

Acknowledgments

This textbook, discussing in hundreds of pages the interdisciplinary science of macromolecular crystallography, could not have been researched and written without the significant involvement, assistance, and also encouragement of the biomolecular crystallography community at large. My grateful acknowledgments therefore are due to numerous individuals providing valuable contributions as follows.

The CCP4 community. Special thanks are due to the numerous contributors to the CCP4 bulletin board who have responded to my postings and volunteered advice and insights as well as ideas and images of crystals, data files, or model coordinates for perusal in my book. I wish to acknowledge them all, even if their material did not make it into final print. When material from these sources is included, I specifically acknowledge the contributors again in the text or figure caption. Thank you for volunteering images, ideas, data, or literature (in historical sequence):

Andrea Schmidt, EMBL Outstation Hamburg; Debanu Das, University of California, Berkeley; Michael Kolbe, MPI for Infection Biology, Berlin; Bernard Collins, National Jewish Medical and Research Center, Denver; Sebastiano Pasqualato, IFOM, Milan; Erik Debler, The Scripps Research Institute, La Jolla; Flip Hoedemaeker, Key Drug Prototyping BV, Amsterdam; Terese Bergfors, Uppsala University; Sergei V. Strelkov, Catholic University of Leuven; Ewa Skrzypczak-Jankun, University of Toledo; Axel Martin, Ruhr-Universität Bochum; Jonathan Grimes, Oxford University; Raquel Lieberman, Harvard University; Juan-Maria Ruiz, Granada; Ehmke Pohl, University of Durham, UK; Dominika Borek, UT Southwestern Medical Center, Dallas; Kenneth Frankel, LBNL; Leonard Banaszak, University of Minnesota, Twin Cities; Graeme Winter, Daresbury Laboratories; Jürgen Bosch, University of Washington; James Whisstock, Monash University, Australia; Mitchell Miller, Stanford University; Andrea Hadfield, University of Bristol; Yvonne Leduc, University of Saskatchewan; Pete Artymiuk, University of Sheffield; Richard Bryant, University of Oxford; Paul Adams, LBNL; Helen Berman, RCSB Rutgers; Frances Bernstein, Bernstein & Sons; Tom Terwilliger, LBNL; Jiamu Du, Shanghai Institute for Biological Sciences; Aiping Dong and Xiaohui Xu, University of Toronto; Henry Bellamy,

CAMD, Louisiana State University, Baton Rouge; Alexander McPherson and Aaron Greenberg, University of California, Irvine; Lukasz Salwinski, University of California, Los Angeles; Peter Zwart, LBNL; Han Remaut, Birkbeck College, London; Dimitri Svergun, EMBL Outstation Hamburg; Simon Colebrook, Oxford University; Joanne Nettleship, Oxford Protein Production Facility; Gunter Stier, MPI Heidelberg; Gloria Borgstahl and Jason Porta, University of Nebraska, Omaha; Artem Evdokimov, Pfizer Global R&D, Groton, CT; Mark Wilson, University of Nebraska, Lincoln; Gyorgy Snell, LBNL; Isabel Usón, Instituto de Biología Molecular de Barcelona, Spain.

I am particularly indebted to all the members of the community of experts who answered, often beyond the scope of the CCP4 bulletin board, the many desperate and poorly articulated questions I have posted, generally at 3 AM California time, on the bulletin board. Amongst those are (in random order) Dale Tronrud, Ian Tickle, Bart Hazes, Kay Diederichs, Randy Read, Garib Murshudov, Eleanor Dodson, Fred Vellieux, Axel Brunger, Alexandre Urzhumtsev, George Sheldrick, Lynn Ten Eyck, Peter Zwart, Gerard Kleywegt, Roberto Steiner, Bernie Santarsiero, Gerard Bricogne, Clemens Vornrhein, Ron Stenkamp, Ethan Merritt, Mark Wilson, James Holton, Chris Hall, Bob Sweet, and Colin Nave.

Commercial vendors. Several commercial vendors have provided trial software, equipment images, and technical drawings for my perusal. I thank Michael Ruf and Sue Byram from Bruker AXS; Ron Hamlin and Chris Nielsen from ADSC Corporation; Jim Pflugrath and Kris Tesh from Rigaku-MSC; and Ruben Abagyan, Molsoft LLC, for the ICM Pro trial license used to produce numerous images of protein structures. Finally, my own company, q.e.d. life science discoveries, has generously supported the online materials and my time devoted during the last four years to the production of this book.

I also wish to acknowledge the University of California, Irvine, and Alexander McPherson for providing me with an adjunct affiliation and Katherine Kantardjieff, CSU Fullerton, for academic library access. During a sabbatical stay in Jim Sacchettini's laboratory at Texas A&M University, some of the ideas for the book evolved from discussions with his lively group of graduate students and postdocs—thank you all, guys!

