Electronic Supplementary Material (ESI) for Molecular BioSystems.

Electronic Supporting Information

for

Signatures of protein thermal denaturation and local hydrophobicity in domain specific hydration behavior: a comparative molecular dynamics study

Prathit Chatterjee and Neelanjana Sengupta[*]

Physical Chemistry Division, CSIR-National Chemical Laboratory, Pune 411008, India

[*] correspondence: n.sengupta@ncl.res.in

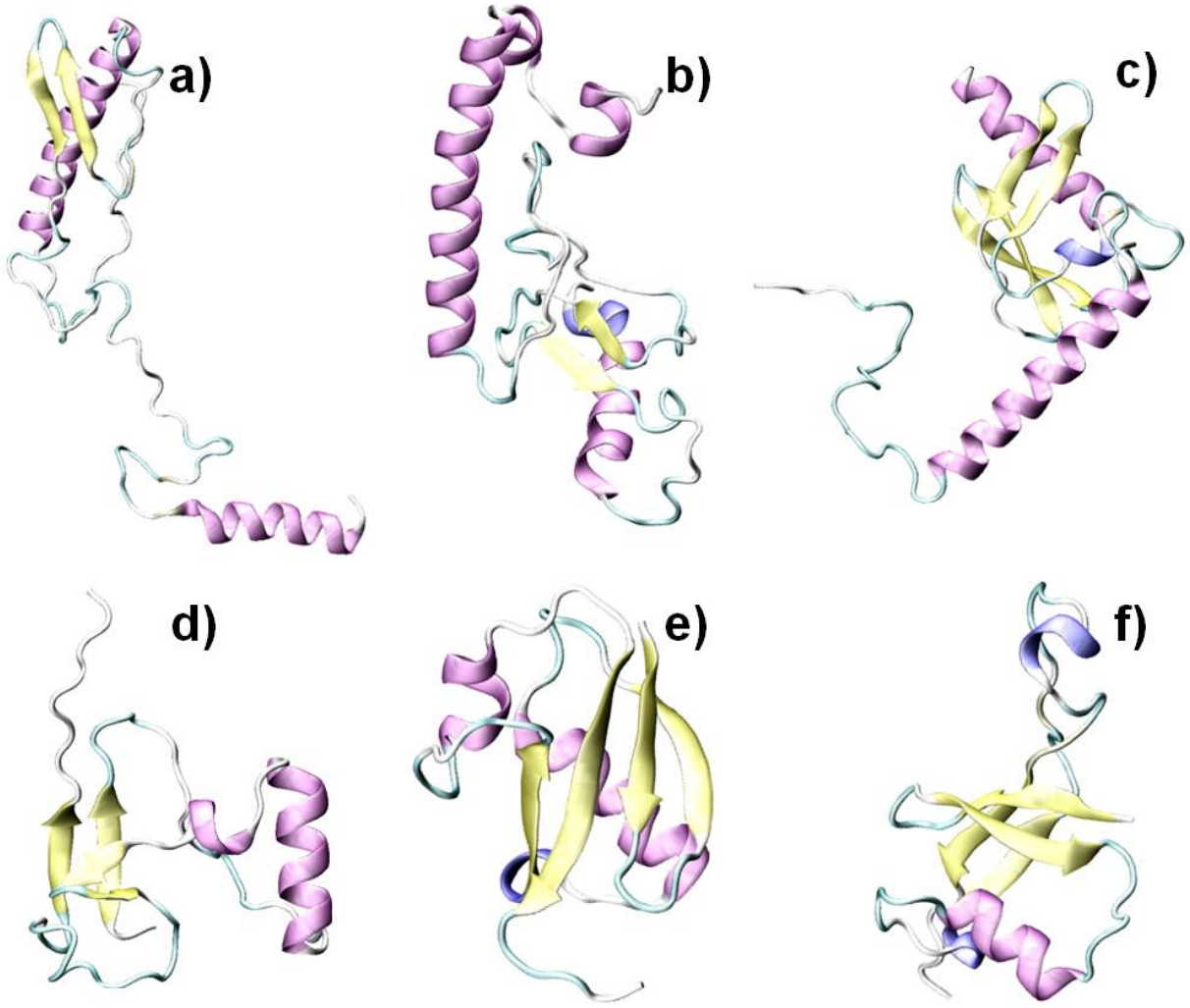

Figure S1: Snapshots of Yfh1 at a) T_{c1}, b) T_{h1}, c) T_{h2}; snapshots of Ubq at d) T_{c1}, e) T_{h1}, f) T_{h2}.

