

## phenix.refine: crystallographic structure refinement in PHENIX

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A combination of highly efficient programming tools and new or improved crystallographic algorithms provides a very high level of automation and robustness in structure refinement. Their implementation in *phenix.refine* – state-of-the-art refinement module of PHENIX package – resulted in a complete set of tools that cover most of refinement needs and scenarios, such as:

- Automatic handling of most data formats (CNS, SHELX, MTZ, etc...)
  - Individual coordinates refinement using minimization or simulated annealing
  - Highly optimized and automated rigid body refinement (multiple-zones algorithm)
  - ADP refinement: individual isotropic or anisotropic, grouped, TLS or any mixture
  - Occupancy refinement (grouped, individual, constrained for alternative conformations or any mixture)
  - Automatic NCS detection and use in refinement as restraints
  - Automatic twinning detection and use in refinement
  - Various refinement targets (maximum-likelihood, maximum-likelihood with experimental phase information, and amplitude least-squares)
  - Robust mask-based bulk-solvent correction and anisotropic scaling
  - $\sigma_A$ -weighted map output with any user-defined coefficients
  - Refinement using X-ray data, neutron data or joint refinement with both
  - Refinement at ultra-high resolution (higher than approx. 0.9 Å) using novel Inter Atomic Scatterers model
  - Use of H atoms in refinement at any resolution
  - Straightforward inclusion of novel ligands
  - Runs on most of platforms (Mac, Linux, Windows)
- More tools are under active development and to appear in future.

*phenix.refine* allows multi-step complex refinement jobs, for example, containing: rigid body refinement, Simulated Annealing, individual or grouped B-factors combined with TLS refinement, constrained occupancy refinement, automatic water picking to be performed in one run. The flexibility of *phenix.refine* allows using different refinement strategies for different selected parts of a model, for example: one part can be refined as a rigid body with B-factors modeled through TLS, individual sites and B-factors can be refined for another part while the rest of the model can be kept fixed.

*phenix.refine* is tightly integrated with other PHENIX components making structure solution, building and refinement a “one-go” process (Automr, Autobuild wizards).

*phenix.refine* is periodically tested by automatic re-refinement of all models in the PDB for which unambiguous experimental data and cross validation flags are available.

The *PHENIX* package, complete documentation and references to relevant publications are available from [www.phenix-online.org](http://www.phenix-online.org).