wwPDB Policies and Processing Procedures Document

Section A: wwPDB Policies

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Mar 2025 version 5.5

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Preface

This document outlines the annotation procedures and policies of the wwPDB. Given the complex nature of some of the issues that can arise during processing, exceptions to policy are considered on a case-by-case basis by the wwPDB Directors/Heads.

The two sections in the complete document are:

A: wwPDB policies

B: wwPDB processing procedures

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

Sept. 2021: major version 5.0, make contact info for entry PI(s) public.

1 PDB Entry Requirements

What are the requirements of acceptance of an entry to the PDB?

OneDep depositions

The wwPDB will accept all experimentally determined structures of biological macromolecules that meet the minimum requirements. These requirements include: three-dimensional atomic coordinates, information about the composition of the structure (studied sample sequence(s), source organism(s), molecule name(s), 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 factor or intensity data are required for X-ray submissions, restraints and chemical shifts are required for NMR submissions. Map volume deposition to EMDB is mandatory for PDB depositions of 3DEM models. If the experimental data deposited with the model coordinates does not follow traditional processing procedures then raw data should be made available by providing a DOI assigned by the existing archives for raw experimental data (eg SBGrid or IRRMC).

Mandatory X-ray structure factor data and NMR restraint data deposition started from Feb 1st, 2008. Mandatory NMR chemical shift data deposition started from Dec 6th, 2020. Mandatory EM map volume deposition started from Sep 5th, 2016.

For structures determined by X-ray crystallography, all atoms must have full B factors. If TLS was used during refinement, the residual B factors must be converted to full B factors. All atoms described by TLS records must have associated ANISOU records.

On occasion, the wwPDB is asked to archive a structure that was determined before deposition of experimental data became mandatory and the experimental data are no longer available. It is difficult to validate such structures without experimental data.

In such cases, the wwPDB Directors/Heads will determine if the structure can be deposited to the PDB. Criteria for accepting structures determined by experimental methods but without experimental data are as follows: there is a peer-reviewed publication prior to January 1st 2008 describing the corresponding structure(s) <u>and</u> either the polymer sequence and/or entities are not represented in the PDB archive or the deposition includes one or more ligand(s) not currently represented in the PDB Chemical Component Dictionary.

Deposition of integrative structures

Integrative structures of biological macromolecular systems are computed by combining different types of information, including varied experimental data, physical theories, statistical preferences, and/or prior models. Experimental data can be produced by traditional structure determination methods (i.e., macromolecular X-ray crystallography (MX), Nuclear Magnetic Resonance (NMR) spectroscopy, and three-dimensional Electron Microscopy (3DEM)), as well as other biophysical and proteomics methods such as small angle scattering (SAS), atomic force microscopy (AFM), chemical crosslinking with mass spectrometry, Förster resonance energy transfer (FRET) spectroscopy, electron paramagnetic resonance (EPR) spectroscopy, and Hydrogen/Deuterium exchange (HDX) with mass spectrometry or NMR spectroscopy.

The PDB accepts integrative structures of biological macromolecules that are at least partly based on experimental data, via the PDB-IHM (PDB-Dev) system. An integrative structure can be depicted using a flexible model representation, including ensembles of multi-scale, multi-state, and ordered models. In addition to atomic and/or coarse-grained coordinates of the modeled system, the deposition needs to include starting models, spatial restraints, modeling protocols, as well as specific metadata information (e.g., citations, authors, software, relevant data in external repositories, and reference sequence information).

What types of experimentally-determined structures are accepted by the wwPDB?

Since October 15, 2006, PDB depositions have been 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, and fiber diffraction can be deposited to the PDB, provided the molecule studied meets the minimum size requirement.