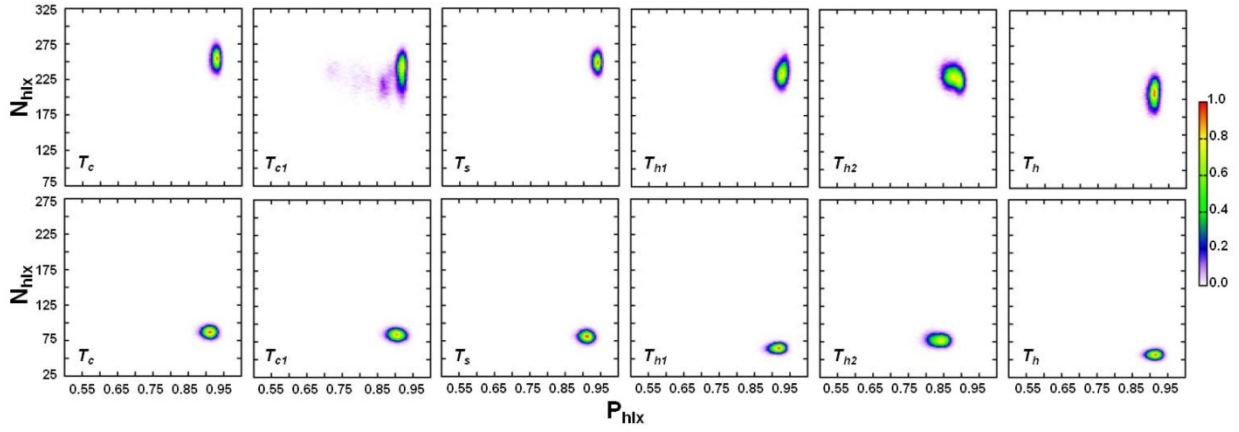

Figure S2: Probability distributions of P_{hlx} *vs.* N_{hlx} (obtained from the last 50 ns of simulations) for Yfh1 (upper row) and Ubq (lower row), at all the simulated temperatures.

