wwPDB OneDep System

Frequently Asked Questions

Starting a deposition session

How to start or access a deposition session using ORCiD?

In addition to login using deposition ID and password (this option is still available), the contact authors can use ORCiDs to login to OneDep system, to start a new deposition session or access the existing deposition sessions. First-time OneDep contact authors will need to verify their email address before being able to create new depositions, this address does not have to be the same as the one registered within ORCiD, and can be updated in future. Once logged-in using ORCiD, OneDep returns a summary table of the entries in which the ORCiD has been provided for the contact author. Users can further access each of their entries' deposition interfaces without the need to login again using a deposition ID or password. The option of 'Start a new deposition' is provided beneath the summary table of existing sessions. You will need to select your country/region from a drop-down menu and then be redirected to the wwPDB member's deposition site corresponding to your location. Follow the procedures on the page, once the new session is created, a notification will be sent to the verified email address associated with your ORCiD, with the deposition ID and the randomly assigned password. The new session will appear in the summary table so you can access it directly from the table. You can also access the session using the deposition ID and the password. A detailed step-by-step tutorial can be found at https://www.wwpdb.org/deposition/tutorial.

Please note that adding a contact author ORCiD in the "Admin > Contact information" in your deposition session will grant this author access to the current deposition, so please check carefully when adding additional contact authors' ORCiDs.

Can I deposit raw data to the PDB?

Depositors are encouraged to deposit raw data of their structure and then provide the corresponding DOI in the "Related Entries" user interface during structure deposition in wwPDB OneDep.

Depositors are strongly encouraged to deposit their raw data in a curated archive.

- X-ray diffraction
  - ProteinDiffraction.org - **https://proteindiffraction.org (https://proteindiffraction.org)**
  - SBGrid - **https://sbgrid.org (https://sbgrid.org)**
  - CXIDB - **http://www.cxidb.org (http://www.cxidb.org)**
  - XRDa - **https://xrda.pdbj.org (http://xrda.pdbj.org)**
- Electron microscopy
  - EMPIAR - **https://www.ebi.ac.uk/pdbe/emdb/empiar/deposition (https://www.ebi.ac.uk/pdbe/emdb/empiar/deposition)**
- NMR e.g., FIDs, in particular those relating to NOESY type spectra
  - please contact BMRB - **help@bmrb.io (mailto: help@bmrb.io)**.

How do I provide raw image DOI to the PDB after deposited to one of the raw image resources?

Go to the "Related entries" page at OneDep interface, in the "Related experimental data sets" section, choose "diffraction image data" as the type of experimental data, and provide image DOI under "DOI for related data set".

What information and files should I have on-hand to deposit?

The information needed for deposition is the same that is required for legacy deposition systems: Gather information about the proteins/nucleic acids in your structure from sequence databases (e.g., using UniProtKB or BLAST) and about ligands in your structure (using Ligand Expo). Instructions for depositing new ligands will be provided during deposition. Collect log file output from the programs that were used for data processing, scaling, MR, refinement, etc., and use **pdb_extract (http://pdb-extract.wwpdb.org/)** to parse these files and gather sequence information for the contents of the sample.

What is the easiest way to deposit many related entries?

Deposit one entry, and then enter the deposition ID for that entry into the "Related depositions" field of the entry page when depositing any related entries. The new system will provide the option to automatically copy information (e.g., author contact information, release status, data collection information, protein name, source organism, sequence information) to the new deposition session.

How can I deposit a new entry based on a previously deposited entry?

Prior to the initial upload of coordinate and experimental data files, enter the Deposition ID (D_xxxxxxxxxx) and password of a previous submission on the File Upload page. Then select the data categories to be copied from the previous submission. Please note that once you have uploaded files and pressed the "populate" button, you will no longer have the option of selecting data from a previous submission. After this point, a new deposition session would need to be started to import information from a previous submission.

I forgot my password. How do I retrieve my password?