Reviewers. I am most indebted to the reviewers who were extremely supportive and did a fantastic job in fine-combing through the manuscript and correcting sloppiness, inaccuracies, and many outright errors. As in almost every first edition, there will be remaining mistakes, errors, and omissions. I wish to declare that I alone take the blame for these and would encourage the readers to report any errors or unclear statements as well as any suggestions for improvements directly to me through the BMC Web site (www.ruppweb.org).

I am particularly indebted to Ian Tickle for extensive technical review and personal discussions of Chapters 7, 10, and 12, assuring adequacy of my statistical and likelihood treatments. Ian has gone beyond anything one could possibly expect from a reviewer in numerous emails and by providing extensive discussions as well as literature references about challenging topics. Dale Tronrud critically worked through Chapter 12, and discussions with him were the inspiration for additional ideas for several figures in Chapter 6. James Holton contributed his expertise by reviewing synchrotron physics and data collection in Chapter 8 and also provided a copy of his awesome *MLFSOM* program. Chapters 6 and 8 have also undergone extensive field review by Jim Pflugrath who provided most valuable suggestions based on his experiences from Cold Spring Harbor Laboratory crystallography boot camp. George Sheldrick, Tobias Beck, Tim Grüne, and Brian Matthews greatly contributed to improvements in Chapter 10 and also provided the data for experimental phasing examples. The personal discussions with George Sheldrick proved exceptionally helpful in tightening up the experimental phasing Chapter 10. During review of Chapters 7, 9, and the mathematical appendix Mark Wilson provided valuable suggestions and review. Chapter 4 would not have been possible without the review, corrections,

and substantial additions by Artem Evdokimov. Gunter Stier has provided additional corrections and figures for Chapter 4. Sections of Chapter 12 dealing with molecular dynamics and *CNS*-specific features were reviewed and corrected by Axel Brunger. Chapter 1 has been edited, reviewed, and shortened by Katherine Kantardjieff, who also provided comments and instructive additions for the ligand structure analysis section in Chapter 13. For this final chapter I thank Gloria Borgstahl for her useful suggestions, Artem Evdokimov for additional review, and Jim Naismith for permission to reproduce his collected experiences about publishing in high impact journals.

Ron Stenkamp, Michael Chapman, and Ehmke Pohl have served as developmental reviewers of numerous chapters, and I thank them for their copious helpful comments and suggestions. Ehmke Pohl has also contributed a draft for the section on DNA-protein complex crystallization.

Many other colleagues have provided assistance ranging from figure preparation to program modifications. Amongst those I thank Jonathan Grimes, University of Oxford, for the beautiful figure of the PRD1 phage head and the phage head crystal images. Peter Briggs has kindly modified the CCP4 mapslicer interface for me, and Garib Murshudov added for me several options to plot reflection statistics in *REFMAC5*. Kevin Cowtan, YSBL York, UK, kindly allowed me to reproduce selected Fourier transform images from his tutorial. Paul Emsley gave me a personalized introduction to his program *Coot*. He and Bernhard Lohkamp patiently responded to my desperate plotting and graphing questions. Gloria Borgstahl and Jeff Lovelace prepared the special figure of an incommensurately modulated protein structure, and I thank Mark Wilson for the TLS figures made with Tim Fenn's *POVscript+*. Artem Evdokimov assembled a figure of HSQC spectrum for Chapter 4. Richard Dickerson kindly provided his amusing electron density figure leading into Chapter 9.

Editorial and production staff. The idea to develop my basic web tutorial into a textbook crystallized when Bob Rogers, senior editor at Garland Science convinced me to take on the project of extending the rudimentary Web contents of *Crystallography 101* into a full text book. It is largely due to his encouragement and his patient but persistent inquiries about progress that the first chapters were ever written. Little did I know then what to expect, and had I known, I am not sure if I would have been foolish enough to embark on this multi-year project. When Bob retired, assistant editor Alex Engels and editor Summers Scholl, together with vice president Denise Schanck, took over and provided patient but unrelenting guidance throughout the process. I wish to acknowledge the great work of the production staff in England under senior production editor Simon Hill. My copyeditor Sally Huish has done a terrific job sorting out my inconsistent language and grammar, and the great layout and typesetting is by Georgina Lucas. The agonizing task of proofing the text and more than 600 equations was thoroughly accomplished by Heather Whirlow Cammarn.

Louise Jones, publishing editor of the International Union of Crystallography, provided me with permissions and reproductions of space group diagrams from the International Tables for Crystallography and figures from IUCr journal publications.