Electronic Supplementary Material (ESI) for Molecular BioSystems

Electronic Supplementary Information

Backbone conformational preferences of an intrinsically disordered protein in solution

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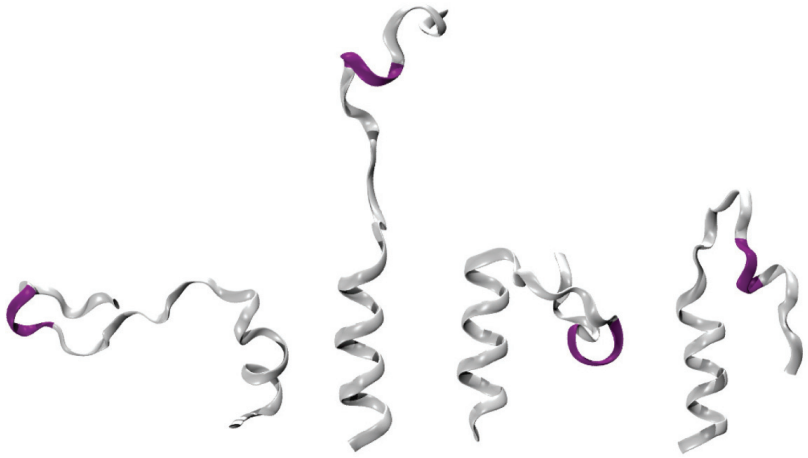

Figure S1. Transient helix formed by residues N139-L142 of KID. We show different snapshots extracted from the 4-μs trajectory of KID. The protein is rendered as ribbons, and the transient helix formed by residues N139-L142 is colored in purple.

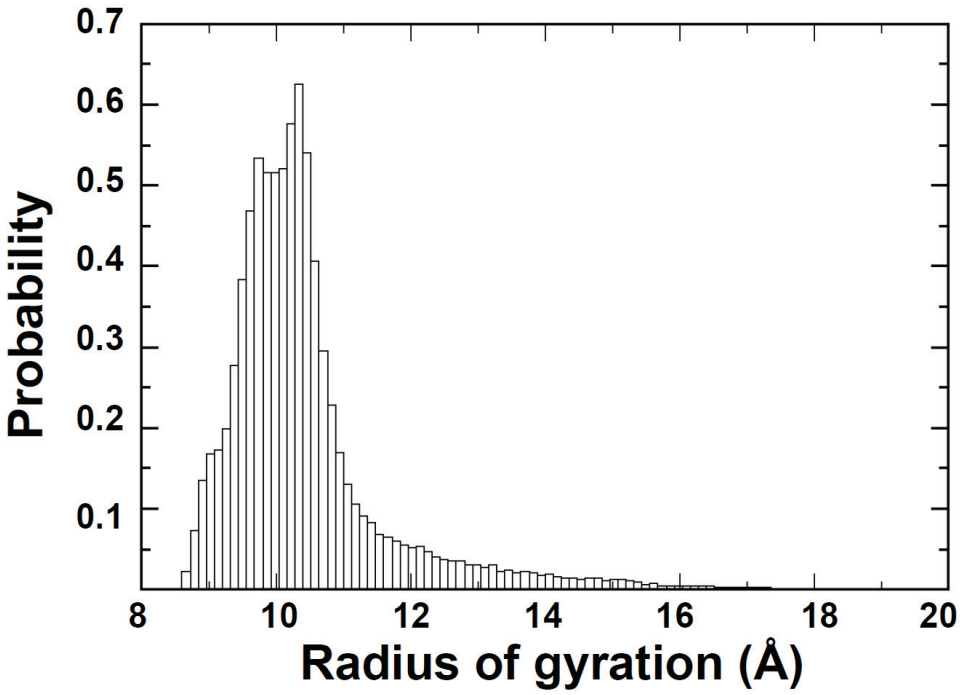

Figure S2. Probability histogram of the radius of gyration of KID. Radius of gyration was calculated for each structure in the 4-μs trajectory using the program VMD (Humphrey, W.; Dalke, A.; Schulten, K., *J Mol Graph* **1996**, *14*, 33).