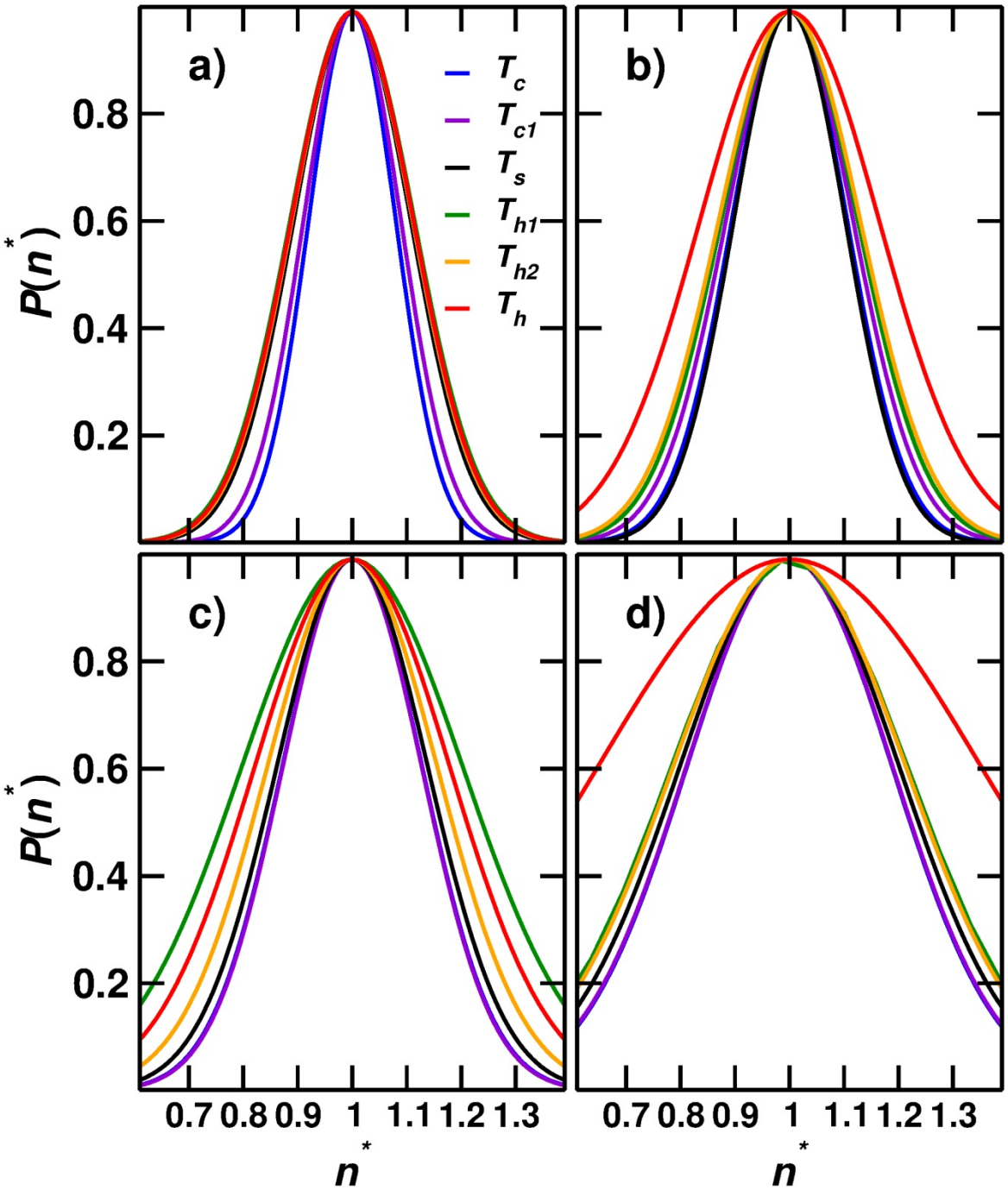

Figure S3: Distributions of $P(n^*)$ (obtained from the last 50 ns of simulations) for a) $beta_H$, and b) $helix_H$ of Yfh1; and c) $beta_H$, and d) $helix_H$ of Ubq; at all the simulated temperatures.

