Crystallography at wavelengths longer than 2.7 A

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The I23 Long wavelength MX beamline at the Diamond Light source is a unique instrument dedicated to experimental phasing and optimised to operate at wavelengths between 1.5 to 4 Å [1]. The beamline enables users to exploit the increased anomalous signal specific to scatterers naturally present in proteins such as S, P, Cl, Ca and K. This renders obsolete the need for selenomethionine incorporation or heavy-atom derivatisation of protein crystals, which represents a significant barrier in the process of experimental phasing. In addition to the long wavelength phasing experiments, I23 is the sole beamline where identification and localisation of biologically important ions, such as K, Ca, Cl is feasible by generation of anomalous difference Fourier maps below and above the element absorption edge [2]. Recent results of native phasing and ion identification/localisation demonstrating the capability and potential of the beamline will be presented.

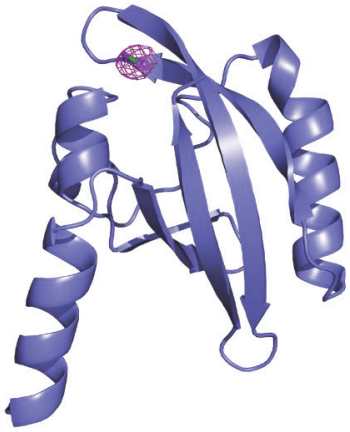

Fig. 1. Sulphur anomalous difference Fourier maps of a 116 residue protein domain solved by S-SAD with a single cysteine.

References

[1] Wagner, A. et al. (2016). *Acta Crystallogr D Struct Biol*. 430-4399

[2] Langan, P.S. et al. (2018). Nature Communications, 9, 4540