Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

book reviews

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Biomolecular Crystallography: Principles, Practice, and Applications to Structural Biology. By Bernhard Rupp. New York: Garland Science, Taylor and Francis Group, 2010. Pp. xxi + 809. Price (hardback) USD 145.00. ISBN 978-0-8153-4081-2.

How many scientists trying to teach crystallography have heard a student ask the question: 'which book do you recommend for learning crystallography' and how many have not struggled with an appropriate answer beyond the mere 'there is none'? There are of course the classics from the last century, Stout and Jensen and Blundell and Johnson from 1960s and 1970s, but they are extremely hard to find nowadays and they are in many aspects outdated. At that time, macromolecular crystallography (MX) was a rather esoteric technique, applied only by a few individuals who were bold enough to embark on protein structure determination projects which could easily take half a decade or more to finish, and the successful outcome of which was not certain at all. Mainly because of modern molecular biology methods, the advent of cryocrystallography, better X-ray sources and detectors, and the efforts of many dedicated researchers who spend their time constantly developing and improving the underlying methods for structure determination, the situation is now vastly different from 40 years ago. Many biologists and biochemists with little or no training in crystallography are now applying MX techniques in order to obtain answers to their mainly biological questions. But back to crystallography books again for a moment: the described changes in the field of MX are not at all reflected by the appearance of suitable textbooks and other teaching material. There are of course books like the famous Glusker and Trueblood from 1985 with its lucid treatment of the Patterson synthesis, which constitutes, in my opinion, still the best material for teaching the meaning and use of the Patterson function in crystallography (if you manage to find it – I still do not know who borrowed my own copy and 'forgot' to return it). Or there are the ones (no more names and titles from now on) all of them great books in their own right, which are frequently perceived to be either too mathematical or too basic, contain too many errors or suffer from whatever shortcoming. In short, as a teacher of crystallography one was forced to assemble the material for a crystallography course from many different sources.

These times are over now. In a formidable five-year endeavour Bernhard Rupp, a member of the US National Academy of Sciences Committee for Crystallography and, after his tenure at the University of California, engaged in private ventures and education (which includes providing certified flight instruction in jet airplanes), embarked upon a project to pull together all relevant crystallographic experience from the literature and the crystallographic community. He made frequent use of the CCP4 bulletin board and posed literally hundreds of questions to the bulletin-board subscribers. This gave him the additional benefits (*a*) of being in constant contact with the practitioners in crystallography and (*b*) of keeping in touch with the current problems and the demands of the MX community. Finally, he wove all of this together and produced a comprehensive treatise of up-to-date MX, in both practical and theoretical aspects. The product of this heroic effort is the recent appearance of *Biomolecular Crystallography* (abbreviated to BMC by the author), an 800-page monograph which covers all aspects of a structure determination by MX, step-by-step, from the decision on which protein to work on, to protein production, crystallization, diffraction data collection and processing, phase determination, model building, refinement and ultimately validation and presentation.

BMC is organized in five parts, which in turn are divided into 13 chapters, which almost follow the flow of a typical structure determination by MX. The only exception is that protein crystallization (Part I, Chapter 3) is treated before protein production (Part II, Chapter 4). This, however, is justified by the simple notion that one needs to know about the requirements for crystallization before one starts to design protein production experiments. Part I of the book also contains an overview chapter and a chapter on the principles of protein structure in general. In part II, covering three chapters, the basics of crystallography are described. Further, this part also contains a whole chapter on statistics and probability, things that are becoming ever more important in MX but are hardly treated in a way digestible for a biological crystallographer elsewhere. Part III with just one chapter is concerned with diffraction data collection, from instrumentation and mounting the crystal to the actual data collection and the processing of the collected data. Part IV, comprising a whopping 320 pages distributed over four chapters, constitutes the heart of the volume. Here, the whole process of structure determination is described thoroughly, step-by-step and in a comprehensible manner. Part V, albeit with 40 pages is not more than a little nightcap chapter, nevertheless constitutes a very important part of the book since it deals with the validation of the structural results obtained and with some issues regarding how to present the structural results to the community. Then, there is an appendix with lots of useful information and an almost 50-page glossary. And yet another feature worth mentioning is the web site of the book (http://www.ruppweb.org/), where typographical and other errors are collected and where updated and supplemental material can be downloaded.

One thing to say about the book is that it is heavy (1898 g). It is so heavy that the only comfortable way of reading it is

when it is lying on a table in front of you. Forget about reading it on the train or in bed – you would be in pain in no time. Fortunately, this is about the only negative thing one can say about it. The actual reading of BMC is a pleasure for every aspiring and for every practicing crystallographer. The book is very well organized, the chapters and the chapter contents follow a logical sequence, and the levels of difficulty in each chapter range from simple and intuitive to formally rigorous. This has the advantage that crystallographers on all experience levels, from student to experienced researcher, will find this book utterly useful: the student and teacher in the classroom that will be using BMC as a textbook as well as the practicing crystallographer who will use it more as a handbook. Each chapter also contains boxes with the essential concepts summarized and sidebars, which may contain historical information, protocols, remarks or additional information. From the technical point, BMC is also top-notch. The illustrations are original and first class (the colour of the chicken-wire electron density representation in some of the figures is a bit too dark and is thus obscuring the structural interpretation underneath it in some places, but this is a minor point and as debatable as taste is debatable). Also, the notations are comprehensive and consistent. While reading the book, I really tried hard to discover something which I thought the author missed but should not have, but I could not. In my opinion, BMC constitutes the first (and maybe the last) comprehensive and easy-to-understand treatise of modern likelihood-based MX. It is a masterpiece. It is the book which the MX community has been waiting for and it is an absolute must-have for everybody in the field.

References

Blundell, T. L. & Johnson, L. N. (1976). *Protein Crystallography*. London: Academic Press.
Glusker, J. P. & Trueblood, K. N. (1985). *Crystal Structure Analysis*. Oxford University Press.
Stout, G. H. & Jensen, L. H. (1968). *X-ray Structure Determination*. New York: Macmillan Publishing Co., Inc.

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