Supplementary material

Table S1. The 39 oligomers studied. All were simulated using the SPC water model (1) and Dang ion parameters (2). Those with stars were also run with the TIP4PEW water model (3).

Name	Sequence	Duration (ns)
AAAA*	GCAAAAAAAAAAAAAAGC	100
AAAC	GCACAAACAAACAAACGC	50
AAAT	GCATAAATAAATAAATGC	50
AGAG*	GCAGAGAGAGAGAGAGGC	50
AGCG	GCCGAGCGAGCGAGCGGC	50
AGCT	GCCTAGCTAGCTAGCTGC	100
AGGA	GCGAAGGAAGGAAGGAGC	50
AGGC	GCGCAGGCAGGCAGGCGC	50
AGGT	GCGTAGGTAGGTAGGTGC	50
AGTC*	GCTCAGTCAGTCAGTCGC	100
AGTG	GCTGAGTGAGTGAGTGGC	100
ATGC	GCGCATGCATGCATGCGC	100
CAAG	GCAGCAAGCAAGCAAGGC	50
CAAT	GCATCAATCAATCAATGC	50
CGCG*	GCCGCGCGCGCGCGCGGC	100
CGGA*	GCGACGGACGGACGGAGC	50
CGGC	GCGCCGGCCGGCCGGCGC	100
CGGT	GCGTCGGTCGGTCGGTGC	50
CGTA*	GCTACGTACGTACGTAGC	100
CGTG	GCTGCGTGCGTGCGTGGC	50
GAAA	GCAAGAAAGAAAGAAAGC	100
GAAC	GCACGAACGAACGAACGC	100
GAAT	GCATGAATGAATGAATGC	100
GATA	GCTAGATAGATAGATAGC	50
GGGA	GCGAGGGAGGGAGGGAGC	50
GGGC	GCGCGGGCGGGCGGGCGC	50
GGGG*	GCGGGGGGGGGGGGGGGC	50

Name	Sequence	Duration (ns)
GGGT	GCGTGGGTGGGTGGGTGC	50
TAAC	GCACTAACTAACTAACGC	100
TAAG	GCAGTAAGTAAGTAAGGC	100
TAAT	GCATTAATTAATTAATGC	100
TATA*	GCTATATATATATATAGC	100
TCGA	GCGATCGATCGATCGAGC	100
TGGA	GCGATGGATGGATGGAGC	50
TGGC	GCGCTGGCTGGCTGGCGC	50
TGGT	GCGTTGGTTGGTTGGTGC	50
TGTA	GCTATGTATGTATGTAGC	50
TGTC	GCTCTGTCTGTCTGTCGC	50
TGTG*	GCTGTGTGTGTGTGTGGC	50

Table S2. Comparison of averages and standard deviations for the base pair A_9 and the central base pair step $A_çG_{10}$ parameters within the ACGT oligomer for three simulations: 0-50 ns with SPC/E water; 50-100 ns with SPC/E water; 0-50 ns with TIP4PEW water. In all tables and figures, translational parameters are in Å and rotational parameters are in degrees.

