Supplementary Materials

Flow-induced β-hairpin folding of the Glycoprotein Ibα β-switch

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1 Supporting Movies

- **Movie S1** shows a trajectory (C1, see Table 1) of backbone rotation of the β-switch under flow condition. To clearly show how the backbone rotates, the frame rate is decreased when movie zooms into specific parts of the backbone.
- **Movie S2** shows a trajectory (C1, see Table 1) of flow-induced β-hairpin folding. Three steps involved in completing β-hairpin folding, namely, hydrophobic collapse (mauve), interstrand hydrogen bond formation (green) and turn formation (cyan) are highlighted.
- **Movie S3** shows the decrease in the number of water molecules during β-hairpin folding (trajectory of C1, see Table 1). Due to the flow, water molecules are not stagnant, but differ from each frame to frame, giving rise to apparently discontinuous jumps of water molecules from frame to frame.

2 Derivation of Eq. (8)

In the freely-jointed chain model of the β-switch, the $\vec{\delta}$ distribution, $\tilde{Q}(\vec{\delta})$, in the presence of flow is given by Eqs. (5, 7) and $W_{\text{flux}}(\vec{\delta}) = -2\vec{f}\cdot\vec{\delta}$. Accordingly, $\tilde{Q}(\vec{\delta})$ can be expressed

$$\tilde{Q}(\vec{\delta}) = A\, Z' \exp\left\{-B\,\delta^2 + 2\,\vec{f}\cdot\vec{\delta}/k_{\text{B}}T\right\} . \tag{S1}$$

where $A = \left[3(N_1 + N_2)/2\pi a^2 N_1 N_2\right]^{3/2}$ and $B = 3(N_1 + N_2)\,\delta^2/2N_1N_2a^2$. Introducing Cartesian coordinates $\vec{\delta} = (x, y, z)^{\text{T}}$ and noting $\vec{f} = (f, 0, 0)^{\text{T}}$ ("T" stands here for "tranposed"), this can be written as a shifted Gaussian

$$\tilde{Q}(\vec{\delta}) = A\, Z' \exp\left\{-B\,(x - \Delta x)^2 - B(y^2 + z^2) + B\Delta x^2\right\} . \tag{S2}$$

where one can readily identify $\Delta x = f/Bk_{\text{B}}T = (2fa/3k_{\text{B}}T)\,[N_1N_2/(N_1 + N_2)]\,a$, i.e., Eq. (8).

3 Supporting Figures

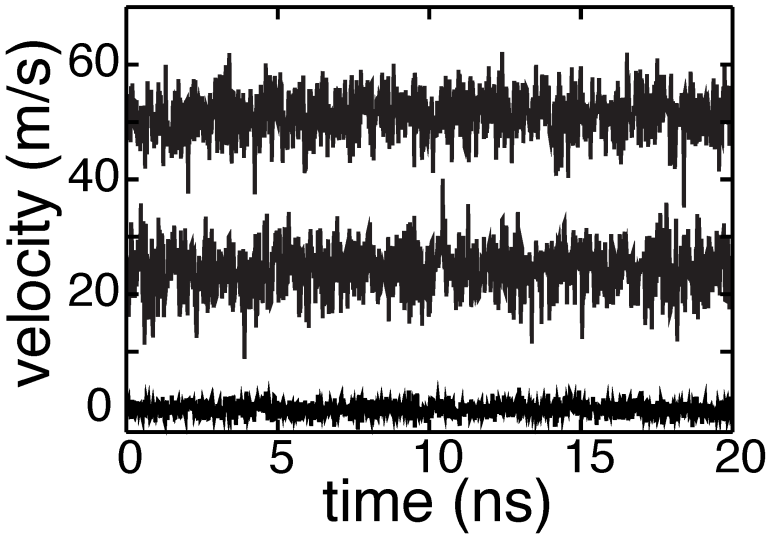

Figure S1: Actual flow velocity arising in simulations.

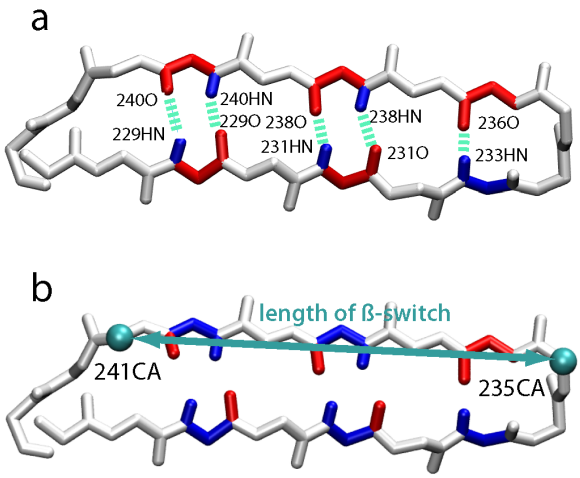

Figure S2: Characteristics of folded β-hairpin. (a) Five hydrogen bonds between strands of the β-switch. (b) Definition of β-switch length.

