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Experimental phasing opportunities for macromolecular crystallography at very long wavelengths

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Despite recent advances in cryo-electron microscopy and artificial intelligence-based model predictions, a significant fraction of structure determinations by macromolecular crystallography still requires experimental phasing, usually by means of single-wavelength anomalous diffraction (SAD) techniques. Most synchrotron beamlines provide highly brilliant beams of X-rays of between 0.7 and 2 Å wavelength. Use of longer wavelengths to access the absorption edges of biologically important lighter atoms such as calcium, potassium, chlorine, sulfur and phosphorus for native-SAD phasing is attractive but technically highly challenging. The long-wavelength beamline I23 at Diamond Light Source overcomes these limitations and extends the accessible wavelength range to $\lambda = 5.9$ Å. Here we report 22 macromolecular structures solved in this extended wavelength range, using anomalous scattering from a range of elements which demonstrate the routine feasibility of lighter atom phasing. We suggest that, in light of its advantages, long-wavelength crystallography is a compelling option for experimental phasing.

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Macromolecular Crystallography

Alexander McPherson

Macromolecular Crystallography:

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