Parameter	0-50 ns SPC/E	50-100 ns SPC/E	0-50 ns TIP4PEW
Shear	0.03 ± 0.29	0.04 ± 0.29	0.02 ± 0.28
Stretch	0.03 ± 0.12	0.03 ± 0.12	0.02 ± 0.12
Stagger	0.15 ± 0.40	0.14 ± 0.40	0.19 ± 0.40
Buckle	7.6 ± 9.9	6.3 ± 10.9	8.1 ± 9.6
Propeller	-8.5 ± 7.8	-8.8 ± 8.0	-8.7 ± 8.1
Opening	4.8 ± 5.8	4.6 ± 5.7	4.5 ± 5.5
Xdisp	-0.62 ± 0.80	-0.66 ± 0.76	-0.69 ± 0.79
Ydisp	0.12 ± 0.47	0.11 ± 0.48	0.02 ± 0.46
Inclination	5.5 ± 4.8	5.3 ± 4.9	5.2 ± 4.7
Tip	4.8 ± 3.6	4.9 ± 3.8	5.1 ± 3.6
Axis bend	2.0 ± 1.1	1.8 ± 1.0	1.9 ± 1.0
Shift	-0.80 ± 0.73	-0.74 ± 0.74	-0.78 ± 0.66
Slide	-0.26 ± 0.56	-0.27 ± 0.57	-0.31 ± 0.57
Rise	3.43 ± 0.29	3.40 ± 0.29	3.44 ± 0.28
Tilt	-4.1 ± 4.0	-4.0 ± 4.0	-3.8 ± 3.9
Roll	1.0 ± 5.7	1.5 ± 5.7	0.6 ± 5.4
Twist	37.1 ± 5.3	36.5 ± 5.6	37.4 ± 4.6
α	-75.5 ± 12.9	-74.7 ± 12.5	-74.6 ± 12.5
β	169.1 ± 11.2	170.2 ± 11.0	169.4 ± 10.5
γ	52.3 ± 10.3	52.9 ± 10.2	53.2 ± 10.2
δ	135.4 ± 12.3	134.9 ± 13.2	134.2 ± 14.2
ε	-113.5 ± 43.3	-119.4 ± 44.0	-114.1 ± 44.6
ζ	175.8 ± 55.6	-175.2 ± 57.4	176.8 ± 57.1
χ	-97.7 ± 16.4	-99.2 ± 16.7	-98.9 ± 17.5
Phase	144.0 ± 19.5	144.1 ± 21.7	142.7 ± 23.7
Amplitude	44.1 ± 6.6	43.6 ± 6.7	43.8 ± 6.7

Parameter	0-50 ns SPC/E	50-100 ns SPC/E	0-50 ns TIP4PEW
Minor groove width	7.47 ± 1.20	7.51 ± 1.10	7.39 ± 1.11
Minor groove depth	4.81 ± 0.99	4.75 ± 0.93	4.91 ± 0.89
Major groove width	11.39 ± 1.57	11.38 ± 1.53	11.58 ± 1.52
Major groove depth	5.54 ± 1.07	5.66 ± 1.09	5.67 ± 1.18

Table S3. Average helical parameters and standard deviations for the A-T and G-C base pairs.

Base pair	A-T	G-C
Shear	0.10 ± 0.29	0.02 ± 0.31
Stretch	0.03 ± 0.12	0.03 ± 0.11
Stagger	0.07 ± 0.42	0.10 ± 0.39
Buckle	3.7 ± 11.7	2.8 ± 12.3
Propeller	-12.9 ± 9.0	-9.1 ± 9.2
Opening	3.1 ± 5.5	1.1 ± 3.3
Xdisp	-1.45 ± 0.82	-1.43 ± 0.96
Ydisp	0.10 ± 0.53	0.00 ± 0.56
Inclination	6.7 ± 5.5	6.9 ± 5.2
Tip	0.2 ± 5.0	0.5 ± 4.9

n.b. Averaging these values for AT and GC base pairs does not give the sequence-averaged parameters listed in Table 1. This is because the signs of shear, buckle, Ydisp and tip change depending on the choice of reference strand - taken here to be the strand carrying the purine. In table 1, since all possible base pairs are considered (AT and TA, GC and CG), the overall average will also include contributions with opposite signs.

Table S4. Average helical parameters and standard deviations for the unique base pair steps

Step	Shift	Slide	Rise	Tilt	Roll	Twist
GG	-0.18 ± 0.73	-0.78 ± 0.79	3.50 ± 0.33	0.0 ± 4.3	4.9 ± 5.6	33.2 ± 6.0
GA	-0.39 ± 0.71	-0.14 ± 0.71	3.38 ± 0.31	-1.5 ± 4.5	1.7 ± 5.9	36.7 ± 6.2
GC	0.11 ± 0.66	-0.45 ± 0.58	3.46 ± 0.29	0.1 ± 4.0	-1.2 ± 5.8	35.6 ± 5.1
GT	-0.11 ± 0.72	-0.64 ± 0.49	3.36 ± 0.31	0.7 ± 3.9	-0.6 ± 5.8	32.1 ± 5.0
AT	0.05 ± 0.66	-0.82 ± 0.43	3.28 ± 0.29	0.2 ± 3.8	-0.5 ± 5.1	30.5 ± 4.2
AG	-0.37 ± 0.74	-0.54 ± 0.65	3.38 ± 0.33	-2.6 ± 4.2	3.1 ± 5.9	33.6 ± 6.0
AA	-0.33 ± 0.64	-0.35 ± 0.62	3.31 ± 0.29	-2.5 ± 4.1	0.2 ± 5.6	35.3 ± 5.5
TG	0.15 ± 0.73	-0.21 ± 0.60	3.13 ± 0.42	-0.2 ± 4.8	10.3 ± 6.3	28.1 ± 9.0
TA	0.04 ± 0.88	-0.29 ± 0.71	3.18 ± 0.38	0.6 ± 5.0	10.0 ± 7.4	29.2 ± 8.4
CG	0.06 ± 0.72	-0.09 ± 0.55	3.09 ± 0.45	0.4 ± 5.1	9.3 ± 6.0	28.5 ± 9.9

