Biomolecular Crystallography:

Principles, Practice and Application to Structural Biology

Bernhard Rupp

Part I: From sequence to crystals

Chapter 1 Introduction: Planning Your Study

- A brief overview of protein crystallography and its method and challenges preparing the ground for the subsequent in-depth chapters.

Chapter 2. Protein structure

- Review of basic protein properties and nucleic acids with emphasis on needs of structural biologist and protein crystallographer.

Chapter 3. Protein crystallization

- Develops theoretical concepts and practical challenges of protein crystallization

Chapter 4. Protein Production and Purification

- After having established that practically all crystallization trouble is rooted in protein properties, we can understand the specific needs for protein engineering for crystallography. This is reversed from actual workflow on purpose.

Part II: Fundamentals of protein crystallography

Chapter 5. Crystal geometry

- The basic concepts of crystal geometry are developed starting from 2-dimensional examples, rapidly demonstrating the first important concepts, which are revisited in necessary detail during the remainder of the chapter.

Chapter 6. Diffraction basics

- The previous chapter about crystal geometry and reciprocal space has introduced the basic concepts of symmetry and reciprocal space which are applied to principles X-ray scattering and diffraction, including anomalous scattering.

Chapter 7. Statistics and probabilities in crystallography

- Many applications in crystallography are based on basic and advanced statistical concepts which are usually not taught - at least not at the right time and in suitable context - in biology-heavy curricula. An introduction to statistical methods and a primer in maximum likelihood and Bayesian inference as used in macromolecular crystallography is provided.

Part III: From crystal to data

Chapter 8. Instrumentation and data collection.

Part IV: Determining your structure

Chapter 9. Reconstruction of electron density and the phase problem

- A basic understanding of how maps are generated and of the phase problem is needed before we can start to learn how to generate phases and solve the structure.

Chapter 10. Experimental phasing

- Begins gently with pictures and phasing circles and progresses into full maximum likelihood treatment. A quick example at the end reinforces the learning objectives by application.

Chapter 11. Non-crystallographic symmetry and Molecular replacement

- NCS and molecular replacement and MR are tightly connected, and this is the best point to review general transformations and NCS averaging. The MR chapter is also technically challenging, but a number of examples illustrate the process.

Chapter 12 Model building and refinement

- Model building and refinement are at the core of crystallography. Theoretical background including maximum likelihood based techniques and examples of god practices in model building are discussed.

Part V: Making sense of your structure

Chapter 13 Validation, analysis and presentation

- Any crystallographic model presents a molecular hypothesis and thus must be critically evaluated against the body of all prior knowledge. Likelihood based validation provides reliable safeguards against misinterpretation.

Appendix
Contains various ancillary materials the exceed side bar volume or tabular material
Math appendices)

Glossary
Index