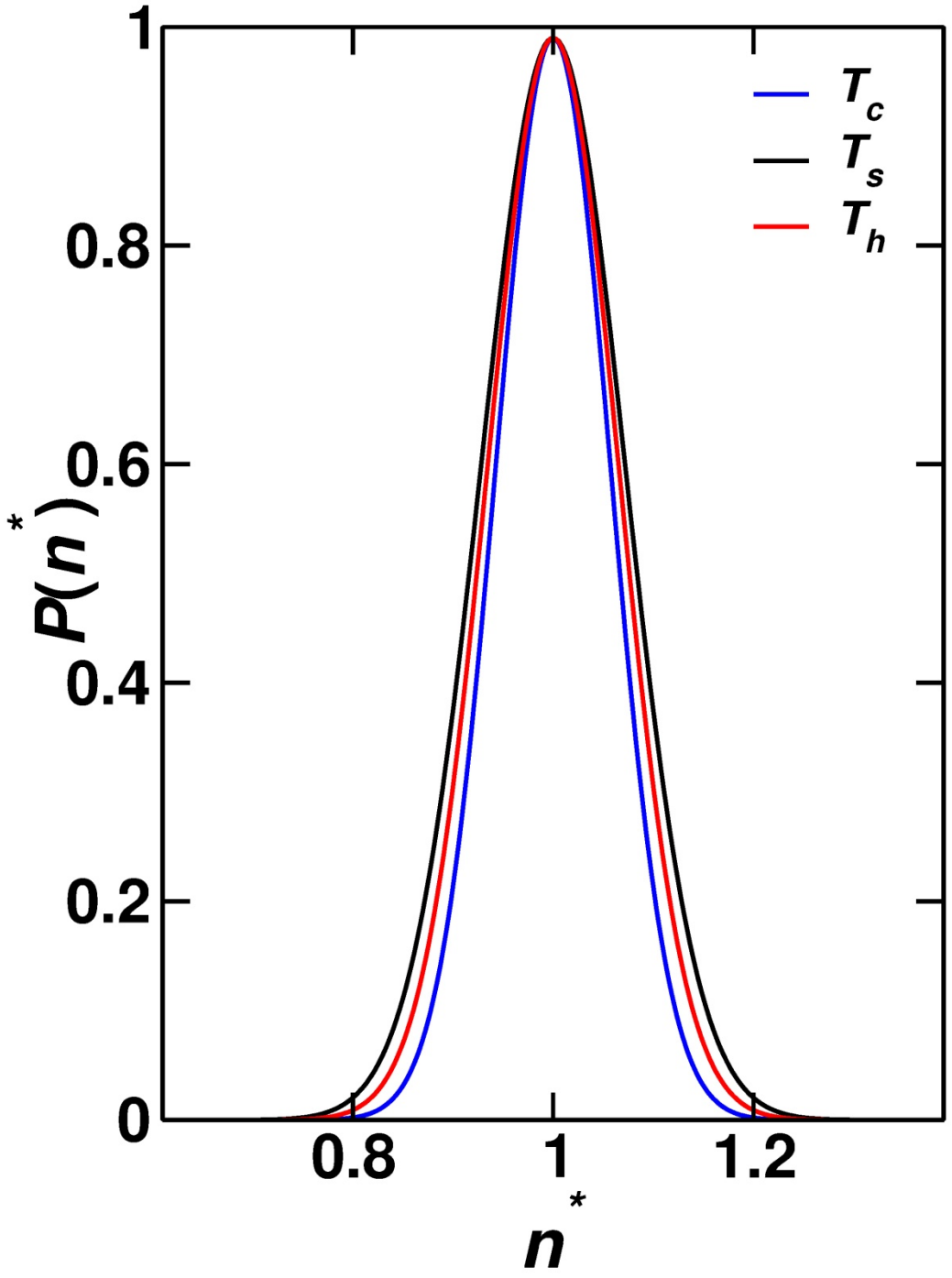

Figure S4: Distributions of $P(n^*)$ (obtained from the last 50 ns of simulations) for $beta_{NH}$ of Yfh1; at temperatures T_c, T_s, T_h.

