Learning by REDOing: Automated macromolecular structure model optimisation in PDB-REDO

Obtaining macromolecular structure models through X-ray crystallography has a long track record of success with about 10,000 new models released in the Protein Data Bank (PDB) every year. Such productivity could not have been achieved without all the automation that has been implemented throughout the crystallographic process.

Here we will discuss the PDB-REDO project that automates many of the steps that crystallographers must take in the last mile of the crystallographic process: moving from a 'solved' structure to a publication quality structure model. After a modest beginning more than a decade ago, PDB-REDO has grown to a comprehensive computational pipeline for crystallographic structure model optimisation. Apart from being provided to practicing crystallographers, the PDB-REDO pipeline is also applied to all available X-ray structures in the PDB. The resulting structure models are freely available for the broader structural biology community of which many members are not crystallographic experts.

We will showcase our latest developments that use the structure models that we made while **REDO**ing the PDB.

What can we learn from these models and how can we apply the new apply our new knowledge in a systematic and efficient way?

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