

Letter to the Editor

Archival Journal Requirements for Data Deposition

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 undersigned 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 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 that referees have sufficient information to prevent incorrect structures from being published.

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

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Received for publication 4 March 1996 and in final form 4 March 1996.

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0006-3495/96/06/2994/01 \$2.00