

Interplay of Hydrogen Bonds and $n \rightarrow \pi^*$ Interactions in Proteins

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Supplementary Information

Supplementary Figure 1

Secondary structure classification of (A) local and (B) non-local Asn groups. Those testing positive for $n \rightarrow \pi^*$ interactions are shown in red; those that test negative shown in black. Secondary structure classifications are those defined by Kabsch and Sander¹ and implemented in Promotif².

Supplementary Figure 2

A copy of Figure 3 in the main text showing the selection of Asn examples from the PDB chosen for NBO analysis.

Supplementary File 1 – ja2013-106122_SI_local_coords_txt.zip. A .ZIP text file archive of all starting local Asn conformations in Gaussian format for NBO calculations.

Supplementary File 2 – ja2013-106122_SI_nonlocal_coords_txt.zip. A .ZIP text file archive of all starting non-local Asn conformations in Gaussian format for NBO calculations.

Supplementary File 3 – ja2013-106122_SI_Data.xlsx. Excel spreadsheet of hydrogen bonding and $n \rightarrow \pi^*$ interaction parameters extracted from PDB files and NBO analyses.

Supplementary Information References

1. Kabsch, W.; Sander, C., Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features. *Biopolymers* **1983**, *22* (12), 2577-2637.
2. Hutchinson, E. G.; Thornton, J. M., PROMOTIF--a program to identify and analyze structural motifs in proteins. *Protein Sci.* **1996**, *5* (2), 212-220.