Figure S1. Distributions of helical parameters for A_9 and A_9G_{10} in the AGTC oligomer: 0-50 ns with SPC/E water (red); 50-100 ns with SPC/E water (blue); 0-50 ns with TIP4PEW water (green). Translational parameters are given in angstroms and rotational parameters in degrees.

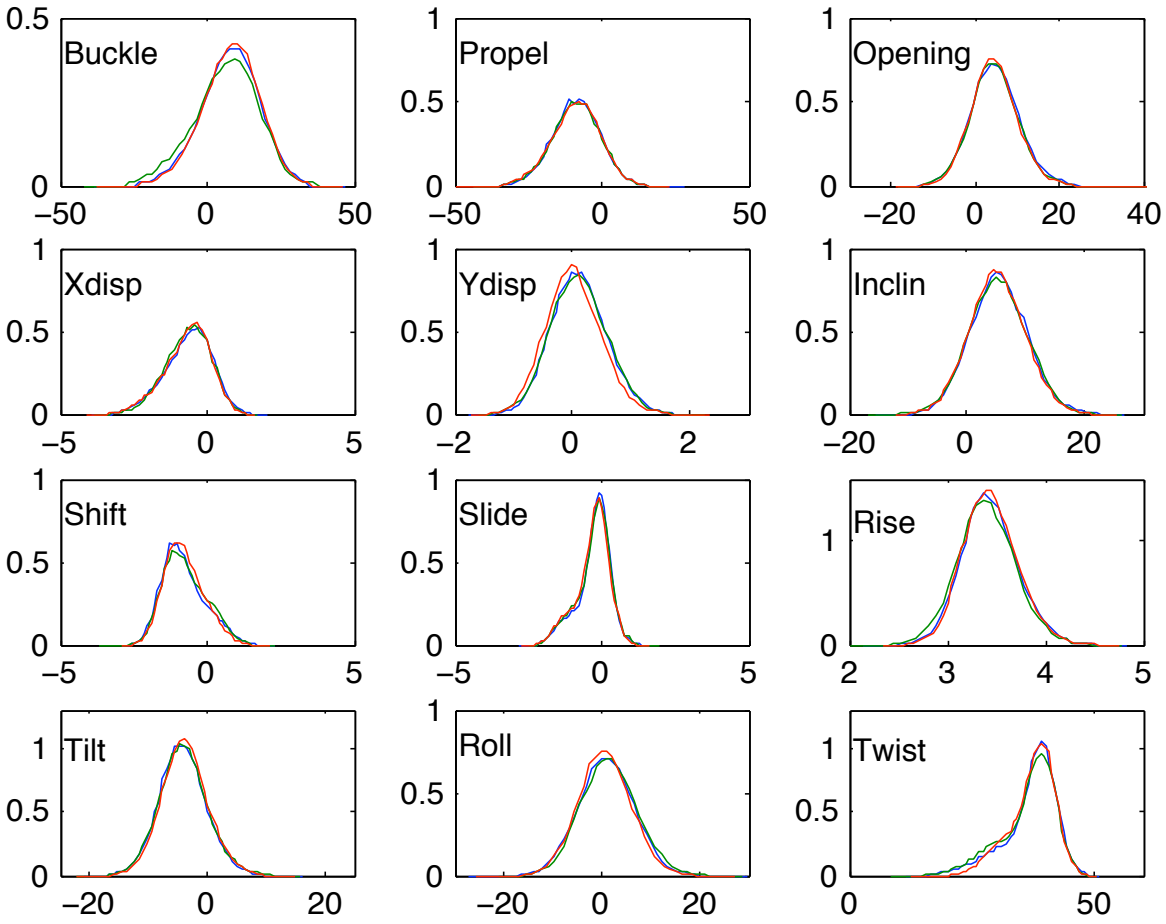
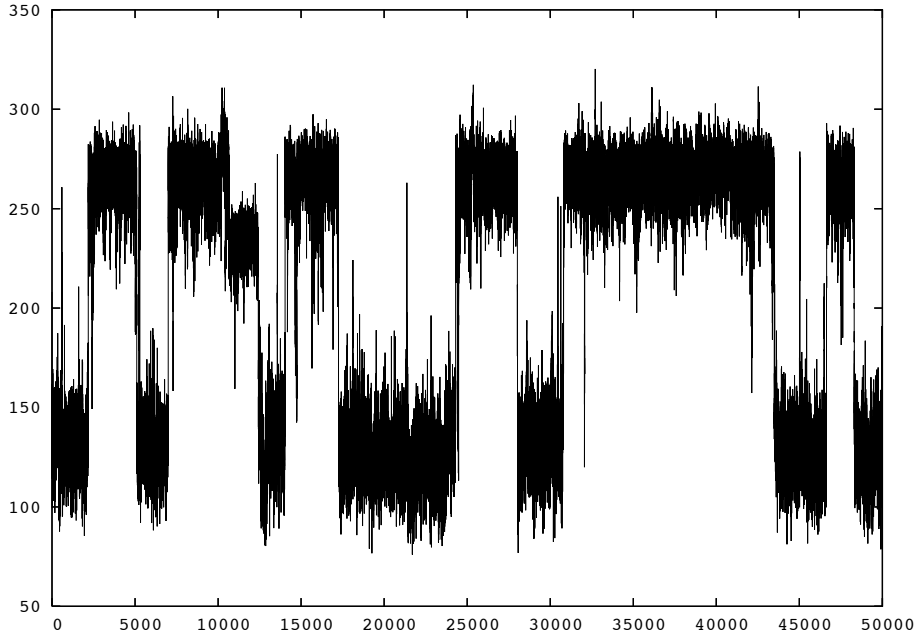


