

## 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

**John R. Helliwell**



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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 Macromolecular Crystallography Charles W. Carter, Robert M. Sweet, 2003 **Macromolecular Crystallography with Synchrotron Radiation** John R. Helliwell, 1992 This highly illustrated monograph provides a comprehensive treatment of the study of the structure and function of the molecules of life proteins nucleic acids and viruses using synchrotron radiation and crystallography Beginning with chapters on the fundamentals of macromolecular crystallography and macromolecular structure the book goes on to review the sources and properties of synchrotron radiation instrumentation and monochromatic data collection There are also chapters on the Laue method on diffuse X ray scattering and on variable wavelength anomalous dispersion methods The book concludes with a description and survey of applications including studies at high resolution the use of small crystals the study of large unit cells and time resolved crystallography particularly of enzymes Appendices are provided that present essential information for the synchrotron user as well as information about synchrotron facilities currently available

Evolving Methods for Macromolecular Crystallography Randy J. Read, Joel Sussman, 2007-06-25 This volume draws on the expertise of leaders in the field of macromolecular crystallography to illuminate the dramatic developments that are accelerating progress in structural biology Their contributions span the range of techniques from crystallization through data collection structure solution and analysis The book shows how modern high throughput methods are contributing to a deeper understanding of medical problems **Macromolecular Crystallography** Maria Armenia Carrondo, Paola

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McPherson, 2002-12-01 *Methods in Macromolecular Crystallography* North Atlantic Treaty Organization. Scientific Affairs Division, 2001 This volume contains 20 papers from two courses Methods for Macromolecular Crystallography and Chemical Prospective in Crystallography of Molecular Biology held during the late spring of 2000 in Reice Italy The papers discuss crystals synchrotrons detector development data processing ab initio phasing and high and low resolution molecular placement experimental phase measurement density modification methods map improvements interpretation of electron

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