

## Update from VMXi – Room-Temperature MX Beamline at Diamond Light Source, UK

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Room temperature protein structures can provide additional information with respect to structures solved at cryogenic temperatures, particularly with regards to inherent flexibility and thermal motion, as well as mode of binding of ligands [1-3]. Understanding how proteins behave at native temperatures has historically been challenging but, thanks to improvements in detector technology, relevant x-ray diffraction data can now readily be collected at the synchrotron. The VMXi beamline [4-6] is one of seven MX beamlines at the Diamond Light Source and offers the unique capability to collect room temperature *in-situ* MX data from crystallisation plates. The beamline is very closely linked with the Protein Crystallisation Facility (PXF), located adjacent to Diamond, in the Research Complex at Harwell building. Users can take advantage of the facility equipment, chemical screens and consumables. A shipping box system has been developed in the US, which has enabled users to send their crystallisation plate experiments to the synchrotron in a safe manner. We have been trialling this system, and so far it appears to be extremely useful. Upon arrival to the VMXi beamline, crystallisation plates are stored in a Formulatrix Rock Imager system and are then automatically transferred to the beamline via a robotic arm when experiments are queued. The process of data collection has been fully automated to provide the highest throughput possible and permits collection of diffraction data on routine samples, as well as those otherwise difficult to harvest or handle. Due to the mechanical limitations of the beamline, datasets are predominantly multi-crystal collections, and data from these experiments are automatically merged [7,8]. This can be taken one step further by creating sample groups, comprising crystals from multiple drops. We present here an update from the beamline and show examples of room temperature ligand-binding studies, as well as advances in sample mounting, which have yielded the first membrane protein structure from the beamline. Updates to downstream data processing pipelines have enabled users to improve the quality of their data, as well as identifying features which may have otherwise gone un-noticed [9]. We briefly describe some plans to add new functionality, which will facilitate studies in dynamic structural biology and will provide the environment for users to better understand the biological systems that they work on.

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