Supplementary Material (ESI) for PCCP

High water mobility on the ice-binding surface of a hyperactive antifreeze protein

Supplementary Information: Further experimental details

Kristofer Modig, Johan Qvist, Christopher B. Marshall, Peter L. Davies and Bertil Halle

Table S1. Amino acid composition of *Tm*AFP samples A and B. [a]

Amino acid	Sequence	Sample A	Sample B
Ala	9	9.0	9.2
Arg	0	0.1	0.1
Asx	11	11.5	11.4
Gly	7	8.1	8.1
Glx	4	6.1	6.4
His	2	2.0	2.1
Ile	0	0.4	0.4
Leu	0	0.3	0.2
Lys	3	3.1	3.1
Met	0	0.7	0.8
Phe	1	1.0	1.0
Pro	2	2.5	3.3
Ser	6	6.6	6.5
Thr	19	18.7	18.6
Tyr	1	0.9	1.0
Val	3	3.4	3.3

[a] Sample B was analyzed 6 years after sample A.

Table S2. Water ^{2}H relaxation rate from *Tm*AFP samples A and B.[a]

	Relaxation rate, R_1 (s^{-1})		
ν_0 (MHz)	Sample A	Sample B uncorrected	Sample B corrected [b]
4.58	2.84	2.76	2.83
6.86	2.80	2.71	2.77
11.96	2.68	2.62	2.68

[a] Sample B was measured 6 years after sample A.

[b] Corrected for lower solvent deuterium fraction by multiplication with viscosity ratio $\eta(X_D=0.476) / \eta(X_D=0.369) = 1.022$ (at 27 °C).

Table S3. Water ^{17}O relaxation rate at 81 MHz before and after emulsification.

	Relaxation rate, R_1 (s^{-1}) [a]	
Sample	Before	After
Reference	1499	1502
Sample B	1569	1572

[a] Estimated experimental uncertainty ± 5 s^{-1}.

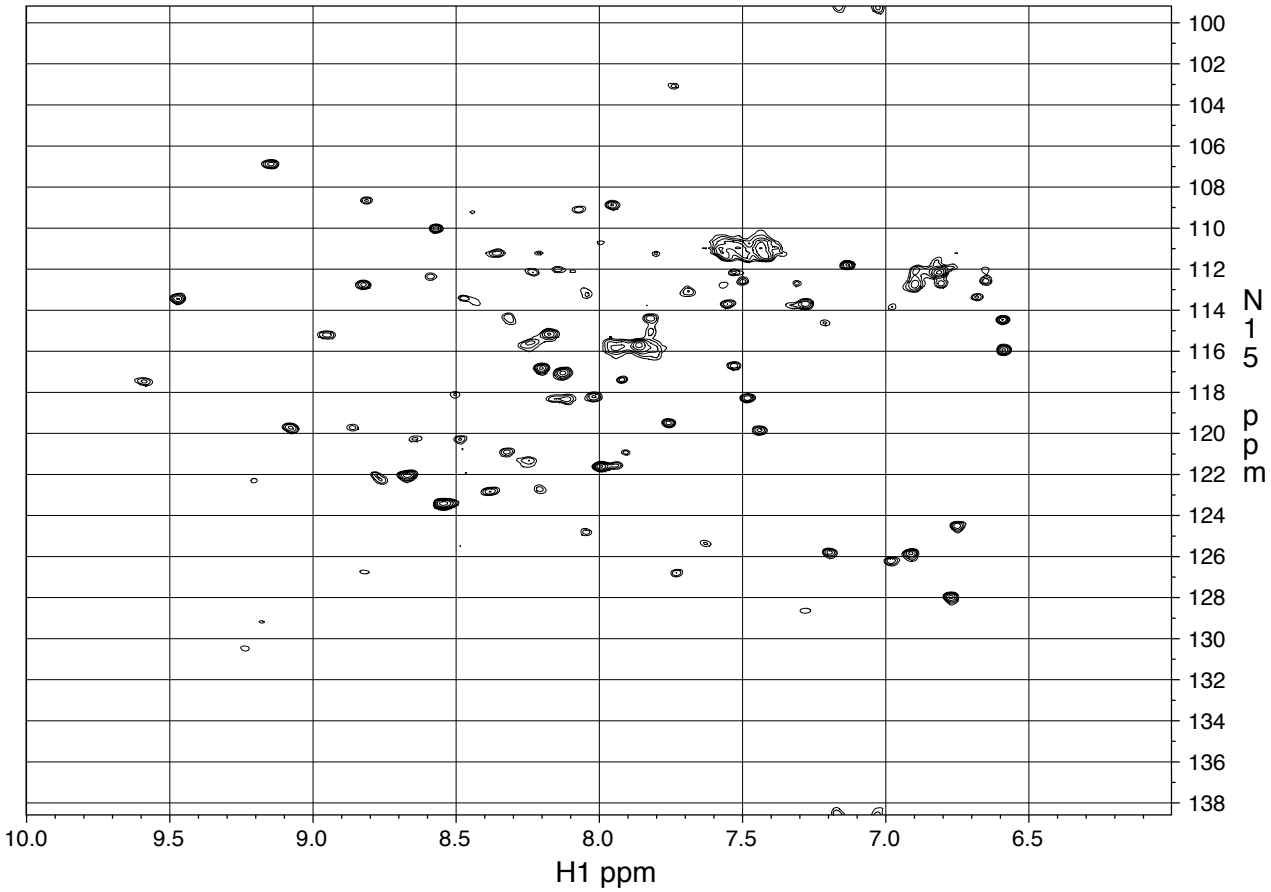

Figure S1. ^{1}H–^{15}N heteronuclear multiple-quantum coherence (HMQC) correlation spectrum of *Tm*AFP sample B (at natural ^{15}N abundance) recorded at 600 MHz after the MRD experiments.