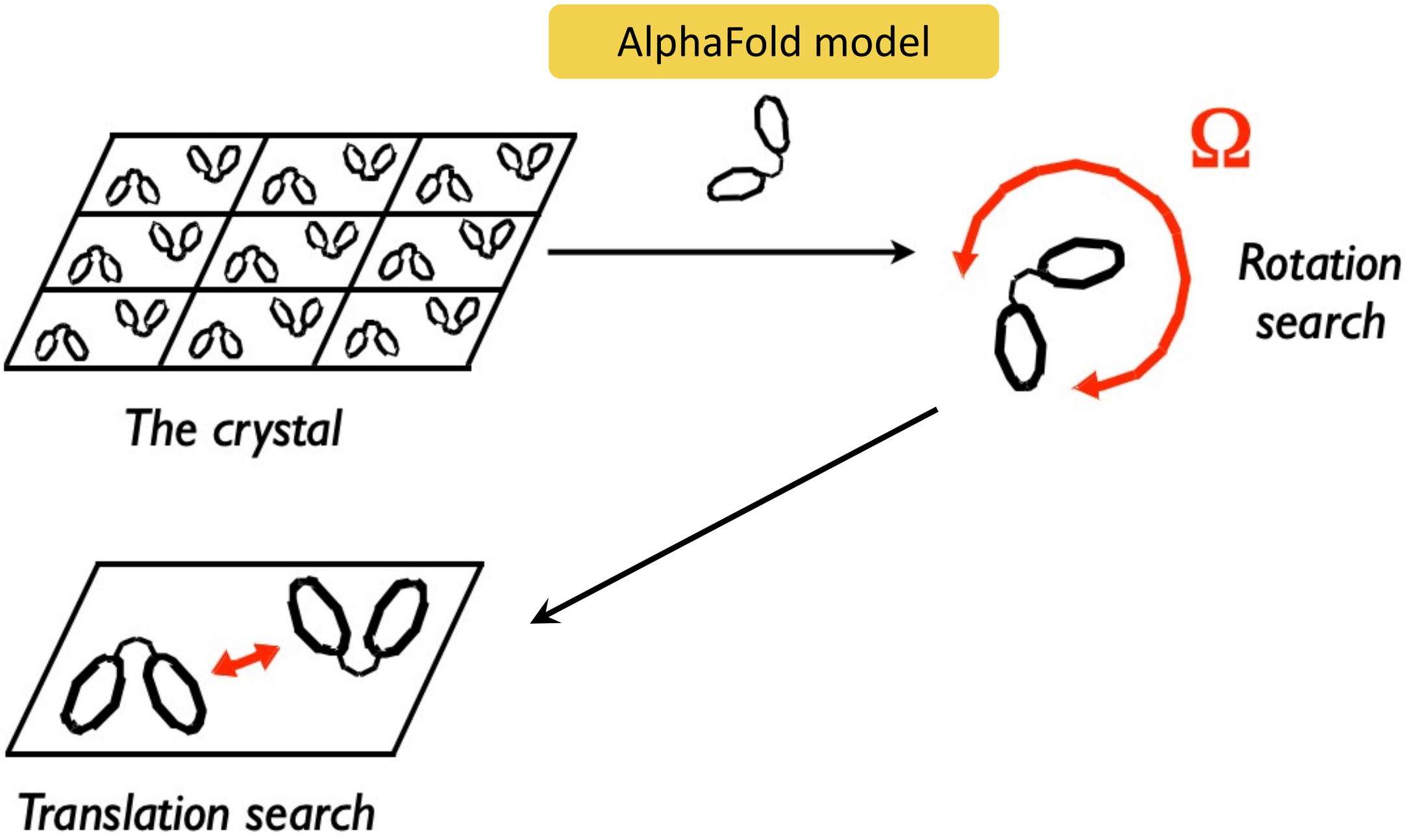
1) Do *multiple sequence alignment* (MSA)
   → find parts of the sequence more likely to mutate and correlations between them
   → find proteins that may have a similar structure (“templates”)
   → guess which amino acids are likely to be in contact with each other

