Supporting Information: Rotational Dynamics of Proteins from Spin Relaxation Times and Molecular Dynamics Simulations

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S1 ~~Supplementary Figures~~Mean square angle deviations of *Pa*TonB-96 simulated with tip4p water model

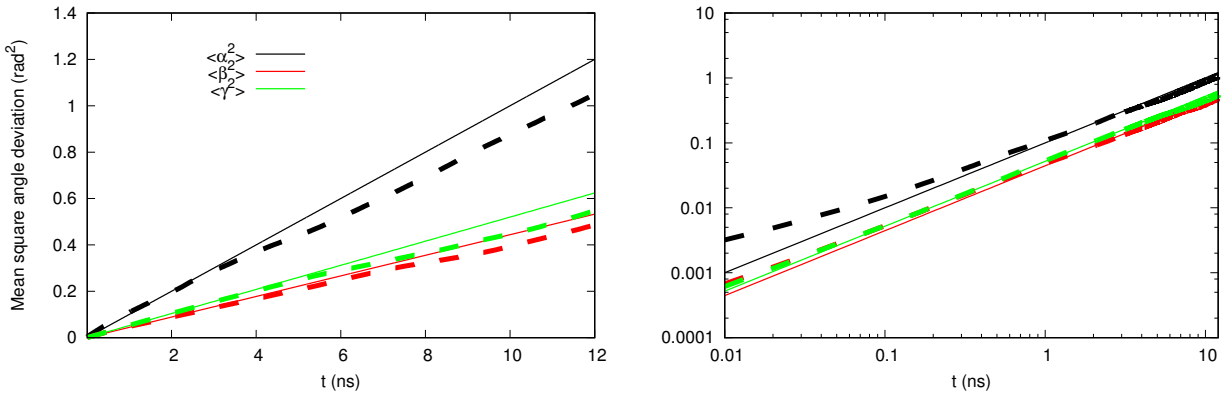

Figure S1: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 310K. The data shown with linear (left) and logarithmic scale (right).

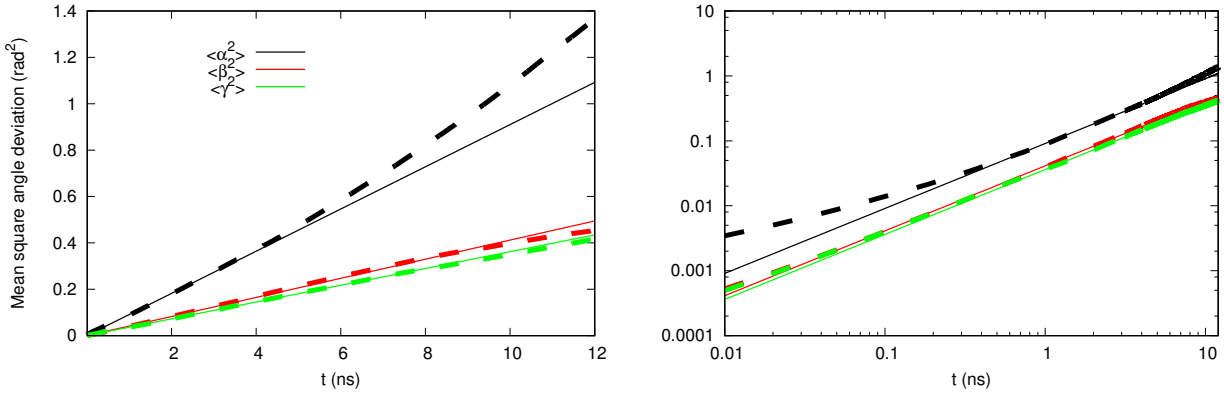

Figure S2: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 298K. The data shown with linear (left) and logarithmic scale (right).

S2 ~~Supplementary table~~Accuracy of the scaling factors for rotational diffusion

Accuracy of the spin relaxation calculations and scaling factors for rotational diffusion were esimated by running three replicas of *Hp*TonB-92 and *Pa*TonB-96 simulations with tip3p. In the first replica, the initial configuration was the lowest energy conformation from the NMR structure bundle. In the second and third replicas, the starting configurations were randomly selected from the bundle. Spin relaxation times calculated from the replicas are compared with the experimental data in Figs. S3 and S4.

General agreement between the calculated spin relaxation times and experiments is essentially similar for all the replicas of both proteins. Optimal scaling factors are also

