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

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S1 Supplementary Figures

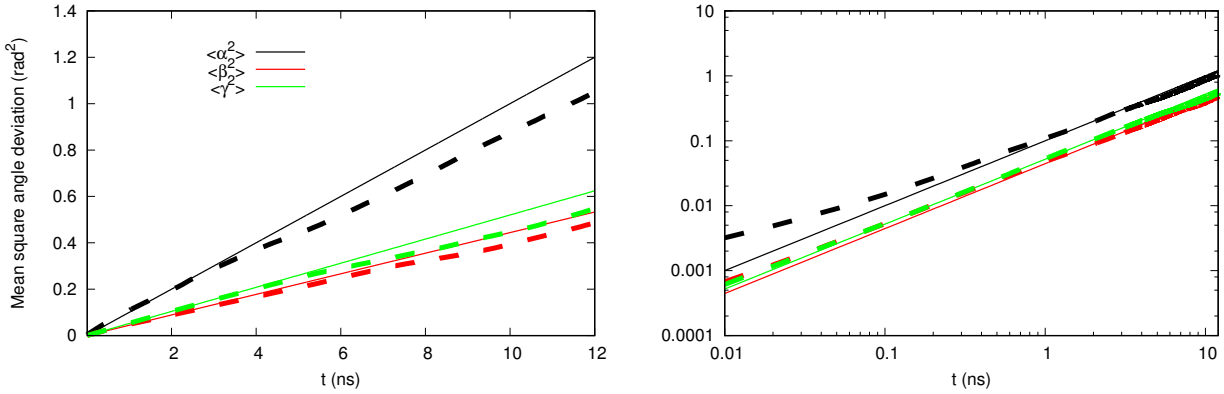

Figure S1: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 310K. The data shown with linear (left) and logarithmic scale (right).

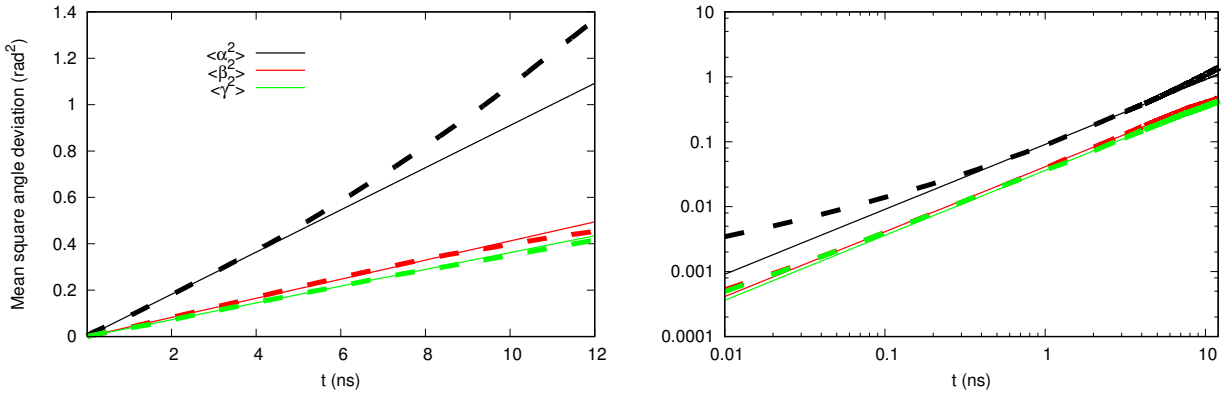

Figure S2: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 298K. The data shown with linear (left) and logarithmic scale (right).

S2 Supplementary table

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

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

References

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