Supporting Figures

Chain Registry and Load-Dependent Conformational Dynamics of Collagen

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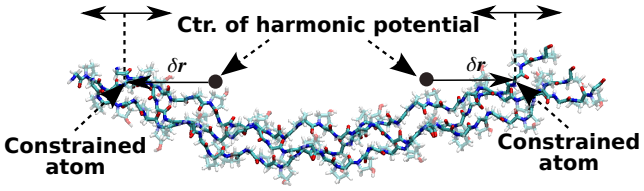

Figure S1: Illustration of the simulation with harmonic constraints at the ends of a peptide. Displacement of the constrained C_α atoms relative to the center of the harmonic potential is $\delta \boldsymbol{r}$. The tug-of-war sampling analyzes the fluctuation of $\delta \boldsymbol{r}$ (double arrow) to calculate the force exerted on the constrained atom at the center of the harmonic potential.

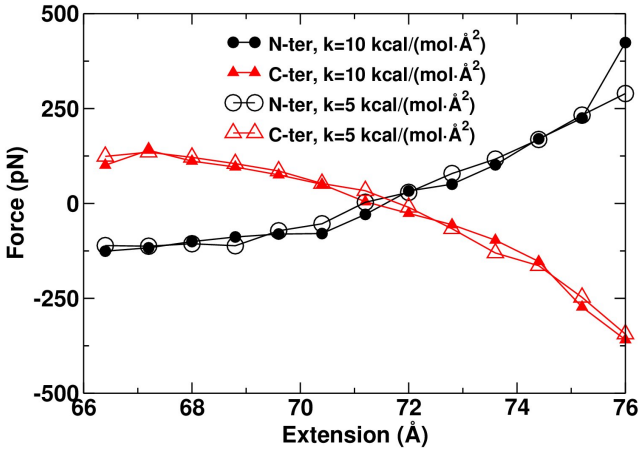

Figure S2: Force-extension relation of *gpo*10 measured using two different spring constants of restraining potentials.

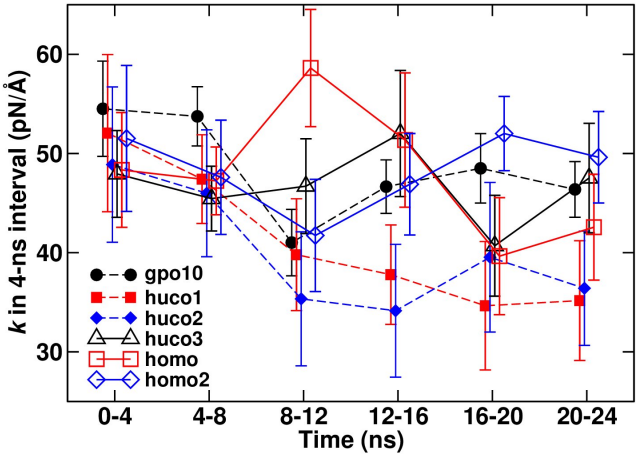

Figure S3: Extensional stiffness k calculated in 4-ns intervals. After 8 ns, *huco*1 and *huco*2 take the two lowest values of k. Due to the nonlinear nature of Eq. 1, values of k over 12–24 ns (Fig. 1c) are not equal to the averages of the last three 4-ns intervals.

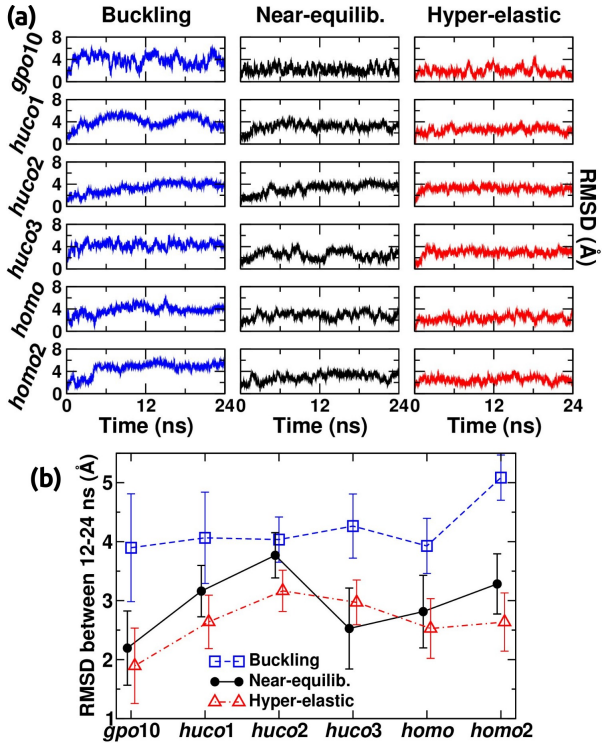

Figure S4: Average root-mean-square deviation (RMSD) of backbone heavy atoms from those at the beginning of the production run. The two GPO triplets at each end of the peptide were excluded from calculation. (a) Time trace. (b) RMSD averaged over 12–24 ns. Error bar: standard deviation. The same representative extensions of the three regimes (buckling, near-equilibrium, and hyper-elastic) in Fig. 3 are used.

