

wwPDB Processing Procedures and Policies Document

Section B: wwPDB Policies

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Preface

This complete document outlines the annotation procedures and policies of the wwPDB.

The two sections in the complete document are:

A: wwPDB processing procedures

B: wwPDB policies

Further information about these sections is available in the introduction to each section.

1 PDB Entry Requirements

What are the requirements of acceptance of an entry to the PDB? The wwPDB will accept all experimentally determined structures of biological macromolecules that meet the minimum requirements. These requirements include: three-dimensional coordinates, information about the composition of the structure (sequence, chemistry, etc.), information about the experiment performed, details of the structure determination steps and author contact information are also necessary for the deposition. In addition, structure factors are required for X-ray submissions and restraints for NMR submissions.

Which type of experimentally determined structures are accepted by the PDB?

Since October 15, 2006, PDB depositions are restricted to atomic coordinates that are substantially determined by experimental measurements on actual sample specimens containing biological macromolecules¹. Currently, coordinate sets produced by X-ray crystallography, NMR, electron microscopy, neutron diffraction, powder diffraction, fiber diffraction, and solution scattering can be deposited to the PDB, provided the molecule studied meets the minimum size requirement. Theoretical model depositions determined purely *in silico* using, for example, homology or *ab initio* methods, are no longer accepted.

Theoretical models that have been previously released or those that were deposited before October 15, 2006 will continue to be publicly available via the historical models archive at <ftp://ftp.wwpdb.org/pub/pdb/data/structures/models/>.

Structures determined by methods new to the PDB will be reviewed in consultation with community of experts to determine if structures determined by the method should in principle be accepted by the PDB. Once a determination is made a new template for the PDB entries from this method will be developed.

How and where are experimental data submitted?

The PDB deposition sites for all the experimental methods are available at the following wwPDB sites:

RCSB <http://deposit.rcsb.org/>

PDBe <http://www.ebi.ac.uk/pdbe-xdep/autodep/index.jsp>

PDBj <http://pdbdep.protein.osaka-u.ac.jp/>

For NMR model coordinates and experimental data an additional access point is located at:

BMRB <http://deposit.bmrw.wisc.edu/bmrw-adit/>

PDBj-BMRB <http://nmradit.protein.osaka-u.ac.jp/bmrw-adit/>

PDBe <http://www.ebi.ac.uk/pdbe-xdep/autodep/index.jsp>

For EM model coordinates and maps data an additional access point is located at:

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) Outcome of a workshop on archiving structural models of biological macromolecules. *Structure*. **14**: 1211-1217

EMDB <http://emdatbank.org/?q=deposition..>

What are the format requirements for deposition? To ensure that all the deposition tools work with minimal error, the format requirements for depositing structures are:

Coordinates and meta data

PDBx format Deposition can be prepared in PDB mmCIF exchange format (PDBx). Definitions and dictionary are available in HTML, ASCII and XML format (see <http://mmcif.pdb.org/> for details).

PDB format Definitions and format content guide are available in PDF and HTML format (see <http://www.wwpdb.org/docs.html> for details).

- Each polymer must be assigned a unique alphanumeric chain ID (A-Z, 0-9, a-z) in column 22.
- Each residue must be assigned a unique residue number within that chain ID.
- If there are alternate conformations in the structure, the alternate conformation indicator must be provided in column 17.
- Atoms with the same coordinates may not be present in the same MODEL.
- All polymer chains should have a TER card at the end. No TER cards should be included at the end of non-polymer residues (such as ions, ligands, waters).
- There should be only one END card at the end of the file.
- Each record must start in the first column.
- Record types (such as COMPND, ATOM, SEQRES) must be capitalized.
- If the entry contains ANISOU, SIGATM, or SIGUIJ lines, there must be a corresponding ATOM record.
- Depositions with multiple models should include MODEL and ENDMDL cards. The models should be listed sequentially in columns 11-14.
- Chain IDs used in the SEQRES records should correspond to those in the coordinates.

Structure factors

- The structure factor file can either be in mmCIF, ASCII, or mtz formats and should include h, k, l, F, SigmaF (and/or I and Sigmal) and test flags.
- Definitions and format are available at <http://www.wwpdb.org/documentation/wwPDB-A-20090317.pdf>.

Restraint Data

- Currently there are no restrictions on the format.
- The common format is NMR-STAR (see <http://www.bmrb.wisc.edu/formats.html> for details).

What types of structure can be deposited to the PDB? PDB contains biomolecular polymers including polypeptides, polynucleotides, polysaccharides, and their complexes.

Polypeptide structures containing 24 or more residues in at least one polymer chain can be deposited to the PDB. Smaller peptides that are complexed with a larger polymer chain (greater than the minimum length defined above) are acceptable to the PDB.

Crystal structures of peptides with fewer than 24 residues within any polymer chain such as antibiotics should be deposited at the Cambridge Crystallographic Data Centre (CCDC, <http://www.ccdc.cam.ac.uk/products/csd/deposit/>). NMR structures of such molecules should be submitted to Biological Magnetic Resonance Data Bank (BMRB) through the Small Molecule Structure Deposition (SMSdep, <http://smsdep.bmrwisc.edu/bmrw-adit/>) system.

