PDB-REDO: high throughput crystallographic model optimisation

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PDB-REDO is an automated pipeline for the optimisation of crystallographic structure models. It has a ten-year track record of model improvement for both PDB entries and work-in-progress models from practicing crystallographers. PDB-REDO combines model refinement in REFMAC with state-of-the-art model (re)building tools and extensive validation routines. These are tied together with robust decision making algorithms.

Here we showcase the new homology-based tools *HODER* and *Loopwhole* that together lead tomore accurate and more complete structure models, even at lower resolution. *HODER* transfers structural knowledge between homologous proteins (or the same protein in a different biochemical state) in the form of hydrogen bond restraints. *Loopwhole* automatically build missing loops in structure models based on homologous templates. We also discuss PDB-REDO features that that cater specifically to high-throughput applications and drug design in an industrial setting.