

W0229

Coot: Model Building Tools for Protein Crystallography. Paul Emsley, Chemistry, Univ. of York, Wentworth Way, Heslington, York, YO10 5YW UK.

Coot[1] is a new CCP4-compatible molecular graphics application intended for protein crystallographers. It is based on the macromolecular coordinate library mmdb [2] and crystallographic object library clipper [3,4].

Despite being relatively immature, it is hoped that the current functionality is in some respects useful. The program includes various fitting procedures, including "interactive" refinement (fitting to density while optimizing geometry).

Features include: embedded fft, "scrollable" electron density, refinement and regularisation, rigid body refinement, mmCIF support, ligand search, water search, symmetry and unit cells, networked accession-code file grabbing, skeletonization, Ca-building, mutations, rotamers, chi angles (including ligand torsions), edit mainchain angles, Ramachandran plots, sequence view, reftmac[5] interface and undo/redo.

More information (and screenshots) are available at: <http://www.yesbl.york.ac.uk/~emsley/cool>

[1] P.Emsley & K. Cowtan (2004) Acta Cryst. Section D-Biological Crystallography (supplement) in press.

[2] E. Krissinel et al. (2004) Acta Cryst. Section D-Biological Crystallography (supplement) in press.

[3] K. Cowtan (2002) Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography vol 40, "The Clipper Project" pub. Daresbury Laboratory, Daresbury, Warrington, UK.

[4] K. Cowtan (2003) Crystallography Reviews (2003) "An overview of Some Developments in Crystallographic Computing Methods Worldwide" 9, 73-80.