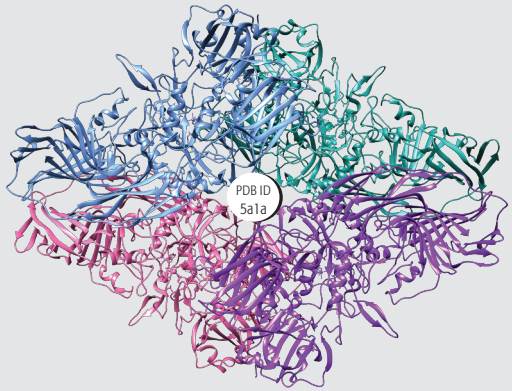
Deposition Checklist

- **Check sample sequence**
  Refer to UniProt
- **Check ligands**
  Are these correctly assigned?
- **Prepare data for deposition**
  Generate PDBx/mmCIF-formatted data files to provide the most complete information about your structure
- **Validate your data**
  Use wwPDB's standalone validation service
- **Deposit your structure using OneDep System**
  When you are ready



Online Resources

PDB_extract: **pdb-extract.wwpdb.org**
Validation: **validate.wwpdb.org**
Deposition: **deposit.wwpdb.org**

Further Information

Tutorials and FAQs for validation and deposition can be found at:

www.wwpdb.org/validation/validation-reports
wwpdb.org/deposition/tutorial
wwpdb.org/deposition/faq

Contact Information

validation@mail.wwpdb.org
deposit-help@mail.wwpdb.org

Citation Information

Cite wwPDB:
Nature Structural Biology **10**, 980 (2003)
doi: 10.1038/nsb1203-980

Cite OneDep:
Structure **25**, 536-545 (2017)
doi: 10.1016/j.str.2017.01.004

wwPDB Members

WORLDWIDE PDB PROTEIN DATA BANK

wwPDB.org

RCSB PDB PROTEIN DATA BANK
PDBe Protein Data Bank in Europe
PDBj Protein Data Bank Japan
BMRB

OneDep

5 EASY STEPS TO PDB DEPOSITION

WORLDWIDE PDB PROTEIN DATA BANK

5 Easy Steps to PDB Deposition with OneDep

1 Check Sample Sequence

Sequence should

- Contain all residues
- Include expression tags and disordered residues

Check against reference database with BLAST

- Proteins ⇨ **UniProt BLAST**
- Nucleic acids ⇨ **NCBI BLAST**

! Any mismatch should correspond to mutation, variant or expression tag in your sequence.

Example of a UniProt alignment with highlighted mismatch

Query

61 RWWANDGRTPGSR

RWW NDGRTPGSR

79 RWWCNDGRTPGSR

P00698
(UniProt Sequence)

2 Check Ligands

Are your ligands already in our Chemical Component Dictionary (CCD)?

Check at:

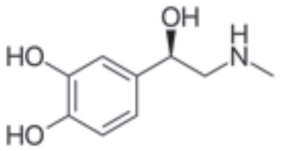
- Ligand Expo **ligand-expo.rcsb.org**
- PDBeChem **pdbe.org/chem**
- Chemie search **pdbj.org/chemie-search**

Is the ligand present in the CCD?

Yes The 3-character code for your ligand should match that in the dictionary

No During deposition you can provide a SMILES or upload a 2D chemical diagram

Example of a chemical diagram that should be provided at deposition



3 Prepare Data

Generate coordinate file in PDBx/mmCIF format

- This can be output directly from some refinement programs (e.g., PHENIX, REFMAC)
- This ensures that the maximum metadata is captured from the file for deposition

pdb_extract can be used to extract information.
Visit **pdb-extract.wwpdb.org**

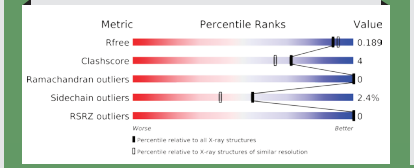
- Creates single PDBx/mmCIF file containing extra meta data (e.g., author info, data collection and refinement stats) using output log files
- Converts SF files to PDBx/mmCIF format for non-MTZ format files

4 Validate! Validate!

The wwPDB provides a standalone validation server for checking your structure
Visit **validate.wwpdb.org**

- Both model and experimental data are validated
- Provides detailed reports (PDF and XML files)

! Attempt to fix major issues highlighted prior to deposition to minimize the requirement for replacement files. It will reduce the time needed to process your entry.



5 Deposit your Structure

Deposition to the OneDep system can be carried out at the wwPDB deposition pages.
Visit **deposit.wwpdb.org**

Deposition is tailored to experimental type:

- X-ray, Neutron, NMR, EM, or any combination of these
- You must upload the relevant coordinate and experimental data files and include mandatory information

A session ID is provided to enable you to continue your deposition at a later date. A PDB ID will be provided upon completion of your deposition.

After Deposition

Entries are annotated, validated, and returned to authors for review

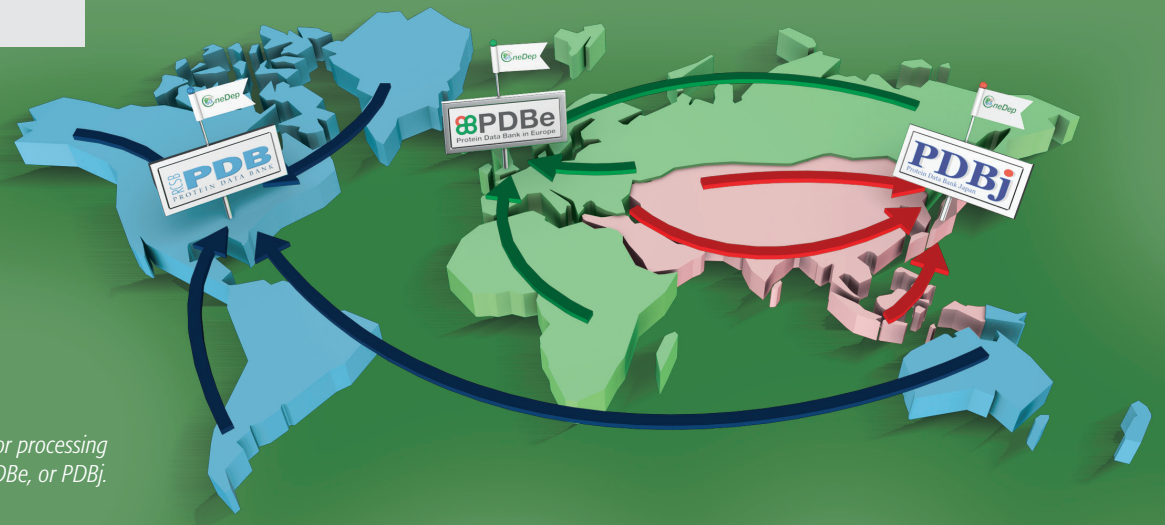
- Processed files and official validation report can be downloaded at communication page

Request entry release and provide citation publication information using OneDep's communication panel.

Coordinate release follows instructions given at deposition

- **REL** - released immediately after processing
- **HPUB** - hold until publication, up to 1 year
- **HOLD** - hold up to 1 year

If the structure is not published within 1 year, you have the option to either release or withdraw the entry.



Depending on the depositor's geographical location, the structure will be assigned for processing to one of the worldwide Protein Data Bank sites: RCSB PDB, PDBe, or PDBj.