PDB\_REDO: lessons from the PDB

During the PDB\_REDO session we’ll discuss the different types of problems in structure models in the PDB and how such problems can be detected by using validation software and by paying a lot of attention to details. We’ll also discuss the PDB\_REDO pipeline1 for structure model optimization which can perform many tasks in model building and refinement fully automatically. The current features are:

* Automated refinement parameterization (using Refmac):
  + Optimize geometric restraint weights
  + Optimize B-factor restraint weights
  + Choose the best B-factor model (one overall value, individual isotropic or anisotropic)
  + Use a simple TLS model, your own model or no TLS at all?
  + Refinement with twinned target, or not?
  + Local NCS restraints or NCS constraints?
* Automated model rebuilding:
  + Rebuild side chains (as rotamers)
  + Peptide plane flipping
  + Delete overenthusiastically built waters
  + Hydrogen bond flipping of ASN, GLN and HIS
  + Fix chirality errors

Running PDB\_REDO on 51,000 X-ray structure models in the PDB showed that:

* Most PDB entries (both old and new) can be improved in terms of (free) R-factor
* Optimizing the fit with the data also leads to improved geometric quality
* Many problems found by validation software can be solved automatically...
* ...but there are still a lot of things in making a good structure model that you have to do by hand

1 See [www.cmbi.ru.nl/pdb\_redo](http://www.cmbi.ru.nl/pdb_redo) for more details

Validation cheat sheet

Structure validation is essential to make a good structure. There is a massive number of available validation tools, but here are a few you should always use before finalizing and depositing your structure model:

Proteins: WHAT\_CHECK, MolProbity and Procheck

RNA/DNA: MolProbity

Waters: WHAT\_CHECK and Coot

Carbohydrates: PDB-care and CARP

Metal ions: WASP, CheckMyMetal and WHAT\_CHECK

Ligands: Validation against geometric restraints and ValLigURL

URLs for software and servers:

WHAT\_CHECK <http://swift.cmbi.ru.nl/gv/whatcheck/>; <http://swift.cmbi.ru.nl/>

MolProbity <http://molprobity.biochem.duke.edu/>

Procheck <http://www.ebi.ac.uk/thornton-srv/software/PROCHECK/>; <http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/Generate.html>

PDB-care <http://www.glycosciences.de/tools/pdbcare/>

CARP <http://www.glycosciences.de/tools/carp/>

WASP <http://xray.bmc.uu.se/cgi-bin/gerard/rama_server.pl>

CheckMyMetal <http://csgid.org/csgid/metal_sites> (down)

ValLigURL <http://eds.bmc.uu.se/eds/valligurl.php>