Figure S2. (A) Fluctuation of ζ in the Crick strand for step C_8G_9 in the GAAC oligomer. Values around 270° corresponds to BI and values around 140° correspond to BII; (B) Fluctuation of twist for the step C_8G_9 in the GAAC oligomer. Data for over 50000 snapshots (50 ns of simulation).

(A)



(B)

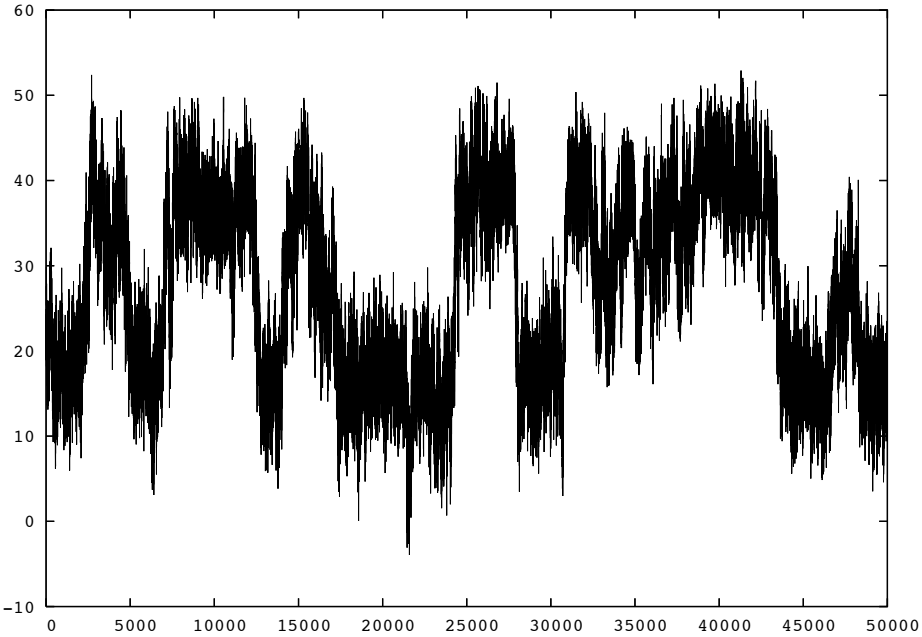


Figure S3. Distributions of helical parameters for the central G base pair and central GT step in three CGTA tetranucleotide fragments in positions 5→8 (red), 9→12 (blue) and 13→16 (green) in the CGTA oligomer. Translational parameters are given in angstroms and rotational parameters in degrees.

