PUBLIC ACCESS TO X-RAY DIFFRACTION DATA

To the Editors:

The undersigned have a long standing concern with the problem of public access to the results of single crystal X-ray diffraction studies on biological macromolecules. The actual data from such research are the measured X-ray intensities, and the primary results are the lists of atomic coordinates derived from those data. While many papers on various proteins and nucleic acids have been published describing and interpreting the results of such a structure analysis, the actual data and results are often not made easily accessible, if at all. We are requesting that the journals which play a major role in the publication of such structural studies adopt and enforce rules for documentation similar to those which apply in all other areas of scientific research. Studies where the structural information has not been made available must be considered incomplete, as would any other piece of research where the data were not provided in published or deposited form.

In the closely related field of small molecule crystallography there is no such problem. The actual X-ray data and the derived structural model are reported directly in the original article in hard copy form. Even for a small protein the amount of data is so large that hard copy publication has occurred only in one or two instances in the early years, but computer readable storage and distribution as currently carried out so effectively by the Protein Data Bank at Brookhaven and its international associated groups is quite practical, and is certainly the preferred form of access today. We note also that a policy requiring coordinate and structure factor deposition would ensure the preservation of important and expensively determined data which otherwise are likely to be lost with the ever-changing personnel and computer installations in numerous laboratories around the world.

There are standard procedures now for the refinement of X-ray structures. Preparation of the data and results for the Protein Data Bank does not constitute a significant burden for authors. The remarks section of the Data Bank file provides plenty of space for any qualifying or expanding remarks that the authors may wish to make. The standard author comment that a structure is not 'finished' or not 'ready' for filing is just nonsense. If a structure is ready to be discussed in a paper, by definition it is ready for filing. Data and coordinate files can always be updated on the basis of future work, as has already happened many times.

We request that you include in the *Notice to Authors* of the journal a statement such as the following or one of equivalent intent.

'Authors of papers describing new structure determinations must be prepared to submit to the Protein Data Bank all of the structural data required to validate the discussion, including both X-ray amplitudes and phases and the derived atomic coordinates. If the paper discusses a protein structure only at the level of the main chain alpha carbon atoms, then only alpha carbon coordinates need be deposited. If the discussion involves higher resolution data, for example all atoms in the active site of an enzyme, then the full set of X-ray data and the coordinate list must be deposited. Following completion of the editorial process and acceptance of the paper, the manuscript will *not* be sent to the printer until confirmation has been received from the author, if not initially supplied, that the required information has been sent to the Protein Data Bank.

If requested by the authors, the editors will ask the Data Bank not to distribute the information until a specified date. For coordinate lists this date may not be more than one year beyond the acceptance date of the manuscript. For the full structure amplitude and phase data the time interval before distribution may not exceed four years. The release date specified by the author will appear in a footnote to the paper along with the statement that the information has been submitted to the Protein Data Bank. In the absence of a specified release date, it will be assumed that the information is available immediately on appearance of the publication.'

Comparable letters have been sent to a number of journals concerned with macromolecular structure. We are aware that several editorial boards are considering this matter, and that a major effort on policy development is underway by the International Union of Crystallography and by certain of its adhering national bodies. We hope that all will act positively (and, if possible, uniformly) on this issue.

A list of the signers of this letter follows. The original signatures are on file in the office of the undersigned.

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