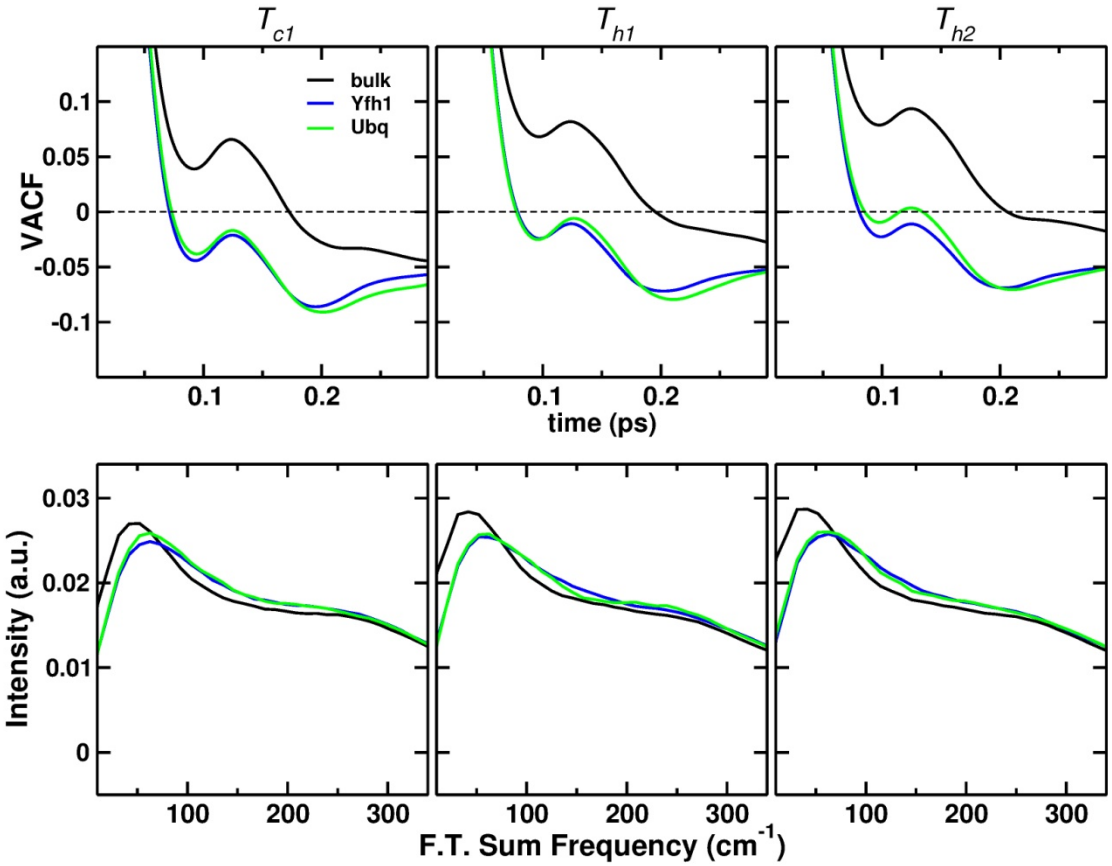

Figure S5: Plots of VACF (upper row), and VDOS (lower row) for the hydration water layer of the whole protein domains of Yfh1 and Ubq, compared with the corresponding bulk behavior, at the selected temperatures (T_{c1}, T_{h1}, T_{h2}).

