

Electronic Supplementary Information

Comparison of hydration behavior and conformational preferences of Trp-cage mini-protein in different rigid-body water models

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Table SI-1 Order parameters for temperatures below and above the unfolding transition for Trp-cage solvated with different water models. Extended simulations upto 50 ns are denoted by asterisk.

	T_{Target} (K)	$\langle T \rangle$ (K)	RMSD (Å)	R_{core} (Å)	R_g (Å)	N_{nc}
mTIP3P	450	449.6	2.6 (0.2)	5.2 (0.03)	7.5 (0.02)	29 (1)
	450*	449.0	2.6 (0.1)	5.3 (0.02)	7.5 (0.01)	29 (0.2)
	460	458.9	5.6 (0.5)	7.3 (0.3)	8.7 (0.2)	22 (1)
	460*	461.9	5.7 (0.4)	7.8 (0.3)	8.3 (0.1)	19(1)
TIP4P	460	462.0	2.6 (0.1)	5.3 (0.1)	7.5 (0.01)	29 (0.1)
	460*	464.3	2.6 (0.1)	5.3 (0.1)	7.5 (0.02)	29 (0.1)
	470	471.4	5.4 (1.0)	7.6 (0.9)	8.8 (0.5)	21 (3)
	470*	478.2	6.3 (0.4)	8.5 (0.4)	9.2 (0.2)	19 (1)
TIP4P-Ew	420	417.2	2.4 (0.04)	5.1 (0.02)	7.5 (0.01)	29 (0.1)
	420*	420.3	2.4 (0.03)	5.1 (0.01)	7.5 (0.01)	29 (0.1)
	430	426.9	7.4 (0.1)	8.3 (0.4)	9.1 (0.3)	14 (1)
	430*	429.8	7.3 (0.09)	8.5 (0.2)	9.0 (0.1)	15 (1)

Table SI-2 Different order parameters for the variants of U1 state solvated with different water models around 250 K. U1 refers to ensemble averaged values over 20 ns run length while U1* refers to ensemble averaged values by extending the former run upto 100 ns. U1a and U1b refers to additional unfolded ensembles around 250 K obtained after repetitive quenching from the same initial configuration at respective high temperatures. Helical content is found to be zero for all these states in all the water models.

Ensemble	D_{end} (Å)	R_g (Å)	RMSD (Å)	N_{nc}	SASA (Å ²)	R_{core} (Å)	RMSD _{core} (Å)	SASA _{core} (Å ²)	
mTIP3P	U1	21.5 (0.6)	11.6 (0.3)	9.2 (0.2)	10 (0.2)	2636 (33)	12.1 (0.4)	10.0 (0.4)	1283 (6)
	U1*	22.4 (0.3)	11.6 (0.1)	9.2 (0.1)	10 (0.2)	2607 (10)	12.5 (0.1)	10.4 (0.1)	1297 (2)
	U1a	20.3 (1.6)	11.6 (0.8)	9.0 (0.6)	10 (0.4)	2616 (36)	13.0 (0.9)	10.8 (1)	1229 (7)
	U1b	21.2 (1.2)	11.2 (0.3)	8.9 (0.3)	15 (0.2)	2587 (17)	10.8 (0.5)	9.1 (0.5)	1182 (12)
TIP4P	U1	19.1 (1.6)	11.9 (0.3)	9.9 (0.3)	6 (0.2)	2768 (32)	12.3 (0.3)	10.6 (0.3)	1296 (3)
	U1*	20.6 (0.6)	12.2 (0.2)	9.9 (0.1)	7 (0.1)	2823 (12)	12.5 (0.2)	10.8 (0.2)	1281 (3)
	U1a	19.2 (0.9)	12.7 (0.3)	9.9 (0.3)	8 (0.2)	2794 (26)	12.5 (0.3)	10.5 (0.3)	1288 (5)
	U1b	23.3 (1.2)	12.2 (0.3)	9.8 (0.2)	12 (1)	2713 (25)	11.6 (0.5)	9.9 (0.5)	1203 (7)
TIP4P -Ew	U1	27.0 (1)	12.9 (0.3)	10.0 (0.2)	3 (1)	2819 (18)	12.9 (0.3)	10.6 (0.3)	1287 (3)
	U1*	23.6 (1)	13.1 (0.1)	10.1 (0.2)	4 (2)	2853 (10)	13.2 (0.2)	10.9 (0.2)	1258 (6)
	U1a	24.0 (1.4)	12.4 (0.3)	9.9 (0.4)	9 (0.2)	2792 (14)	13.6 (0.4)	11.5 (0.5)	1295 (2)
	U1b	28.7 (1)	13.0 (0.2)	9.8 (0.2)	6 (0.3)	2861 (18)	13.6 (0.2)	11.3 (0.3)	1300 (3)