In order to retrieve your password, please click the "Forgot Password" button located on the left-hand panel ("Existing Deposition") of the deposition page. You will be prompted for your Deposition ID and e-mail address. When you have provided this information, your password will be e-mailed to you. In order to maintain security and confidentiality of the on-hold submissions, passwords are only sent to those email addresses that were added to the contact information at the time of deposition. The email address needs to be an exact match of what is currently present in the deposition i.e. email aliases will be treated as a different email address and hence you won't receive the password.

I did not receive an email containing my password after attempting to retrieve my password. Why might this have happened?

There are several possible reasons: (1) There was a typo in the email address or/and deposition ID that were provided; (2) the email address provided for password retrieval is not associated with the deposition session; (3) the email was filtered into the spam folder. Deposition-related email messages are sent from noreply@mail.wwpdb.org; you may need to adjust your mail settings so that this address is not filtered.

Can I reset or change my password?

At this time, deposition session passwords cannot be reset or changed. We will implement this feature in our future updates.

How do I add an author to an entry or citation author list?

Click the "+" button next to the author name after which the new author name is to be placed. This will add a new blank form for new author's name. To reorder the author list, drag the up/down arrow icons. Choose the trashcan icon to remove a name from the list.

How long will my deposition session be saved?

Un-submitted sessions will expire 3 months after last login. Un-submitted sessions and uploaded files will be removed once they expire.

Where can I designate my deposition for structure prediction competition?

At "Release Status" page, set "Y" to designate your deposition for prediction target, then select a proper development method such as CASP for the prediction if it has sequence identity to available structures below 50% or you expect it to be interesting for prediction otherwise.

How do I provide information for a re-refined structure of an alternative interpretation using the same experimental data from an existing PDB entry?

If you are depositing an alternative interpretation of a structure which was determined using an original experimental data set (e.g., structure factors) of an existing PDB entry either coming from the same or different research lab, you should provide PDB id of the original entry that the experimental data was used and choose “re-refinement” as content_type.

If you have used data from a different research lab, please see additional requirements at http://www.wwpdb.org/documentation/procedure#toc_15.

Experimental methods

How do I submit hybrid method structures?

At the start of deposition, you will be asked to provide information about the experimental methods employed to determine the structure. Multiple experimental methods may be selected. For example, select both X-ray diffraction and neutron diffraction if the X-ray/neutron hybrid method was used.

All relevant accession codes will be assigned when the deposition is submitted. For example, a structure determined using a combination of X-ray diffraction and solution NMR will be assigned both PDB accession codes and BMRB accession codes upon submission.

As a deposition session proceeds, depositors will be asked to provide experimental details such as data collection and refinement information for each experimental method.

I can't find a software name in the pull-down list for data processing. How do I add information about software used for data processing?

Use the Communication page to submit the missing information. An annotator will instruct you how to proceed with your deposition and will add the software information to the list during entry processing.

File Formats

How do I collect the data from the refinement program log file necessary to generate a complete PDBx/mmCIF format file?

Pdb_extract (http://pdb-extract.wwpdb.org/) can be used to harvest data from your fully refined coordinate file, experimental data file (e.g., structure factor file), refinement program log file, and author information template file (if available). **Pdb_extract (http://pdb-extract.wwpdb.org/)** can produce fully populated coordinate and experimental data files in PDBx/mmCIF format that can then be used for validation or deposition.

How do I convert PDB format file into PDBx format file?

In the new deposition system, files uploaded in PDB format will be automatically converted to PDBx/mmCIF format. The uploaded PDB and converted PDBx/mmCIF format files will be available via the "Download files" link at the bottom of the left hand panel.

Alternatively, if you want to convert your PDB format file to PDBx format prior to deposition, you may use **pdb_extract (http://pdb-extract.wwpdb.org/)** to convert and prepare the files for deposition.

How can I upload a file in PDB format?

Please make sure that an uploaded PDB format file meets the following requirements:

a) There must be a complete TER record after the end of each polymeric chain
Example:

```
ATOM   2705  CB  HIS A 337      -2.421  -9.493  35.428  1.00 30.90           C
TER
ATOM   2707  N   ALA B   3      14.064   2.135  20.580  1.00 15.71           N
```

b) All the ligands/compounds present in your PDB coordinate file must have a HETATM at the start of the atom coordinate line

```
HETATM 1574  C1  GOL A 104      -1.268 -20.812  15.070  0.75 21.78           C
```

How do I convert my structure factor file to mmCIF format?

