Supporting Information

for

Chiral Structure Fluctuations Predicted by a Coarse-Grained Model of Peptide Aggregation

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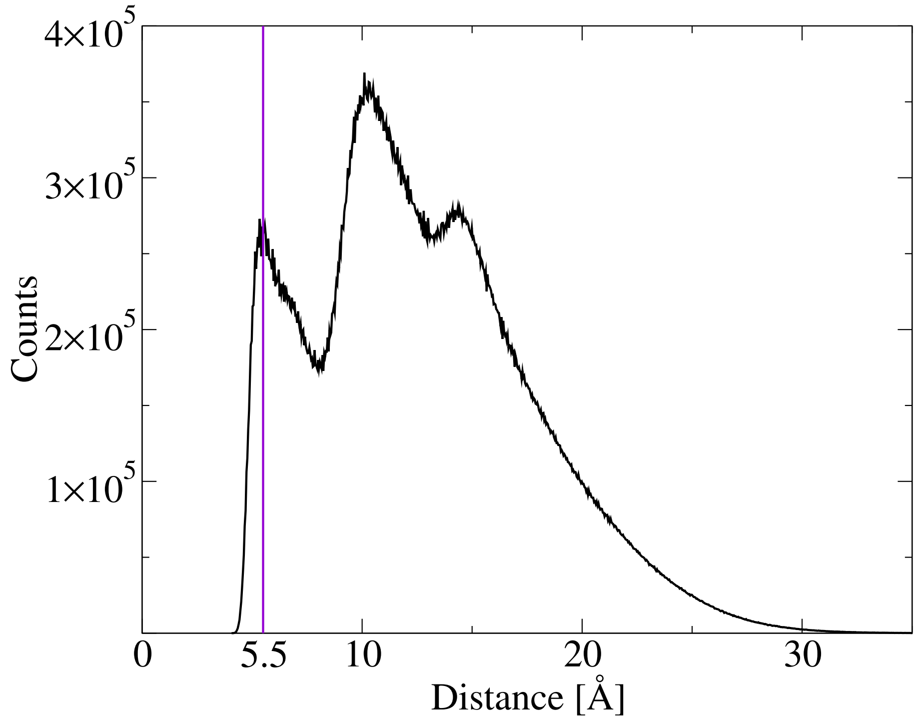


Figure S1: Example histogram of atom distances in all clusters for a simulation with $N = 9$, $\varepsilon = 2$ kJ/mol, $k_\theta = 1000$ kJ/mol. The first maximum at 5.5 Å marked by a vertical line determines the cluster cut-off distance.

