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 ROTAMERS

In x-ray crystallography, crystallographers use the occupancy to evaluate the amount of each conformation that is detected in the crystal. Sadly, most molecular modelling and visualization software programs have no mechanism to distinguish rotamers, and simply display both on top of each other. The crystal structure of Crambin (PDB ID: 1CBN) in **Fig. 1** shows Thr, Glu and Arg rotamers displayed on top of each other, showing spurious bonds. In molecular dynamics simulation or docking, a researcher will have to use one conformation and since rotamers are studied for various reasons, PRAS users can decide which rotamer to keep by selecting appropriate option in the drop-down menu. Subsequently, the server assigns full occupancy to the rotamer the user chooses to study and ignores the rest.

It should be noted that rotamer does not occur in every PDB file. PRAS provides this option just in case there are rotamers.
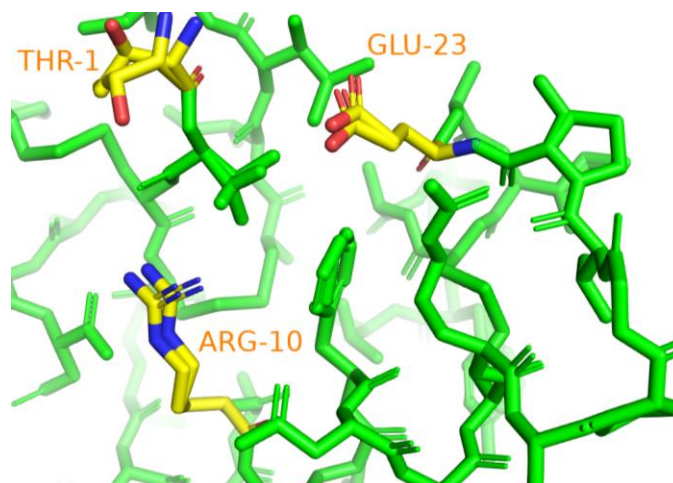

Fig.1. Crystal structure of Crambin (PDB ID: 1CBN). Image created with PyMOL

ABOUT MICROHETEROGENEITY OR POINT MUTATION

Sequence microheterogeneity or point mutation is present in a PDB file when two residues with partial occupancy are assigned the same position or sequence number. This can be seen in **fig. 2** where Pro and Ser both occupy the same position. The hugely popular PyMOL software program has no mechanism to distinguish point mutations, and simply displays both on top of each other, showing spurious bonds as a consequence. The PRAS server deals with microheterogeneity by assigning full occupancy to the amino acid residue the user chooses to study and ignores the rest.

It should be noted that point mutation does not occur in every PDB file. PRAS provides this option just in case there is point mutation.
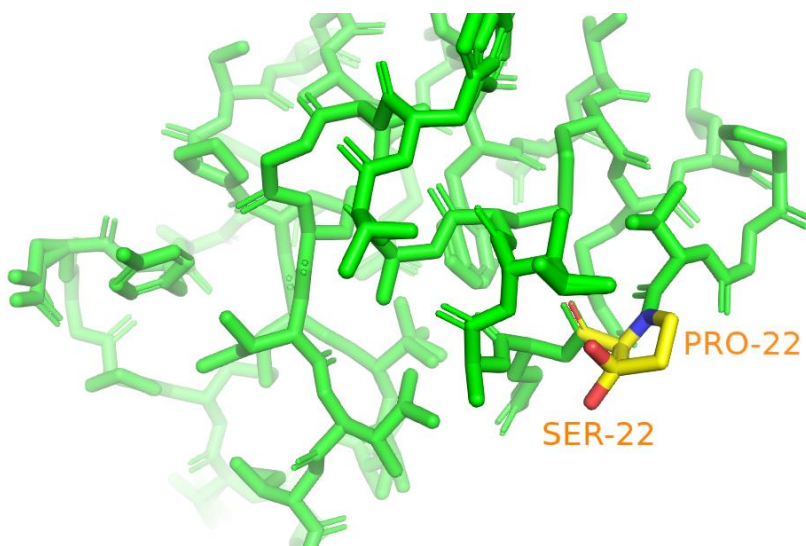

Fig.2. Crystal structure of Crambin (PDB ID: 1CBN). Image created with PyMOL.