Use of non-crystallographic symmetry (NCS):

For crystal structures, coordinates for the complete asymmetric unit should be provided, even if non-crystallographic symmetry (NCS) is used. The only exceptions are models that produce highly symmetric assemblies (e.g., viruses, helical symmetry, etc.) in which only a portion of the asymmetric unit is used in refinement. Depositors must provide the model in the standard crystal frame along with the NCS matrices.

For microscopy methods, if symmetry operators are required to create the complete biological assembly from the modeled coordinates, such operators must be provided.

Example: in PDB entry 2wbh, the complete MS2 bacteriophage capsid biological assembly is generated from the three deposited chains (A, B, C) by applying the 60 operators provided in _pdbx_struct_oper_list (REMARK 350) records. The crystal asymmetric unit of 2wbh, which corresponds to 1/3rd of the complete capsid, is generated from the three deposited chains by applying the 20 NCS operations provided in the _struct_ncs_oper (MTRIX) records.

ftp://ftp.wwpdb.org/pub/pdb/data/structures/divided/pdb/wb/pdb2wbh.ent.gz ftp://ftp.wwpdb.org/pub/pdb/data/structures/divided/mmCIF/wb/2wbh.cif.gz

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/.

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

Structures determined by methods not currently supported by 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 such a determination is made, a new template for PDB entries derived from this method will be developed.

How and where are experimental data submitted?

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

RCSB http://deposit.wwpdb.org/deposition/

PDBe https://deposit-pdbe.wwpdb.org/deposition/

PDBj http://deposit-pdbj.wwpdb.org/deposition/

For deposition of additional NMR experimental data, an access point is located at:

BMRB https://bmrb.io/deposit/

PDBj-BMRB http://deposit.bmrb.pdbj.org/

For deposition of integrative structures, access PDB-IHM (PDB-Dev) at:

https://pdb-dev.wwpdb.org/deposit.html

What are the format requirements for deposition?

To ensure that all wwPDB and related deposition tools function with minimal loss of data fidelity, depositors should output PDBx/mmCIF format files from their refinement program, if supported. A PDBx/mmCIF preparation guide is available. The format requirements for depositing structures are as follows:

Coordinates and meta-data

- **PDBx/mmCIF format:** Deposition can be prepared in PDBx/mmCIF exchange format. Definitions and dictionary are available in HTML, ASCII, and XML format (see http://mmcif.wwpdb.org/ for details).
- **PDB format:** Definitions and format content guide are available in PDF and HTML format (see http://wwpdb.org/documentation/file-format for details).

Structure factors

- The structure factor file can either be in mmCIF or mtz formats and should include h, k, I, F, SigmaF (and/or I and SigmaI) and test flags.
- Definitions and format are available at http://wwpdb.org/documentation/procedure#toc_appendicsB.

Restraint Data

- Currently there are no restrictions on the format.
- The common format is NMR-STAR (see https://bmrb.io/formats.shtml for details).

What types of structure can be deposited to the PDB?

Biomolecular polymers, including polypeptides, polynucleotides, polysaccharides, and their complexes that meet the following criteria are accepted:

- Biologically relevant polypeptide structures of at least 3 residues with consecutive standard peptidic bonds
 - Gene products
 - Naturally-occurring peptides that are non-ribosomal in origin
 - o Peptidic repeat units of larger polymers (such as fibrous and amyloid polymers)
 - Biologically-relevant synthetic oligopeptides
- Non-biologically relevant synthetic polypeptide structures of at least 24 residues within a polymer chain
- Polynucleotide structures of four or more residues
- Polysaccharide structures of four or more residues

Crystal structures of peptides with fewer than 24 residues within any polymer chain that do not meet the criteria above 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.protein.osaka-u.ac.jp/bmrb-adit/) system.

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

Can a re-refined structure be deposited to the PDB?

A re-refined structure based on the data generated by a research group or laboratory different from the contributors can only be deposited to the PDB if there is an associated peer-reviewed publication available describing the details of the re-refined structure.

