

Reason for Exclusion	# Excluded	Examples (BMRB ID, PDB ID)
DNA/RNA entries, entries with ligands, oligomers and protein complexes	1756	(50269, 7JXG)
Severe residue index mismatch between PDB and BMRB	1194	(50268, 6XB7)
No restraint file	710	(50015, 6YJ0)
No distance restraints in restraints file	190	(50263, 6Z0G)
No aromatic residues in sequence	152	(50202, 6YFY)
>3500 distance restraints *	151	(36176, 5ZMR)
Restrained amide-aromatic pairs > 8Å apart *	141	(36000, 5B7A)
Residue index mismatch between restraint and structure files	81	(36097, 5XR1)
Structure not yet released in PDB	21	(50842, 7MC3)
BMRB entry only exists in NMR-STAR 2.0	6	(19704, 2MJ4)
Empty restraint file	4	(25068, 2MRC)
Misformatted restraint file	3	(4540, 1QTG)
Miscellaneous	15	(34476, OTWG), (25510, 2N00), (25508, 2MZY), (25499, 2MZT), (25497, 2MZR), (25493, 5ODD), (25489, 2MZI), (25496, 2MZQ), (17985, 2LK9), (6187, 1SF0), (25984, 2NBN), (5864, 1P9F), (6059, 1RFH), (16665, 2KSI), (19214, 2M7V)

Supp. Table 1: 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.