Supporting Information

The effects of flexibility on dsDNA-dsDNA interactions

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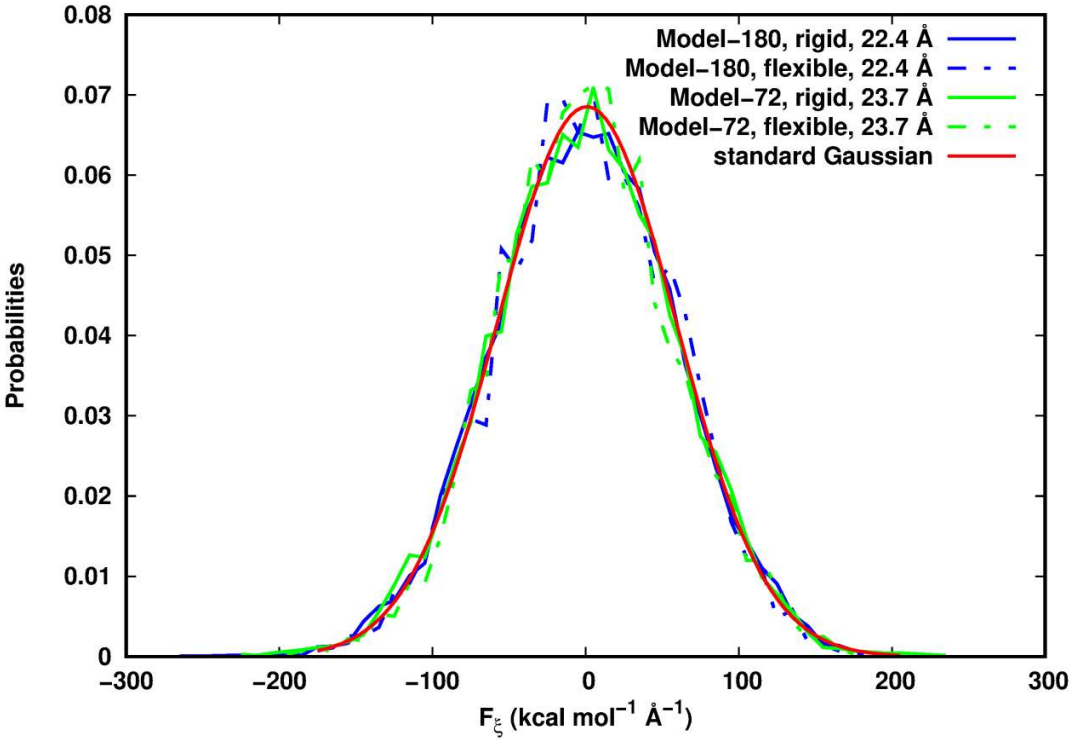

Figure S1. Distribution of instantaneous force at chosen separation distances for both flexible and rigid systems.