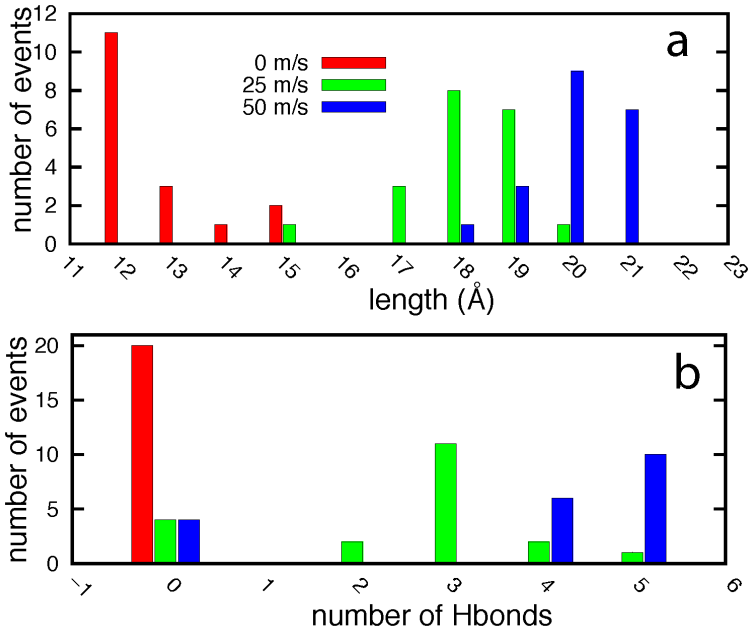

Figure S3: Hairpin formation statistics for 60 simulations. (a) Length distribution under different flow conditions. (b) Interstrand hydrogen bonds formed under different flow conditions.