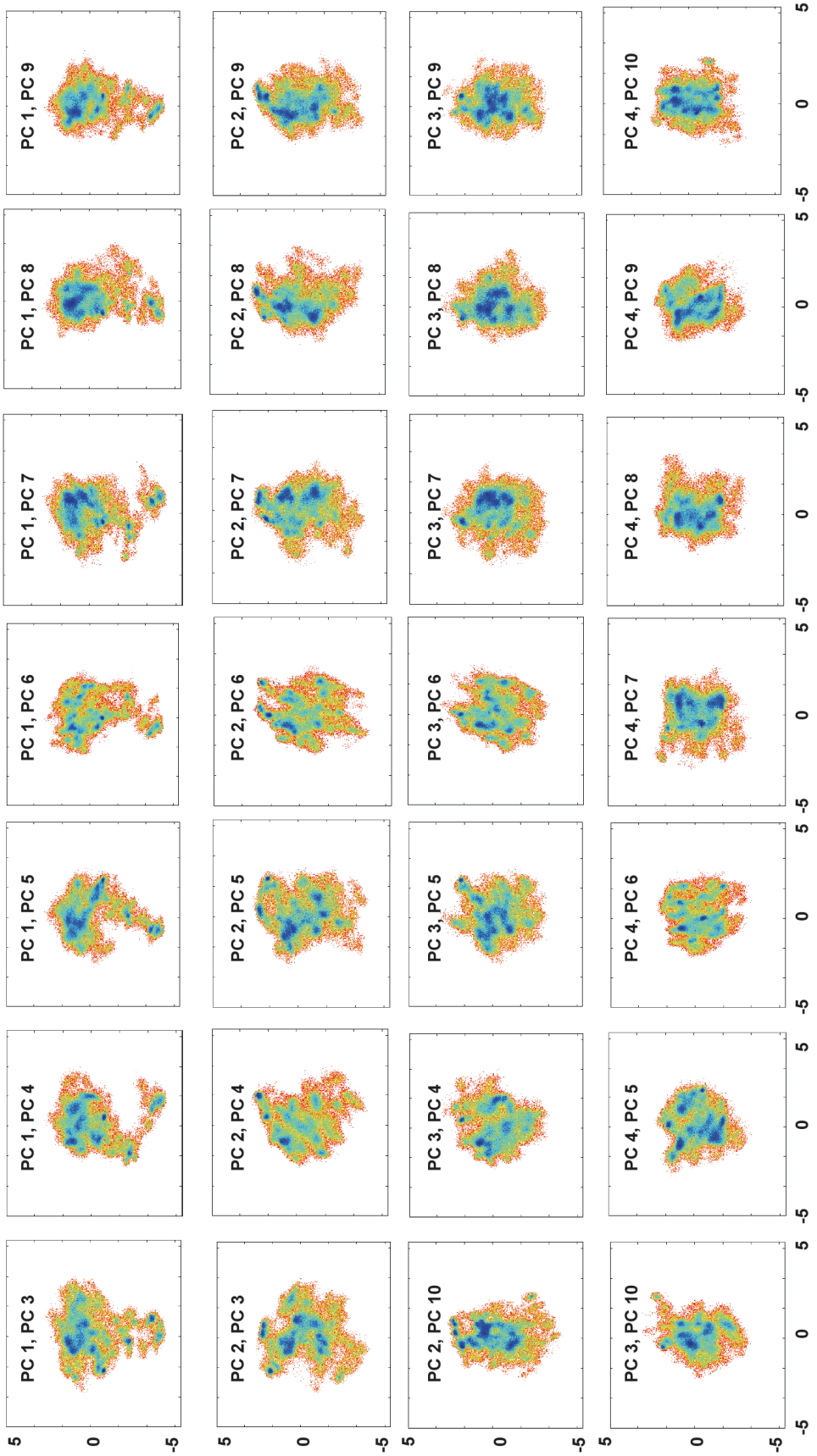

Figure S3. Free energy landscapes of KID. We used all possible pair combinations of the first ten principal components as reaction coordinates to construct two-dimensional free energy landscapes. The legend inside each plot indicates the pairs of principal components (in the format PC*a*,PC*b*) that were used to construct the energy landscapes. We used the color scale dark blue → light blue → green → yellow → red, where dark blue and red colors correspond to the lowest and highest free energy. The scale unit along the x- and y-axes is in Angstroms (Å).

