Supplementary material for: Free Energy Landscape and Characteristic Forces for the Initiation of DNA Unzipping

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SUPPLEMENTARY MATERIAL

We include in Supplementary Fig. 1 a plot of the average number of hydrogen bonds for each of the first three base pairs against the separation distance, as seen through the all atom simulations. The first base pair is completely open at roughly 2 Å separation, and the second one at $\sim$ 11 Å. The simulations are not carried out at larger separations to observe the opening of the third base pair.

We present an additional analysis the force components and the torque on the terminal base pairs upon unzipping (see Simulation Methods in the main text). They are plotted in Supplementary Fig. 2 and show that there are large forces applied in x and y directions on C1:O3′ and G12:O3′ atoms (i.e., between the O3′ atoms on the first Cyt residue on one strand its complementary base, base Gua12 on the other strand), see Figs. 2-a,b) for the first base-pair opening and they are smaller during the second base-pair unzipping. These force components on C1:O3′ atom is in +x and -y directions whereas they are in -x and +y directions on G12:O3′ atom. Thus, the total torque in z direction (sum of torques on C1:O3′ and G12:O3′ atoms) is also larger for the the first base-pair unzipping than the one seen for the second base-pair opening (see Supplementary Fig. 2c).

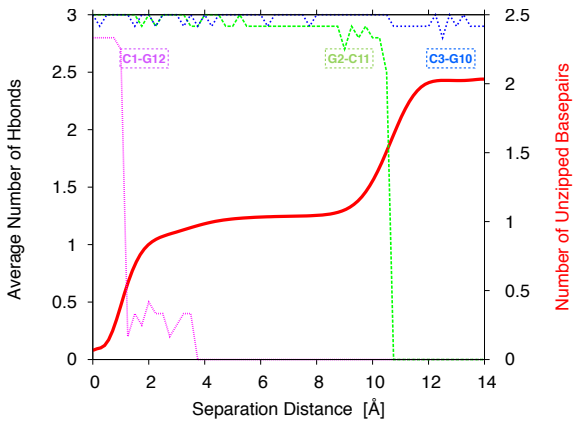

Figure 1: Supplementary Figure 1: Number of unzipped base pairs (solid red line) and average number of hydrogen bonds for the first three base-pairs (pink, green and blue dotted lines) as a function of separation distance. A base pair is considered to be unzipped when the average number of hydrogen bonds decreases below 0.5.

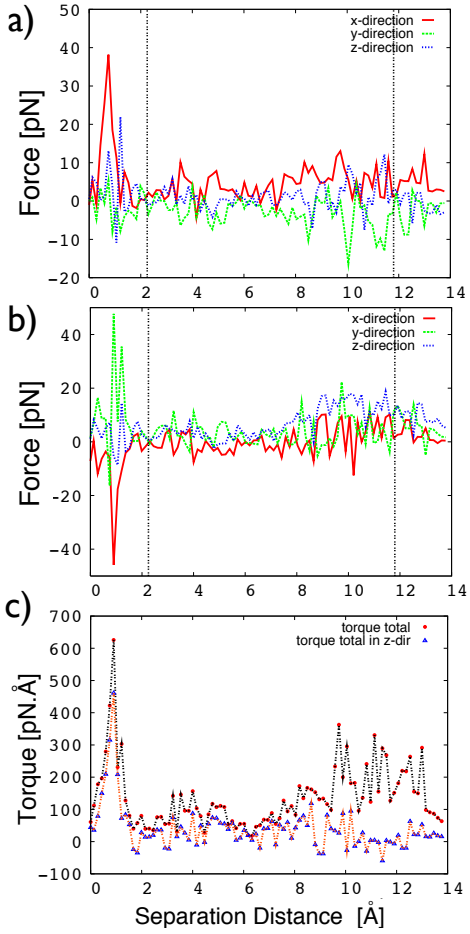

Figure 2: Supplementary Figure 2: Vector components of force acting on **a)** C1:O3′ atom and **b)** G12:O3′ atom, **c)** total torque and torque in z direction acting on atoms C1:O3′ and G12:O3′