The macromolecular crystallography beamline I04 at Diamond [1] is a versatile variable and microfocus beamline aiming to provide the best quality diffraction data from crystals of macromolecules mainly at cryo temperatures. Beam delivery is achieved through the combination of a double crystal monochromator (DCM) with a F-switch which houses compound refractive lenses (CRL) that can be brought individually into the beam path. Both devices were designed inhouse and this combination allows variable focus of a very stable beam from the microfocus regime (8 µm x 5 µm (h x v)) to larger beam sizes (up to 110 µm x 100 µm) over the whole energy range of 6-18 keV. Beam delivery within 3% RMS of the beam size is achieved by making use of a dedicated feedback system using X-ray beam position monitors (XBPMs). In June 2022 the original U23 insertion device has been replaced with a cryocooled permanent magnet undulator (CPMU) and this has resulted in a significant flux increase which has opened up new opportunities, including faster data collection and the ability to address more challenging data collections, in particular for microcrystallography.

Related to the insertion device upgrade we are carefully monitoring any heat load effects on the optics and are further characterising the performance of our F-switch device with the aim to optimise beam delivery.

The combination of the stable beamline optics with the SmarGon multi-axis goniometer and Eiger2 XE 16M detector provides a versatile yet very stable setup that allows to optimise the experiment based on sample properties and the scientific aim as well as providing new scientific capability. The beamline can be used in interactive or remote mode making full use of the tools available to tackle even the most challenging samples in the microfocus regime. More recently we have added functionality which allows to run a dose-driven data collection rather than providing an exposure time. For experimenters it is very difficult to understand the I04 beam properties given the recent insertion device upgrade and the possibility to focus the beam to various beam sizes and this can easily lead to too low or too high exposure times for a given sample. The dose-based approach is taking away the decision about the correct exposure time and rather tries to direct towards the experimental aim and if implemented on other beamlines will also allow an easier comparison of data sets. The current implementation is based on assuming a crystalline sample with standard composition, but further developments are ongoing to include more sample-based information. The dose-driven data collection is also used in our unattended data collection (UDC) mode where we offer fully automated data collection protocols depending on the scientific aim and data collection requirements based on user input to the ISpyB/Synchweb interface. We intend to provide this combination of crystallographic expertise system and dose-aware data collection also via the graphical user interface. Multi-sweep, multi-orientation data collection protocols are routinely used with the multi-axis SmarGon goniometer resulting in high multiplicity high quality data sets [2].

We are constantly developing and improving our tools for beamline quality and speed monitoring, and this allows us to easily diagnose any changes in performance after a hardware or software configuration change. Furthermore, we are looking into providing additional tools and ancillary techniques that would provide additional sample information while keeping a streamlined user experience. An outlook will also be given about plans to improve beam delivery further.

1 https://www.diamond.ac.uk/Instruments/Mx/I04.html

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