EMBL beamlines for macromolecular crystallography at PETRA III. Thomas R. Schneider, Gleb Bourenkov, Michele Cianci, Johanna Kallio, Guillaume Pompidor, Stefan Fiedler,

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Since 2012, EMBL Hamburg is operating three beamlines for structural biology applications at PETRA III at DESY (Hamburg, Germany). Two beamlines (P13, P14) provide excellent condition for diffraction data collection on macromolecular crystals; one beamline (P12) offers automated small-angle X-ray scattering experiments on solutions of biological macromolecules. P13 offers a photon flux of $>10^{13}$ ph/sec from 16 keV to 6 keV. Energies between 4 and 6 keV are accessible with a photon flux between $>10^{12}$ ph/sec providing unique conditions for experimental phasing. Using adaptive focusing mirrors, the full beam ($\sim 1.5 \times 1\text{ mm}^2$) can be focused to a size of ca. 30 x 20 µm$^2$. An MD2 diffractometer with a mini-kappa goniostat allows for rapid and accurate rotation of crystals in the X-ray beam. P14 offers a photon flux of $>10^{13}$ ph/sec between 7 and 20 keV. Using adaptive focusing mirrors, a beamsize of $7 \times 4 \text{ µm}^2$ with a total flux of $>10^{12}$ ph/sec can be used for crystallographic experiments. The focusing mirrors can be moved into and out of the beam in less than half a minute allowing to rapidly toggle between a fully focused small beam and an unfocused large ($\sim 1.5 \times 1 \text{ mm}^2$) beam to optimize data collection parameters for differently sized crystals. A high-precision vertically mounted MD3 diffractometer with a sphere of confusion of less than 100 nm is available for data collection. Both MX beamlines are equipped with PILATUS 6M detectors and dedicated data processing computers. The beamlines are embedded into the 'Integrated Facility for Structural Biology' offering facilities for sample preparation and characterization, a laboratory specifically equipped for the preparation of heavy atom derivatives, and downstream facilities for data evaluation. Applications for beamtime can be made at smis.embl-hamburg.de. Access support can be obtained via www.biostruct-x.eu. We will report about the status of the beamlines, describe typical experimental situations and present early results.

Keywords: synchrotron radiation; beamline optics; data collection