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Data collection and analysis

Gwyndaf Evans[a] and Martin Walsh[b]

[a]Diamond Light Source, Chilton OX11 0DE, England, and [b]MRC France, ESRF, Grenoble, France

The CCP4 Study Weekend held at the University of Reading in January 2005 turned its attention to methods and techniques for the measurement and analysis of X-ray diffraction data from crystals of biological macromolecules. The primary aim of the meeting was to provide the audience with insight into the workings of modern software packages for data analysis and the current thinking on data-collection strategies both in-house and at synchrotron facilities.

The programme has been organized to take the audience through the stages of sample preparation, sample screening, data collection and preliminary data analysis and at all stages attempts to provide details of the underlying theory of the computational methods being employed as well as offering practical insight for the experimenter, whether they be conducting experiments at home on conventional X-ray sources or at state-of-the-art third-generation undulator beamlines.

An introductory session on the first day set the scene with two talks presenting the current status and future perspectives of the field of macromolecular crystallography from two points of view; Zbyszek Dauter from the software and methodological viewpoint and Andrew Thompson from that of an X-ray instrumentation developer.

A small excursion into methods for expression and crystallization saw presentations how best to increase the chances of obtaining the best diffraction-quality crystals from protein material and then on how best to treat the crystal prior to and during a diffraction experiment.

Subsequent lectures covered the ins and outs of diffraction data indexing, data integration, data-collection strategies and X-ray area detector technology.

The second day presented the audience with more practical considerations in data collection for in-house and synchrotron experiments. The key steps which allow experimenters to validate experiments and prepare data for subsequent phasing or refinement were then presented in three talks, two of which covered the special topics of twinned crystals and the treatment of data displaying the effects of radiation damage.

The final session focused on more diverse ‘real-life’ topics in the form of the perspectives of an industrial crystallographer, the structure determination of a particularly awkward crystal structure and how protein can be encouraged to crystallize by rationalized mutation.