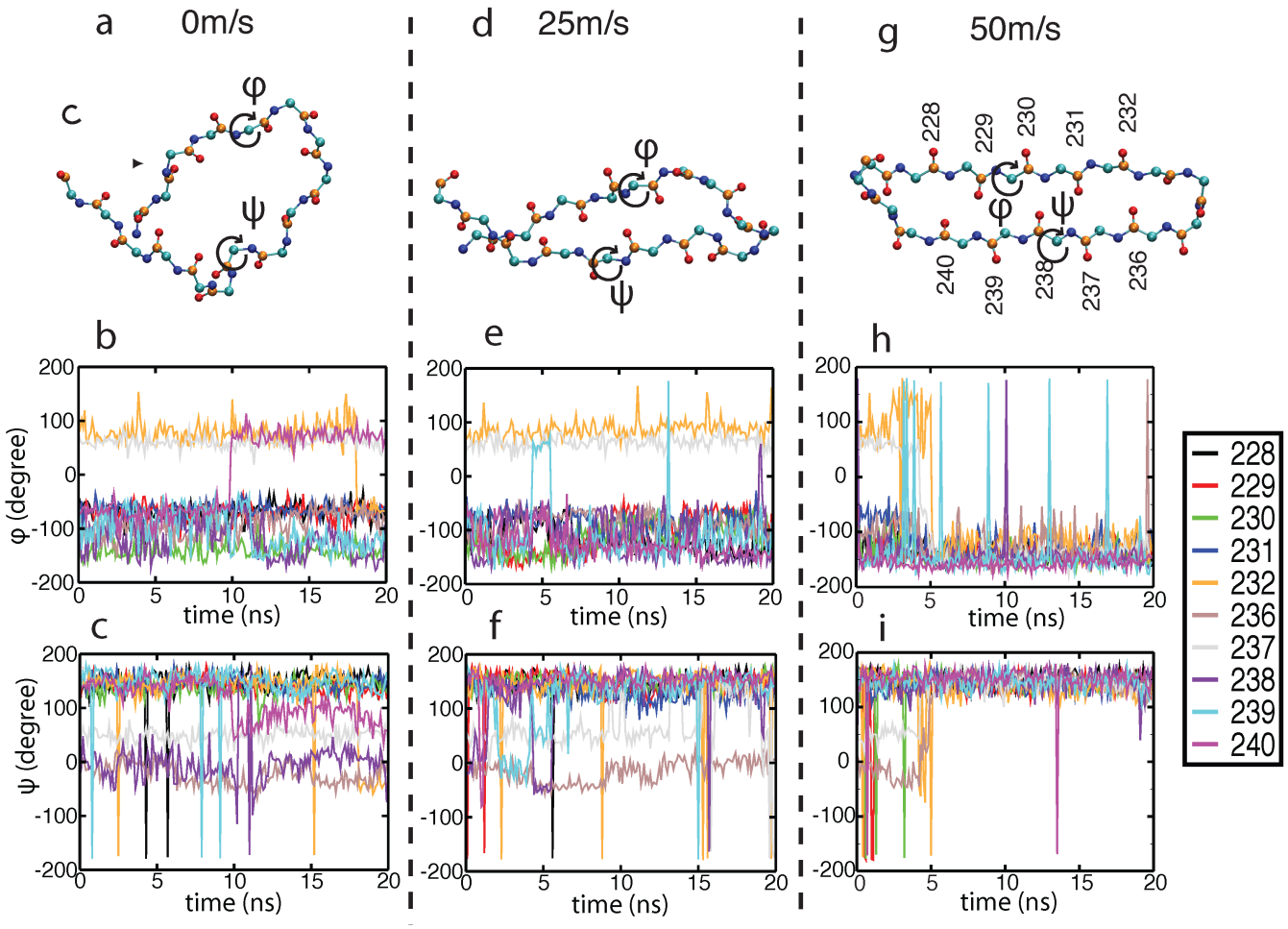

Figure S4: Rotation of backbone dihedral angles ϕ (C'-N-C_α-C') and ψ (N-C_α-C'-N) from simulations A1, B1, and C1 (see Table 1). (a), (b), (c) show the torsion angles at zero flow (A1). The distribution of angles are wide and fluctuations are large. (d), (e), (f) show that for 25 m/s-flow (B1) the torsion angles fluctuate less than in case of zero flow. The torsion angles of residues, involved in hydrogen bond formation, like that of THR240, converge to 150° after 7 ns. (g), (h), (i) show that for 50 m/s-flow (C1) ϕ and ψ assume values of $\pm 170°$ consistent with maximum β-switch extension. The torsion angles of residues (VAL229, THR240, LYS231, ALA238), which form the first three hydrogen bonds, rotate to 150° first. The dihedral angles proximate to hydrogen bond 233HN-236O rotates at 5 ns synchronously with the formation of that hydrogen bond.