A re-refined entry may be deposited prior to publication, but will not be processed (will have REFI status) or released until the associated peer-reviewed publication has become publicly available. The depositor must provide the relevant publication details to the wwPDB and allow for extra time required for the processing and release of these entries. Authors who require early entry processing in order to facilitate journal manuscript submission should contact the wwPDB and processing of these entries will be handled on a case-by-case basis.

In addition, a dedicated remark (_pdbx_database_remark with id = 0) will be added to the PDBx/mmCIF file along with the primary citation of the original PDB entry (under _citation with id = original_data_1).

Details on the annotation of a re-refined PDB entry can be found at http://wwpdb.org/documentation/procedure.

2 Entry Authorship

There are 3 types of authorship associated with a PDB entry: Entry Author, Contact Author, and Citation Author.

The supervisor of the research group where the structural determination work began, known as the Principal Investigator (PI) or Team Leader equivalent, is responsible for the authorship represented in the final PDB entry. If more than one PI/Team Leader equivalent is responsible for the entry, they will need to come to a mutual decision on all issues.

Contact Authors

The Contact Authors indicated at the time of deposition are responsible for depositing the structure, responding to any queries from the wwPDB during processing, and indicating when entries can be released.

At least one Contact Author should be designated "responsible for correspondence" including data submission and responses to questions from the wwPDB. The PI/Team Leader equivalent must be listed as a Contact Author and will be copied on all communications. In some cases, the PI/Team Leader equivalent may be contacted with questions directly. It is the responsibility of the depositor to label author roles correctly.

All Contact Authors will be notified of any changes or requests for changing/obsoleting/removing entries. In the case of a conflict between Contact Authors, the wwPDB will follow requests from the PI/Team Leader equivalent who ultimately makes the final decision. The PI/Team Leader equivalent is the individual(s) specified as PI/Team Leader in the PDB entry that was approved by the contact authors.

Entry Authors

The PI/Team Leader equivalent should be included as Entry Author. In addition, it is recommended that all who contributed to the structural determination as identified by the PI/Team Leader equivalent, be designated as Entry Authors. Commercial entities should include the company name along with any other relevant names.

Entry Authors can be the same as those listed in the primary citation, or a subset of Citation Authors. Alternatively, there may be more Entry Authors listed than there are Citation Authors.

It is the responsibility of the PI/Team Leader equivalent to ensure that the listing of Entry Authors is appropriate and that all listed Entry Authors have approved the final version of the data and have agreed to PDB submission.

For the entries deposited or revised starting September 24th 2021, name(s), email address(es), and ORCiD id(s) of principal investigator(s) are made publicly available when these entries are released.

Citation Authors

Citation Authors are those listed on the primary publication describing the entry. The Citation Author list may be different from the Entry Author list as described above.

If an entry is to be obsoleted, it is the responsibility of the PI/Team Leader equivalent to notify the corresponding author of the paper.

Authorship and Re-refined Entries

A re-refinement of data available in the PDB must acknowledge the original data set by citing the PDB entry (and corresponding citation, if available) in the re-refined PDB entry. This information can be noted at the time of deposition. A re-refined entry may be deposited prior to publication but will not be processed (will have REFI status) or released until the associated publication has become publicly available. See the wwPDB Processing Procedures Document for further information (Section A.9).

3 Release of PDB Entries

What are the author-requested status codes for PDB entries?

REL entries are to be released as soon as the authors have approved the processed files.

HPUB (Hold until PUBlication) entries are placed on hold until publication or until one year from the date of deposition, whichever comes first.

HOLD entries are placed on hold for up to one year from the date of deposition.

What are the release policies for PDB entries?

REL entries are scheduled for release after authors have approved the processed files. If no reply is received within three weeks after the validation report is made available to the authors, the wwPDB will consider the entry to have been approved by the authors. If at that point there are no outstanding issues² with the entry, the entry will be released. For entries with outstanding issues see the *Problem Structures* section below. Entries can be released without citation information and updated with this information at a later date.

