LETTERS

Immediate Release of Crystallographic Data: A Proposal

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For several years, *Science* policy has required that published X-ray crystallographic coordinates be deposited with a publically accessible database (e.g., Brookhaven Protein Data Bank). That policy recognized the high costs and risks of solving important structures to accord those who have made such investments successfully the time to reap their intellectual benefits. Wlodawer *et al.* (below) assert that recent technical enhancements have reduced "the time needed to solve a structure (to less than) than the allowed hold period" and have called for immediate release of the data. In cooperative discussions with

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There has been an incredibly rapid increase in the rate of determination of three-dimensional (3D) structures of biomacromolecules, as reflected by the deposition of a new structure in the Protein Data Bank (PDB) at the Brookhaven National Laboratory (1), on average, every 5 hours. Unfortunately, in parallel, an increasing proportion of depositors take advantage of the PDB's policy of allowing structures to be kept “on hold” for up to a year after coordinate deposition. Despite a recent drop in the number of structures put “on hold,” nearly half the entries deposited are not released immediately. The policy of the PDB is based on rules drawn up by the International Union of Crystallography (IUCr) in the late 1980s for papers published in IUCr journals. These rules (2) also provide the basis for the policies of most other scientific journals and of a number of government funding agencies, such as the National Institutes of Health, for work undertaken with grant support.

It is time to consider whether this policy is still appropriate. When it was debated and accepted by the community 10 years ago, the time needed to solve a macromolecular structure was often measured in years and was rarely less than 1 year. The time needed for detailed analysis of such structures was also fairly long. The 1-year hold on coordinates was therefore instituted to allow the authors to reap the fruit of their tremendous investment of time and effort. Because of recent advances in protein expression and purification, crystallization procedures, x-ray instrumentation, and computer software, the time needed to solve a structure is often shorter than the allowed hold period. In light of such developments, it is difficult to justify withholding coordinates for any period once the paper has been published.

Biomolecular structure analysis has succeeded in bringing 3D structures to the forefront of molecular biological research. This success has expanded both the interest in and utility of the information being deposited in the PDB. The molecular modeling community has grown and evolved considerably, due to the expansion of this source of experimental data. The value of the data rests in their availability to the broader community. Methods are continuously being developed to analyze new structures and their relationships to the

who have access to them. Three-dimensional structural information is also a crucial link elucidating the role of a translated region of a DNA sequence of unknown function.

The time has come to change the rules of deposition so as to ensure that the coordinates are released concomitantly with publication of the paper (or papers) describing the structure. We are convinced that without access to the coordinates, the structures cannot be used for comparison with other proteins, for theoretical analysis or, more and more important, for drug design.

We propose that coordinates deposited at the PDB should be marked as either “for immediate release” or “to be released upon publication.” We also recommend that the maximum hold for primary data (that is, x-ray structure factors, and nuclear magnetic resonance proton-proton distance and dihedral angle restraints) be reduced from 4 years to 1 year. The PDB is already working on a “layered approach” to deposition so that it will be possible to release entries as submitted, after the authors have checked for outliers and errors through the PDB's WEB-based AutoDep procedure, on the same day that they are deposited (with the permission of authors), or when the article related to the structure is published, if the authors request “release on publication date” rather than “hold for a year.” It is clear that such a change in policy will require cooperation of both the granting agencies and the scientific journals, as well as the overwhelming support of the scientists doing the research. It should be stressed that even the current policy is not uniformly enforced. These changes would bring macromolecular crystallography into line with the requirements of other fields, such as gene sequencing, which have never allowed extended hold periods. We hope that this proposed change in the deposition policy will be publicly debated and ultimately accepted.

References

1. ↵ **http://pdb.pdb.bnl.gov/**. Google Scholar

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