Appendix

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