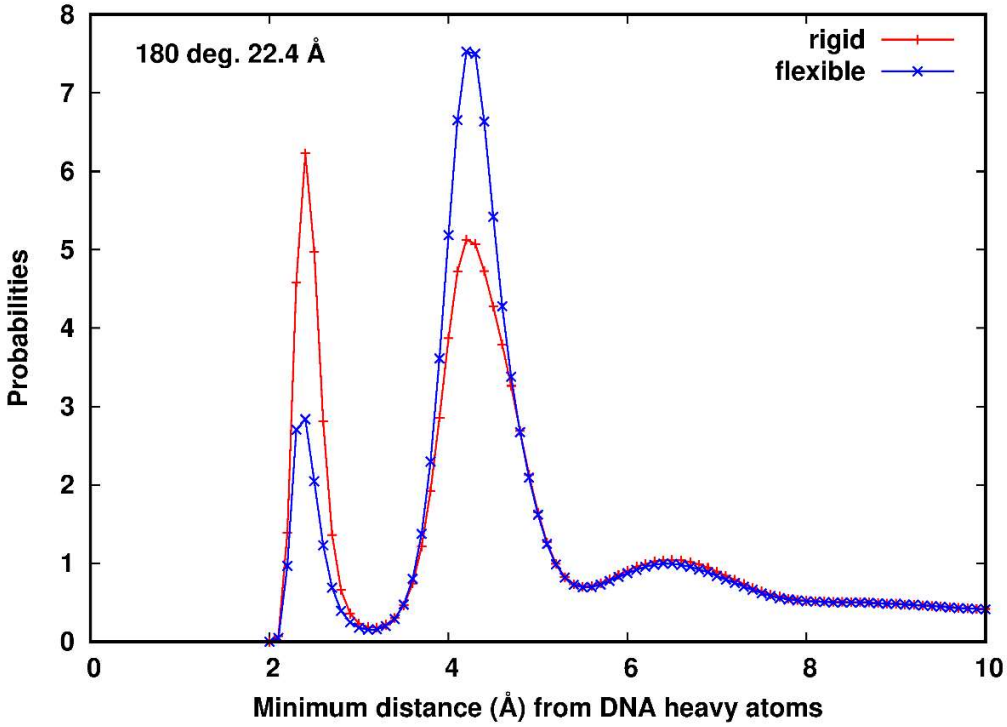

Figure S2. Minimum distance distribution of Na^+ ions from heavy atoms of dsDNAs in the rigid and flexible structures of Model-180 with the inter-helical distance at 22.4 Å. The distributions for the other configurations with different distance separations are similar. A first sharp peak centered at 2.4 Å corresponds to a direct contact of sodium ions to DNA phosphates or base group oxygen atoms, and a second broader peak at ~ 4.2 Å corresponds to the interaction of the hydrated Na^+ ions with the negatively charged atoms.

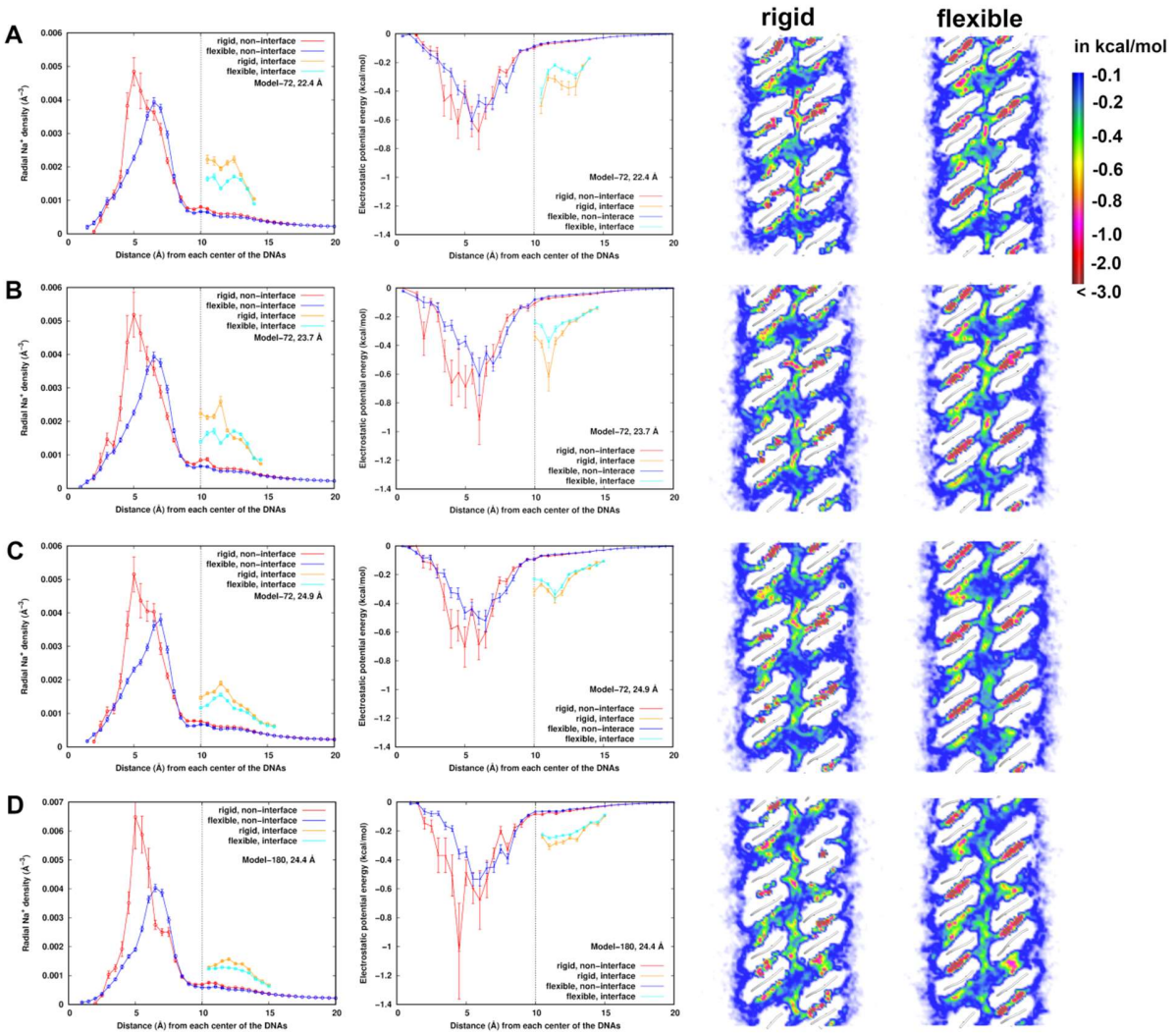

Figure S3. From left to right are radial distribution of Na^+ ions number density from the helical center of the dsDNAs, radial distribution of electrostatic potential energy of Na^+ ions with dsDNAs, a cross section of electrostatic potential energy in rigid structures and flexible structures, respectively. (A) Model-72 with the inter-helical distance d = 22.4 Å; (B) Model-72 with d = 23.7 Å; (C) Model-72 with d = 24.9 Å and (D) Model-180 with d = 24.4 Å. Backbones of dsDNAs are in color of white.

