

On the prompt update of literature references in the Protein Data Bank

Alexander Wlodawer

Updating literature references in the Protein Data Bank is discussed.

Macromolecular Crystallography Laboratory,
National Cancer Institute, Frederick, MD 21702,
USA

Correspondence e-mail: wlodawer@nih.gov

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One of annoying and potentially serious problems encountered during analysis of the macromolecular structures deposited in the Protein Data Bank (PDB) is the difficulty of finding where the research that resulted in the creation of some of the deposits was published. Conversely, although release of the coordinates upon publication of the relevant papers is now the law of the land, it is often difficult for the PDB to know that publication has taken place, since they have to search the whole literature for a specific PDB code. Typically, if the title of the future publication indicated during coordinate deposition differs from the final one, PDB has no way to know that the relevant paper has been published. Thus, many structures are not immediately released upon publication if the authors themselves do not promptly notify the PDB that their paper is already out.

I would like to make a simple suggestion that might help to rectify both problems. It should not be very difficult for a journal to generate a message to be sent to the PDB when a paper that refers to a newly deposited structure is actually published. 'Publication' would mean that any version of the paper becomes available to the readers, whether preliminary or final, depending on the editorial policy. If all journals that publish macromolecular structures would adhere to this recommendation, both problems mentioned above would become moot. Since the IUCr journals (mostly *Acta Crystallographica Section D*, *Acta Crystallographica Section F* and *IUCrJ*) publish a large fraction of papers that report new macromolecular structures, it would be particularly appropriate if they would spearhead such a policy.

Helen M. Berman,^{a*} Stephen K. Burley,^a Gerard J. Kleywegt,^b Haruki Nakamura^c and John L. Markley^d

^aDepartment of Chemistry and Chemical Biology, Center for Integrative Proteomics Research, Rutgers, The State University of New Jersey, 174 Frelinghuysen Road, Piscataway, NJ 08854, USA, ^bPDBe, European Molecular Biology Laboratory–European Bioinformatics Institute, Cambridge CB10 1SD, UK, ^cPDBj, Institute for Protein Research, Osaka University, 3-2 Yamadaoka, Suita, Osaka, 565-0871, Japan, and ^dBioMagResBank, Department of Biochemistry, University of Wisconsin-Madison, Madison, WI 53706, USA

Correspondence e-mail:
berman@rcsb.rutgers.edu

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Response to *On prompt update of literature references in the Protein Data Bank*

The wwPDB responds to the article *On the prompt update of literature references in the Protein Data Bank* [Wlodawer (2014), *Acta Cryst.* **D70**, 2779].

The wwPDB receives publication dates and citation information from authors, several journals, the user community, and additionally scans the literature for publications. The journals that currently provide related citation information either in advance or at the time of publication include IUCr Journals (*Acta Crystallographica Sections A–F*, *IUCrJ*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); *Journal of Biological Chemistry*; *Journal of Molecular Biology*; *Proceedings of the National Academy of Sciences*; *Nature* journals; *Science*; *Proteins: Structure, Function, and Bioinformatics*; and *Protein Science*.

For each weekly update of the PDB archive, all files scheduled for release or modification are checked and validated one final time. Authors may be contacted to resolve any issues that may arise while preparing the entries for release. If this is not accomplished in time for that release cycle, the entry may be scheduled for release at a later date.

The preparation and packaging of the weekly PDB update begins Thursday afternoon (local time at each wwPDB member site), and the files are publicly released on the following Wednesday at 00:00 UTC (Coordinated Universal Time).

The wwPDB encourages journals to provide citation information [paper title, author list, related PDB ID(s), DOI, and publication date] to deposit@wwpdb.org, ideally at least two weeks in advance of publication of a structure report so that the release of the corresponding PDB entry can be timed accordingly.

References

Wlodawer, A. (2014). *Acta Cryst.* **D70**, 2779.