

# Treatment of Theoretical Models in the Worldwide Protein Data Bank Archive

August 15, 2006

## 1. Introduction

On November 19-20, 2005, a workshop was held at the RCSB Protein Data Bank in Rutgers University to discuss the archiving of theoretical models. It was attended by a cross-section of the structural biology community including modelers, cryo-electron microscopists and structural genomicists as well as representatives of wwPDB. The outcome of this workshop was a set of recommendations and implementation plans. The key recommendation is:

***PDB depositions should be restricted to atomic coordinates that are substantially determined by experimental measurements on specimens containing biological macromolecules.***

This includes, for example, structures determined by X-ray crystallography, NMR and cryo-electron microscopy. It does not include models determined purely *in silico* using, for example, homology or *ab initio* methods. A paper describing the outcome of the Workshop on Archiving Structural Models of Biological Macromolecules available in the August 16 issue of *Structure*.<sup>1</sup> At the request of the PDB Advisory Committee, an implementation plan was written. The plan outlined below has been reviewed and approved by that body and the wwPDBAC.

## 2.0 Implementation Plan

### 2.1 Archiving of Current Models

Theoretical models that have been previously released or that are released under the provisions of the transition process described below will continue to be made publicly available only via the existing models archive, which is maintained as a distinct and

separate archive from that for experimental structures.

## **2.2 Archiving of Models after October 15, 2006**

Archiving of theoretical models will be phased out such that theoretical model depositions will no longer be accepted after October 15, 2006. On October 15, the theoretical model deposition views on all wwPDB deposition servers will be removed.

## **2.3 Transition Plan (August 15-October 15, 2006)**

**2.3.1** All existing un-processed theoretical model entries as well as entries deposited from August 15 through October 15, 2006 will not be validated and will not be processed. The PDB format file will be generated only from the information the author supplied during deposition and the entry will be released as-is without author review or corrections. The authors will have the choice of correcting their entries by withdrawing the original entry and then re-submitting the corrected version before October 15, 2006.

The details of this implementation are:

**2.3.1.1** At the RCSB, PDBj and MSD-EBI: The PDB format files for theoretical models will not be validated and thus will not include remark 500 (geometry and stereochemistry). Instead, the following statement would be added in remark 220 in the header section of the PDB format file:

*“This theoretical model entry was not annotated and not validated by the wwPDB staff and therefore may not conform to the PDB format.”*

**2.3.1.2** The authors of theoretical models that have already been deposited will receive email to state that the PDB format files will be released as-is on the web site according to the status set at the time of deposition. Author corrections will not be incorporated. Authors will have the option of withdrawing the entry. The status authors may choose for newly deposited theoretical models is either REL or HOLD until a certain date. HPUB will no longer be an allowed option.

**2.3.1.3** Entries that have previously been processed and returned to the authors for review (on AUTH) status will be updated and released.

**2.3.1.4** Theoretical models already on HPUB or HOLD status will continue to be released after the October 15, 2006 date into the theoretical model archives, which is separate from the experimental structures.

1. H.M. Berman, S.K. Burley, W. Chiu, A. Sali, A. Adzhubei, P.E. Bourne, S.H. Bryant, J. Roland L. Dunbrack, K. Fidelis, J. Frank, A. Godzik, K. Henrick, A. Joachimiak, B. Heymann, D. Jones, J.L. Markley, J. Moult, G.T. Montelione, C. Orengo, M.G. Rossmann, B. Rost, H. Saibil, T. Schwede, D.M. Standley, and J.D. Westbrook (2006) Archiving structural models of biological macromolecules: outcome of a workshop on biological macromolecular structure models. *Structure*. **14**: 1211-1217.