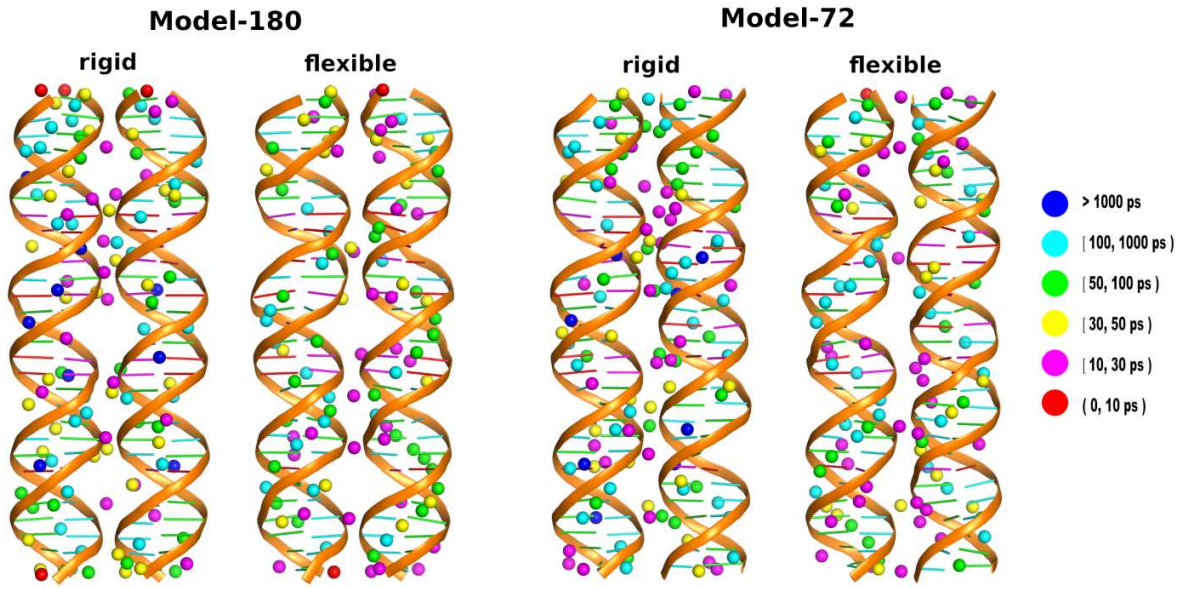

Figure S4. The effective sodium sites in the grooves and interface zone in the rigid and flexible Model180 and Model-72 with the inter-helical distance d = 22.4 Å, respectively. The sites are colored with respect to residence time. The sites were finally identified until the separation of the sites is larger than 2.8 Å. The DNA bases are colored: A, red; T, magenta; G, green; and C, cyan. To identify effective sodium sites in a particular region, we first divided the trajectory into several blocks and generated sodium density map using a grid size of 0.5 Å for each block; then for the grid points whose densities are larger than a threshold (> 0.01 # / point), we extracted the points which are ~70% overlapped; we smoothed the points by density-weighted averaging the 6-closest neighbors.[1] A residence time at a site was approximated as the inverse slope of the linear region in log(C(t)) by linear least-squares fitting, in which C(t) is a survival time correlation function representing the average number of Na^+ ions that remain in a site for a duration of time.[2]

Table S1. Probabilities that a location randomly chosen from the flexible system has higher diffusion coefficient than a location randomly chosen from the rigid one.

	minor groove	major groove	interface
Model-180, 22.4 Å	0.66	0.59	0.61
Model-180, 24.4 Å	0.69	0.59	0.59
Model-72, 22.4 Å	0.67	0.60	0.65
Model-72, 23.7 Å	0.69	0.58	0.61
Model-72, 24.9 Å	0.69	0.57	0.61

References

1. Lai, C. L.; Chen, C.; Ou, S. C.; Prentiss, M.; Pettitt, B. M., Interactions between identical DNA double helices. *Phys Rev E* **2020,** *101* (3-1), 032414.
2. Feig, M.; Pettitt, B. M., Sodium and chlorine ions as part of the DNA solvation shell. *Biophys J* **1999,** *77* (4), 1769-81.