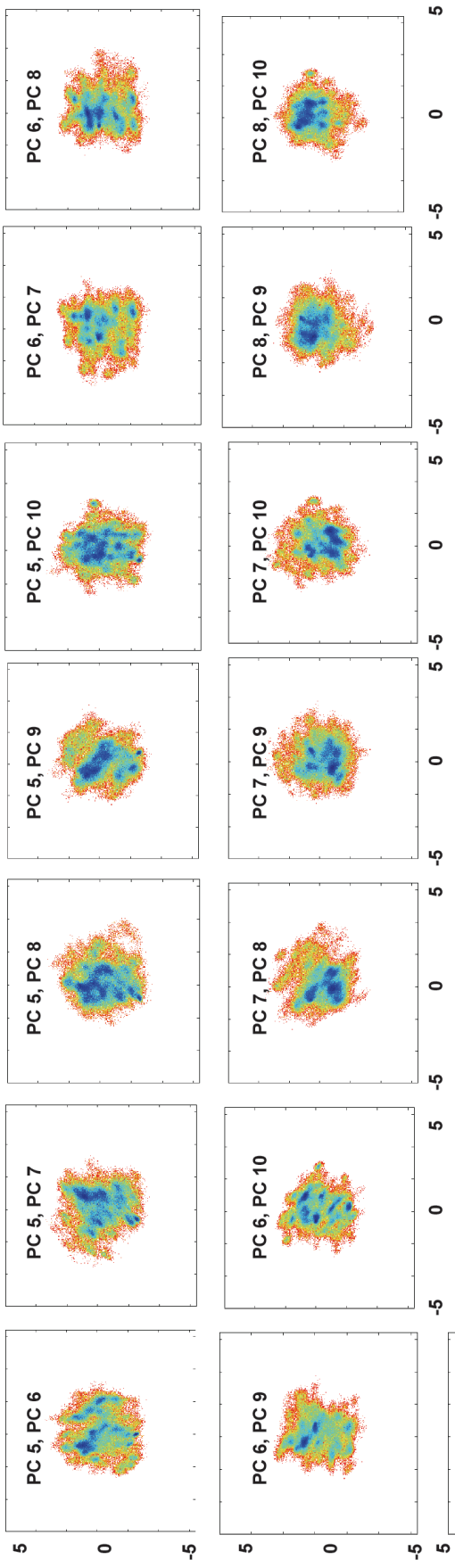

Figure S3. Continued.

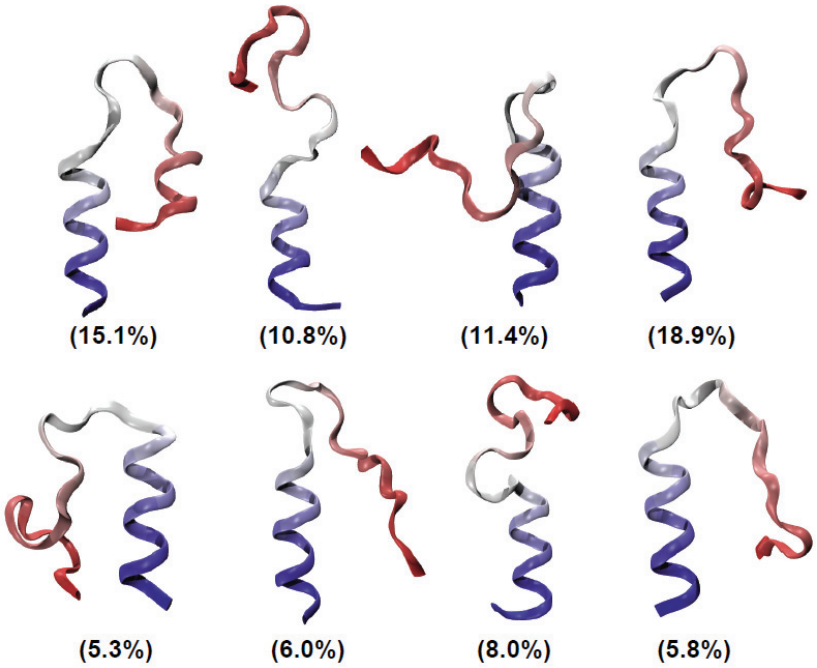

Figure S4. Representative conformations of KID obtained from clustering analysis using the first three principal components obtained from PCA. The numbers in parenthesis indicate the propensity of individual conformational states in the 4-ms trajectory. The N-terminus of KID (around domain α_A) is shown in blue, while the C-terminus (around domain α_B) is shown in red.

