

I. EM Deposition & Retrieval Tutorial

Deposition

Workshop participants can view a completed deposition and can create practice depositions at the demo site: <http://emdep-staging.rutgers.edu>. To initiate a *bona fide* joint submission of a map + fitted model, use one of the map deposition servers listed at <http://www.emdatabank.org/deposit.html>.

1. View a completed deposition (example: transcription initiation complex):

Go to the demo site: <http://emdep-staging.rutgers.edu>

click on “start session”

click on “continuation”

enter submission reference number: 60040 / password: emdb

Use the left-hand menu to navigate the map deposition entry pages.

To view entry pages for the coordinate deposition, first go to the “Deposit Coordinates at the PDB” page. Scroll down to bottom of the page and click on the blue-underlined link.

2. Create your own practice deposition:

Go to the demo site: <http://emdep-staging.rutgers.edu>

click on “start session”

click on “new submission”

Follow the instructions in the “CryoEM Map + Model Deposition Guide” on the following pages. This guide is also available online on the EMDataBank.org site under the “Help” tab.

Important: Please do not upload map files larger than ~25 Mbyte to the practice deposition server. **Practice depositions will not generate valid EMDB or PDB entries.** You may receive one or more emails indicating that your practice entry has been assigned an id; please disregard.

Retrieval

3. Find EM Maps and Models using the emdatabank.org site:

- New map entries are listed on the front page, updated weekly.
- “Search” tab provides links to USA (RCSB) and UK (PDBe) EMSEARCH services, also alpha version of EMDB full text search at PDBe.
- Search results point to atlas pages that provide summary information and details for map entries and links to fitted PDB models.

4. Search EMDB directly using UCSF Chimera (from v. 1.4)

- Under “file” menu, select “fetch by id,” click “EMDB” or “EMDB & fit PDBs” and enter a search term in the search box at bottom of the window (example search terms: Rossmann, ribosome). You can also directly fetch a map with fitted PDB entries by entering the numerical part of the EMDB id (XXXX of EMD-XXXX).

5. Find EM PDB entries using Search Services of wwPDB partners (RCSB, PDBe, PDBj)

II. CryoEM Map + Model Deposition Guide

This is an overview of the steps required to make a joint map + fitted coordinate model deposition to the EM DataBank (EMDB) and Protein Data Bank (PDB). Please contact help@emdatbank.org with any questions.

1. [Preparation](#)
2. [Start an EMDEP session](#)
3. [Create the EMDB Map Deposition](#)
4. [Depositing Fitted Model Coordinates](#)
5. [What happens after EMDB map + PDB model submission](#)

1. Preparation

You'll want to have the following items on hand.

- **Map File:** One map file is allowed per EMDB entry. Accepted map upload formats are MRC, Spider, and CCP4. Check that pixel sizes and origin are correct. File uploads can be compressed (tar, zip, gzip).
- **Model File:** Atomic coordinates can be provided in PDB or mmCIF format. The coordinates should be in the same experimental coordinate frame as the map. Detailed information about acceptable formats and annotation and processing policies can be found at <http://www.wwpdb.org/docs.html>.
- **Experiment Info:** Basic information about your experiment, including a description of the assembly, specimen preparation, microscope imaging, image processing and reconstruction, and coordinate fitting. This is the same information you would include in a manuscript.
- **External database ids:**
 - GO -- gene ontology -- <http://genontology.org>
 - INTERPRO -- protein sequence family -- <http://www.ebi.ac.uk/interpro>
 - PDB -- reference coordinates used for fitting -- <http://wwpdb.org>
 - ICTVdB -- virus classification -- <http://www.ncbi.nlm.nih.gov/ICTVdb>
 - PUBMED -- published citation -- <http://www.pubmed.gov>
- **Optional:** Masks, Images (tif, jpg, png), Structure Factors, Layer-line data, Fourier Shell Correlation xml, Harvest xml.

2. Start an EMDEP session

EM maps and their fitted coordinate models can be submitted to joint deposition sites at PDBe (UK) or RCSB-PDB (USA). At these sites, a model can be deposited to PDB after the map is submitted to EMDB with automatic transfer of experiment metadata (sample description, microscope type, etc). Go to <http://emdatbank.org/deposit.html>, click on "Deposit" and select the deposition site you wish to use. To begin, click on "Start Session."

