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Book Review

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X-Ray Crystallography of Biomacromolecules: A Practical Guide

Wiley-VCH; November 2006

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The first part of this book is about "principles and methods", whereas the second part consists of "practical examples". Although the book title refers to "macromolecules", the content almost exclusively concerns proteins. In fewer than 300 pages of text and illustrations, the author has covered all major topics in modern macromolecular crystallography in moderate depth. It includes everything from preparation of samples for crystallisation trials to structure solution and refinement. However, the depth of coverage varies greatly from topic to topic. It is evident that the author is passionate about the mathematical aspect of X-ray crystallography because this is described in more detail. The word "practical" in the title of this book is used in the context of "hands-on situation" and not "relating to experiments". Readers may be disappointed to find little guidance on laboratory work.

The "Principles and Methods" part consists of nine chapters. It begins with an introductory chapter on crystal morphology, symmetry and the crystallisation process. Chapter 2 is concerned with X-ray sources, hardware and data collection. Theoretical treatment of X-ray diffraction follows (Chapter 3), then a chapter on data processing. Chapters 5 and 6 are devoted to solving the phase problem and phase improvement and the contents of these chapters are inevitably highly mathematical. Chapter 7 covers the major algorithms employed in computational refinement of structures. Chapter 8 is a brief introduction to time-resolved Laue diffraction experiments. The final chapter of part one takes on "structural genomics". It is a huge topic in itself, so here the focus is mainly placed on protein production that is adaptable to high-throughput methodologies and automation.

The second part of the book, "Practical Examples", takes the format of a "walkthrough" of case studies and serves to illustrate several key computational steps in crystallography. Here, the use of some of the most popular crystallographic software is briefly mentioned, and is illustrated with computer screen outputs. To begin with, Chapter 10 contains examples of data processing with *MOSFLM* and *SCALA*. Chapter 11 is about solving heavy atom positions with *SnB* and *RSPS,* whereas Chapter 12 is about MAD phasing with *SHARP*. Molecular replacement with *Molrep* is described in Chapter 13. Density modification by exploiting non-crystallographic symmetry is discussed in Chapter 14. The last chapter covers manual model building with *O* and very briefly, computational refinement using *CNS*.

The real strength of this book is that it gives a panoramic view of the field of protein crystallography. It has a very clearly organised structure and it helps readers, especially newcomers of this research area, to put individual stages of X-ray crystallography into perspective. Structural scientists will find this book a useful all-in-one portal for general referencing. The comprehensive collection of references at the end of each chapter in the first part is a very handy resource. Students will find the practical examples section especially helpful. Another merit of this book is its up-to-date theories, experimental methods and software tools. Practising researchers will find themselves most at home because all the methods and tools referred to are among the most popular ones used in the wider research community.

To keep the book to a reasonable length, the author has had to be extremely selective in materials and in maintaining a balance between coverage and depth. However, one obvious omission is fibre diffraction. The author has made substantial effort in many places to try to accommodate lay readers by minimizing the use of technical terms. Still, in some cases, expert language is used without any introduction or further elaboration. Although an ample number of figures are included, several of these are adopted from other sources without adequate annotation or explanation in the text. In the theoretical chapters, an advanced mathematical background is required to follow the reasoning at a rather sophisticated level. It is fair to say that the book is not for an absolute beginner. However, graduate students with some prior exposure to X-ray crystallography will find this book most beneficial. In summary, there is something for everyone in there but not everyone will be able to grasp everything.

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