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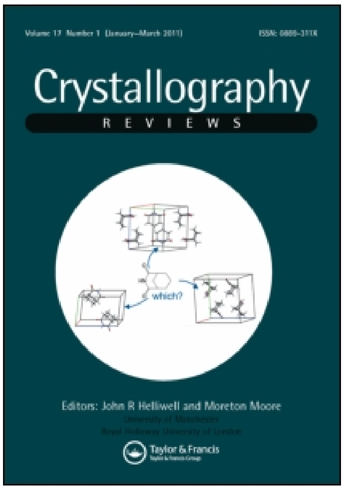

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Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, by Bernard Rupp

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BOOK REVIEW

Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, by Bernard Rupp, Garland Science, Taylor & Francis Group, 2009, xxi + 809 pp., £60 (hardcover), ISBN 978-0-8153-4081-2

As stated by Brian Matthews in his Foreword, this new work by Bernard Rupp is a true and worthy successor to the classic text *Protein Crystallography* by Thomas Blundell and Louise Johnson that served as the protein crystallographers' bible for a generation of practitioners of the art. However, much has changed since the 1970s in the methodology, practice and most of all the nature of the people who undertake biomolecular crystallography. Thirty years ago, most newcomers to protein crystallography had a background in chemical crystallography but lacked familiarity with the practical aspects of handling protein crystals, recording diffraction data from crystals with a limited lifetime (before cryocrystallography), the use of multiple isomorphous replacement to determine experimental phases, molecular replacement or model building with the use of a Richards' box. These days many protein crystallographers come to the field when they have found a structural biology problem as a result of their researches in molecular biology, immunology or other area of biological or medical science. For these people especially, but for all protein crystallographers, this new work is an invaluable introduction to the field for the novice and reference volume for the experienced researcher. It is a worthy successor to Blundell and Johnson.

Along with its up-to-date contents, this book is presented in the style of a modern biochemical or biology undergraduate text. The illustrations are colourful and informative and liberal use is made of sidebars and boxes to introduce extra material and to emphasize important concepts. Many texts on protein crystallography have been written since Blundell and Johnson's original work. Some have thoroughly covered fundamental and theoretical aspects of the subject such as *Principles of Protein X-ray Crystallography* by Jan Drenth, and others have been written especially to introduce non-experts to practical aspects of the field such as *Crystallography made Crystal Clear* by Gale Rhodes, *Outline of Crystallography* by David Blow and many others. Rupp's work is comprehensive in the form of a text book covering both the theoretical background and practical aspects but liberally threaded with tips from an experienced user. In fulfilling a role as the comprehensive text for an in-depth graduate level course in macromolecular crystallography, Rupp's book uses a presentation style that integrates the experimental approaches throughout the text. For example, in the chapter that describes protein structure, the appearance of amino acids in electron density maps appears alongside their chemical and structural descriptions.

The volume is arranged in five parts. The four chapters in Part I introduce the subject emphasising the overall requirements for a protein crystal structure analysis. This leads to some necessary forward referencing where concepts are introduced early but are only defined later in the text. While this makes reading the work in a linear fashion slightly more difficult, it is more than compensated for by the way that important material is

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introduced early, allowing the reader to see the significance of the concepts without wading through reams of dry theory. The remainder of Part I covers protein crystallization and a basic description of protein structure. The emphasis is towards the need to prepare proteins for structure analysis and includes sections on the treatment of purification tags, membrane proteins and protein engineering. The section on the analysis of protein stability and conformational state is a very valuable addition. The description of protein structure is not intended to be a comprehensive replacement for a dedicated work on the subject but gives sufficient information for the understanding of structure solution and refinement.

The three chapters in Part II cover the basics of crystallography including crystal geometry, symmetry and space-groups, diffraction physics and very importantly for a modern text, an entire chapter on statistics and probability. Given the widespread use of direct methods in structure solution by SAD phasing methods, inclusion of a section on direct methods phasing in protein crystallography is novel and important. The use of full colour makes the diffraction and symmetry diagrams very easy to follow.

Part III contains a single chapter that focuses on the diffraction experiment itself. All aspects of instrumentation from X-ray sources and detectors to robotics are covered in some detail. Although one would normally expect the discussion of twinning to be included in the Chapter on Crystal Geometry in Section II, it is included along with other aspects of integrating diffraction data. This is in keeping with the philosophy of the text that keeps experimental aspects of the subject together. The detailed treatment of mosaicity and splitting of reflections is very valuable and is too often not given the prominence it deserves.

Part IV in four Chapters first deals with the theoretical aspects of generating electron density from the diffraction amplitudes. Once again, it is the practical aspect that distinguishes this work from other volumes. The question of data completeness is addressed in detail covering both the random deletion and systematic omission of segments of data, which result in quite different outcomes. The second chapter in this section deals with the question of experimental phasing, once again the use of full colour illustrations is especially informative. The widespread use of maximum likelihood methods in phasing and refinement receives extensive coverage. Some of the more spectacular, though thankfully very infrequent, errors in protein structure that have occurred are referenced in sidebars. The chapter on molecular replacement includes coverage of the choice of search models and the use of non-crystallographic symmetry and the locked rotation function. It is very pleasing to see the attention given to the treatment of coordinate errors in a refined structure. This area is too often overlooked in macromolecular crystallography. The difference between the use of constraints and restraints to reduce the number of parameters and to increase the number of observations, respectively, is discussed, but might have warranted a fuller treatment in regard to their practical application. The section on the recognition and interpretation of electron density is very useful and provides practical examples of the addition of solvent to the model and of the modelling of multiple conformations.

The final part deals with questions of structure validation and presentation that are far too often taken for granted. In many cases the analysis of a structure takes longer than data collection, structure solution and preliminary refinement. Nowadays a structure may be solved and partly refined at the synchrotron while data on other samples are still being recorded. It would be a loss to structural biology if protein structures were to be treated merely as a form of structure verification without an attempt to fully exploit the available data thus emphasising the need for good data collection and refinement practices. The uses for Ramachandran plots to highlight differences in non-crystallographically related molecules and real-space correlation plots are discussed as well as their normal use for checks on geometry.

In summary, this text should be an essential member of any protein crystallographer's library. It is modern and up-to-date and fulfils its aim of providing the theoretical underpinnings of the subject in the context of a how-to guide or comprehensive text book. This work puts into print many years of protein crystallography folklore currently distributed across websites and bulletin boards. As the author states in his preface, in any first edition of a work as extensive as this there will be errors. In this case, these are generally minor questions of presentation and I am sure that people will respond to the author's invitation to report these on his website. This is a book whose time has come. It is superbly executed and relatively inexpensive for such a large and high-quality publication.

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