

MS08 Serial crystallography, obtaining structures from many crystals

MS08-1-9 Routine room-temperature structure determination from protein crystals in situ on Diamond beamline VMXi using the Crystallisation Facility at Harwell
#MS08-1-9

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Abstract

The need for rapid turnaround times from the appearance of protein crystals to the determination of high quality crystal structures has driven many aspects of automation. Moreover, it is increasingly recognised that room temperature structures allow access to protein dynamics, may reveal ligand binding modes not apparent at cryogenic temperatures and allow for time resolved structures to be determined. We present the current pipeline of the Crystallisation Facility at Harwell and Diamond Beamline VMXi [1] and the capability of the pipeline to produce high quality structures at room temperature from small numbers of crystals in situ, for example within crystallisation plates. Protein samples in solution are provided by users, with automated crystallisation and data collection offering datasets and structure solution in many cases within days. In situ data collection allows for rapid feedback on crystallisation conditions for further optimisation and is particularly suitable for crystals challenging to cryo-protect or that are not robust to mechanical handling or other stresses. Operation is typically completely remote with data measured using a queueing system, providing convenience for the scientist. Recent developments in sample delivery and data analysis will also be described. We will also present illustrative examples in which the approach described above has led to effective structure solution on user projects.

References

1. VMXi: a fully automated, fully remote, high-flux in situ macromolecular crystallography beamline (2019) Juan Sanchez-Weatherby, James Sandy, Halina Mikolajek, Carina M. C. Lobley, Marco Mazzorana, Jon Kelly, Geoff Preece, Rich Littlewood and Thomas L.-M. Sørensen. *Journal of Synchrotron Radiation*. 26, 291-301.