SF-tool (http://sf-tool.wwpdb.org/) can be used to convert your structure factor file to mmCIF format.

Can I submit an entry that has more than 99,999 ATOM lines and/or more than 62 chains (and is therefore incompatible with the PDB format)?

Large entries (>99,999 atoms and/or >62 chains) should be deposited in the PDBx/mmCIF format. A **PDBx/mmCIF (/deposition/preparing-pdbx-mmcif-files)** preparation guide is available.

For large structures generated using exact symmetry operations (e.g., strict helical, point, or non-crystallographic symmetry (NCS)), authors should deposit only those chains that were fitted and/or refined and supply a PDB file containing the operators (matrix transformations) that can be used to generate the complete assembly.

File Upload

How do I upload files for deposition? Which files are required for deposition?

Go to "Upload files" page of the deposition interface. Select one coordinate file using "browse" button and choose a proper file type (PDB or mmCIF).

Select experimental data file(s) using "browse" button again and choose a proper file type (e.g., mmCIF or mtz for structure factors).

Follow the instructions provided on the file upload page regarding which file types are required for deposition. Press "Continue deposition" button at the bottom to proceed with the deposition.

X-ray depositions require one coordinate file and one structure factor file.

NMR depositions require one coordinate file, one chemical shift file, and at least one restraint file. Depositors are also encouraged to upload a peak list file.

3DEM depositions require one coordinate file, one map image file, and one primary map file. Depositors are also encouraged to upload half maps, additional maps, FSC curves, structure factor data, and layer line data.

There were problems with the file I uploaded. Where can I see a list of those problems?

Errors encountered upon file upload will be presented in two places: (1) on the diagnostic screen (headed by a graphic showing a pair of red gears) that appears after pressing the "Continue deposition" button on the file upload page, and (2) on the Upload summary page of the deposition interface.

Why did my file upload fail?

Some possible reasons for the upload failure include:

- Uploaded file has incorrect file type selected (make sure that the correct file type is selected for each uploaded file)
- Incorrect file format (common errors include missing TER cards in PDB format files and cif items in PDBx/mmCIF files that do not conform to standard formatting/definition **http://www.wwpdb.org/documentation/file-format (http://www.wwpdb.org/documentation/file-format)**).

Review the error messages at the "Upload files" page, correct the file accordingly, and re-upload the file on the "Upload files" page.

Chemical Components (ligands)

How do I provide information for a new chemical component (ligand)?

The deposition interface searches the Chemical Component Dictionary (CCD) for matches between submitted ligands and the contents of the dictionary. Summary information will be displayed for any chemical components (ligands) detected in the uploaded file. Authors should review this information and note any missing data.

If no CCD match is available, authors must provide complete chemical information by 1) uploading or sketching a 2D chemical drawing using the deposition tool, or 2) providing the appropriate SMILES string or InCHI key, or 3) providing a ligand ID existing in the CCD that should be the match but is not presented as a hit due to geometry ambiguities or other reasons.

Where can I upload a ligand image or ligand definition file prior to or after submission?

Prior to submission, the ligand verification page will display the message "Address mismatched instances of" for ligands without matches in the CCD. After confirming the ligand type, please provide a ligand image (required) and/or a ligand definition file (optional). If you need to provide a ligand image or definition file after an entry has been submitted for annotation, you can request that the session is

unlocked using the Communication page. In your request, please inform the annotation staff that you wish to upload a ligand image or ligand definition file. Once the session has been unlocked, the procedure will be the same as that of prior to submission.

I already provided mandatory ligand information, but the interface still indicates that a ligand mismatch requires attention. What do I do?

Return to the instance-level verification page (click the "Inspect Selected Ligands" button on the ligand summary page) and make sure that the "Save" button near the bottom of the page has been clicked. When this button is clicked, it should change from a "Save" button to an "Undo" button and all mismatched instances of the ligand should switch from a yellow header to a light blue header that reads "Mismatch(es) now addressed." Make sure that all the ligands that require attention have been addressed by visiting all of the available tabs (one ligand type per tab). You will need to press the "Finish (all issues addressed)" button after you have pressed the "Save" button. If there are any additional problems, you can use the Communication page to contact the wwPDB annotation staff for assistance.

