Supporting information for Aggeli et al. (2001) Proc. Natl. Acad. Sci. USA 98 (21), 11857–11862. (10.1073/pnas.191250198)

Table 1. Comparative molecular parameters and macroscopic properties of the aqueous solutions of the two *de novo* designed self-assembling β -tape-forming peptides P₁₁-I and P₁₁-II, shown schematically in a β -strand conformation.

	Peptide P ₁₁ -I			22222			
	β-Tapes	OOOO Ribbons	⊖ Fibrils	β-Tapes	Ribbons	Fibrils	
	p-rapes			p-rapes			
<i>c</i> _{cr} / μΜ	8*	1,000*	<i>c</i> > 25,000*	< 90*	90*	700 ± 200*	
E trans		6.5 ± 1.5			3 ± 1		
€ _{tape}	31.0 ± 1.5			24.5 ± 1.0			
Eribbon		$(3.5\pm1.5)10^{-3}$			0.6 ± 0.3		
Efibril			< 10 ⁻³			$(2.0 \pm 0.3)10^{-4}$	
Pitch <i>h /</i> nm	30 ± 15*	$50 \pm 20^{*}$			160 ± 40	160 ± 40*	
Twist angle $\gamma_{\theta}/^{\circ}$	3*	3*		1	1	1*	
Bend angle $\gamma_{\rm v}/^\circ$	3*	0*			0*	0*	

ĩ / μm	< 0.3*	$0.6 \pm 0.2^*$		$1.0 \pm 0.3^{*}$	20–70*	
L / μm (<i>c</i> = 6 mM)	10 ⁻¹	$10^{-1} - 10^{0}$	10 ⁻³	10 ⁰	10 ¹⁷	
Properties of aq. solution	Isotropic fluid(c < 13 mM) Nematic fluid / gel(c >13 mM)		Isotropic fluid ($c < 0.9 \text{ mM}$) Nematic fluid ($c \approx 0.9 - 6 \text{ mM}$) Nematic gel ($c > 6 \text{ mM}$)			

Open and filled circles represent polar and apolar amino-acid residues, respectively. The upper side of the β -strand is identical for both peptides. c_{cr} is the threshold concentration above which the corresponding type of self-assembling structure emerges in substantial quantities. For explanation of the various energetic parameters ε_j , see the text and Fig.1A. All values of ε_j are given in $k_B T$. The errors in the values of ε_j arise from the errors in the value of v_{tape} , and from the uncertainty of measurements of the real lengths of the polymers in solution at a given concentration. The values of ε_{trans} and ε_{tape} for both peptides, and ε_{ribbon} for P₁₁-II are received from the fits of the self-assembly curves (Figs. 2*c* in the text and 4*c* in supporting information), and the observed tape/ribbon lengths, with $v_{tape} \approx 5 \cdot 10^{-6}$ nm³ (this value is estimated from the observed persistence lengths of the ribbons). ε_{fibril} is estimated from c_{cr}^{fibril} and ε_{ribbon} for P₁₁-I from the corresponding c_{cr}^{ribbon} . \tilde{l} , h, γ_{ν} , and γ_{θ} are either directly measured from electron micrographs or calculated with the help of the model similar to Fig.1*B*. Elastic constants are estimated from the observed persistence lengths of ribbons and fibrils. The contour lengths *L* agree with both the data and the predictions of the theory (see *Theoretical Model* in the text). Directly measured constants are indicated with an asterisk.