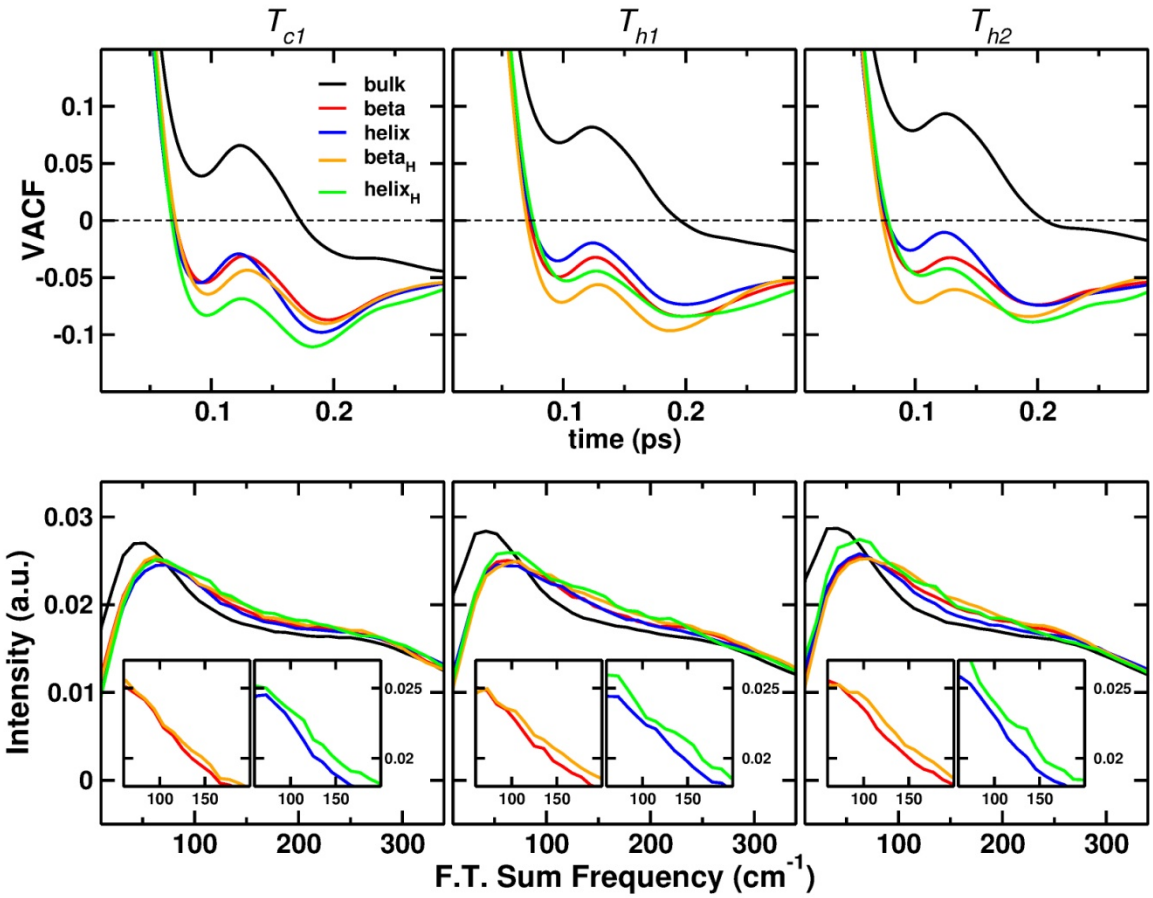

Figure S6: Plots of VACF (upper row), and VDOS (lower row) for the hydration water layer of the beta, helix, beta$_H$, and helix$_H$ domains of Yfh1, compared with the corresponding bulk behavior, at the selected temperatures (T_{c1}, T_{h1}, T_{h2}); differences in VDOS for beta & beta$_H$ and helix & helix$_H$ are represented by the magnified plots in the respective insets.