Sequence Information

How do I provide a polymer sequence containing non-standard or modified residues?

When providing a protein or nucleic acid sequence, depositors should provide the full sequence that was present in the experimental sample. This sequence should contain any expression tags or other unobserved regions that were not modeled in the final coordinate file.

For polypeptide chains containing standard amino acids, please provide the sample sequence using one-letter codes for all standard amino acid residues present in the polymer chain (e.g., Y for tyrosine).

Similarly, for nucleic acid chains, provide the one letter codes for standard nucleotides present in the polymer chain (e.g., U for uracil). Please refer to the list of standard amino acid and nucleic acid one-letter codes.

If the polymer chain contains non-standard amino acids or nucleotides, please provide the three-letter code of the residue as it appears in your coordinate file in parentheses. For instance, use "(MSE)" in the sample sequence if it contains selenomethionine.

Example of a sample sequence containing modified residue:
VQDKTT(MSE)ELFISEKTV

I have two (or more) copies of the same protein in the coordinates, but the deposition interface displays two (or more) macromolecules. How do I correct the number of unique polymers and/or chain IDs on the Macromolecules pages?

If sample sequences were not provided in the uploaded coordinate file, the deposition system automatically generates unique polymer entities based on sequences extracted directly from the coordinates themselves. As different instances of the same polymer might have different subsets of their sequences modeled, multiple entities might be generated for a single polymer.

To associate these entities (each of which will have a different page under the "Macromolecules" header) so that they can be identified as the same polymer during processing, go to the page for one of the polymer entities, e.g., "Molecule 1." Provide any information available for the polymer, including molecule type, provenance, and source (and host, if applicable) information. Most importantly, provide the full polymer sequence that was used for the experiment. This sequence should include any expression tags and any residues that were present but may not have been modeled in the coordinates.

Then, on each page under the "Macromolecules" header for a polymer entity that is the same polymer as the one just identified, you can enter the molecule number at the top of the page and click the "Copy every field from Molecule" button to copy all of the entered information from that entity, including the sequence.

During the annotation process, identical polymers identified in this manner will be consolidated from multiple entities into a single entity encompassing multiple chains. No further action on the part of the depositor should be necessary.

An example:

An X-ray crystal structure of lysozyme is deposited. There are two molecules of lysozyme modeled in the asymmetric unit in the coordinates. Because of poor electron density, a loop that is modeled in the first molecule is not modeled in the second molecule. The uploaded coordinate file did not happen to contain the sequence of the experimental lysozyme construct that was crystallized, so the deposition system extracts the sequences from the coordinates. Because of the un-modeled loop in the second molecule, different sequences are extracted for the two molecules and they are identified as different polymer entities, Molecule 1 and Molecule 2, in the Macromolecules section.

On the Molecule 1 page, the depositor provides all of the required information for the polymer including the experimental sequence, which includes not only the problematic loop, but also some N-terminal residues present in the sequence that were not modeled in either instance of the polymer. The depositor then moves to the Molecule 2 page. He or she enters "1" in the box at the top of the page and clicks the "Copy every field from Molecule" button.

The depositor has now done what is necessary. During annotation, Molecule 1 and Molecule 2 will be consolidated into a Molecule 1 that includes both molecules of lysozyme.

Where can I provide details about a polymer or sequence?

Each unique macromolecule in a submission will have its own page under the Macromolecules header in the left-side menu. Any particular details regarding the nature or sequence of the macromolecule that do not fit in any of the other available data fields can be included in the "Compound details" box located under the sequence alignment.

I got a mismatch error during sequence alignment. How I do fix this problem?

To correct a mismatch error in the sequence alignment, it is necessary to determine whether the error is in the provided sequence or in the uploaded coordinate file. If the error is in the sequence, then the corrected sequence can be entered in the appropriate field and the alignment refreshed. If the error is in the uploaded coordinate file, a corrected coordinate file must be uploaded on the Replacement Upload page.