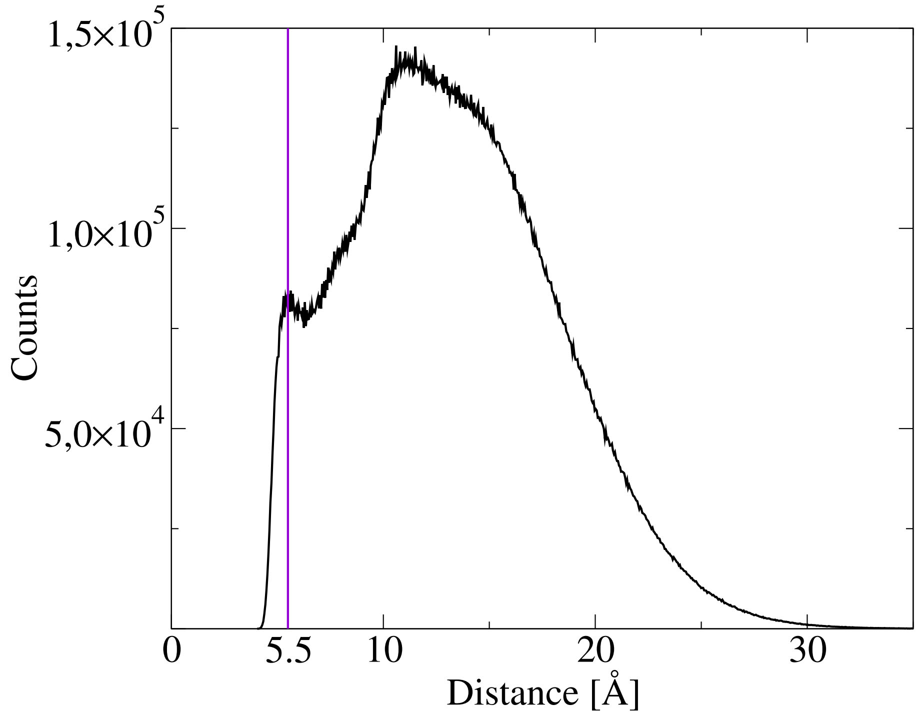


Figure S2: Example histogram of atom distances in all clusters for a simulation with $N = 9$, $\varepsilon = 2$ kJ/mol, $k_\theta = 10$ kJ/mol. The first maximum at 5.5 Å marked by a vertical line determines the cluster cut-off distance.

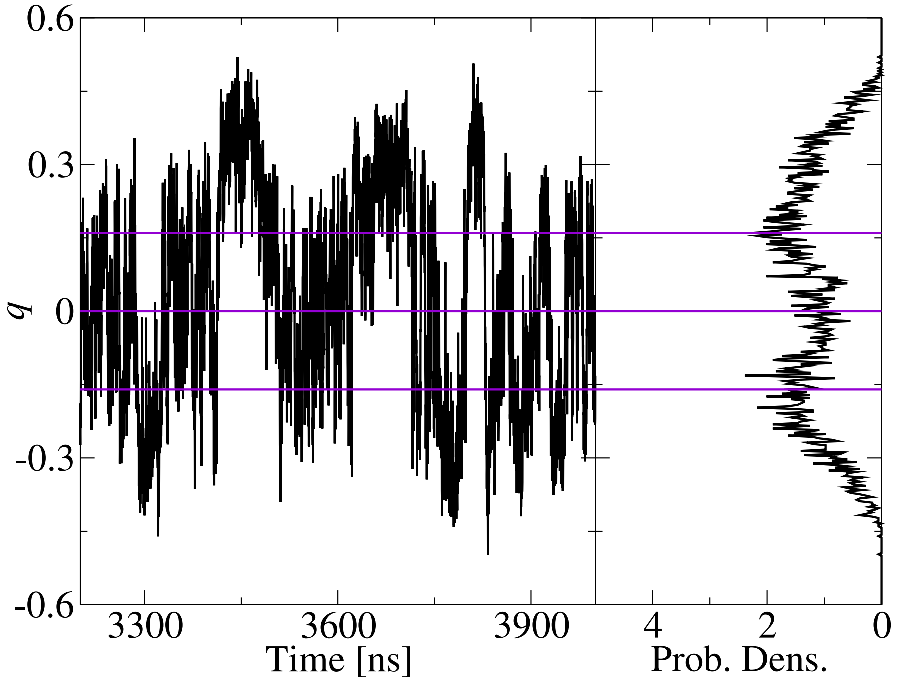


Figure S3: Cluster twist trajectory $q(t)$ for an aggregate of size $M = 41$. The normalized trajectory histogram (estimated probability density) is presented on the right panel. Three maxima marked by violet lines are visible on the histogram at $q\approx$ 0.16, $q\approx$ 0.0, and $q\approx$ -0.16.