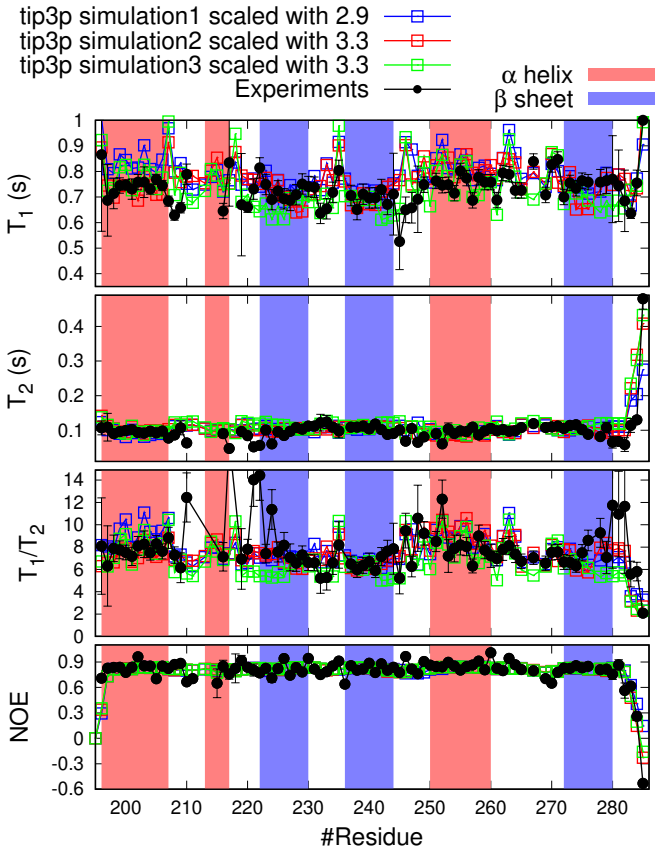

Figure S3: ^{15}N spin relaxation times for *Hp*TonB-92 from experimental data (circles) and MD simulations with different initial configurations (squares).

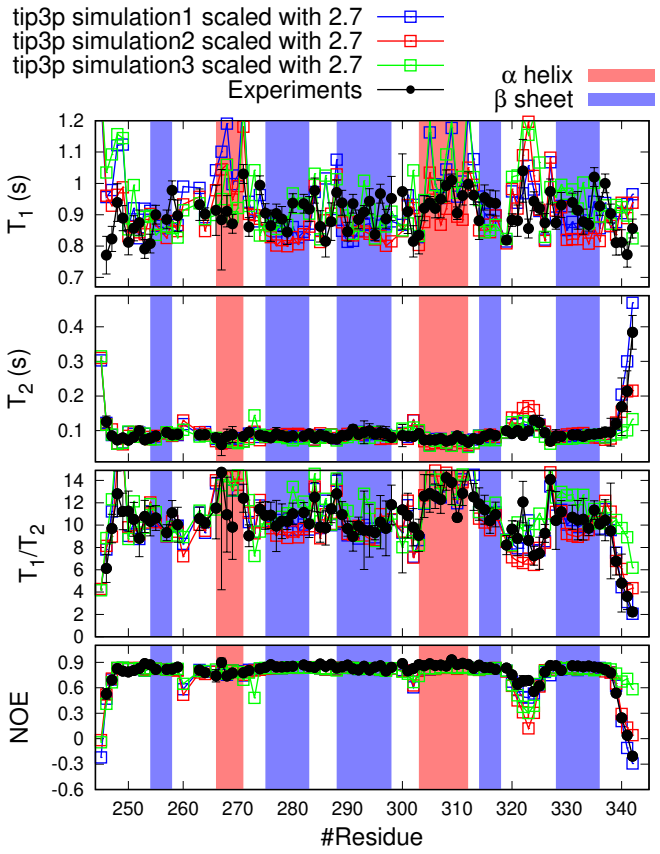

Figure S4: ^{15}N spin relaxation times for *Pa*TonB-96 from experimental data (circles) and MD simulations with different initial configurations (squares).

the same for different replicas, except for the simulation1 of *Hp*TonB-92 which gives slightly lower scaling factor than the other two replicas. Optimal values of the scaling factors for rotational diffusion from different simulations are summarized in Table S1. The scaling factors for simulations with tip3p water model vary between 2.7–3.3, while the scaling factors for simulations with tip4p, OPC4 and SPC/E water models are closer to 1. The results are in line with the self-diffusion coefficients of water calculated from different water models [1], also shown in Table S1.

Table S1: Scaling factors used to correct the overall rotational diffusion coefficients for different proteins simulated with different water models. [a] **CMB64 protein from *Spirochaeta thermophila*** [b] **Calcium recoverin was 12 residues shorter in simulations than in experiments.** [b] [c] **Ratio of isotropic rotational diffusion coefficients from simulations and experiments from Ref. 2.** [c] [d] **Ratio of simulated and experimental self-diffusion constant of water calculated from Ref. 1.**

	tip3p	tip4p	OPC4	SPC/E
*Hp*TonB-92	2.9 – 3.3	1.0	-	-
*Pa*TonB-96	~~-~~2.7	1.2	-	-
~~CBM-64~~ *St*CBM64[a] [3]	-	-	1.3	-
65K C-RRM [4]	-	1.0	-	-
Calcium recoverin[a] [b] [5]	3.2	-	-	-
GB3[b] [c]	-	1.1	-	1.3
Ubiquitin[b] [c]	2.7	1.1	-	1.1
Binase[b] [c]	-	-	-	1.2
Lysosome[b] [c]	2.7	-	-	1.3
Water self-diffusion[c] [d]	2.4	1.1	1	1.3

References

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