
Contents

Preface	v
Contributors	ix
Contents of Volume 1	xi
1 Cryocrystallography of Macromolecules: <i>Practice and Optimization</i> Elspeth Garman and Robin L. Owen	1
2 Determination of Reaction Intermediate Structures in Heme Proteins Kelvin Chu	19
3 Annealing Macromolecular Crystals B. Leif Hanson and Gerard J. Bunick	31
4 First Analysis of Macromolecular Crystals: <i>Biochemistry and X-Ray Diffraction</i> David Jeruzalmi	43
5 X-Ray Data Collection From Macromolecular Crystals Elspeth Garman and Robert M. Sweet	63
6 Characterizing a Crystal From an Initial Native Dataset Michael R. Sawaya	95
7 Molecular Replacement Eric A. Toth	121
8 Phase Determination Using Halide Ions Miroslawa Dauter and Zbigniew Dauter	149
9 The Same But Different: <i>Isomorphous Methods</i> <i>for Phasing and High-Throughput Ligand Screening</i> Mark A. Rould	159
10 Substructure Determination in Multiwavelength Anomalous Diffraction, Single Anomalous Diffraction, and Single Isomorphous Replacement With Anomalous Scattering Data Using <i>Shake-and-Bake</i> G. David Smith, Christopher T. Lemke, and P. Lynne Howell	183
11 Substructure Determination in Isomorphous Replacement and Anomalous Diffraction Experiments Ralf W. Grosse-Kunstleve and Thomas R. Schneider	197

12	Automated Structure Solution With autoSHARP <i>Clemens Vonnrhein, Eric Blanc, Pietro Roversi, and Gérard Bricogne</i>	215
13	Introduction to Macromolecular Refinement <i>Dale E. Tronrud</i>	231
14	Quality Control and Validation <i>Gerard J. Kleywegt</i>	255
15	Crystallographic Software: <i>A Sustainable Resource for the Community</i> <i>Stephen J. Everse and Sylvie Doublié</i>	273
	Index	279

Macromolecular Crystallography Protocols, Volume 2

Structure Determination

Doublie, S. (Ed.)

2007, XII, 284 p. 70 illus., Hardcover

ISBN: 978-1-58829-902-4

A product of Humana Press