Tutorial: Validation with Coot

CCP4 Workshop New Delhi 2010

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1 Preamble

We will validate the structure in which we fitted the 3-aminobenzamide ligands.

2 Difference Map Peaks

One of the best tools for finding problems is the difference maps peaks tool. So let's use that that.

You should be able to see the ligand sites and other interesting features. What the problem here? (For me it is peak 5, but if you have run refmac with the model from the ligand fittingq, then it may be peak number 1.) Fix the problem.

3 Rotamer Analysis

Another useful tool is the Rotamer Analysis. Use that tool (in the Validate menu) to find problematic residues (note: not all big bars are necessarily wrong).

4 Ramachandran Plot, and Difference Plots

The Ramachandran Plot is a classic model-based validation tool. The Kleywegt Plot (*i.e.* Ramachandran NCS difference Plot) is often used to examine NCS-related mainchain differences.

Use these tools on this model to find Rotamers with problematic phi/psi values. What is the Kleywegt Plot telling you? Is there a problem? If there is a problme, how might you fix it? (Hint is there anything in Refinement/Regularization Control (R/RC) that might be of use?)

5 NCS and NCS Ghosts

Another way of showing NCS differences is using the NCS Ghosts, NCS Maps and NCS skipping.

5.1 NCS Skipping

Press `"P"` to go to the nearest and then `"O"` to jump between NCS-related models preserving the relative (NCS-compensating) view.

5.2 NCS Ghosts

Draw → NCS Ghosts Control... Then for the chosen molecule turn on the NCS ghosts.

5.3 NCS Maps

NCS maps (Calucalate → NCS maps) are useful addition to the NCS Ghosts because they show the maps corresponding the the NCS ghost molecules in the context of the NCS master (typically "A") chain.

6 Sequence Validation

Sometime people make sequence-based errors in building models. Coot has a tool that allows you to compare the sequence in the model with a reference sequence.

Validate → Alignment vs. PIR

Read in the sequence file and press OK.

Is there a sequence problem? How might you fix it?