HPUB/HOLD entries will be released either when release is requested by the authors or by a journal, or when the wwPDB becomes aware of a publication describing the entry.

HPUB/HOLD entries cannot be held for more than one year beyond the date of deposition. If an entry remains unreleased at the end of the hold period, it must either be released or withdrawn. Ten months following deposition, the wwPDB will communicate with the authors of unreleased entries, asking whether they wish to release or withdraw the entry before the one-year anniversary of the deposition date.

The wwPDB promotes open science and immediate release of data when associated publications appear online (identified by detection of wwPDB Core Archive [PDB, EMDB, BMRB] accession codes in those publications). wwPDB policies state that if a wwPDB Core Archive database accession code is identified in a publication (pre-print or peer-reviewed) the on Hold for Publication entry will be released. If a Depositor has questions or concerns regarding a specific entry, she/he should directly contact the leader of the appropriate wwPDB data center. Any revision of the PDB entry following release will be managed under the PDB

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.

archival versioning system - please see the section 'What changes can be made after release?' for more details.

Publication dates and citation details are obtained through a combination of direct communications from authors, journals, and members of the scientific community (communicated via OneDep or deposit-help@mailto:deposition and PubMed searches (automated comparison of title and author lists included with the deposition and manual review for PDB, EMDB, and BMRB IDs).

It is normal practice for authors to review and approve curated entries before they are released. If the contact author does not reply within three weeks after the validation report is made available to them, and assuming that there are no outstanding issues with the deposition, the wwPDB will deem this entry to have been approved by the authors. The entry will be released when the wwPDB is aware that the publication describing the entry is available. Entries with outstanding issues will be handled as per the *Problem Structures* section below.

Authors may withdraw their unreleased entries, provided the publication citing the entry has not been published. When an entry is withdrawn, the latest version of the processed files will be made available to the authors in case they wish to re-deposit the entry in the future. Withdrawn entries will remain in the list of unreleased entries in the PDB archive (status **WDRN**).

Problem Structures, as identified by the wwPDB biocuration staff or from the contents of the wwPDB validation report, will be discussed with the authors in order to resolve issues such as unusual structural chemistry, distant water molecules, long/short covalent bonds, certain sequence mismatches, or other conflicts. An entry for which these issues cannot be resolved will be withdrawn upon expiration of the one-year hold unless a publication describing the entry is available. In that case, the entry will be released by wwPDB staff with a database_PDB_caveat record. If a publication describing a withdrawn entry appears in the literature, the withdrawn status of an entry may be reversed by the wwPDB (as determined by the wwPDB staff).

Can the experimental data be released separately from the coordinate file?

Coordinates and experimental data share the same release status (REL, HPUB, or HOLD). Thus, coordinate and experimental data files can only be released simultaneously.

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 revision are subjected to a final data integrity check. Contact Authors may be asked to resolve issues arising while entries are prepared for release.

When release of HPUB structures is requested, wwPDB staff routinely check for the primary citation. To be included in the upcoming update, any required author correspondence should be sent to the appropriate wwPDB member by 12:00 noon on Thursday (local time at processing site). Occasionally the request cutoff date may be changed under certain circumstances. Requests received after these cutoff times will be processed during a later update cycle.

Depositors should contact the wwPDB through the web communication within the relevant deposition while general PDB users should contact the wwPDB at deposit-help@mail.wwpdb.org regarding publication and/or release.

All entries set for release are transferred to the RCSB-PDB (the current Archive Keeper) for final packaging into the master PDB ftp archive. Data entries are added to the PDB archive on a weekly schedule and synchronized among FTP sites at RCSB-PDB, PDBe, and PDBj.

The process for weekly PDB archive data release, with the advice and concurrence of the Advisory Committee to the Worldwide Protein Data Bank, is as follows:

Phase I: Every Saturday from 3:00 UTC, for every new entry, the following will be provided from the wwPDB website: sequence(s) (amino acid or nucleotide) for each distinct polymer and, where appropriate, the InChI string(s) for each distinct ligand and the crystallization pH value(s).

