Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Microscopic Significance of Hydrophobic Residues in the Protein-Stabilizing Effect of Trimethylamine N-oxide (TMAO)

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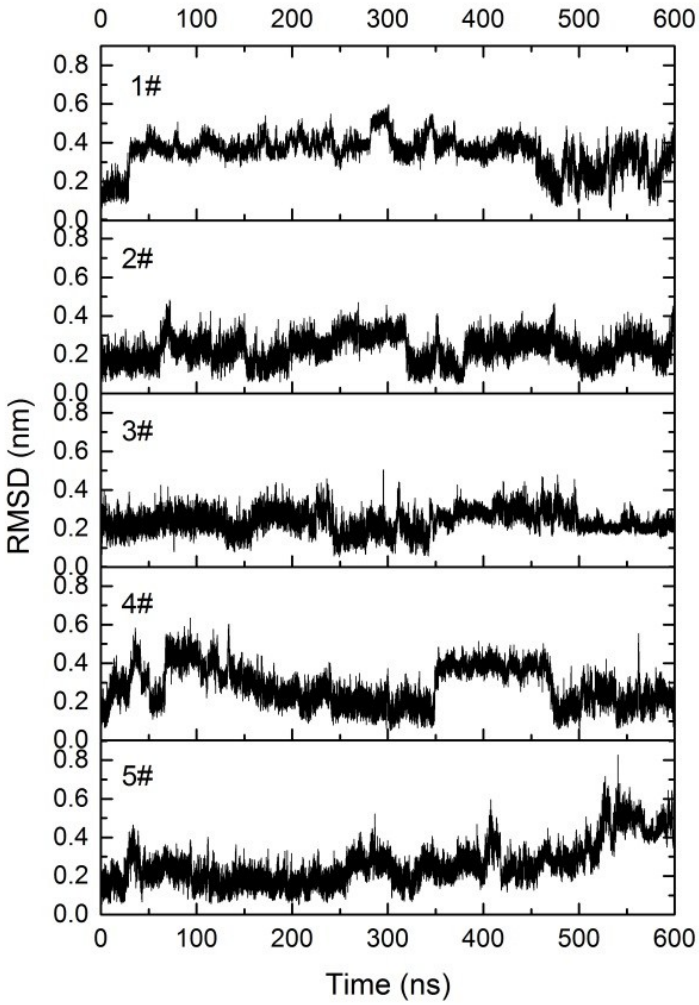

Figure S1. Root mean square deviation (RMSD) of HP35 backbone heavy atoms with reference to the starting structure in pure water (five parallel trajectories).

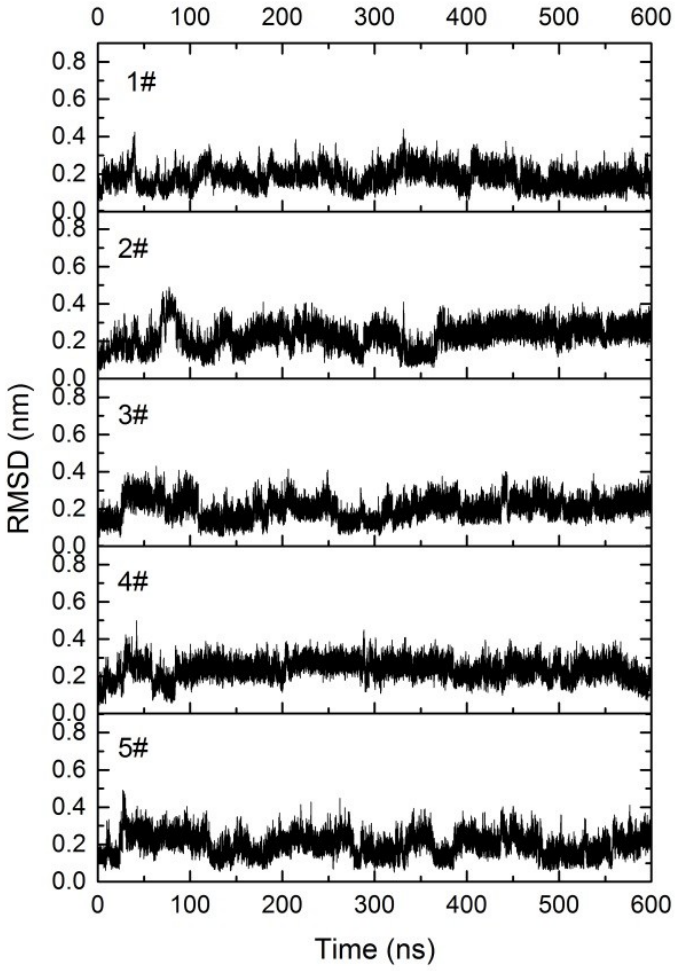

Figure S2. RMSD of HP35NN backbone heavy atoms with reference to the starting structure in pure water (five parallel trajectories).