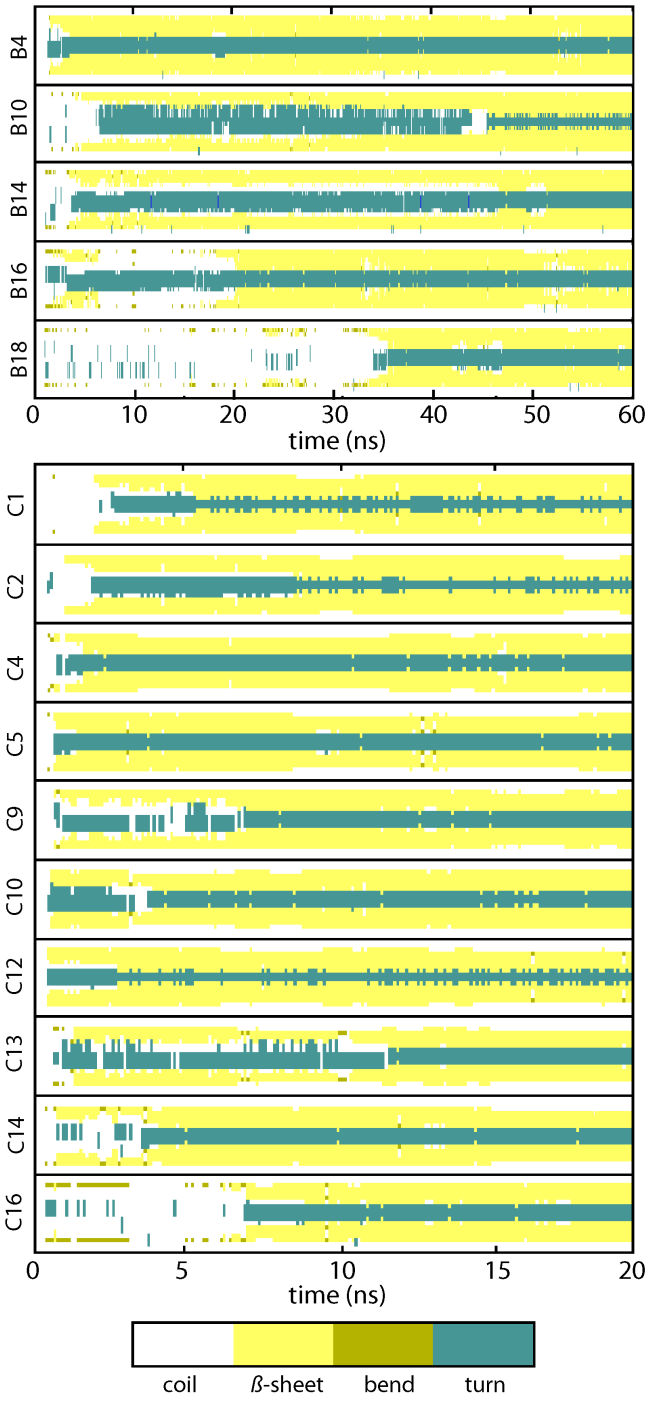

Figure S5: Secondary structure seen in β-hairpin folding trajectories at 25 m/s-flow and 50 m/s flow. Under 25 m/s-flow (top), two interstrand hydrogen bonds either formed before turn formation (B10 and B18), or the formation of turn and interstrand hydrogen bonds occurred at the same time (B4, B14 and B16). Under 50 m/s-flow (bottom), five β-hairpin foldings were initiated by interstrand hydrogen bond formation (C1, C2, C13, C14, C16); in other β-hairpin foldings, the formation of turn and interstrand hydrogen bonds occurred simultaneously.

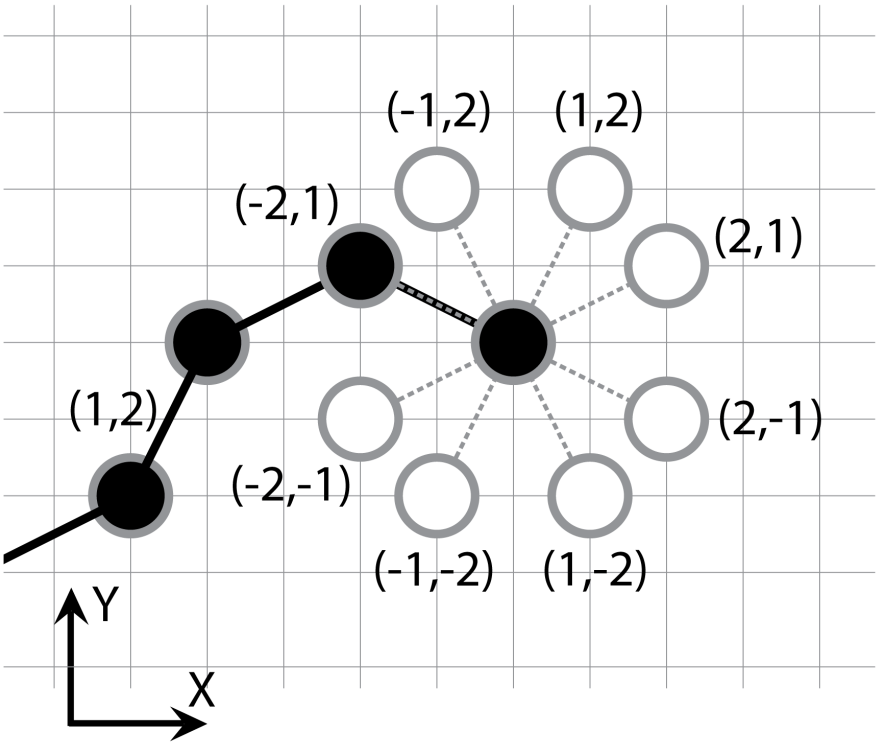

Figure S6: Two-dimensional lattice model describing conformation and dynamics of proteins. Each amino acid is represented by a bead placed on a lattice point; peptide bonds between amino acids are represented by a vector of length $\sqrt{5}$. Every bead has eight neighbors, e.g., a bead at lattice point (0,0) has neighbors at (1,2), (2,1), (2,-1), (1,-2), (-1,-2), (-2,-1), (-2,1), and (-1,2).