**Supplementary File 1**

1. **Editing a PDB file: removing remarks.** Remove all remarks preceding the protein coordinates.



1. **Editing a PDB file: removing connectivity data.** Remove the connectivity data following the coordinates.



1. **Editing a PDB file: inserting a TER card.** A TER card indicates that a new molecule (protein chain) is to be started. It should also be inserted between the protein and ligand coordinates (if present).



1. **Editing a PDB file: replacing the residue name HIS with HIE, HID, or HIP.**