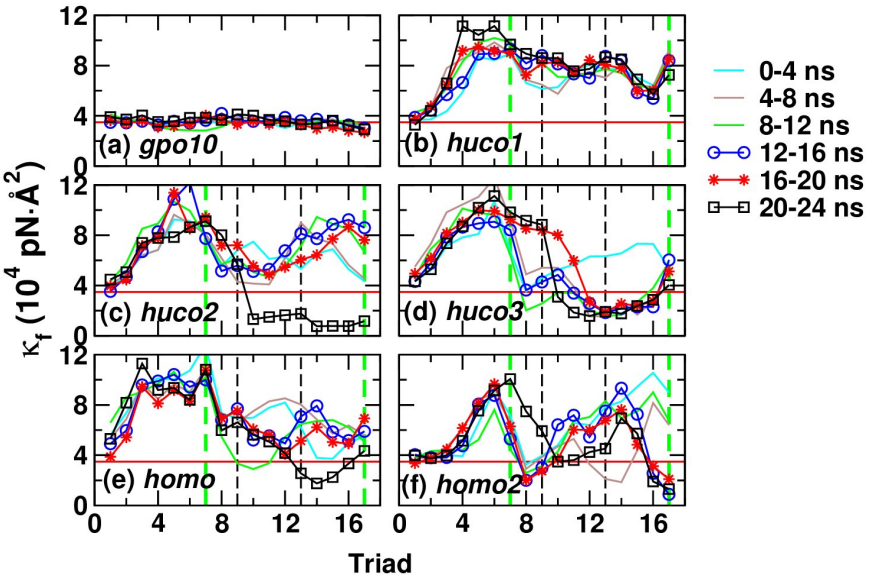

Figure S5: Local bending stiffness κ_f calculated in 4-ns intervals. Red horizontal line and vertical dashed lines are explained in Fig. 2. Among *huco*1, *huco*2, and *huco*3, the latter two have κ_f in the cleavage region (triad 9–13) consistently lower than that of *huco*1 after 12 ns. The large decrease in κ_f of *huco*2 in triads 9–17 during 20–24 ns is due to unfolding of this region that occurred at around 22.5 ns, as shown in Fig. 3c.

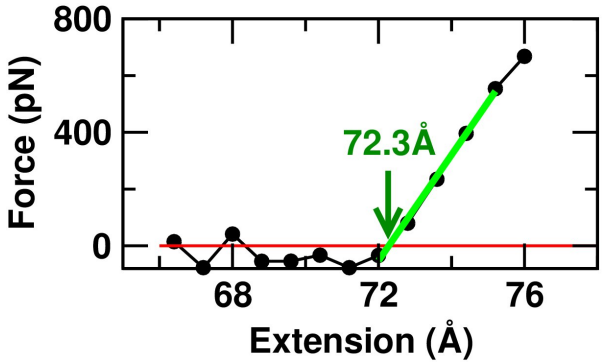

Figure S6: Force-extension relation of *huco*2 with ends of all three chains constrained. Lines and symbols are defined in Fig. 1b. The stiffness, 187 pN/Å (slope of the thick green line), is much higher than the case of *huco*2 with only one α chain restrained (37.1 pN/Å).

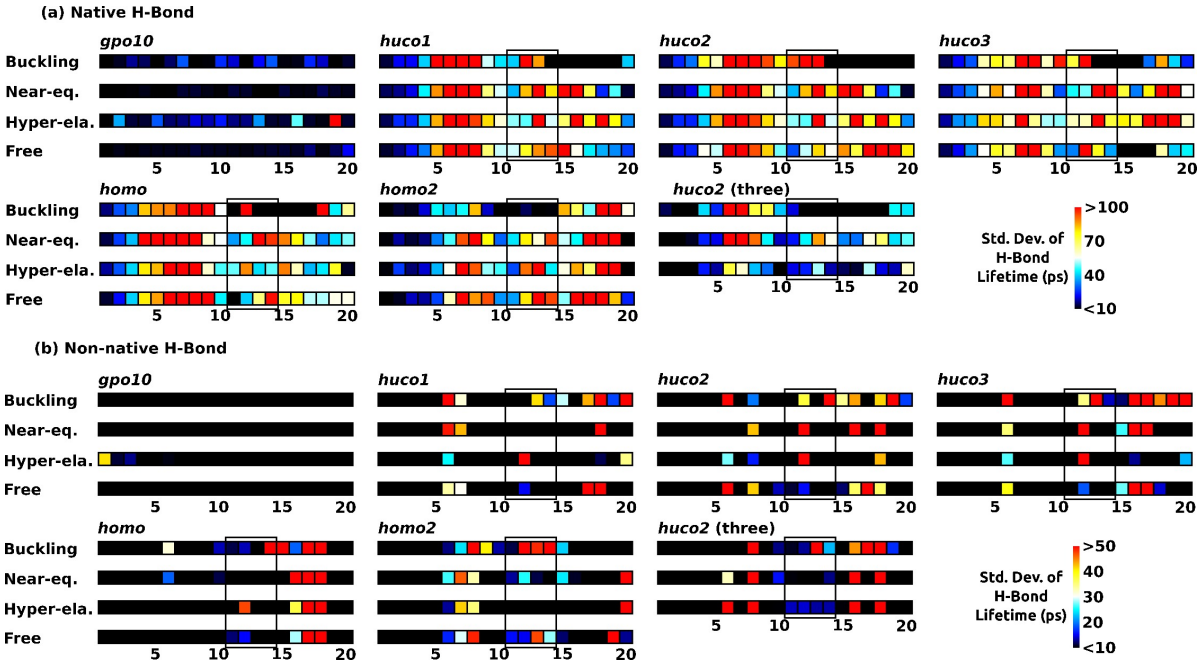

Figure S7: Standard deviation in the hydrogen bond lifetime. (a) Native and (b) non-native. *cf.*, Figs. 4 and 5.