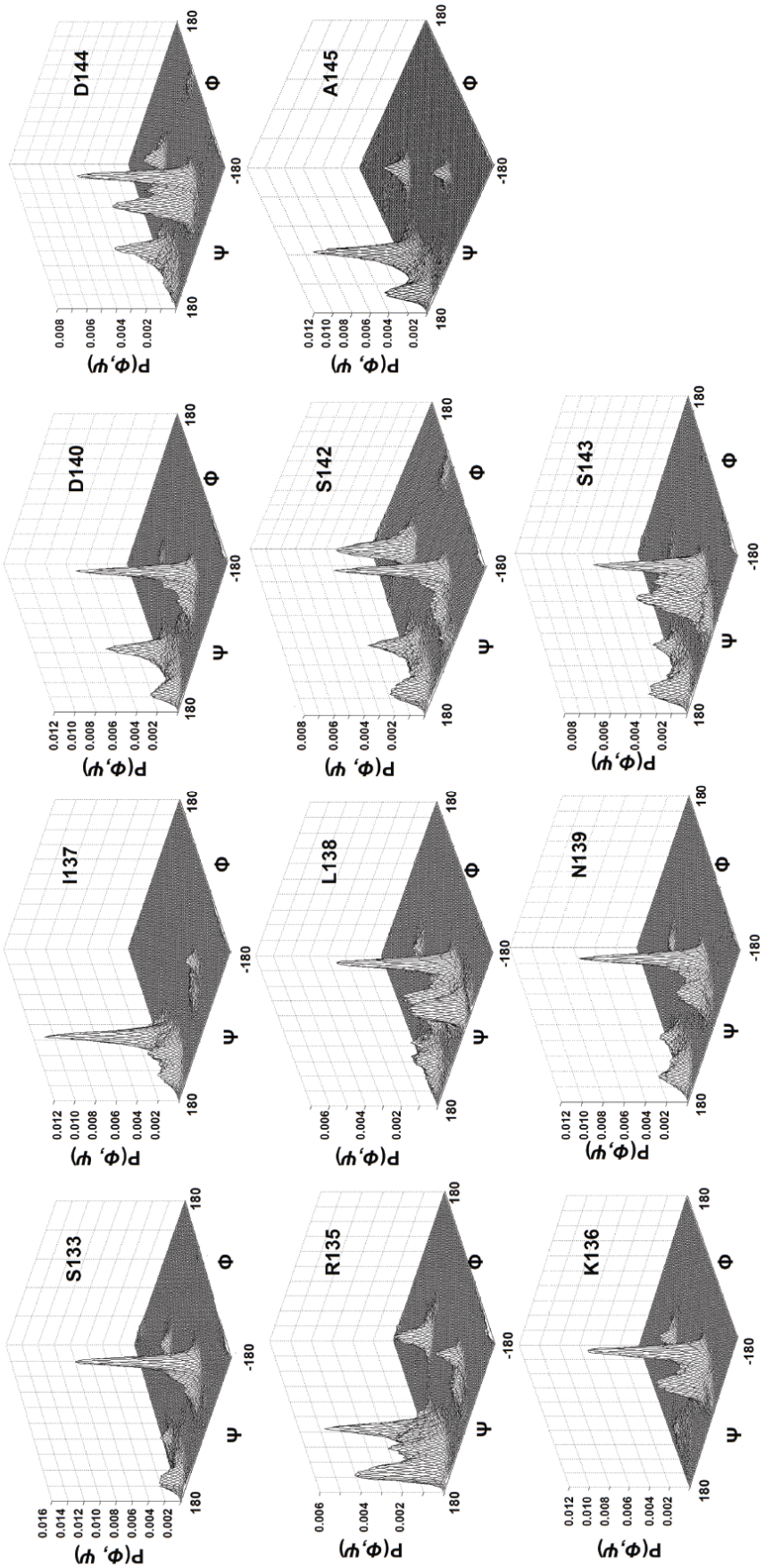

Fig. S5. Probability histograms of the (Φ,Ψ) dihedral angles of residues S133-A145 (segment α_B). The histograms show a preference for specific conformations in the (Φ,Ψ) space over the 4-μs trajectory. Histograms of residues Y134 and L141 are shown in Fig. 3 of the manuscript.