

Better protein structure models with homology-based hydrogen bond restraints

Bart van Beusekom, (b.v.beusekom@nki.nl), NKI, Plesmanlaan 121, 1066 CX Amsterdam

Abstract:

Producing high quality protein structure models from low-resolution crystallographic datasets is relatively difficult. A high-resolution ‘reference’ model from the Protein Data Bank (PDB) adds extra information to the model refinement process. But why use one reference when the average protein has twenty homologs in the PDB?

We describe an automated method that finds all suitable high-resolution homologs and uses them to derive case-specific hydrogen bond restraints. If few homologs are available, hydrogen bond restraints are generated based on PDB-wide high-resolution data. Applying these restraints in the PDB_REDO framework gives more plausible low-resolution structure models, for both published and work-in-progress cases.