

W0277

Model-Building and Validation with Coot. Paul Emsley, emsley@ysbl.york.ac.uk.

Coot[1] is a molecular graphics application providing electron density map fitting functions in a modern user interface. It is fair to say that Coot has been influenced by O.

Coot is built on CCP4 library components: Kevin Cowtan's clipper and Eugene Krissinel's mmdb as well as other Free Software libraries. It is a GUI-driven system with the aim of providing both powerful tools and ease of use. Coot displays maps, skeletons, symmetry atoms and allows model manipulations such as idealization, refinement, rigid-body fitting, ligand search, solvation, mutations, rotamers, least-squares and secondary structure-based matching.

Coot includes Ramachandran plots and other validation tools, using both the model and the fit to density. These functions also provide annotated interactive graphs. The close relationship between validation and model correction in Coot delivers a considerably quickened validate-rebuild-refine cycle. It is therefore realistic to create a deposition-quality structure in less than 1 day.

There is more information, documentation, screenshots, a FAQ and a mailing list available at the web site [2]. There are binaries for various Red Hat and Fedora Core Linuxes, SGI IRIX and Mac OS X.

[1] Emsley & Cowtan (2004) *Acta. Cryst. D*, 60, 2126-2132

[2] <http://www.ysbl.york.ac.uk/~emsley/cool>