

Appendix

Appendix.....	1
A.1. Coordinate file formats.....	1
A.1.1. The PDB file header section	2
A.1.2. The CRYST1 and SCALE records	2
A.1.3. The coordinate section of the PDB file.....	3
A.2. Basic linear algebra.....	5
A.1.1. Matrix representations.....	6
A.1.2. Sum, difference, and multiplication of matrices	6
A.1.3. Transpose, inversion, determinant, and trace of a matrix	7
A.1.4. Vector operations as matrix operations.....	8
A.3. Crystallographic coordinate system and fractional coordinates.....	10
A.1.1. Direction cosines.....	11
A.1.2. The metric tensor G, bond distances and bond angles	11
A.1.3. Basis transformations	13
A.1.4. Reindexing of diffraction data	13
A.1.5. Coordinate system transformations.....	14
A.1.6. Reciprocal space metric relations	15
A.1.7. Reciprocal lattice vectors	16
A.4. Cosine rule.....	18
A.5. Proof of Euler's formula	19
A.6. Electron density is real	20
A.7. Directional cosine matrix in spherical coordinates	21
A.8. Crystallographic restriction theorem.....	21
A.9. Anatomy of a ligand restraint file	22
A.10. The 44 indexing possibilities and possible space groups	24
A.11. Protein – metal coordination and distances	25
A.12. Selected physical constants and conversions.....	26
A.13. References	26

The Appendix contains supplemental material and information necessary for basic crystallographic computing. Explanation of the PDB file records is provided, and a small linear algebra refresher follows, limited to what is needed to follow or to verify most of the derivations provided in the main text. Useful are also a reminder of the cosine rule and the proof of Euler's equation by MacLaurin series expansion. The explicit proof that electron density is real is provided as an exercise. Various useful tables and definitions follow.

A.1. Coordinate file formats