Funding agency information

How do I provide funding agency information?

The funding agency information can be provided at the "Grant information" page of the deposition interface. Select "Y" under "Was this work funded by a grant?" and select country from the pulldown menu. Once you start typing your funding organisation name in the provided box, a list of organisations will appear for you to select from.

What if my funding organisation name is not in enumeration list?

Select "Other private" or "Other government" from the list, whichever applies, and provide funding details using Communication page of the deposition interface. The funding organisation name will be added to the enumeration list during entry processing.

Assembly information

How do I properly fill in the "Assembly" page of deposition interface?

Assembly page is designed to capture the quaternary structure information for the deposition. For X-ray structures, for example, quaternary assembly can be 1. the same as the asymmetric unit, 2. part of the asymmetric unit when a symmetry needs to be applied to the content of the asymmetric unit to generate the complete assembly or 3. several units contained within the asymmetric unit.

On the Assembly page of the deposition interface "Assembly details" box can be used to include a brief description of the assembly. If there is experimental evidence that supports this assignment, then it can be provided in the "Experimental evidence for the assembly" section.

And finally a detailed assignment of each chain in the assembly can be provided in the "Chains and matrices for the assembly" section.

If all chains in the asymmetric unit are involved in assembly #1 then select "Y" under "Does this assembly apply to all chains?".

Otherwise select "N" and provide the relevant chain ids under "List of chain IDs in this assembly".

If there is no additional symmetry needed to generate the assembly then select "Y" under "Can you generate the assembly without applying matrices?" and the unitary matrix will be selected automatically. Otherwise select "N" and provide the necessary symmetry matrix under "Provide 3x4 rotation with translation matrices in the format".

Then select "+" if more assemblies are needed to be described.

Official validation report

The journal requested that I provide a fully annotated validation report, but I only have the "Preliminary Validation Report". How do I get the report?

Prior to the entry annotation only the preliminary validation report is available. This version is produced by the deposition system upon successful file upload. The official confidential validation report will be sent to you after the entry is processed by a member of the wwPDB biocuration team. You will also receive a validation letter which includes any questions that may have arose during entry processing and the processed data files. The confidential validation report will also be available at the Validation Reports page of the deposition interface (after the entry is processed by a biocurator and the processed files are sent for your review).

Finishing a Deposition Session

How will I know when all mandatory data have been submitted?

The progress bar in the upper left-hand corner of the deposition interface tracks mandatory data items. Click on the progress bar at any time to view any missing mandatory data items.

Once all mandatory data items have been provided, the progress bar will become the Submit button.

When a deposition is complete and the Submit button is clicked, PDB/EMDB/BMRB accession code(s) will be issued and the entry will be submitted for wwPDB annotation and processing.

I have already provided complete contact author information for the PI and corresponding author, but the navigation panel still indicates that the data on the page are still incomplete. Why?

By default, the deposition system provides extra blanks for additional contact author information. If there are no additional contact authors, select "N" as the answer to the question "Are there other authors you wish to add?" This will remove the extra blanks and complete the page, providing principal investigator and corresponding author information has been properly filled in.

All of the indicators on the navigation panel are green and the "Submit" button is available, but when I click the "Submit" button, it tells me that I have not clicked on the validation report. Why?

The deposition interface requires that the wwPDB validation report be downloaded before a deposition session can be completed. You are expected to read the validation report and correct any obvious errors before submission. When the report has been generated, you will receive an email notification. You can then return to the Validation Reports page within the deposition interface and click on the link for the PDF validation report. After the report has been downloaded and accepted, you will be permitted to complete the deposition process.

Replacing Data

When can I replace an uploaded file?

An uploaded file can be replaced either pre-submission (before a PDB accession code has been issued for the deposition) or post-submission (after a PDB accession code has been issued and the entry is either being processed or has been processed by the wwPDB biocuration staff). Please note that the files for withdrawn or obsoleted depositions cannot be replaced.

How can I replace an uploaded file pre-submission?