Phase II: Every Wednesday from 00:00 UTC, all new and modified data entries will be updated at each of the wwPDB FTP sites.

Revision dates (database_PDB_rev.date, pdbx_version) The revision date indicates the date of release of the entry. Revision date will be set to the date of scheduled release, which is on Wednesday.

Who has access to unreleased data?

Unreleased coordinate sets, experimental data and metadata are distributed only to the authors of that entry. In cases where the author has given explicit permission some metadata is released to the public prior to the entry release, including entry title, entry author list and sample sequences. Reviewers of the journal submissions and wwPDB users may not obtain unreleased data from the wwPDB. The wwPDB strongly encourages journal editors and referees to request wwPDB validation reports from authors as part of the manuscript submission and review process.

What information is available for unreleased entries?

Unreleased entries at the PDB archive contain the title, authorship, status, PDB ID, experimental data status and sequence availability. Entry titles and authorship may be suppressed at the request of the Contact Author, but status and PDB ID cannot be publicly suppressed.

4 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 may be requested. The wwPDB reserves the right to change author's ligand codes. PDB ID and ligand codes are automatically assigned and do not carry identifying information.

When are PDB IDs assigned?

PDB IDs are automatically assigned by the deposition software tool, 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.)

5 Changes to Entries

What changes can be made before release?

Authors can update the coordinates, experimental data, and related header information any time before release.

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 subject to delay because the file must be reprocessed.

Once an entry is marked for release, the author has until the deadline time listed above (see Section 3, *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 metadata 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.

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) can be made through depositor-initiated or wwPDB-initiated updates. Major revisions include:

- Replacement of any existing coordinates (the x,y,z values themselves).
- Changes in chemical composition (e.g., SO4→PO4 or SER→CYS).
- Changes in coordinate section including chain ID, numbering, atom name, ordering of molecules and/or ligands.
- Changes in sample sequence including add or remove a region that is unobserved in the coordinates such as terminal or loop region.

Depositor-initiated or wwPDB-initiated update to the coordinates will be versioned while retaining the same PDB accession code. Entries will be processed and released immediately. If there is a change to the experimental data (they are new, or in some way modified), an entry must be replaced by a new deposition needing a new PDB ID. The old entry is then obsoleted (if the depositor wishes) and replaced (superseded) by the new one.

Obsolete entries remain available to the public through the ftp archive. Users who search for an obsolete structure through the main web search interface will be automatically redirected to the superseding entry. Under no circumstances can a released structure be withdrawn.

There are some rare circumstances in which an obsolete structure is not superseded by a new structure. The entry must contain a statement specifying the reason for obsoleting the structure (under pdbx database PDB obs spr.details).

 The publication is retracted. The associated PDB entry will be obsoleted if requested by the journal. If a request has not been received, the wwPDB will do its best to contact the

depositor and co-authors, (former) PIs, journal editors, etc. when made aware of the retraction. If the reason(s) for retraction were such that the associated PDB entry needs to be made obsolete, the wwPDB will obsolete the entry. The citation in the obsoleted entry is the published journal retraction.

- There is no associated publication and the entry author obsoletes the entry (e.g., the structure is incorrect).
- A third-party (such as the employer) requests that the entry is obsoleted (e.g., in case of malfeasance). In such cases, the wwPDB will obsolete the entry if either the primary citation for the structure is retracted or a formal report by an appropriate government or supranational agency in the region (e.g., US Office of Research Integrity) is published.

wwPDB Remediation

The wwPDB reviews the entire archive on a regular basis and remediates PDB data as required. The coordinates themselves are never 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 is 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 and recorded in _pdbx_version mmCIF category in every file. The older version is maintained as a snapshot on the FTP site.