

Foreword	p. xi
Preface	p. xv
Acknowledgments	p. xix
Contributors	p. xxi
Data Collection, Analysis, and Visualization	p. 1
Defining Bioinformatics and Structural Bioinformatics	p. 3
Fundamentals of Protein Structure	p. 15
Fundamentals of DNA and RNA Structure	p. 41
Computational Aspects of High-Throughput Crystallographic Macromolecular Structure Determination	p. 77
Macromolecular Structure Determination by NMR Spectroscopy	p. 93
Electron Microscopy in the Context of Structural Systems Biology	p. 143
Study of Protein Three-Dimensional Structure and Dynamics Using Peptide Amide Hydrogen/Deuterium Exchange Mass Spectrometry (DXMS) and Chemical Cross-Linking with Mass Spectrometry to Constrain Molecular Modeling	p. 171
Search and Sampling in Structural Bioinformatics	p. 207
Molecular Visualization	p. 237
Data Representation and Databases	p. 269
The PDB Format, mmCIF Formats, and Other Data Formats	p. 271
The Worldwide Protein Data Bank	p. 293
The Nucleic Acid Database	p. 305
Other Structure-Based Databases	p. 321
Data Integrity and Comparative Features	p. 339
Structural Quality Assurance	p. 341
The Impact of Local Accuracy in Protein and RNA Structures: Validation as an Active Tool	p. 377
Structure Comparison and Alignment	p. 397
Protein Structure Evolution and the Scop Database	p. 419
The Cath Domain Structure Database	p. 433
Structural and Functional Assignment	p. 457
Secondary Structure Assignment	p. 459
Identifying Structural Domains in Proteins	p. 485
Inferring Protein Function from Structure	p. 515
Structural Annotation of Genomes	p. 539
Evolution Studied Using Protein Structure	p. 559
Macromolecular Interactions	p. 573
Electrostatic Interactions	p. 575
Prediction of Protein-Nucleic Acid Interactions	p. 593
Prediction of Protein-Protein Interactions from Evolutionary Information	p. 615
Docking Methods, Ligand Design, and Validating Data Sets in the Structural Genomics Era	p. 633

Structure Prediction	p. 663
Casp and Other Community-Wide Assessments to Advance the Field of Structure Prediction	p. 665
Prediction of Protein Structure in 1D: Secondary Structure, Membrane Regions, and Solvent Accessibility	p. 679
Homology Modeling	p. 715
Fold Recognition Methods	p. 733
De Novo Protein Structure Prediction: Methods and Application	p. 755
RNA Structural Bioinformatics	p. 791
Therapeutic Discovery	p. 807
Structural Bioinformatics in Drug Discovery	p. 809
B-Cell Epitope Prediction	p. 847
Future Challenges	p. 879
Methods to Classify and Predict the Structure of Membrane Proteins	p. 881
Protein Motion: Simulation	p. 907
The Significance and Impacts of Protein Disorder and Conformational Variants	p. 937
Protein Designability and Engineering	p. 961
Structural Genomics of Protein Superfamilies	p. 983
Index	p. 1019

Table of Contents provided by Blackwell's Book Services and R.R. Bowker. Used with permission.