Table S1. Final RMSD values averaged over the last 5 ns of ten trajectories for HP35 and HP35NN in urea solution. The results are expressed in descending numerical order.

	Trajectory No.	RMSD(nm)		Trajectory No.	RMSD(nm)
HP35	1#	1.90	HP35NN	1#	1.74
	2#	1.51		2#	1.23
	3#	1.50		3#	0.99
	4#	1.14		4#	0.96
	5#	0.88		5#	0.96
	6#	0.86		6#	0.90
	7#	0.82		7#	0.81
	8#	0.76		8#	0.79
	9#	0.68		9#	0.79
	10#	0.39		10#	0.42

Table S2. Final RMSD values averaged over the last 5 ns of ten trajectories for HP35 and HP35NN in urea+TMAO mixed solution. The results are expressed in descending numerical order.

	Trajectory No.	RMSD(nm)		Trajectory No.	RMSD(nm)
HP35	1#	1.39	HP35NN	1#	0.82
	2#	1.24		2#	0.72
	3#	1.01		3#	0.52
	4#	0.83		4#	0.37
	5#	0.80		5#	0.37
	6#	0.54		6#	0.34
	7#	0.43		7#	0.32
	8#	0.42		8#	0.31
	9#	0.34		9#	0.29
	10#	0.33		10#	0.21

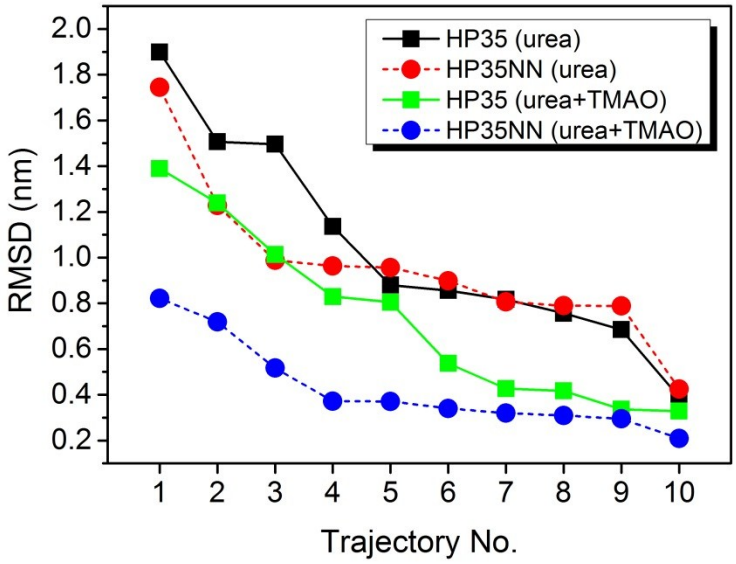

Figure S3. Final RMSD of protein backbone heavy atoms after simulation with reference to the starting structure, data can be found in Table S1 and S2.

