

Development of Powder Diffraction Methods for Macromolecular Crystallography

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Modern developments of the powder diffraction technique have allowed the investigation of systems with large unit cells like proteins [1]. Powder diffraction measurements can give a range of complementary information beyond that which can be obtained from a single crystal. For example, the peak shapes depend on the microstructure of the material, accurate unit cell parameters can easily be determined, and the sample generally survives under more varied or extreme conditions. In the present work, we aim in establishing the full potential of powder diffraction technique in the research of macromolecular systems. Specific examples that will be presented refer to: **(a)** structural modifications of the hen and turkey egg-white lysozymes (HEWL & TEWL) with crystallisation conditions and temperature [2-3]. **(b)** in-situ observation of crystal growth of HEWL **(c)** the development of a successful cryoprotection protocol for powder diffraction, with an almost complete suppression of radiation damage in pancreatic porcine elastase & **(d)** heavy atom derivatives of HEWL and elastase. A key point of the current work is to carefully assess various instrumental configurations and experimental strategies for the recording of protein powder data, either with high-resolution scanning instruments or with area detectors.

[1] Von Dreele R. B. *Acta Cryst.*, 2005, D61, 22-32. [2] Margiolaki I., et al., *Acta Cryst.*, 2005, D61, *in press*, see also: *ESRF Scientific Highlights*, 2004, 24. [3] Basso S. et al., *in preparation*.

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