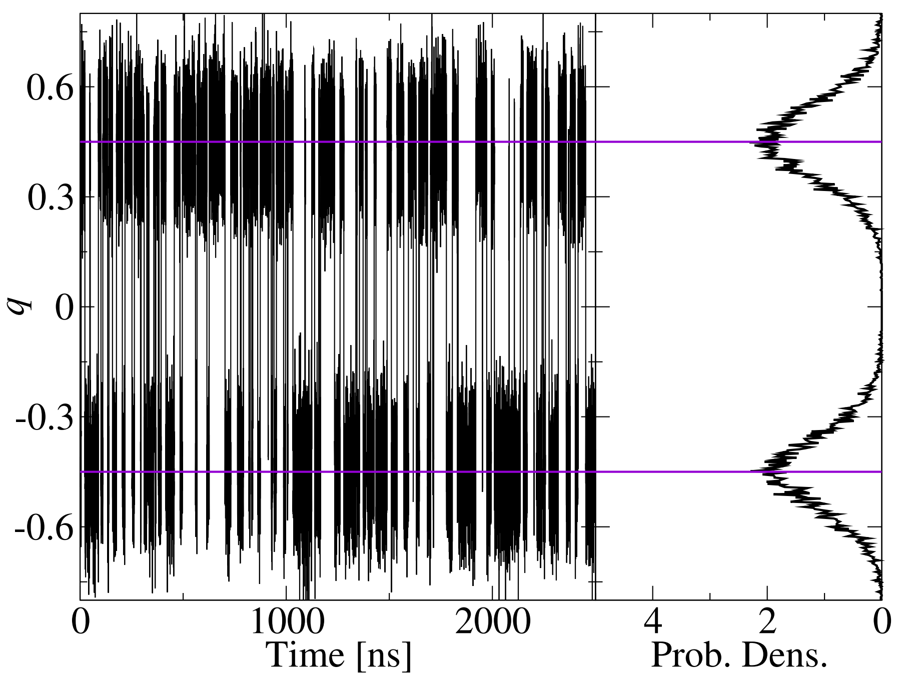


Figure S4: Cluster twist trajectory $q(t)$ simulated by the stochastic diffusion model for an aggregate of size $M = 20$. The normalized trajectory histogram (estimated probability density) is presented on the right panel. Two maxima marked by violet lines are visible on the histogram at $q\approx$ 0.45 and -0.45.

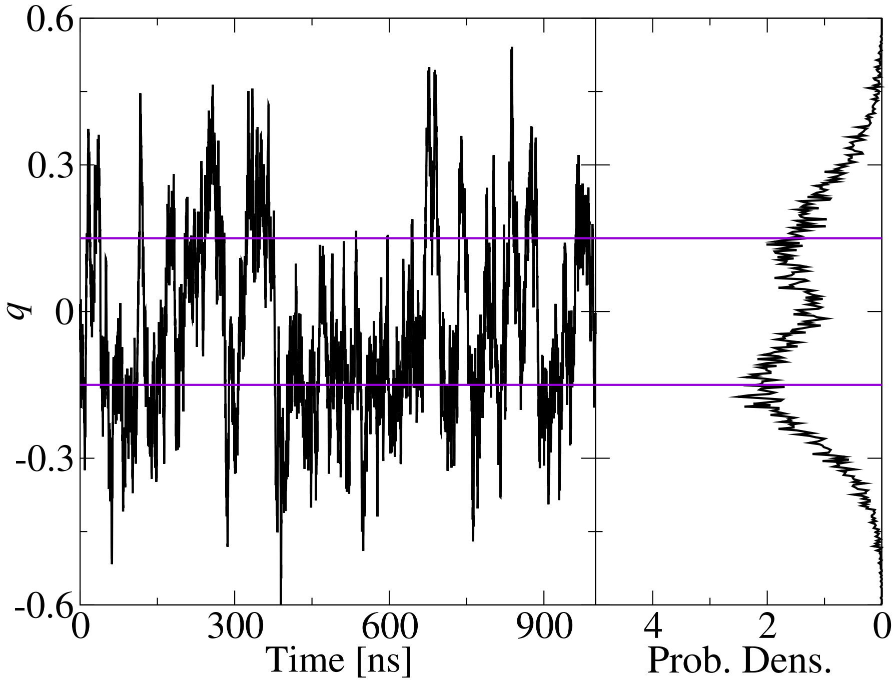


Figure S5: Cluster twist trajectory $q(t)$ simulated by the stochastic diffusion model for an aggregate of size $M = 41$. Normalized histogram (estimated probability density) is presented on the right panel. Two maxima marked by violet lines are visible on the histogram at $q \approx$ 0.15 and -0.15.