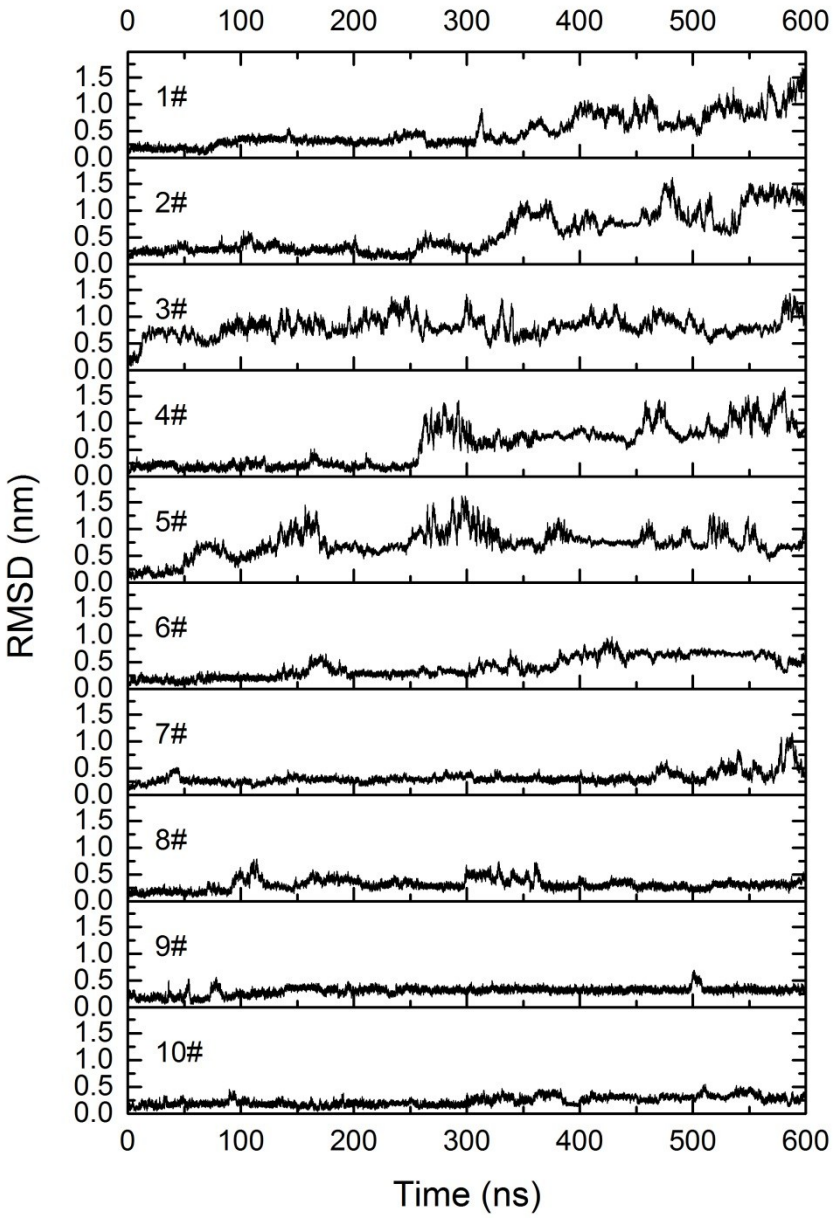

Figure S4. RMSD of HP35 backbone heavy atoms with reference to the starting structure in urea+TMAO mixed solution (ten parallel trajectories).

