

# Protein Repair and Analysis Server: A Web Server to Repair PDB Structures, Add Missing Heavy Atoms and Hydrogen Atoms, and Assign Secondary Structures by Amide Interactions

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## ABOUT KEEPING LIGAND

The default behavior of PRAS is to generate clean PDB structures (neglecting all ligands), since in most MD simulation and molecular docking tasks, the ligand is specially treated. However, if user checks this box, PRAS will keep all non-water ligands in the structure after the repairs. PRAS does not repair ligands and will just append the data as it is in the output file.

**Important!** Modified amino acids (e.g., O-SULFO-L-TYROSINE and SELENOMETHIONINE) whose entries start with “HETATM” will be kept if user checks the box “**keep ligands**”. Because PRAS does not repair ligands, these modified amino acids would cause atom clashes (PRAS does not consider their position when adding missing H-atoms). To resolve these clashes, delete the entries for ligands bonded covalently to the protein.

Note that if user selects a particular chain, then PRAS will keep only the ligand bound to that chain (if there is). If user checks this box but there happens to be no ligand in the PDB structure, PRAS will ignore user’s selection and continue with the repairs.