Select "new deposition", or select "based on previous submission" if the experiment is closely related to a prior deposition. On the next page you are assigned an EMDEP session id and you are asked to provide a password. Record both the id and password in a safe place to enable future access to your deposition session data.



3. Create the EMDB Map deposition

The map deposition is completed by filling in a series of pages (forms). Pages that need to be completed are shown in the left hand menu with red arrows (see image at left). When all required information in a page is saved, the symbol on the left hand menu changes from a red arrow to a green circle. You can then move to the next page, until all pages are completed. You can also go back and change answers on completed pages. Help text can be displayed for each individual data item by clicking on the item title.

- **Depositor Info: Supply YOUR contact info, not the info of your PI.** If you are a prior depositor, type in your email address and press “save” to retrieve your contact info on file. Please provide and/or update your contact information.
- **Instructions to EMDB:** Choose the release instructions for your deposition—release immediately, hold until publication, or hold for 1 year. Indicate if the entry replaces a prior deposition, and provide any additional processing instructions or comments on this page.
- **File Uploads:** On this page, please upload the map for the entry, as well as any associated files (see [step 1, Preparation](#)). Files can be in compressed format. The maximum file size that can be handled through our http server is 1.5 GB. For large files, please notify the processing site annotation staff by email.
- **Title, Author, Citation:** In most cases deposition occurs before publication. Please provide the most complete citation information possible.
- **Sample Details:** Aggregation state is “Icosahedral” for icosahedral single particle reconstructions but “Single Particle” for other point symmetries. Use “Individual structure” for tomograms or subtomogram averages. Fill out a sample component section for each unique sample component. e.g. for an Fab:virus complex, fill out two component sections.
- **Fitting:** Provide the PDBids and chain ids of any reference coordinates used for map interpretation, plus the refinement protocol and other fitting details. For example, if your map describes a virus:receptor complex, provide the PDBids for X-ray structures of virus and receptor used for fitting/interpretation of the map. Note: the final atomic coordinates obtained from the fitting experiment (fitted model coordinates) are deposited later in [step 4, depositing fitted model coordinates](#), below.
- **Submit:** Please review all of the pages of your entry and especially the entry hold instructions before depressing the submit button.

4. Depositing Fitted Model Coordinates

After you have completed the EMDB deposition using EMDEP at either the PDBe or RCSB-PDB sites, a link for depositing model coordinates to PDB will appear in the left-hand menu. At the PDBe site, the link opens an AutoDep session; at the RCSB-PDB site, the link opens an EM-Adit session. In either case, the metadata entered during the map deposition is automatically transferred to the coordinate deposition. Also, the EMD-id assigned to the map is automatically included in the PDB deposition as an associated database entry.

Please keep in mind:

- The fitted coordinates should be deposited in the same frame as the map.
- Coordinates can be either full residue or alpha-carbon/phosphate backbone traces.

The sequence information provided for each protein or nucleic acid entity should include the entire sequence of the imaged material, including any mutations or expression tags. Currently there is one exception to this rule: if the fitted coordinates are from a related species (e.g., chicken actin coordinates obtained from X-ray crystallography are being deposited after fitting them into a fly muscle actin filament), please supply the sequence of the related species (in the example given, this would be the chicken sequence). In every case, the genus/species description for each entity should be that of the imaged sample.

If the structure has regular point or helical symmetry, the coordinates for one asymmetric unit may be deposited along with a set of transformation matrices to build the assembly. For more information about annotation of symmetry information please see <http://emdatbank.org/pdbsymmetry.html>.

5. What happens after EMDB map + PDB model submission

Map deposition: you will receive an automated email from the EMDB deposition site with your session id and the assigned EMD-id. The latter is the public id that should be included in your publication.

Within two weeks you should receive a second email from the annotator handling your entry informing you that your deposition has been curated, and requesting that you review the entry (login via saved deposition id and password as in step 2, selecting “continue session”). If any further changes are needed, please let the annotator know. Otherwise, please reply with approval of the entry. The header for the entry will then be released.

Maps and any associated layer line or structure factor data will be released later, according to your release instructions. Please send your annotator an email with the PubMed id of your publication, when available.

PDB deposition: you will be assigned a PDB id after completion of the coordinate deposition. Maps and models deposited through the joint deposition systems will be annotated/validated together.

Questions? Please take a look at our FAQ (<http://emdatbank.org/faq.html>) or contact us at help@emdatbank.org.