Microsymposium

Protein-Ligand Analysis and Validation

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A number of tools related to handling of ligands have been added to Coot in recent years - these include 2D depictions, ligand binding pocket layout and a ligand scoring system. Coot also incorporates a number interface to other tools (CCP4's Refmac, Molprobity's probe and reduce and the CCDC's Mogul) to generate score for protein ligand complexes. This scoring system has been applied to models (with data) from the PDB. The details of the ligand scoring, and its application to one's own complex structure will be discussed.

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Keywords: Ligand, Electron Density, Validation