

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

**Randy Read, Alexandre G.
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Sanderson, Jane V. Skelly, 2007-08-23 Macromolecular crystallography is the study of macromolecules using X ray crystallographic techniques to determine their molecular structure This title synthesises contributions from a team of internationally recognized leaders offering chapters on conventional and high throughput methods *Macromolecular Crystallography, Part D* Charles W. Carter Jr., Charles W. Carter, Robert M. Sweet, 2003-12-10 Accurate molecular structures is vital for rational drug design and for structure based functional studies directed toward the development of effective therapeutic agents and drugs Crystallography can reliably predict structure both in terms of folding and atomic details of bonding Phases Map interpretation and refinement Analysis and software **Macromolecular Crystallography**

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crystalline form Volume 2 complements the first volume by addressing laboratory techniques for crystal handling and structural characterization as well as computational techniques for data collection phasing and refinement The volume concludes with a detailed and insightful survey of available crystallographic software These volumes will be an indispensable reference for obtaining macromolecular crystals and determining their three dimensional structure

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