Building the Structural Model: Protein, Ligands, Metals and Other ions.

Ivan Shabalin, University of Virginia

Crystal structures of proteins and their complexes with small molecules and ions are at the core of structure-based drug discovery. Careful and informed building of the atomic model is crucial for understanding of intermolecular interactions and biological processes. We will cover the following aspects of model building for protein crystal structures:

- Automated model building with Buccaneer, ARP/wARP, RESOLVE, REFMAC, and HKL3000; getting the most complete model; building a model with very poor phases
- Placement of macromolecular models inside the unit cell with ACHESYM and Coot
- Automated improvement of side-chain conformations with FITMUNK
- When and how to slash side-chains
- When and how to model an alternative confirmation
- Identification and restraining of metal ions with Coot, CMM, and REFMAC; distinguishing metal ions and halogens
- Do I really have my ligand? Identification and modelling of small molecules.