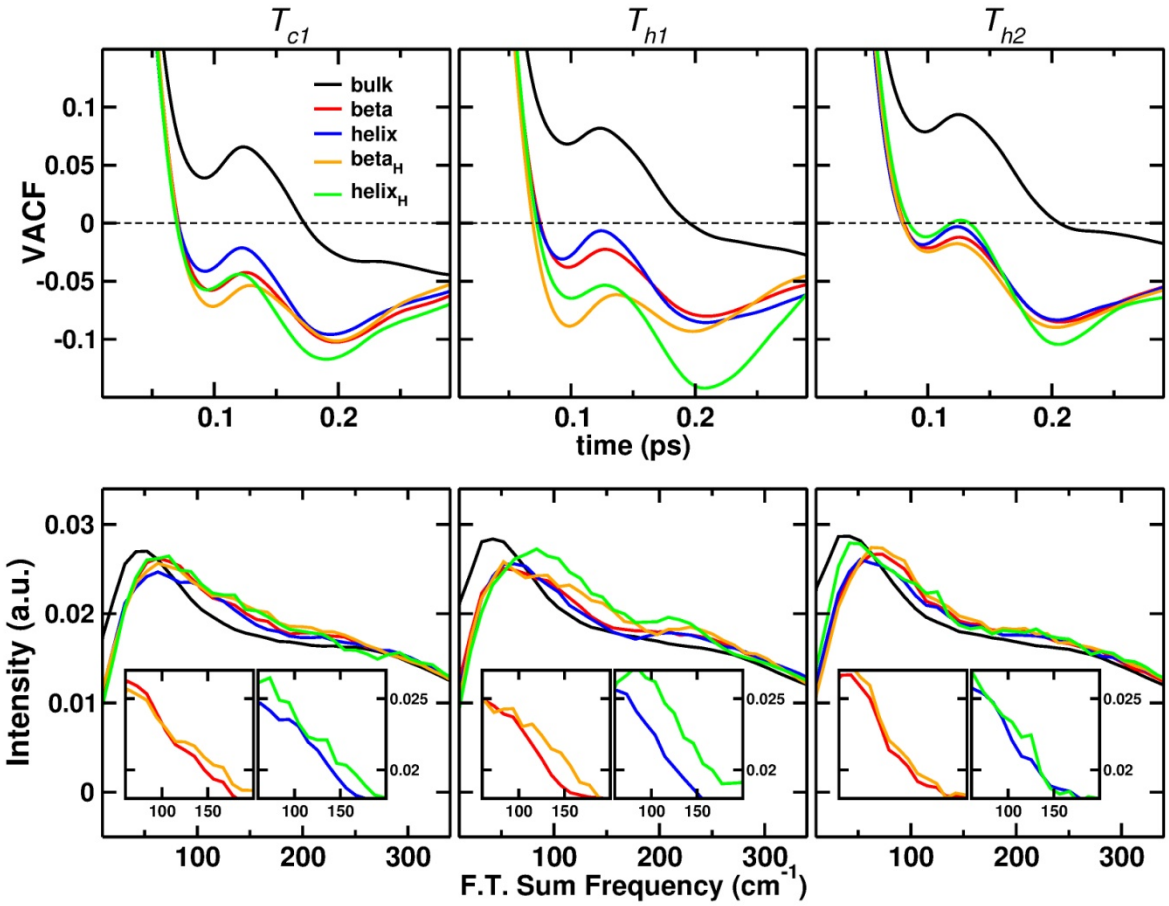

Figure S7: Plots of VACF (upper row), and VDOS (lower row) for the hydration water layer of the beta, helix, beta$_H$, and helix$_H$ domains of Ubq, compared with the corresponding bulk behavior, at the selected temperatures (T_{c1}, T_{h1}, T_{h2}); differences in VDOS for beta & beta$_H$ and helix & helix$_H$ are represented by the magnified plots in the respective insets.