Coordinate files can be replaced at any time prior to submission using the "Re-upload files" page on the left side menu of the deposition interface. Browse the new coordinate file and specify its type (PDB or mmCIF). Be sure to select the new coordinate file within the list, deselect any previously uploaded coordinate files and press the "Process selected files" button at the bottom of the page to initiate the upload and incorporation of the new coordinate file.

The system will ask you to wait while the files are checked and converted. If there are no issues, the system will allow you to continue with your deposition. The validation process will start running after the new file is successfully uploaded. After all deposition requirements are fulfilled be sure to click the "Submit deposition" button.

If you encounter any error messages, please check the "Upload Summary" page and read the answer to the question **"Why did my file upload fail?" (https://www.wwpdb.org/deposition/faq#upload)** in this FAQ if necessary.

You can make the requested corrections and try again. If you have made corrections to a file, you should re-upload it, define its type, and de-select the coordinate file you are replacing before you click the green "Process selected files" button.

If your file upload failed and you would like to return to the previous state of the deposition click "Undo failed upload" button at the bottom.

My file has no problems yet the deposition system can not proceed with file replacement. What do I do?

In cases when the new files have no errors, but the system cannot process them because of the major changes made (for instance, change to the number of polymer chains or chain ids) a button called "Clear deposition data" at the bottom of the page should be used to reset the entry. Clicking this button will result in the deletion of much of the information associated with your deposition and will require that you re-enter all the deleted information. You should re-upload the coordinate file, select it, define its type, and de-select the coordinate file you are replacing. Click the "Clear deposition data" button. When the system has accepted the new file, you can then proceed to re-enter any metadata that has been deleted in the process.

How can I replace an uploaded file post-submission?

After a submission has been completed, your deposition session (including the "Re-upload files" page) will be locked. Go to the Communication page within the left-hand panel of the deposition interface and send a request to a PDB biocurator to unlock the deposition session. After you have received a message

confirming that the session has been unlocked, you will be able to upload the new file following the steps described in **How can I replace an uploaded file pre-submission?** in this FAQ.

I want to replace only a coordinate file or only experimental data file. How do I proceed?

If only the coordinate file needs to be replaced, upload the new file at the "Re-upload files" page, deselect the previously selected coordinates file and keep other previously uploaded files selected. Similarly, if only experimental data file (for example structure factor file) needs to be replaced, upload the new file at the "Re-upload files" page, deselect the previously selected experimental data file and keep other previously uploaded files selected.

Can I replace the coordinates for my previously released entry and keep the original PDB ID, how to proceed?

Yes, the authors (PIs) of released PDB structures can update the model coordinates while retaining the same PDB accession code, thereby preserving the link with the original publication. For entries deposited via OneDep, depositors should log into the corresponding session at **deposit.wwpdb.org (http://deposit.wwpdb.org/)** and submit the request via the OneDep communication panel. For entries deposited via legacy systems, requests should be initiated by sending an email to **deposit-help@mail.wwpdb.org (mailto:deposit-help@mail.wwpdb.org)** and including the PDB code in the subject and body of the email. Once submitted, the revised model will be processed by wwPDB biocurators and the updated version released immediately upon depositor's approval. Versioning of PDB entries will be limited to changes in the coordinate files, with no changes permitted to the deposited experimental data. To limit the impact on the wwPDB biocuration resources, PDB versioning is currently restricted to one replacement per PDB entry per year, and three entries per Principal Investigator per year.

Communication

How do I get help during and after deposition?

If you have any questions about deposition, you can log in to your deposition session and use the Communication page to communicate with wwPDB annotation staff. The Communication page is available toward the bottom of the left menu in the Deposition Tool.

How can I provide feedback about the system in general?

We welcome your feedback on the Deposition System and on the information provided in the FAQ. Use "Communication" web form at deposition interface to let us know if the available instructions need clarification or if you have encountered any problems during deposition.

Deposition and Release Policies

The paper has been published, why the corresponding structure is not released?

Visit our PDB release policy here (/documentation/policy#toc_release).

Electron Microscopy

Where can I find EM data deposition and access information?

Visit **how to deposit EM MAP (/deposition/tutorial#electron-microscopy-volume-map-depositions)** or **EM Data Resource (https://www.emdataresource.org/faq.html)** for other EM data depositions and access questions.