Polynucleotide structures with 4 or more residues are accepted at the PDB. Smaller oligonucleotides (dinucleotides and trinucleotides) can be deposited at Nucleic Acid Database (NDB, <http://ndbserver.rutgers.edu>).

Coordinates for the repeating unit of fibrous and amyloid polymers may be deposited to the PDB.

Polysaccharide structures with 4 or more sugar residues are accepted at the PDB.

Molecules that do not conform to these guidelines but have been previously deposited in the PDB will not be removed.

2 Release of PDB files and information

A journal policy of "release upon publication" takes precedence over the 6-month or one-year hold PDB policy.

What are the status codes for PDB entries?

REL entries are processed and released as soon as authors have approved the processed files. If we do not hear from the authors within three weeks from the mailing of the annotation report and assuming there are no major issues with the submission, we will consider this entry to be author approved. The entry will then be released. If the corresponding paper has been published and there are outstanding issues², the entry will be released by wwPDB staff with CAVEAT record. If the corresponding paper has not been published and the entry has outstanding issues which have not been addressed, the entry will be withdrawn by the wwPDB at the end of the 12-month period after deposition.

Entries can be released without citation information and updated with the complete citation information later.

HPUB entries released upon publication. The wwPDB receives publication dates and citation information from the authors, some journals as well as user community. In addition, the wwPDB scans the literature for publications. While the wwPDB makes every effort to track citations and release files accordingly, it is ultimately the responsibility of the depositors to notify the wwPDB when the citation has been published.

HPUB structures are released when they have been published, either in electronic or paper publication, whichever is sooner. If the manuscript is first released electronically, the entry will be released at that time. The author cannot request to delay the release of the entry until paper

² Note: Any issues that arise during annotation that prevent the standard processing of submissions are considered to be outstanding issues. These could include, for example, unusual geometry and stereochemistry, sequence-related problems, solvent structures, to name but a few.

publication of the manuscript. The author cannot withdraw an entry once the paper of the corresponding structure is published. It may be obsoleted a new entry created with replacement coordinates.

Normally authors approve before entries are released. If the contact author does not reply and assuming there are no major issues with the submission, we will consider this entry to be author approved. The entry will be automatically released when the corresponding paper has been published. If the paper has been published and there are outstanding problems with the entry, it will be released with CAVEAT record.

In the case of HPUB for which there is no publication, there is a one-year hold limit. Entries cannot be held for more than one year past the date of deposition. If authors do not respond to our first reminder, then further reminders will be sent every 30 days after the initial processing date until the author approves of the entry or one year from the date of deposition or paper publication, whichever is sooner. By the end of 10 months after deposition, a letter will be sent to the authors of the deposition asking if they wish to release or withdraw the entry by the 1 year anniversary of the deposition date. If the e-mail sent to the contact author(s) bounces or the author does not reply, the entry will be automatically released at 12 months after deposition if there are no outstanding issues. If there are outstanding problems with the entry and it has not been published, it will be withdrawn.

HOLD entries are placed on hold until and are released on the date specified by the author. When the corresponding electronic or paper publication occurs, the entry must be released if the journal requires release upon publication. Once the paper is published the entry cannot be withdrawn. It can be obsoleted with replacement coordinates.

Normally authors approve before entries are released. If the author does not reply and assuming there are no major issues with the submission, we will consider this entry to be author approved. The entry will be automatically released when it reaches specified hold date.

There is a one-year hold limit on all the entries. Entries cannot be held for more than one year past the date of deposition. If there are outstanding problems, further reminder will be sent. By the end of 10 months after deposition, a letter will be sent to the authors of the deposition asking if they wish to release or withdraw the entry by the 1 year anniversary of the deposition date. If authors do not respond by the 1 year anniversary of the deposition date, it will be withdrawn if the corresponding paper has not been published or will be released with CAVEAT record if the corresponding paper has been published.

WDRN (withdrawn) Authors may withdraw their unreleased entries at any time as long as the paper has not been published, following the same deadlines as written in the release section. Withdrawn entries will appear in the unreleased entries search as withdrawn.

Problem structures will be discussed with the depositors to resolve issues such as unusual structural chemistry, many distant waters, long/short covalent bonds, many sequence mismatches or other conflicts. Entries for which these issues can not be resolved (as determined by the wwPDB staff) will be withdrawn if the paper has not been published.

What are the deadlines for requesting release of entries? PDB entries are processed by the members of the wwPDB (RCSB PDB, PDBe and PDBj). They are either released immediately (REL), when the corresponding paper is published (HPUB), or on a particular date (HOLD).

Each week, 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.

When the release of HPUB structures is requested, the PDB staff routinely confirms the primary citation. If this is not accomplished within that release cycle, the entry may be scheduled to be released in a later update.

