

MS44-1-2 The High-throughput Macromolecular Crystallography Beamline P11
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Abstract

P11 at PETRA III (DESY, Hamburg) is a high-throughput instrument for macromolecular crystallography (1). P11 has tuneable photon energy between 5.5 - 28 keV having the Eiger2 X 16M as the stationary detector and the possibility of using a CdTe-detector for higher energies. Beam size from 200 x 200 µm to 4 x 9 µm can be used with a maximum photon flux of 1.3 x 10¹³ ph/s at 12 keV energy. The automatic sample changer at P11 is based on the unipuck format with a total capacity of 23 pucks (368 samples) having a mount-unmount cycle of approximately 36 s, which brings the beamtime spent per sample down to ca. 2min. Furthermore, in close proximity of the beamline, P11 has a user laboratory with e.g. a crystal shifter for semi-automated crystal harvesting.

During the past two years mode of operation at P11 has changed from fully on-site to almost exclusively remote. Remote connection using FastX-access via a dedicated remote machine was established in 2020, which has enabled near normal user operation throughout the pandemic. Users are supported by a virtual meeting and the scientific accounts can be used during and after the beamtime for manual data processing on Maxwell, the central computational cluster, where the autoproccessing is also migrated to the dedicated P11 nodes.

P11 is a very diverse environment and allows the adjustment to various non-standard experiments e.g. via the long term proposal (LTP) scheme. For example, serial synchrotron crystallography at P11 is enabled with sample delivery through various types of solid supports or the tape-drive setup, which enables time-resolved experiments by the mix-and diffuse method (2), and has been developed through the LTP scheme along with the real-time autoproccessing of serial data with CrystFEL (3).

This year MXCuBE will be employed as the default control software with the integration to ISPyB for tracking shipments, communicating the sample details to MXCuBE, as well as acting as a data archive. The establishment of parallel autoproccessing pipelines in addition to the currently used, XDSAPP-based (4) pipeline, and the implementation of strategy calculation including dose estimation are also planned. Furthermore, these software developments are synchronising P11 with the EMBL PETRA III beamlines for the future foundation of a uniform structural biology village at PETRA IV.

References

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