Supplement of

Anomalous amide proton chemical shifts as signatures of hydrogen bonding to aromatic sidechains

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| Reason for Exclusion                                      | # Excluded | Examples (BMRB ID, PDB ID) |
|----------------------------------------------------------|------------|-----------------------------|
| DNA/RNA entries, entries with ligands, oligomers and protein complexes | 1767       | (50411, 7JK8)               |
| Severe residue index mismatch between PDB and BMRB       | 1199       | (50842, 7MC3)               |
| Restraint file not in ReBoxitory                         | 716        | (36368, 7CQ1)               |
| No distance restraints in restraints file                | 190        | (50264, 6Z0H)               |
| No aromatic residues in sequence                         | 152        | (50202, 6YFY)               |
| >3500 distance restraints *                               | 151        | (36176, 5ZMR)               |
| Restrained amide-aromatic pairs > 8Å apart *              | 136        | (36008, 5GHD)               |
| Unable to match residues from structure to restraints    | 99         | (36097, 5XR1)               |
| mmCIF file not in ReBoxitory                             | 18         | (50886, 7MLL)               |
| STR file not in ReBoxitory                               | 7          | (36326, 6M6K)               |
| Empty restraint file                                     | 3          | (25068, 2MRC)               |
| Misformatted restraint file                              | 3          | (4540, 1NLA)                |
| Miscellaneous                                            | 7          | (2NBN, 25984), (2M7V, 19214), (2LK9, 17985), (2KSI, 16665), (1SF0, 6187), (1RFH, 6059), (1P9F, 5864) |

Table S1: Reasons for the exclusion of BMRB/PDB entries from the analysis. Most reasons make analysis difficult (e.g. index mismatches) or impossible (e.g. no restraint file). Reasons with a * were implemented to maintain quality. An entry having > 3500 distance restraints or restraints between amide-aromatic pairs that were > 8 Å apart was in some cases indicative of deeper problems with the restraint assignments, such as restraints being assigned between all atoms.