

## Experimental phasing opportunities for macromolecular crystallography at very long wavelengths

Kamel El Omari<sup>1,2</sup>, Ramona Duman<sup>1,2</sup>, Vitaliy Mykhaylyk<sup>1,2</sup>, Christian M. Orr<sup>1,2</sup>, Merlyn Latimer-Smith<sup>1</sup>, Graeme Winter<sup>1</sup>, Vinay Grama<sup>1</sup>, Feng Qu<sup>2,3,14</sup>, Kiran Bountra<sup>2,3</sup>, Hok Sau Kwong<sup>2,3</sup>, Maria Romano<sup>2,3,15,16</sup>, Rosana I. Reis<sup>4</sup>, Lutz Vogele<sup>5,17</sup>, Luca Vecchia<sup>6,18</sup>, C. David Owen<sup>1,2</sup>, Sina Wittmann<sup>7,19</sup>, Max Renner<sup>4,20</sup>, Miki Senda<sup>8</sup>, Naohiro Matsugaki<sup>8,9</sup>, Yoshiaki Kawano<sup>10</sup>, Thomas A. Bowden<sup>6</sup>, Isabel Moraes<sup>4</sup>, Jonathan M. Grimes<sup>6</sup>, Erika J. Mancini<sup>11</sup>, Martin A. Walsh<sup>1,2</sup>, Cristiane R. Guzzo<sup>12</sup>, Raymond J. Owens<sup>6,13</sup>, E. Yvonne Jones<sup>6</sup>, David G. Brown<sup>5</sup>, Dave I. Stuart<sup>1,6</sup>, Konstantinos Beis<sup>2,3</sup> & Armin Wagner<sup>1,2,14</sup>

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.

<sup>1</sup>Diamond Light Source, Harwell Science and Innovation Campus, • OX110DE, UK. <sup>2</sup>Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot OX11 0FA, UK. <sup>3</sup>Department of Life Sciences, Imperial College London, London SW7 2BZ, UK. <sup>4</sup>National Physical Laboratory, Hampton Road, Teddington TW11 0LW, UK. <sup>5</sup>Charles River Discovery Research Services UK, Chesterford Research Park, Saffron Walden CB10 1XL, UK. <sup>6</sup>Division of Structural Biology, Wellcome Centre for Human Genetics, University of Oxford, Oxford OX3 7BN, UK. <sup>7</sup>Department of Biochemistry, University of Oxford, Oxford, UK. <sup>8</sup>Structural Biology Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan. <sup>9</sup>Department of Materials Structure Science, School of High Energy Accelerator Science, The Graduate University of Advanced Studies (Soken-dai), 1-1 Oho, Tsukuba, Ibaraki 305-0801, Japan. <sup>10</sup>Advanced Photon Technology Division, RIKEN SPring-8 Center, Hyogo 679-5148, Japan. <sup>11</sup>School of Life Sciences, University of Sussex, Falmer, Brighton BN1 9QG, UK. <sup>12</sup>Department of Microbiology, Institute of Biomedical Sciences, University of São Paulo, São Paulo 05508-000, Brazil. <sup>13</sup>The Rosalind Franklin Institute, Harwell Campus, Oxford OX11 0FA, UK. <sup>14</sup>Present address: Department of Biochemistry, University of Oxford, Oxford, UK. <sup>15</sup>Present address: Institute of Biostructures and Biomedicine, IBB, CNR, 80131 Naples, Italy. <sup>16</sup>Present address: Department of Pharmacy, University of Naples "Federico II", 80131 Naples, Italy. <sup>17</sup>Present address: Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany. <sup>18</sup>Present address: Friedrich Miescher Institute for Biomedical Research, Basel, Switzerland. <sup>19</sup>Present address: Institute of Molecular Biology (IMB), Ackermannweg 4, 55128 Mainz, Germany. <sup>20</sup>Present address: Department of Chemistry, Umeå University, 901 87 Umeå, Sweden.

\*email: [armin.wagner@diamond.ac.uk](mailto:armin.wagner@diamond.ac.uk)

# Macromolecular Crystallography

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## **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

**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 Spadon, 2011-12-01 This volume is a collection of the contributions presented at the 42nd Erice Crystallographic Course whose main objective was to train the younger generation on advanced methods and techniques for examining structural and dynamic aspects of biological macromolecules The papers review the techniques used to study protein assemblies and their dynamics including X ray diffraction and scattering electron cryo electron microscopy electro nanospray mass spectrometry NMR protein docking and molecular dynamics A key theme throughout the book is the dependence of modern structural science on multiple experimental and computational techniques and it is the development of these techniques and their integration that will take us forward in the future

**Introduction to Macromolecular Crystallography** 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

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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 andinappropriately 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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## **Table of Contents Macromolecular Crystallography**

1. Understanding the eBook Macromolecular Crystallography
  - The Rise of Digital Reading Macromolecular Crystallography
  - Advantages of eBooks Over Traditional Books
2. Identifying Macromolecular Crystallography
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Macromolecular Crystallography
  - User-Friendly Interface
4. Exploring eBook Recommendations from Macromolecular Crystallography
  - Personalized Recommendations
  - Macromolecular Crystallography User Reviews and Ratings
  - Macromolecular Crystallography and Bestseller Lists
5. Accessing Macromolecular Crystallography Free and Paid eBooks
  - Macromolecular Crystallography Public Domain eBooks
  - Macromolecular Crystallography eBook Subscription Services
  - Macromolecular Crystallography Budget-Friendly Options

6. Navigating Macromolecular Crystallography eBook Formats
  - ePub, PDF, MOBI, and More
  - Macromolecular Crystallography Compatibility with Devices
  - Macromolecular Crystallography Enhanced eBook Features
7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Macromolecular Crystallography
  - Highlighting and Note-Taking Macromolecular Crystallography
  - Interactive Elements Macromolecular Crystallography
8. Staying Engaged with Macromolecular Crystallography
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Macromolecular Crystallography
9. Balancing eBooks and Physical Books Macromolecular Crystallography
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Macromolecular Crystallography
10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
11. Cultivating a Reading Routine Macromolecular Crystallography
  - Setting Reading Goals Macromolecular Crystallography
  - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Macromolecular Crystallography
  - Fact-Checking eBook Content of Macromolecular Crystallography
  - Distinguishing Credible Sources
13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
14. Embracing eBook Trends
  - Integration of Multimedia Elements



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