s9.m31.o1 **GUI Design of the Graphical Tools in Coot**. Paul Emsley, *YSBL, University of York, Wentworth Way, Heslington, York, YO10 5YW UK, emsley@ysbl.york.ac.uk*

Keywords: GUI Design; Protein Crystallography; Molecular Graphics

Coot[1] is a 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]. The program includes fitting procedures, such as "interactive" refinement and other tools for molecular graphics protein model building. The success and failure of these and other GUI issues will be discussed.

More information (and screenshots) are available at: http://www.ysbl.york.ac.uk/~emsley/coot

[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

s9.m31.o2 **Design and development of the Mercury visualiser.** Clare Macrae, *Cambridge Crystallographic Data Centre, UK. E-mail: macrae@ccdc.cam.ac.uk*

Keywords: Mercury; Visualisation; Hydrogen Bonding

The application Mercury [1] provides a comprehensive range of tools for crystal structure visualisation and the exploration of crystal packing. Facilities include the automated study of hydrogen bonding and other user-defined short-range interactions, the generation of least squares and Miller planes, and the display of slices through crystals. Mercury is distributed as part of the Cambridge Structural Database (CSD) system [2], and is also available as a free download for various platforms from http://www.ccdc.cam.ac.uk/mercury/. The program's design, including the use of in-house object-oriented crystallographic and visualisation C++ libraries, and the Qt cross-platform Graphical User Interface toolkit [3] will be presented. This will be followed by a summary of both recent improvements to Mercury, such as the display of simulated X-ray powder diffraction patterns, and of planned future additions. An overview will also be given of a range of other applications, e.g. enCIFer, that have been developed at the Cambridge Crystallographic Data Centre, using these same development tools.

[1] Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M. K., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst*. **B58**, 389-397.
[2] Allen, F. H. (2002). *Acta Cryst*. **B58**, 380-388.
[3] www.trolltech.com