

## Prepare files for PDB deposition

The final PDB file and the cleaned MTZ file are required.

In the PDB files the first lines should be deleted, up to the line written

**REMARK IF THIS FILE IS FOR PDB DEPOSITION: REMOVE ALL FROM THIS LINE UP.**

Only polymer chains should finish with a *TER*, remove all other *TER* present for the ligands or water molecules.

Coordinates may be deposited as either mmCIF or PDB formatted files. We encourage you to use `pdb_extract` to prepare mmCIF formatted file. If you are using a PDB formatted coordinate file, please check the following PDB format requirements prior to file upload:

- A TER record is placed at the end of every polymeric chain.
- TER records are not present within a polymeric chain. Some refinement packages insert extra TER records at gaps within a chain. Please remove the extra TER records.
- No TER records should be included at the end of non-polymer residues such as ions, ligands, or waters.
- PDB format files with misplaced TER records will result in incorrect format translation and data extraction - which may result in data loss during annotation.
- Depositions comprised of multiple models should include MODEL and ENDMDL records. The models should be listed sequentially in columns 11-14.
- If there are alternate conformations in the structure, the alternate conformation indicator must be provided in column 17 of ATOM and HETATM records.
- There should be only one END record at the end of the file.

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