

## First results from the long-wavelength macromolecular crystallography beamline I23 at Diamond Light Source

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Over the past years technical developments such as single-photon counting detectors and improved stability from synchrotron sources and beamline equipment have led to an increased number of protein and nucleic acid structures being solved by experimental phasing techniques at longer wavelengths around  $\lambda = 2 \text{ \AA}$  [1]. Single wavelength anomalous diffraction (SAD) utilizes therein the increase of the anomalous signal from sulfur or phosphorus towards their K absorption edges which are around 5  $\text{\AA}$  and 6  $\text{\AA}$ , respectively. Solving the crystallographic phase problem directly in the absence of a know protein model similar to the one under investigation and without additional labelling of the protein or nucleic acid has the potential to become the method of choice for phasing macromolecular crystals.

At Diamond Light Source, over the past years, the long-wavelength MX beamline I23 [2] has been designed, constructed and has recently started operation with “friendly” users. The beamline differs radically from the existing well developed and established MX beamlines. To eliminate air absorption, the complete beamline is operated in vacuum, including the sample environment and the detector. Several technical issues had to be addressed, leading to a variety of pioneering new developments, like the large in-vacuum semi-cylindrical Pilatus 12M detector and the dedicated kappa goniometer.

The beamline covers a wavelength range from 1.1 to 5.9  $\text{\AA}$  (2.1 – 11.5 keV) which allows accessing several K absorption edges of biological relevance like phosphorus, sulfur, chlorine, potassium and calcium, elusive on other MX beamlines. Apart from experimental phasing experiments, anomalous contrast can be used to identify and distinguish these light atoms in the electron density and use their positions to help model building at low resolution.

First data has been successfully collected and several structures have been solved using SAD phasing based on phasing information from phosphorus, sulfur and calcium. An overview on the current status and first results from this novel instrument will be presented.

[1] J. Rose, B.-C. Wang, M. Weiss, *IUCrJ* 2 (2015) 431.

[2] A. Wagner, R. Duman, K. Henderson, V. Mykhaylyk, *Acta Cryst. D* 72 (2016) 430.