# SUPPORTING INFORMATION

## N-H…N Hydrogen Bonds Involving Histidine Imidazole Nitrogen Atoms: A New Structural Role for Histidine Residues in Proteins

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## Figure S1

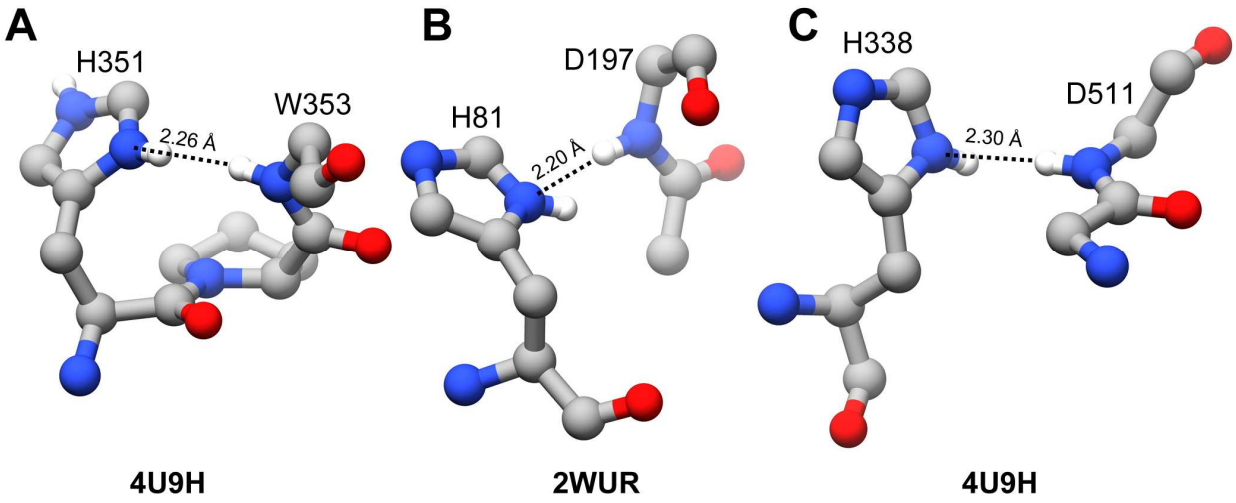


**Figure S1:** The three examples of histidine residues from ultra high-resolution structures that satisfied the hydrogen bond geometric criteria for N-H…Nδ/Nε type of interaction. All three examples resulted in positive interaction energies in quantum chemical calculations (see Table 1 in the main text). In all these three cases, the Nδ atom of imidazole ring is protonated and this protonated nitrogen is also close to main-chain N-H hydrogen atom. The unique PDB IDs and the residue numbers are indicated in the figure.

## Figure S2

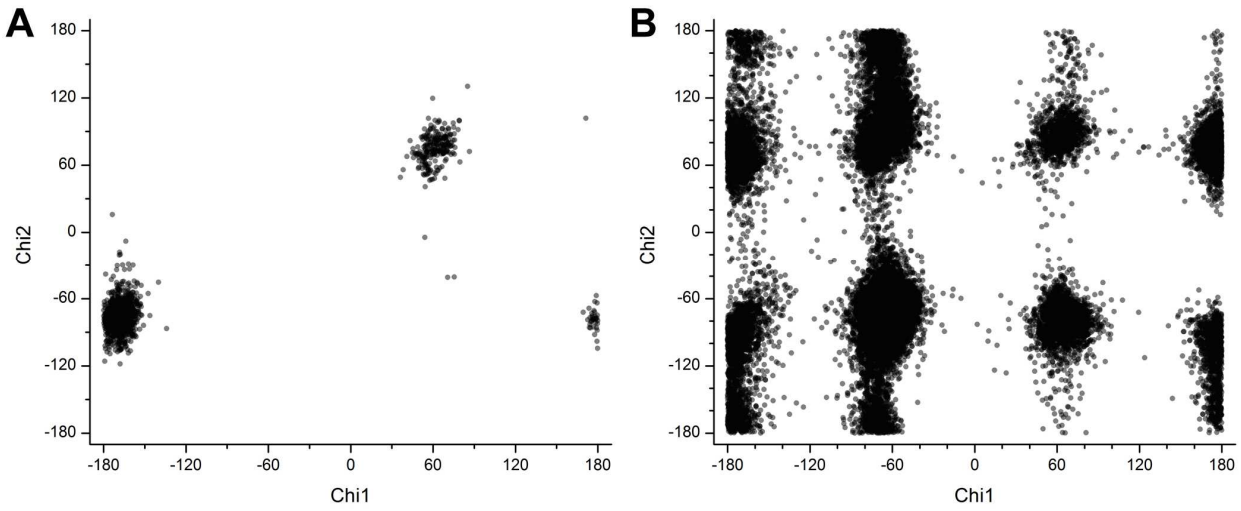


**Figure S2:** Plot of $\chi 1$ versus $\chi 2$ distribution of histidine side-chain dihedral angles for (A) all histidine residues participating in $N_{i+2}$-$H_{i+2}$…$N\delta_i$/$N\varepsilon_i$ hydrogen bonds and (B) for all histidine residues whose imidazole nitrogen is not involved in N-H…N hydrogen bonds.