

Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin (HZB)

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HZB operates three beamlines for Macromolecular Crystallography (MX) at the electron storage ring BESSY II [1,2]. Beamlines BL14.1 and BL14.2 are dedicated to multi-wavelength anomalous dispersion (MAD) phasing methods, operating between 5.5-15.5 keV (2.25 to 0.75 Å) which cover the absorption edges of most commonly used heavy atom derivatives. State-of-the-art detector technologies, including the PILATUS 6M (BL14.1) and PILATUS3S 2M (BL14.2) detectors (Dectris, Switzerland) enable high quality and rapid data collection.

BL14.1 provides a high degree of automation with an MD2 microdiffractometer equipped with a mini-kappa axis and reliable sample changing is realized by a CATS sample changing robot. This beamline also features an in situ plate screening option.

On the fully refurbished beamline BL14.2 an automated sample changer G-ROB, which has a high capacity sample dewar hosting up to 294 samples, supporting both, SPINE and UNIPuck standard allows high-throughput data collection. Beamline BL14.3 is a fixed energy station operating at 13.8 keV (0.89 Å).

Located in the middle of Europe, the MX group at BESSY II serves more than 100 research groups from across Europe. More than 2000 protein structures have been deposited to the Protein Data Bank (PDB), from data collected on one of the beamlines. With 450 depositions in 2016, the HZB-MX beamlines are currently among the most productive MX-beamlines in Europe.

Both MAD beamlines are running MXCuBE V2 as control software, allowing fast and efficient data collection. Collected data is live processed using various programs, including the data processing expert system XDSAPP [3].

The beamlines support all standard data collection procedures, including SAD and automated MAD data collection. BL14.2 is also dedicated for long-wavelength data collection due to its minimal sample-detector distance. Further experiments are available: radiation induced phasing; on- and off-line UV-Vis micro-photo-spectroscopy, e.g. to detect radiation damage; controlled crystal dehydration using an HC1 dehydration device. Furthermore, the MX-groups operates a S1 BioLab which supports the complete workflow from “gene to crystal”.

[1] Mueller, U. et al. (2012). *J. Synch. Rad.* 19, 442-449.

[2] Mueller, U. et al. (2015). *Eur. Phys. J. Plus* 130, 141.

[3] Sparta, K. et al. (2016). *J. Appl. Cryst.* 49, 1085-1092.