2) Neural network 1: identify which parts of the MSA are more informative

3) Neural network 2: build a model

Structural model

Use AlphaFold model for MR

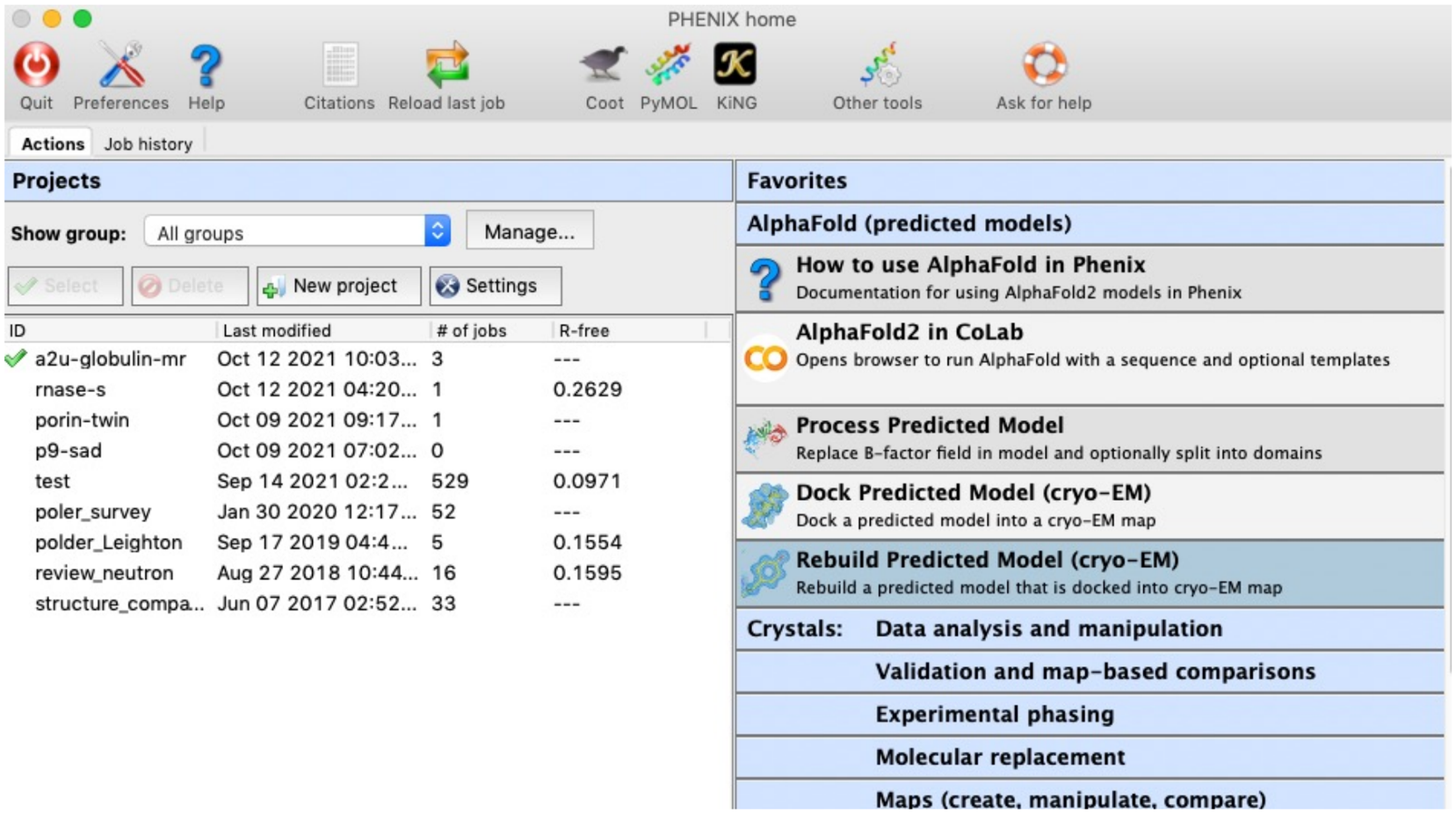


AlphaFold for MR

Use the tutorial data for the A2U-globulin structure (MR tutorial)

1) Run the tutorial with supplied search model

2) With the sequence, do a prediction and run MR again



The Phenix 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

Acknowledgements

Berkeley Laboratory
Pavel Afonine, Youval Dar, Nat Echols, Jeff Headd, Richard Gildea, Ralf Grosse-Kunstleve, Dorothee Liebschner, Nigel Moriarty, Nader Morshed, Billy Poon, Ian Rees, Nicholas Sauter, Oleg Sobolev, Peter Zwart

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

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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