

Supporting Information:

Rotational Dynamics of Proteins from Spin Relaxation Times and Molecular Dynamics Simulations

O. H. Samuli Ollila,^{*,†,‡} Harri A. Heikkinen,[†] and Hideo Iwai[†]

[†]*Research Program in Structural Biology and Biophysics, Institute of Biotechnology,
University of Helsinki*

[‡]*Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague 6,
Czech Republic*

E-mail: samuli.ollila@helsinki.fi

S1 Supplementary Figures

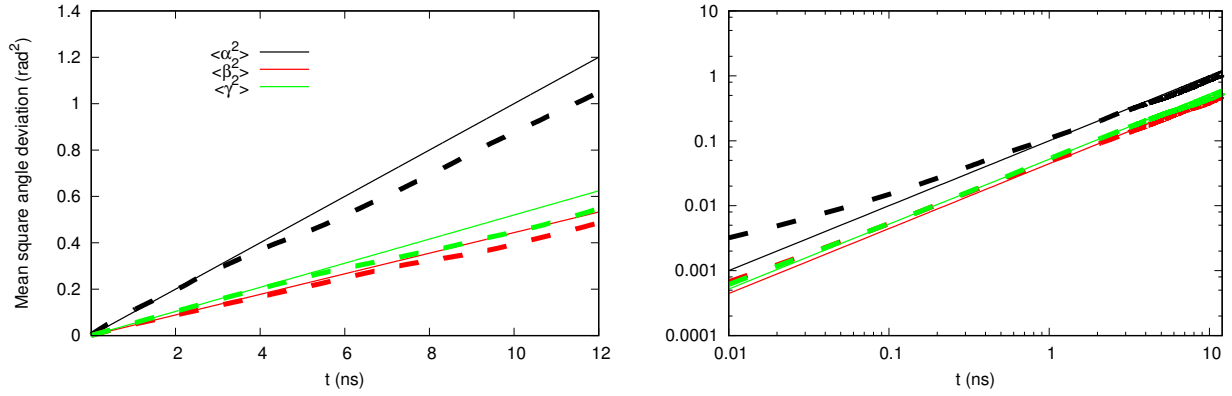


Figure S1: Mean square angle deviations of inertia tensor axes calculated from *PaTonB-96* simulation with tip4p water model at 310K. The data shown with linear (left) and logarithmic scale (right).

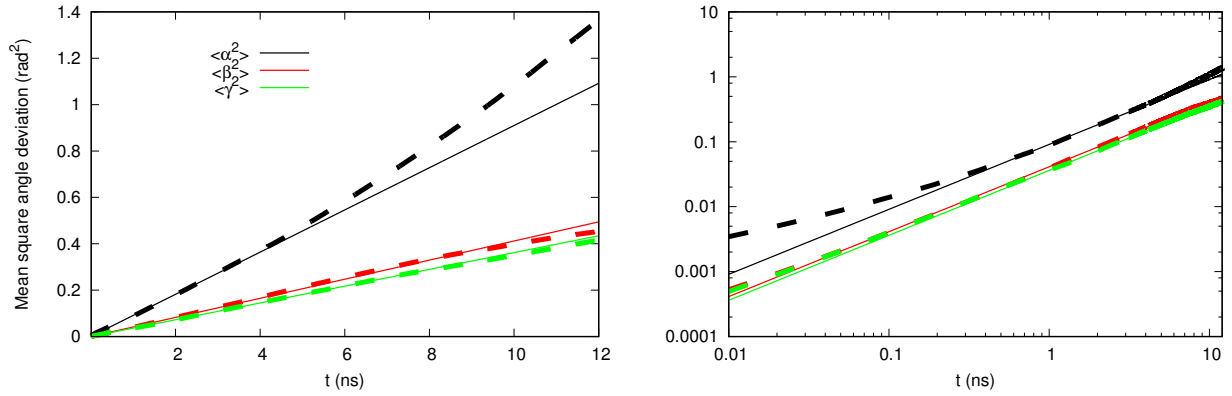


Figure S2: Mean square angle deviations of inertia tensor axes calculated from *PaTonB-96* simulation with tip4p water model at 298K. The data shown with linear (left) and logarithmic scale (right).

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

- (1) Wong, V.; Case, D. A. Evaluating Rotational Diffusion from Protein MD Simulations. *J. Phys. Chem. B* **2008**, *112*, 6013–6024.
- (2) Izadi, S.; Anandakrishnan, R.; Onufriev, A. V. Building Water Models: A Different Approach. *J. Phys. Chem. Lett.* **2014**, *5*, 3863–3871.
- (3) Heikkinen, H. A.; Iwai, H. In Preparation.
- (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

lead to structural destabilization and impaired binding of U12 snRNA. 2017; 10.1261/rna.062844.117.

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