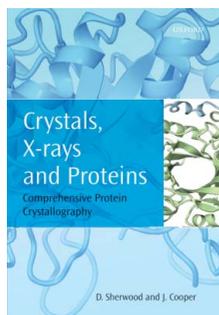


## book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.



### **Crystals, X-rays and Proteins: Comprehensive Protein Crystallography.**

By Dennis Sherwood and Jon Cooper.

Oxford University Press, 2010.

Pp. 626. Price USD 98.50. ISBN 978-01995-5904-6.

A new book on macromolecular crystallography (MX) by Sherwood and Cooper entitled *Crystals, X-rays and Proteins* appeared at the end of 2010. It is a new edition of the original book of the same title by Sherwood, which was published in 1976, the same year that the famous text by Blundell and Johnson appeared. At that time, MX was still in its infancy, only about few dozen protein structures had been determined, crystallographic equipment was often not available commercially and had to be custom-made, and researchers in the field needed to write most of the computer programs to handle their crystallographic data and results themselves. Consequently, whoever was bold enough to embark on an MX project, had to have a profound knowledge of the theory of diffraction and all the underlying fundamental mathematical concepts. This need was perfectly met by the text published by Sherwood. In clear and concise language, the fundamental crystallographic concepts were explained comprehensively and comprehensibly. The recently published new edition under the joint authorship of Dennis Sherwood and Jon Cooper retains most of the fundamentals but supplements them with a number of more modern aspects of experimental macromolecular crystallography.

The book is divided into three main parts which cover some of the fundamental concepts needed for understanding crystallography (chapters 1–6, 220 pages), diffraction theory (chapters 7–9, 120 pages) and the course of a macromolecular structure determination (chapters 10–16, 280 pages). The part on fundamentals covers everything concerning crystals, vector algebra, symmetry, waves, Fourier transforms and diffraction. These concepts are introduced thoroughly with plenty of mathematical basics, so that even students with little mathematical background will find it useful. In the diffraction-theory part, the principles of diffraction are worked out starting from a level that is familiar to most students. As stated above for the fundamentals part, any student with a decent background of high-school mathematics will find it easy to follow. In the third and largest part, the steps of a macromolecular structure solution from sample preparation, crystallization, diffraction data collection and processing to solving the phase problem all

the way to refinement are explained. The book then finishes off with a chapter on complementary diffraction techniques such as neutron diffraction and Laue crystallography.

In its 626 pages, which include about 250 black-and-white or halftone illustrations, the book provides a comprehensive description of the theory of the diffraction of X-rays by crystals. As implied by the title the emphasis is put upon the processes of structure determination of biological macromolecules. Although the book is complete in the sense that it covers everything from theory to the whole process of structure determination, it does fall short in several places. The part on cloning, protein expression and purification is too short to be of any significant use and is, in many ways, outdated. The chapter on crystal mounting starts with mounting into capillaries, which is hardly ever done anymore. In contrast, new concepts for crystal mounting, *e.g.* loopless or dry mounting, are not mentioned at all. There is no discussion on diffraction data collection strategy and there is no mention of multi-circle goniometers, which are now in use more and more. Another omission concerns modern phase-determination techniques such as sulfur-SAD (S-SAD) or X-ray and ultraviolet radiation damage induced phasing (RIP, UV-RIP). The chapter on refinement largely neglects modern likelihood-based methods, or concepts such as DEN-refinement or jelly-body-refinement, which are all essential, particularly if the data resolution is limited as is often the case in macromolecular crystallography projects nowadays. The perils and pitfalls of building an atomic model into electron-density maps are not even touched upon and a chapter on validation is also sorely missed. The one and half pages of text on structure validation stuffed into the refinement chapter are clearly insufficient given the importance of this issue in structural science these days. I also missed having a glossary and a much more comprehensive index.

The question remains, who is the target audience of this book? Biologists and biochemists, who are mainly interested in crystallography as a tool to understand their biological problem, will probably prefer more descriptive texts such as Blow (2002) or Rhodes (2006). Practicing crystallographers will most likely turn to the comprehensive and up-to-date text by Rupp (2010). Students or expert crystallographers who are interested in understanding the deep intricacies of MX will resort to even more advanced works such as Drenth (2007) or Giacovazzo *et al.* (2002). Now, who does this leave? In my opinion, this book would be the perfect textbook for a theoretical course on macromolecular crystallography taught to students of biochemistry, chemistry or physical sciences, who are in their second, third or fourth year and who have a strong interest in understanding the structures of large biomolecules. However, in times when macromolecular

crystallography is mainly performed by biologists and when its main purpose seems to be to add more macromolecule structures to the collection of already known ones, it almost looks like a futile effort to put such a book on the market. However, it does fill an important gap and maybe it even has the potential to spark an interest among teachers and professors in chemistry and physical science departments to offer courses on macromolecular crystallography, and to educate young chemists and physicists in this important field. There is still so much more to be learned about macromolecule structures than just what they look like.

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