Supplementary Material for:

Entropic bonding of the type 1 pilus from experiment and simulation Fabiano Corsetti, Alvaro Alonso-Caballero, Simon Poly, Raul Perez-Jimenez, Emilio Artacho

EXAMPLES OF REJECTED TRACES

Fig. S1 shows some examples of force-extension traces rejected by the automatic processing procedure.

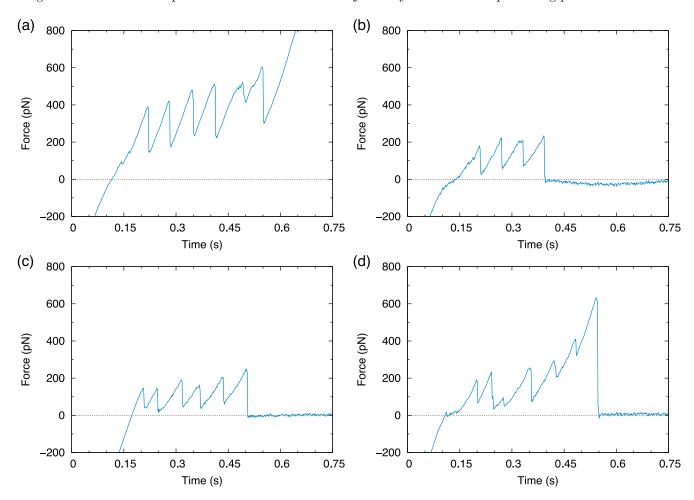


FIG. S1. Examples of rejected experimental traces. The reasons for rejection are: (a) no flat region at the end of the trace; (b) too few peaks; (c) fitted WLC curves not close enough to the real trace; (d) unreasonable values for the domain contour lengths.

WORM-LIKE CHAIN AND FREELY-JOINTED CHAIN MODELS

The worm-like chain (WLC) model used to fit the branches of the experimental traces is that of Bouchiat et al. [1], given by:

$$f = \left(\frac{k_{\rm B}T}{P}\right) \left[\frac{1}{4(1 - x/s)^2} - \frac{1}{4} + \sum_{i=1}^{7} \alpha_i \left(\frac{x}{s}\right)^i \right],\tag{S1}$$

where f is the force, x is the end-to-end extension, s is the contour length, P is the persistence length, $k_{\rm B}$ is Boltzmann's constant, T is the temperature, and the coefficients of the polynomial expansion are $\alpha_1=1,\ \alpha_2=-0.5164228,\ \alpha_3=-2.737418,\ \alpha_4=16.07497,\ \alpha_5=-38.87607,\ \alpha_6=39.49944,\ \alpha_7=-14.17718.$

The freely-jointed chain (FJC) model used to fit the last part of the simulated traces is that of Smith et al. [2], given by:

$$x = s \left[\coth \frac{2Pf}{k_{\rm B}T} - \frac{k_{\rm B}T}{2Pf} \right] \left(1 + \frac{f}{K} \right), \tag{S2}$$

where K is the elastic modulus.

^[1] C. Bouchiat, M. D. Wang, J.-F. Allemand, T. Strick, S. M. Block, and V. Croquette, Biophys. J. 76, 409 (1999).

^[2] S. B. Smith, Y. Cui, and C. Bustamante, Science 271, 795 (1996).