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for

Exploring the Conserved Water Sites and Hydration of a Coiled-Coil Trimerization Motif: A MD Simulation Study

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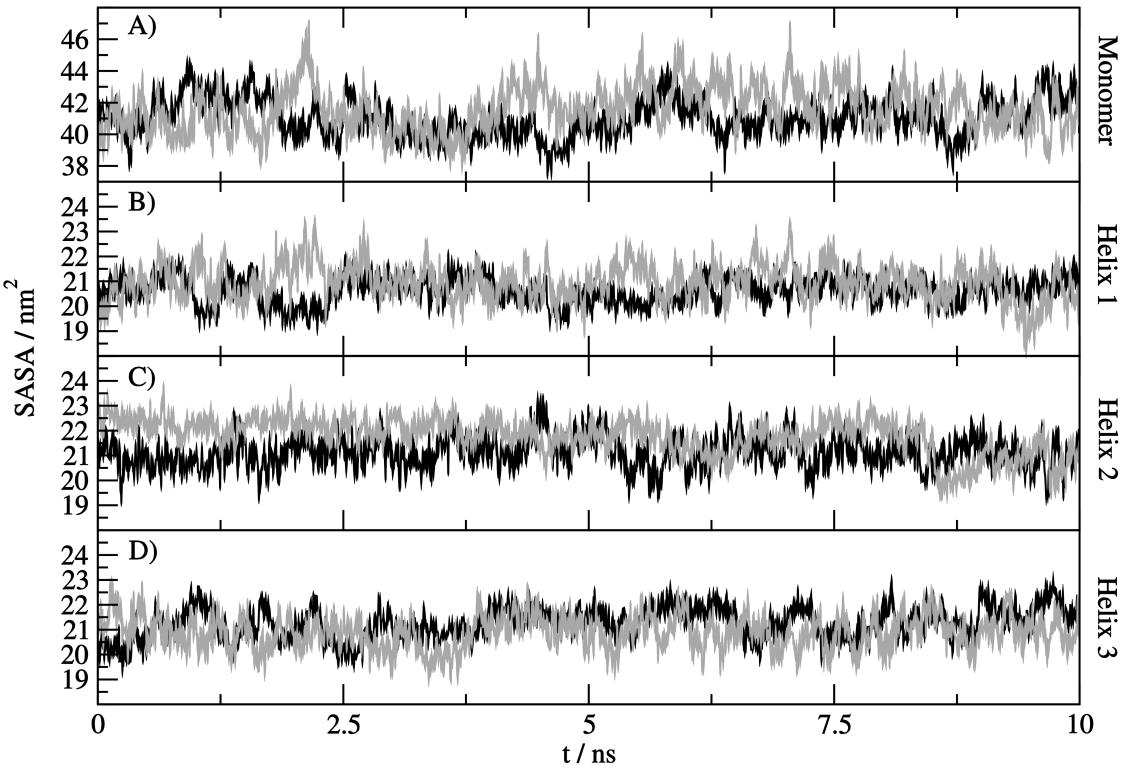

Figure S1: Solvent accessible surface area (SASA) computed as a function of simulation time for the ccβ-p monomer (A) and the three helices of the coiled coil trimer (B, C, D) at 278 K (dark) and 330 K (light). Notice the difference in scales.

Table S1: The rate of exchange of water molecules (in ps^{-1}) in the first hydration shell of the carbonyl oxygen atoms for the ccβ-p monomer and the three helices of the ccβ-p coiled-coil.

	Monomer		Helix 1		Helix 2		Helix 3	
	278 K	330 K	278 K	330 K	278 K	330 K	278 K	330 K
Ser1	2.7	3.6	0.3	3.8	4.4	0.9	0.5	1.1
Ile2	0.8	0.5	0.2	0.3	0.0	0.8	0.5	0.4
Arg3	1.2	3.6	1.2	1.6	1.4	1.4	1.5	2.0
Glu4	0.4	1.6	0.7	0.7	0.8	0.8	0.6	0.8
Leu5	0.4	3.2	0.0	0.0	0.0	0.0	0.0	0.0
Glu6	0.3	4.4	0.3	0.4	0.5	0.4	0.2	0.5
Ala7	0.9	1.0	1.0	1.5	0.0	1.3	1.0	1.4
Arg8	0.7	0.2	0.6	0.8	0.8	0.7	0.8	2.3
Ile9	0.2	2.4	0.4	0.5	0.3	0.4	0.5	0.4
Arg10	1.1	2.8	0.7	1.3	1.2	1.3	1.4	1.2
Glu11	2.4	0.8	0.8	0.8	1.2	1.0	0.8	1.0
Leu12	3.1	0.5	0.0	0.0	0.0	0.0	0.2	0.0
Glu13	4.0	3.1	1.6	1.8	1.9	1.6	2.1	1.9
Leu14	0.1	0.1	5.2	5.2	5.0	4.7	3.5	4.2
Arg15	4.9	3.2	4.3	4.6	4.1	4.7	1.5	4.6
Ile16	1.8	1.8	1.3	1.9	1.3	1.9	1.3	2.8
Gly17	4.2	5.1	2.2	4.7	2.6	4.5	3.0	5.5