# LETTERS TO THE EDITOR

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## Deposition of macromolecular data

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A formal discussion of the archival journal requirements for data deposition was held at the International Seminar-cum-School on Macromolecular Crystallographic Data at Calcutta, India in November.

The current policy of the International Union of Crystallography (IUCr) is that on publication of a crystal structure determination of a macromolecule the atomic parameters used or represented in the publication must be deposited in the Protein Data Bank. The deposition of structure amplitudes is recommended but not insisted on. The policy provides crystallographers with the option to delay the release of atomic parameters for one year and of structure amplitudes for up to four years from the date of publication. Participants strongly supported this policy and felt it should be strictly applied by the journals (referees).

Recent developments in X-ray crystallographic experimental and refinement techniques and the huge expansion in computing power and networking however necessitate the review of deposition arrangements.

It was noted that the new validation procedures are much more effective but require the experimental structure amplitudes as well as the atomic parameters. In addition the technical arrangements for deposition analysis and validation of macromolecular crystal structures are now much easier.

The aforementioned consider it vital for the macromolecular crystallographers to respond to these developments in their deposition practices. *We recommend therefore that publication of macromolecular crystal structures should be accompanied by deposition of atomic parameters and also structure amplitudes.* Amongst the many reasons identified for this practice the two following are critical.

(1) Rigorous validation of the structure determinations results can only be carried out using both atomic parameters and experimental structure amplitudes. It is important that journals ensure referees have sufficient information to prevent incorrect structures being published.

(2) Archival of this data will ensure they are not lost. There were numerous reports at this meeting of data being lost. This most probably reflects a general problem in the crystallographic community.

*Note from the Section Editor.* It has always been the policy of *Acta Crystallographica Section D* to have both atomic coordinates and structure factors deposited in the Protein Data Bank before a paper is published. This policy is reinforced by the official notice published here.

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