

Preface

BY MICHAEL G. ROSSMANN AND EDDY ARNOLD

International Tables for Crystallography, Volume F, *Crystallography of Biological Macromolecules*, was commissioned by the International Union of Crystallography (IUCr) in recognition of the extraordinary contributions that knowledge of macromolecular structure has made, and will make, to the analysis of biological systems, from enzyme catalysis to the workings of a whole cell. The volume covers all stages of a crystallographic analysis from the preparation of samples using the techniques of molecular biology and biochemistry, to crystallization, diffraction-data collection, phase determination, structure validation and structure analysis. Although the book is written for experienced scientists, it is recognized that the modern structural biologist is more likely to be a biologist interested in structure than a classical crystallographer interested in biology. Thus, there are chapters on the fundamentals, history and current perspectives of macromolecular crystallography, as well as on the availability of useful programs and databases including the Protein Data Bank. Each chapter has been written by an internationally recognized expert.

Macromolecular crystallography is undergoing a revolution. Just as crystallography became central to the study of chemistry, macromolecular crystallography has become a core science in biology. Macromolecular crystallography has shaped our view of biological molecular structure, and is providing a broader understanding of biological ultrastructure and the molecular interactions in living systems. As reflected by the exponential increase in entries in the Protein Data Bank over the past decade, there has been an explosion in the number of macromolecular structures determined, the majority by X-ray crystallography. Knowledge of the sequences of entire genomes, from bacteria to human, has sparked a structural genomics effort that aims to determine 10 000 new macromolecular structures in the next decade. Crystallography is expected to yield the largest share of this new crop of structures. The field of macromolecular crystallography is still evolving rapidly, and capturing its essence in a single volume is a challenge. Therefore, the volume emphasizes durable knowledge, but also contains articles on somewhat more volatile topics.

This project had its inception when Ted Baker (at that time President of the IUCr) approached one of us (MGR) about writing a book on macromolecular crystallography for the IUCr. Not only were there already some excellent books that covered most aspects of the subject, but the breadth of the subject was now so vast that no single person could possibly be an expert in all relevant topics. After further exchanges of e-mails, MGR realized that the officers of the IUCr were tacitly assuming that he would be willing to carry out the advice he had given so freely. He then asked his former post-doc and coauthor of an earlier article on molecular replacement in Volume B of *International Tables*, Eddy Arnold, to help him get out of a tight corner. After some serious deliberations of his own, Eddy agreed to be co-editor.

Together we fleshed out an outline that was broader than MGR's original plan, which had focused largely on crystallographic theory and technique. We felt that it would be valuable to briefly cover related techniques beyond X-ray diffraction, as well as to give an overview of the current field of structural biology. Although basic crystallography is also presented in the other volumes of *International Tables*, chapters describing fundamental crystallographic principles and practices have been included in an attempt to make the volume as coherent and self-contained as possible. We established an advisory board, developed a list of required chapters and obtained promises of participation from potential authors. In a departure from the style of previous volumes of *International Tables*, which have fewer articles and authors, we sought contributions for nearly 100 articles from an even larger number of contributing authors. The members of the advisory board reviewed the proposed outline of chapters and authors. We were pleasantly surprised when so many experts generously agreed to write articles for this volume, and delighted that the vast majority fulfilled their promises.

Significant events punctuating the process were the 1996 and 1999 IUCr congresses. At the 1996 IUCr Congress in Seattle, we convened a meeting with many of the authors. There we described the overall project design and received valuable suggestions. At that time, we hoped that the volume could be completed by 1999. At the 1999 IUCr Congress in Glasgow, we reviewed the detailed contents of the volume at an open meeting on the volumes of *International Tables* under development. By that time, we had received most of the articles and typesetting began in late 1999. The complexities of handling a large number of articles from so many authors led to delays at a number of stages. Ultimately, the completion date became mid-2001.

We are especially grateful to the staff at the IUCr and at our own institutions for their dedicated help in bringing this project to fruition. At the IUCr, we thank Nicola Ashcroft for an outstanding job on overall production of the volume, and for her patient correspondence and attention to detail. We also thank Peter Strickland, Sue King, Theo Hahn, Uri Shmueli, Mike Dacombe and Ted Baker for their help in coordinating the project. At Purdue University, we thank Cheryl Towell and Sharon Wilder for constant assistance, and Fay Chen for editorial suggestions. At the Center for Advanced Biotechnology and Medicine and Rutgers University, we thank Susan Mazzocchi and Barbara Shaver for their help in handling correspondence and galley proofs from the authors.

We are also especially indebted to the authors for their generous contributions and for documenting relevant expertise. We also thank the advisors and the members of the advisory board for their help. We are saddened to note that Paul Sigler, a member of the advisory board, passed away during the project. Paul was a towering figure who, with his medical background, recognized the role structure plays in providing insights into fundamental chemical and biological processes.