

## 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**



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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

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**Advancing Methods for Biomolecular Crystallography** Randy Read, Alexandre G. Urzhumtsev, Vladimir Y. Lunin, 2013-04-03 This work presents a snapshot of the state of the art of modern biomolecular crystallography from crystallisation through structure determination and even interactive presentation on the web Methods driving the latest automated structure determination pipelines are explained as well as how to deal with problems such as crystal pathologies that still demand expert analysis These methods are illustrated through their application to problems of great biological interest such as the molecular machinery underlying the complement pathway the mechanism of action of monoamine oxidase inhibitors and the structure of the eukaryotic ribosome Complementary approaches such as neutron diffraction small angle X ray scattering coherent diffraction and computational modelling are also explored      **Structural Biology in Drug Discovery** Jean-Paul Renaud, 2020-01-27 With the most comprehensive and up to date overview of structure based drug discovery covering both experimental and computational approaches Structural Biology in Drug Discovery Methods Techniques and Practices describes principles methods applications and emerging paradigms of structural biology as a tool for more efficient drug development Coverage includes successful examples academic and industry insights novel concepts and advances in a rapidly evolving field The combined chapters by authors writing from the frontlines of structural biology and drug discovery give readers a valuable reference and resource that Presents the benefits limitations and potentiality of major techniques in the field such as X ray crystallography NMR neutron crystallography cryo EM mass spectrometry and other biophysical techniques and computational structural biology Includes detailed chapters on druggability allostery complementary use of thermodynamic and kinetic information and powerful approaches such as structural chemogenomics and fragment based drug design Emphasizes the need for the in depth biophysical characterization of protein targets as well as of therapeutic proteins and for a thorough quality assessment of experimental structures Illustrates advances in the field of established therapeutic targets like kinases serine proteinases GPCRs and epigenetic proteins and of more challenging ones like protein protein interactions and intrinsically disordered proteins      **Macromolecular Crystallography Protocols** Sylvie Doublé, 2007 In the decade since publication of the first edition of Crystallographic Methods and Protocols the field has seen several major developments that have both accelerated the pace of structure determination and made crystallography accessible to a broader range of investigators Volume I Preparation and Crystallization of Macromolecules is

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Crystallography of Protein Dynamics, 2023-09-25 Approx 400 pages Approx 400 pages **Crystallography Made Crystal Clear** Gale Rhodes, 2010-08-04 Crystallography Made Crystal Clear makes crystallography accessible to readers who have no prior knowledge of the field or its mathematical basis This is the most comprehensive and concise reference for beginning Macromolecular crystallographers written by a leading expert in the field Rhodes uses visual and geometric models to help readers understand the mathematics that form the basis of x ray crystallography He has invested a great deal of time and effort on World Wide Web tools for users of models including beginning level tutorials in molecular modeling on personal computers Rhodes personal CMCC Home Page also provides access to tools and links to resources discussed in the text Most significantly the final chapter introduces the reader to macromolecular modeling on personal computers featuring SwissPdbViewer a free powerful modeling program now available for PC Power Macintosh and Unix computers This updated and expanded new edition uses attractive four color art web tool access for further study and concise language to explain the basis of X ray crystallography increasingly vital in today s research labs Helps readers to understand where models come from so they don t use them blindly and inappropriately Provides many visual and geometric models for understanding a largely mathematical method Allows readers to judge whether recently published models are of sufficiently high quality and detail to be useful in their own work Allows readers to study macromolecular structure independently and in an open ended fashion on their own computers without being limited to textbook or journals illustrations Provides access to web tools in a format that will not go out of date Links will be updated and added as existing resources change location or are added

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predict structure both in terms of folding and atomic details of bonding Methodological methods in crystals Methodological methods data analysis

## Unveiling the Power of Verbal Artistry: An Emotional Sojourn through **Macromolecular Crystallography**

In a world inundated with monitors and the cacophony of instantaneous interaction, the profound power and psychological resonance of verbal artistry usually diminish in to obscurity, eclipsed by the constant barrage of noise and distractions. However, situated within the musical pages of **Macromolecular Crystallography**, a charming work of fictional beauty that pulses with raw thoughts, lies an wonderful journey waiting to be embarked upon. Published by way of a virtuoso wordsmith, that enchanting opus guides viewers on an emotional odyssey, delicately exposing the latent possible and profound impact stuck within the intricate internet of language. Within the heart-wrenching expanse of the evocative evaluation, we can embark upon an introspective exploration of the book is key styles, dissect their fascinating writing design, and immerse ourselves in the indelible impact it leaves upon the depths of readers souls.

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