

Supporting Information:

**Rotational dynamics of proteins from spin
relaxation times and molecular dynamics
simulations**

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S1 Supplementary Figures

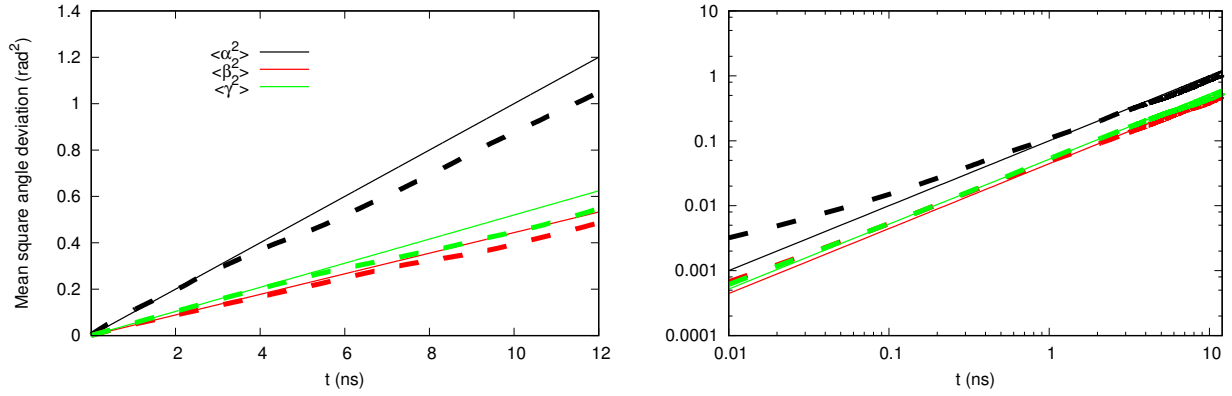


Figure S1: Mean square angle deviations of inertia tensor axes calculated from *PaTonB-96* simulation with tip4p water model at 310K. The data shown with linear (left) and logarithmic scale (right).

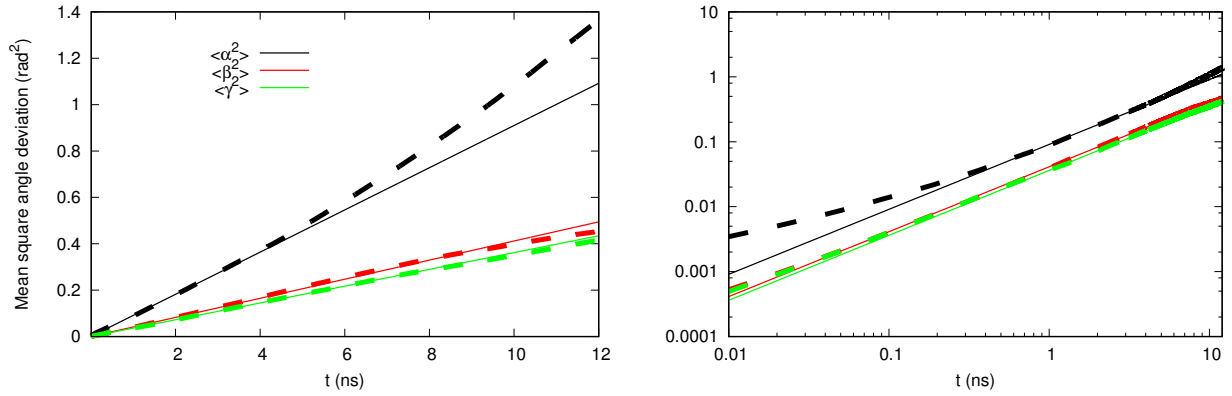


Figure S2: Mean square angle deviations of inertia tensor axes calculated from *PaTonB-96* simulation with tip4p water model at 298K. The data shown with linear (left) and logarithmic scale (right).

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
<i>Hp</i> TonB-92	2.9	1.0	-	-
<i>Pa</i> 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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- (4) Norppa, A. J.; Kauppala, T. M.; Heikkinen, H. A.; Verma, B.; Iwai, H.; Frilander, M. J. Mutations in the U11/U12-65K protein associated with isolated growth hormone deficiency

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- (5) Timr, S.; Kadlec, J.; Srb, P.; Ollila, O. H. S.; Jungwirth, P. Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity. In Preparation.