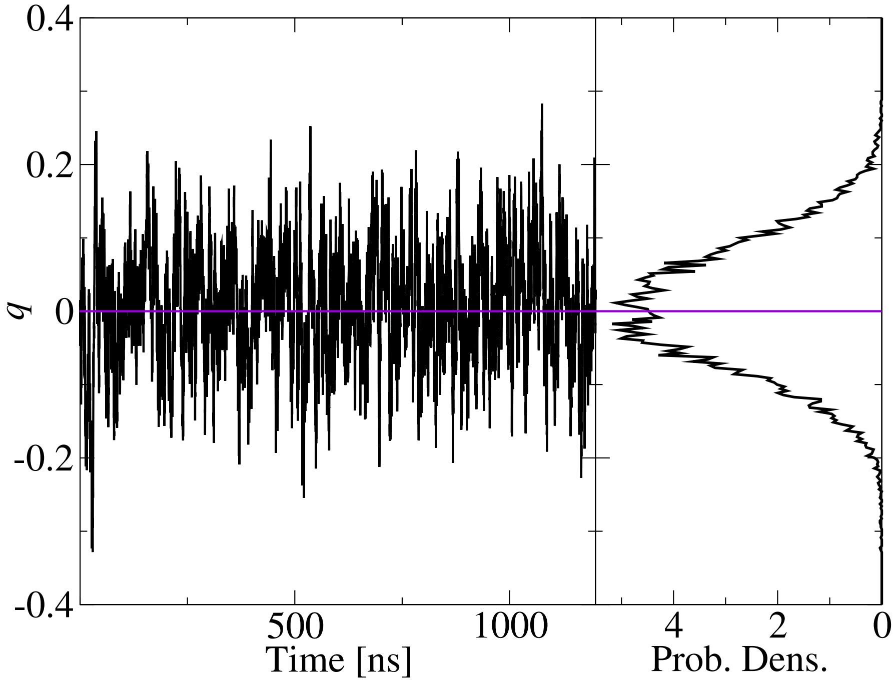
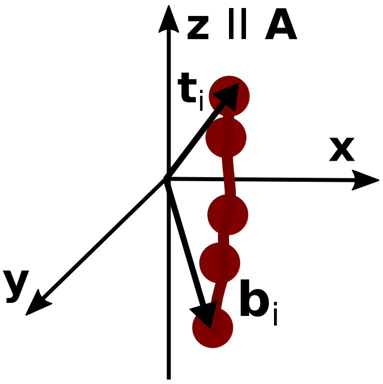
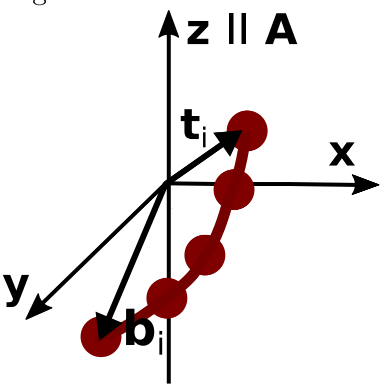
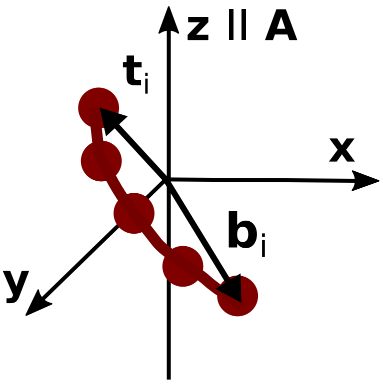


Figure S6: Cluster twist trajectory $q(t)$ simulated by the stochastic diffusion model for an aggregate of size $M = 68$. Normalized histogram (estimated probability density) is presented on the right panel. The maximum marked by violet line is located at $q \approx$ 0.

Table S1: The chain twist $\cos(\tau) = (\mathbf{b} \times \mathbf{t}) \cdot \mathbf{A}$ for three cases: achiral, right and left-handed chain twists.

Achiral	
	$\mathbf{A} = (0, 0, 1)$ $t_x = b_x$ $t_y = b_y$ $t_z = -b_z$ $\mathbf{b} \times \mathbf{t} = (-2b_y b_z, 2b_x b_z, 0)$ $\cos(\tau) = (\mathbf{b} \times \mathbf{t}) \cdot \mathbf{A} = 0$
Right-handed	
	$\mathbf{A} = (0, 0, 1)$ $t_x = -b_x$ $t_y = b_y$ $t_z = -b_z$ $\mathbf{b} \times \mathbf{t} = (-2b_y b_z, 0, 2b_x b_y)$ $\cos(\tau) = (\mathbf{b} \times \mathbf{t}) \cdot \mathbf{A} = 2b_x b_y$ $b_y > 0; b_x < 0;$ $\cos(\tau) < 0$
Left-handed	
	$\mathbf{A} = (0, 0, 1)$ $t_x = -b_x$ $t_y = b_y$ $t_z = -b_z$ $\mathbf{b} \times \mathbf{t} = (-2b_y b_z, 0, 2b_x b_y)$ $\cos(\tau) = (\mathbf{b} \times \mathbf{t}) \cdot \mathbf{A} = 2b_x b_y$ $b_y > 0; b_x > 0;$ $\cos(\tau) > 0$