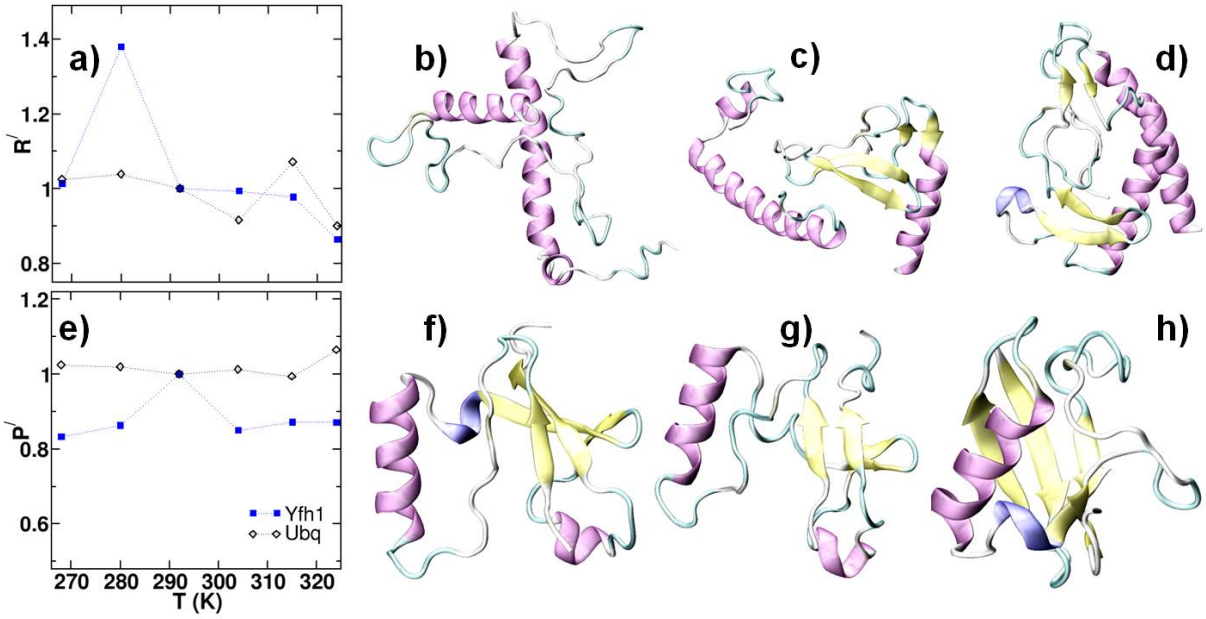

Figure S8: Plots of $R^{/}$ and $P^{/}$ for Yfh1 and Ubq as a function of temperature, as well as representative snapshots of Yfh1 and Ubq at selected temperatures, with TIP4P/2005 water model. a) evolution of $R^{/}$ of Yfh1 at all the simulated temperatures; snapshots of Yfh1 at b) T_c, c) T_s, d) T_h; e) evolution of $P^{/}$ of Yfh1 at all the simulated temperatures; snapshots of Ubq at f) T_c, g) T_s, f) T_h.

Table S1: α values (10^{-2}) corresponding to the beta_{NH} (α_{bN}) residues, at temperatures T_c, T_s, T_h; for Yfh1.

T (K)	α_{bN}
T_c	0.65
T_s	1.03
T_h	0.85

Table S2: First minima (ps, 10^{-2}) of VACF for the secondary structural domains (beta, beta_H, helix, helix_H) of Yfh1; as well as respective differences between the ordinates (depth of the minima) of beta & beta_H (Δ_1), and helix & helix_H (Δ_2).

T (K)	beta	beta_H	Δ_1	helix	helix_H	Δ_2
T_c	(0.094, –5.90)	(0.096, –6.63)	0.73	(0.092, –5.47)	(0.1, –7.87)	2.40
T_{c1}	(0.094, –5.45)	(0.098, –6.46)	1.01	(0.09, –5.46)	(0.096, –8.31)	2.85
T_s	(0.098, –5.10)	(0.098, –6.26)	1.16	(0.094, –4.07)	(0.102, –5.15)	1.08
T_{h1}	(0.096, –4.94)	(0.098, –7.17)	2.23	(0.096, –3.54)	(0.102, –5.30)	1.76
T_{h2}	(0.1, –4.52)	(0.104, –7.22)	2.7	(0.096, –2.61)	(0.106, –4.81)	2.2
T_h	(0.104, –2.83)	(0.108, –5.05)	2.22	(0.098, –2.84)	(0.11, –8.30)	5.46

Table S3: First minima (ps, 10^{-2}) of VACF for the secondary structural domains (beta, beta_H, helix, helix_H) of Ubq; as well as respective differences between the ordinates (depth of the minima) of beta & beta_H (Δ_1), and helix & helix_H (Δ_2).

T (K)	beta	beta_H	Δ_1	helix	helix_H	Δ_2
T_c	(0.09, –6.89)	(0.09, –9.89)	3.0	(0.094, –4.91)	(0.098, –9.11)	4.20
T_{c1}	(0.098, –5.79)	(0.98, –7.17)	1.38	(0.092, –4.15)	(0.094, –5.75)	1.60
T_s	(0.1, –5.35)	(0.102, –6.16)	0.81	(0.094, –4.65)	(0.098, –9.85)	5.20
T_{h1}	(0.098, –3.81)	(0.098, –8.87)	5.06	(0.094, –3.09)	(0.1, –6.48)	3.39
T_{h2}	(0.1, –2.14)	(0.1, –2.47)	0.33	(0.096, –1.86)	(0.098, –1.18)	–0.68
T_h	(0.108, –2.98)	(0.1, -5.32)	2.34	(0.102, –2.74)	(0.1, –7.74)	–5.0

Table S4: Mean values of R_g obtained from the TIP4P/2005 simulations, for Yfh1 (R_g^Y) and Ubq (R_g^U).

T (K)	R_g^Y	R_g^U
T_c	18.21	13.52
T_{c1}	24.78	13.71
T_s	17.96	13.20
T_{h1}	17.85	12.09
T_{h2}	17.56	14.14
T_h	15.52	11.88