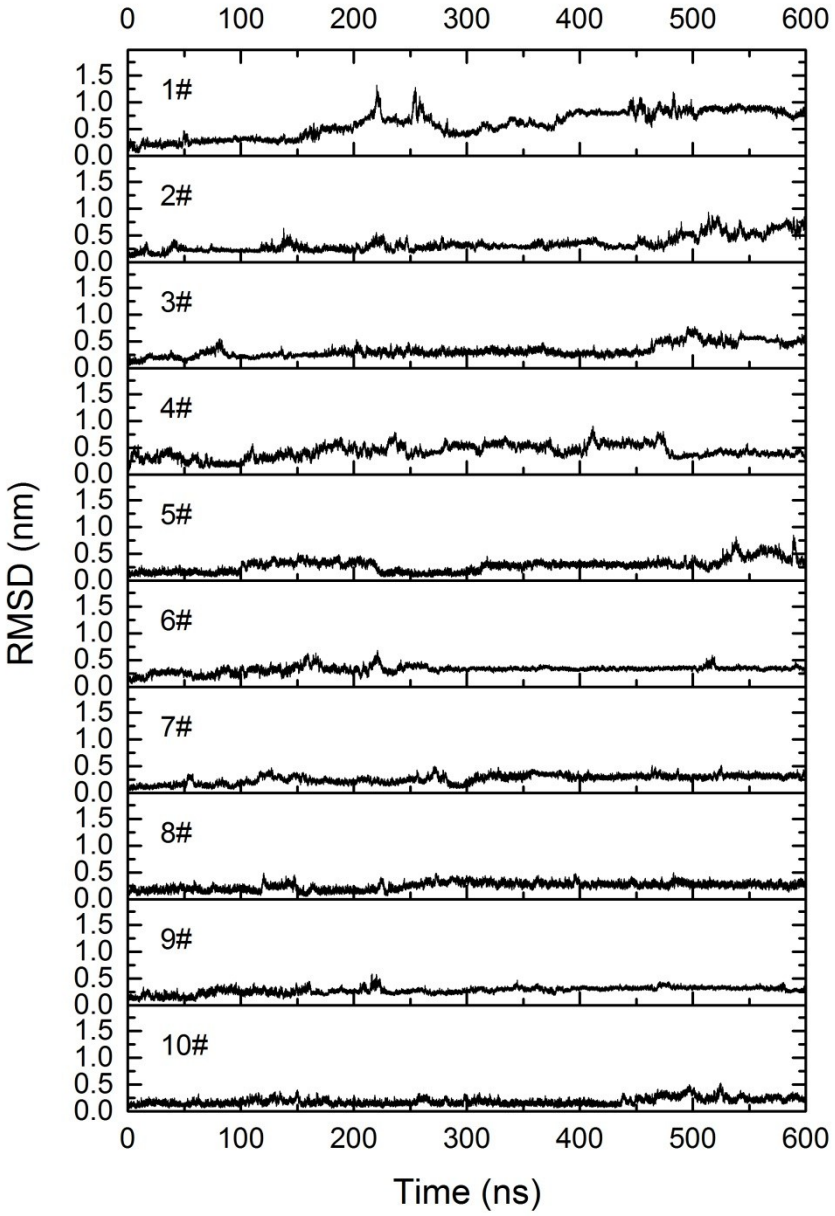

Figure S5. RMSD of HP35NN backbone heavy atoms with reference to the starting structure in urea+TMAO mixed solution (ten parallel trajectories).

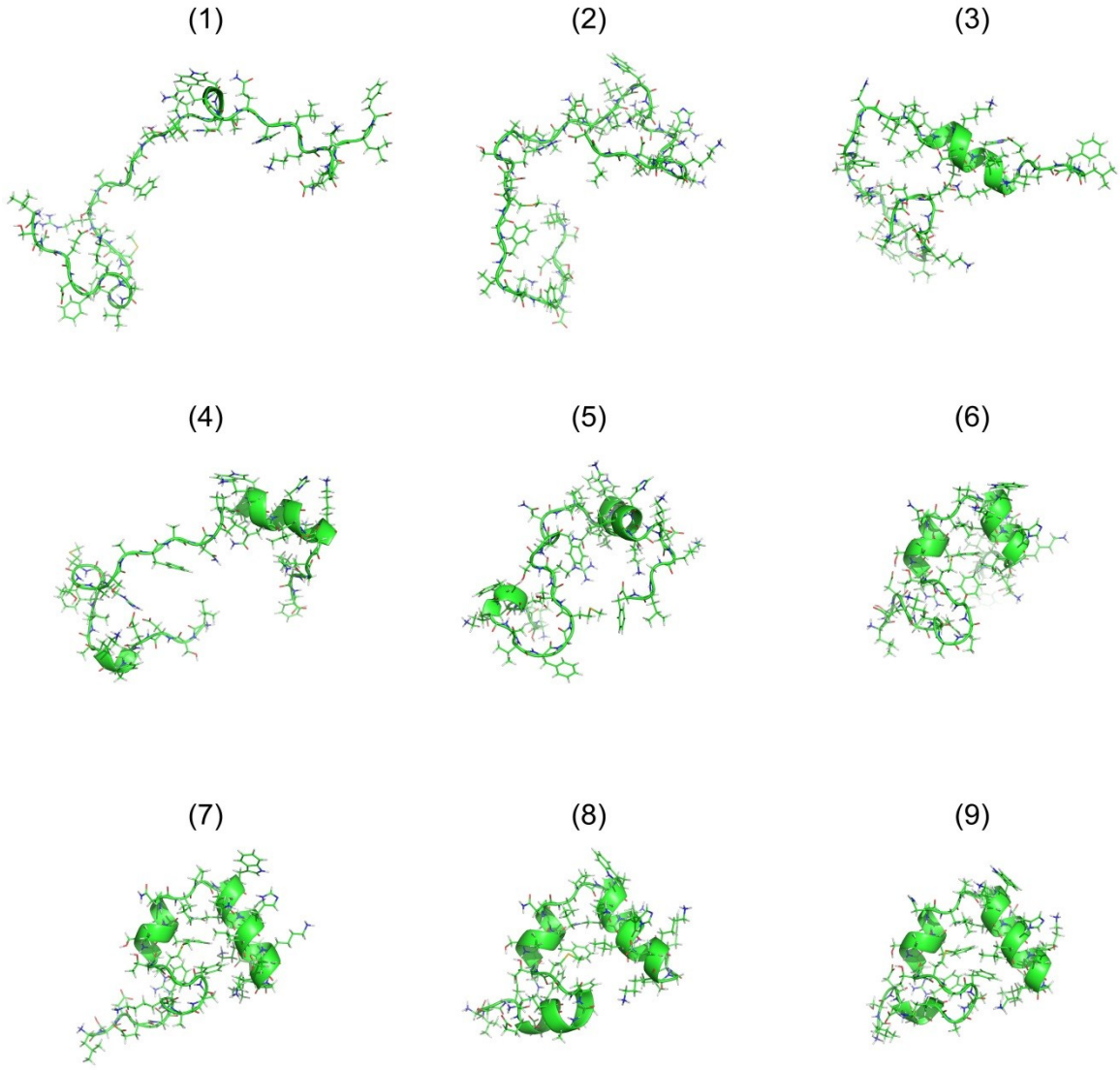

Figure S6. The final structures (after 600 ns simulation) of HP35 in urea+TMAO mixed solution for trajectory 2-10 labelled in Table S2.

