Data collection tools for challenging samples at the MX beamlines at Diamond

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Diamond Light Source [1] is the UK third generation synchrotron facility located south of Oxford and it started with the user programme in early 2007. Currently, there are five operational macromolecular crystallography (MX) beamlines that provide state of the art facilities to the user community and eventually there will be seven beamlines dedicated to MX [2]. All MX beamlines provide tools for standard data collection but given the increasing complexity and associated challenges with bigger macromolecular complexes, membrane proteins, smaller crystals, and radiation damage, different approaches are often required to get the best possible data out of these samples. Tools for sample location and characterization are a first step. Often, because of radiation damage and sample deterioration, multiple crystals are needed in order to obtain a complete data set and a number of tools and different experiment setups that help to address this problem will be described, including use of suitable software tools to get the best data set, fast data collection, crystal humidity control, in situ screening and use of a mini kappa goniometer. These tools enable new data collection strategies which can make the difference towards a successful structure determination. A special focus will be on the use and potential of multi-axis goniometers. Given the limited amount of beam time and ever faster data acquisition rates, quick decision making during the beam time becomes more important. Therefore, data collection strategies and crystal and diffraction image characterization are provided automatically. Very shortly after the data collection has finished the results from our automatic data processing routines are available and we also provide difference electron density map, molecular replacement and experimental phasing pipelines.


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