To be included in the next update, any required author correspondence should be sent to the appropriate wwPDB member by 12:00 hrs noon on Thursday (local time at processing site). Requests received after these cutoff times will be processed during the next update cycle.

The email addresses to contact the wwPDB centers are:

- RCSB (deposit@deposit.rcsb.org)
- PDBe (pdbdep@ebi.ac.uk)
- PDBj (adit@adit.protein.osaka-u.ac.jp)

All entries due for release are transferred to the RCSB for final packaging into the master PDB ftp archive. The PDB archive can be accessed at FTP sites at the RCSB PDB, PDBe, and PDBj. The update schedules for these sites have been coordinated to be simultaneous. All updates now occur at the target time of Wednesday, 00:00 UTC (Coordinated Universal Time).

REVDAT dates The REVDAT date indicates the date of release of the entry. Entries processed from the Wednesday after the last release to the Tuesday of the current release have Tuesday as the REVDAT date.

Who has access to unreleased data? Unreleased coordinate sets are distributed only to the authors of the particular entry. Reviewers of the paper may not obtain unreleased coordinate sets from the PDB. If a reviewer wishes to access the validation report, the reviewer should contact the journal editor, who in turn will obtain the validation report from the author and forward them on to the reviewer.

Are Email addresses of authors publicly available? The email addresses of authors who deposit PDB entries are not made publicly available and will not, individually or in bulk, be distributed to those who request them.

What information is available for unreleased entries? The unreleased entries search of the wwPDB web sites contains the title, authorship, status, PDB ID, experimental data status and sequence availability for each entry. Titles may be suppressed at the request of the author, but the authorship, status and PDB ID can not be publicly suppressed.

3 Assignment of PDB IDs and Ligand codes

Can a PDB ID or ligand code be requested? Neither a single PDB ID/ligand code nor a range of PDB IDs/ligand codes can be requested. PDB ID and ligand codes are automatically assigned and do not carry intrinsic information.

When are PDB IDs assigned? PDB IDs are automatically assigned by software when the author has completed his/her deposition (i.e. the author has filled out at least the minimal information for deposition and has pressed the deposit & confirmation buttons.)

4 Changes to entries

What changes can be made before release? Authors can update the coordinates, structure factors, as well as the related header information any time before release as long as the data is not collected after deposition. If the author has collected new data after deposition

and wishes to replace the original deposited data, the author will have to withdraw the old entry and deposit the new entry using the online deposition tools to obtain a new PDB ID. This is because the new data set will be entirely different from the original for data collection, structure factors, refinement, and will need to be completely re-processed. Authors can base the new deposition on the old data in regards to sequence and taxonomy.

If the depositor sends new coordinates for an entry shortly before or at the time of electronic or paper publication, the release of the entry may be delayed because the file must be re-processed.

Once an entry is marked for release, the author has until the deadline time listed above (see Section 2, *Deadline for requesting release of entries*) to submit revisions or to request the entry not to be released.

What changes can be made after release?

Minor changes may be made. These are defined as:

- Update on header section such as citation, author's name, etc.
- Update or change on structure factor or constraint file due to format corrections or addition of data set while coordinates remain unchanged.
- Changes to chain ID, numbering, atom name, ordering of molecules and/or ligands.

A REVDAT appear in the file with a description of the change

Major revisions to coordinates that change the structure's geometry or chemical composition (such as a change in the sequence of the polymers or ligand identity) require the entry to be *obsoleted and superseded* by a new deposition. The major revisions include:

- Replacement in any existing coordinates (the x,y,z values themselves).
- Changes in chemical composition (i.e. from SO₄ to PO₄ or SER to CYS) which change the identity of the current ligands.
- Changes in sequence such as adding or removing terminal residues.

Typically a released entry is obsoleted when the authors have collected new data or re-refined the structure. A released entry must be obsoleted by the author; it can not be withdrawn. When an entry is obsoleted, both experimental data and coordinates must be obsoleted together. Obsolete structures are still available to the public through the ftp archive. In the normal case an obsoleted structure is replaced by a new entry that receives a new PDB ID. Users who search for an obsolete structure through the main web search interface will be automatically redirected to the superceding entry.

There are some rare circumstances in which an obsolete structure is not superceded.

- The structure is incorrect and the author retracts the publication. The citation in the obsoleted entry is the published journal retraction.
- The structure is incorrect and the author obsoletes the entry. The entry must contain a statement as to the reason for obsoleting the structure.
- A PDB entry has been found to be fabricated. If the author does not agree to obsolete the entry, the employer of the author may request that PDB entry be obsoleted. This request must be fully documented. The citation for the obsolete entry must be a published explanation of the circumstances that led to having the entry being obsoleted.

wwPDB Remediation

The wwPDB reviews the entire archive on a regular basis and remediates the data. The coordinates themselves are not changed but there may be changes in the meta data and nomenclature to assure consistency and uniformity in the files. The nature of the changes are described in a public document on the wwPDB site. In the case of global remediation the individual authors are not contacted. A version number is assigned. A REMARK with this version number and date is in every file. The older version is maintained as a snapshot on the FTP site.