MS01-P05

First steps towards routine serial crystallography at the VMX-i beamline

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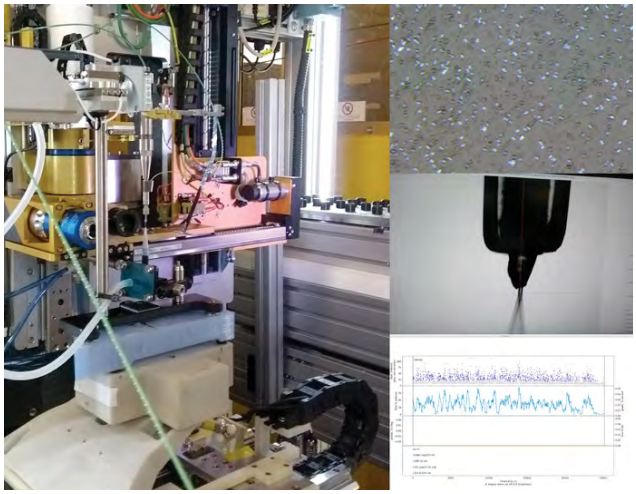
MXi is the most recent addition to the portfolio of macromolecular crystallography beamlines at Diamond Light Source. VMXi was built in place of the previously existing tuneable I02 beamline and was built as an entirely remote, high throughput in-situ crystallography beamline. The beamline operates in a fully automated fashion and the users input data collection parameters and evaluate results via a remote web interface. The beamline is in the initial phases of user operation but its unique optical properties and very high flux make it particularly well suited for serial crystallography. During the past few months, several proof of principle experiments have been carried out at VMXi in collaboration with members of the XFEL hub. These experiments highlight the scientific opportunities that this beamline will offer and enable us to shape the best model for the VMXi user program that better suits the needs of the user community. The results from these experiments will also provide the test bed for improving the autoprocessing pipelines needed for the high volume of data produced by this beamline and XFEL beamlines around the world. We will present examples of the different sample delivery systems tested, how the resulting data are collected and processed, and discuss the options of how the beamline could be best used by the growing UK XFEL community.References:



Keywords: in-situ, serial crystallography, multilayer monochromator

MS02 - From data collection to structure finalization: getting the most from your crystal

Chairs: Dr. William Shepard, Dr. Katherine McAuley

MS02-P01

Identification of contaminants with SIMBAD: A Sequence-independent molecular replacement pipeline

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In protein crystallisation it is not uncommon for contaminant proteins to crystallise instead of the protein of interest. Solving structures with molecular replacement in such cases can be difficult since the search models, assumed to be similar to the protein of interest, are not necessarily related to the proteins that have actually crystallised. SIMBAD is a pipeline to solve crystal structures without prior sequence information that can provide a route to identify the presence of a contaminant in a crystal and lead to structure solution. Early users of SIMBAD have unearthed several examples of unintentional crystallisation of previously known and unknown contaminant proteins. Other successful user cases have highlighted the problem of the mis-identification of crystals, where a mix-up has occurred (e.g. swapped crystallisation trays) and a dataset has been incorrectly assigned as being a different target structure. In all of these cases, mis-directed efforts in attempting to solve the structure of the target crystal could have been avoided through the use of SIMBAD at the point of data collection or through more rigorous annotation and experimental assessment of the crystal prior to data collection.

Keywords: SIMBAD, MR, contaminants