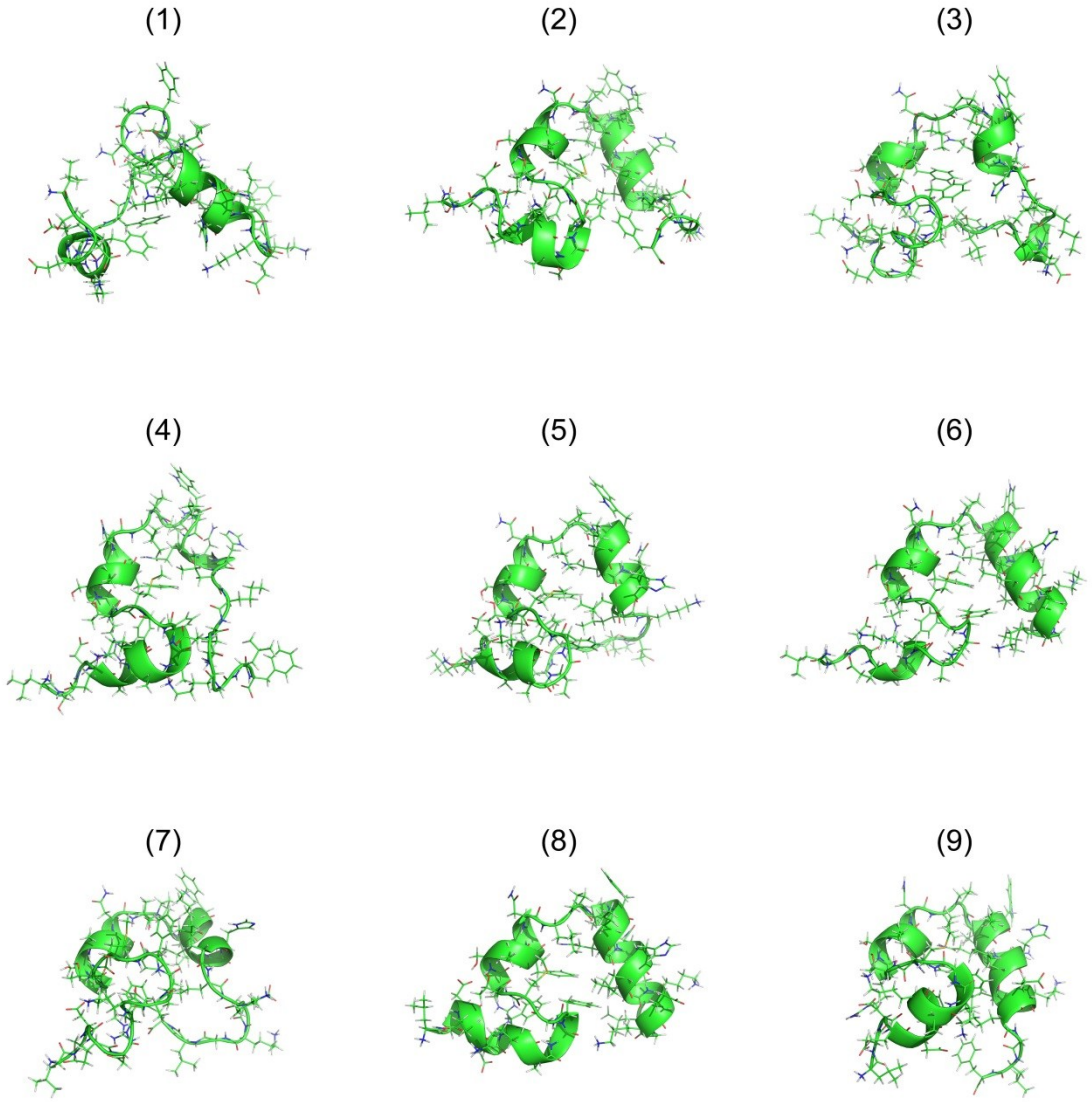

Figure S7. The final structures (after 600 ns simulation) of HP35NN in urea+TMAO mixed solution for trajectory 2-10 labelled in Table S2.