

Design and development of the Mercury visualiser,
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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