ELECTRONIC SUPPLEMENTARY INFORMATION:THE EFFECT OF PROTEIN COMPOSITION ON HYDRATION DYNAMICS

O.RAHAMAN, S.MELCHIONNA, D.LAAGE, F.STERPONE

1. Protein composition

System/AA	Meso- (1EFC,T8-E203) [%]	Hyper- (1SKQ,K4-V229) [%]
Arg	3.6	4.9
Lys	4.1	10.2
His	4.1	2.6
Asp	8.2	5.8
Glu	7.7	9.3
Asn	2.6	4.0
Gln	2.6	2.2
Ser	2.1	4.0
Thr	8.2	5.7
Cys	1.0	0.0
Pro	5.6	4.4
Gly	8.2	6.6
Ala	10.2	6.2
Val	8.2	8.0
Ile	6.7	5.8
Leu	8.2	8.4
Met	2.6	3.5
Phe	2.0	4.9
Tyr	3.6	3.1
Trp	0.5	0.4

Table 1. Amino-acid composition of the two G-domains.

System/Sites	Mesophile	Hythermophile
Acceptor	16.4% (23.0%)	12.0% (18.0%)
Donor	6.3% (7.0%)	7.6% (10.0%)
Hydrophobe	77.3% (70%)	80.4% (72.0%)

TABLE 2. Fraction of the hydration shell localized next to HB acceptor, HB donor and hydrophobic groups of the amino acid side chains. Data in parenthesis are calculated including the acceptor and donor sites of the back-bone.

2. Water riorientation

System	τ_{st} (ps)	γ	$< \tau_R >$(ps)
Meso- T300	2.76	0.40	9.01
Meso- T330	1.27	0.39	4.54
Meso- T360	0.69	0.37	2.85
Hyper- T300	2.63	0.39	9.03
Hyper- T330	1.19	0.37	4.63
Hyper- T360	0.66	0.36	2.89

TABLE 3. Fit parameters for the average reorientational correlation function computed for water molecules in the protein hydration shell. We report the data for representative configurations and temperatures. We fit the decay of the time correlation function with a stretched-exponential function $f(t) = exp(-(t/\tau_{st})^{\gamma})$. The characteristic time for the average reorientation is computed as $< \tau_R >= \frac{\tau_{st}}{\gamma} * \Gamma(\frac{1}{\gamma})$.

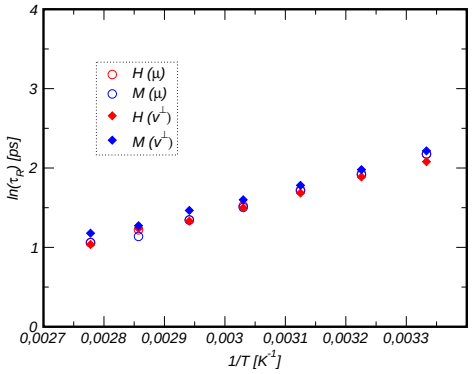

FIGURE 1. Reorentational characteristic times extracted from the time correlation function $P_2(t)$ computed for the water dipole (μ) and the orthogonal vector to the water plane ($\nu^{\perp}$).

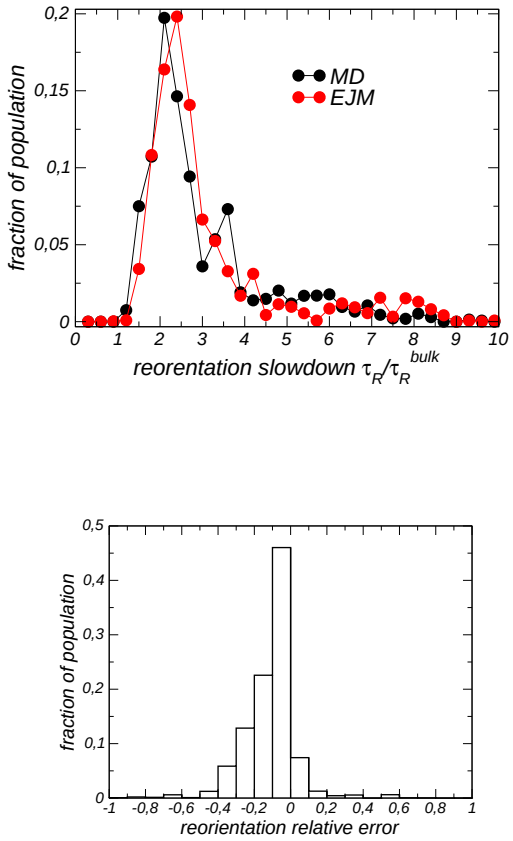

FIGURE 2. Top Panel: distribution of the slowdown factor computed for water reorientation directly from the MD trajectory (black) and via the EJM (red). Bottom Panel: distribution of the relative error $\tau_R^{EJM}/\tau_R^{MD} - 1$. The distributions are obtained by weighting the reorientation times with the number of water molecules that solvate each site.