

Crystallographic Guidelines

Authors of crystallographic manuscripts are requested to note the following guidelines:

1. The study must meet the standard criterion for publication in the Journal of providing substantial novel insights into the biochemical mechanism of a major biological process.
2. The manuscript should include the following:
 - a. An electron density map of critical regions discussed in the text, so that the quality of the phasing can be assessed. This may be part of the text or submitted as an appendix.
 - b. A summary of the Ramachandran plot.
 - c. The space group and number of molecules in the asymmetric unit.
3. Stereographic pairs of electron densities or structural details that are difficult to comprehend in mono are encouraged. The spacing between left and right views should generally be 5.5 - 6.0 cm
4. Structure refinements:
 - a. The number of reflections and cutoff (for example $F > 0\sigma F$ or $F > 3\sigma F$) used in the refinement should be specified.
 - b. The degree of data completeness at the highest resolution is expected to be at least 75%.
 - c. For refinements at 2.0 Å or better, with good data, $R_{\text{working}}-R_{\text{free}}$ should generally be $<10\%$. If this is not the case, an explanation should be provided.
 - d. The average atomic B-factor for protein, ligand, and solvent atoms, as well as the Wilson B factor should be provided.
 - e. Cell constants and computed parameters should be specified only to the number of significant figures justified by the data.
5. Depending on the method used to solve the phase problem, the following data should be provided:
 - a. Molecular replacement:
Program employed, search model (PDB code), resolution range of data, correlation coefficient and R_{factor} of the correct solution and the second unrelated peak.
 - b. Multiple anomalous diffraction and single/multiple isomorphous replacement:
Program employed, derivative(s), number of sites, resolution range of data, initial figure of merit/phasing power, and figure of merit after density modification and/or averaging.
6. Superpositions: The number of atoms used should be specified.
7. Because the experimental section should include the crystallographic methods, prepublication of these methods (crystallization, data collection, or structural determination) will generally preclude publication in the Journal.