

# 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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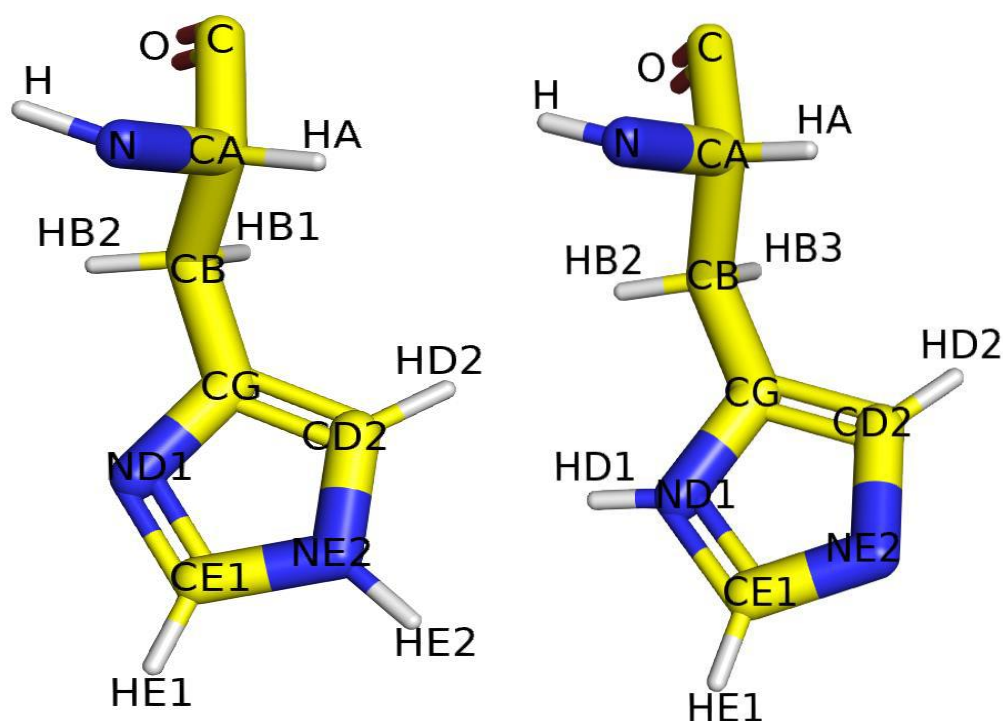
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## HISTIDINE PROTONATION

Histidine (HIS) side-chain pKa is approximately 6.0 – 6.1 and at the pH of 7 assumed by PRAS, a fraction of the residue may be charged. Depending on the hydrogen-bonding network or local environment, the neutral side-chain has a hydrogen attached on either NE2 or ND1 as shown in Fig. 1.

For a neutral histidine side-chain, PRAS assigns one hydrogen atom to NE2. If user checks the box “Consider histidine protonation”, PRAS protonates 20% of total HIS residues on both NE2 and ND1, otherwise all HIS side-chain will remain neutral. PRAS does not consider the hydrogen-bonding network due to ambiguities in X-ray crystal structures. HIS residue can adopt a number of rotameric states (flipped HIP, flipped HID, or flipped HIE). Alternatively, user can download the source code and decide how many HIS to protonate or whether to place the hydrogen atom(s) on NE2 or ND1 or both.



**Fig.1.** A representation of HIS-337 of BSA (PDB code: 4f5s). The image was created using PyMOL