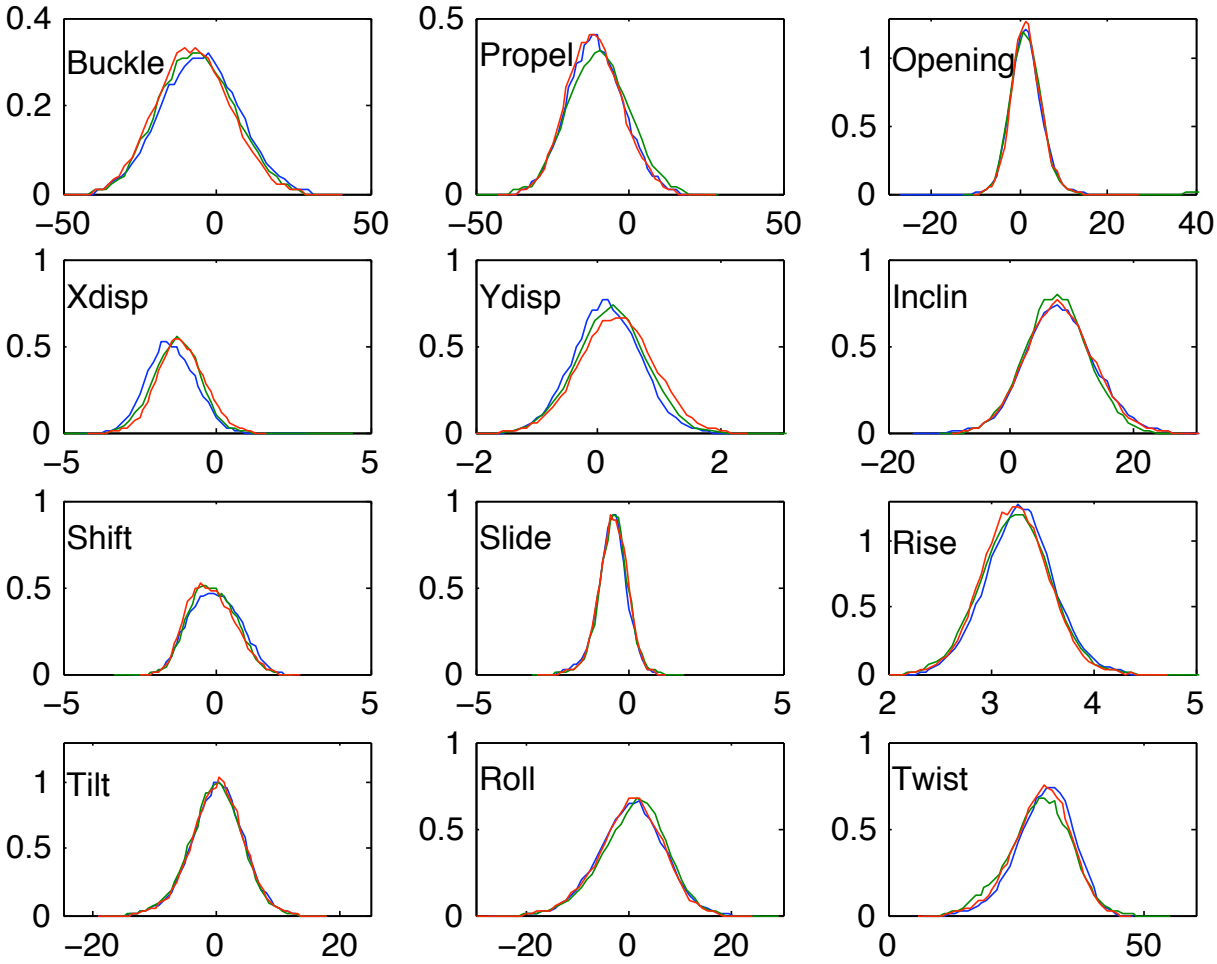


Figure S4. Base pair opening measured using the R(N1)-Y(N3) distance (Å) for three base pairs in the CGCG oligomer sampled at 100 ps intervals during 50 ns of simulation: G_1 (red), G_6 (green) and C_{18} (black). Terminal base pairs, such as G_1 and C_{18} can show large, occasionally long-lived openings, but away from the ends the openings are small and rapidly reversible.

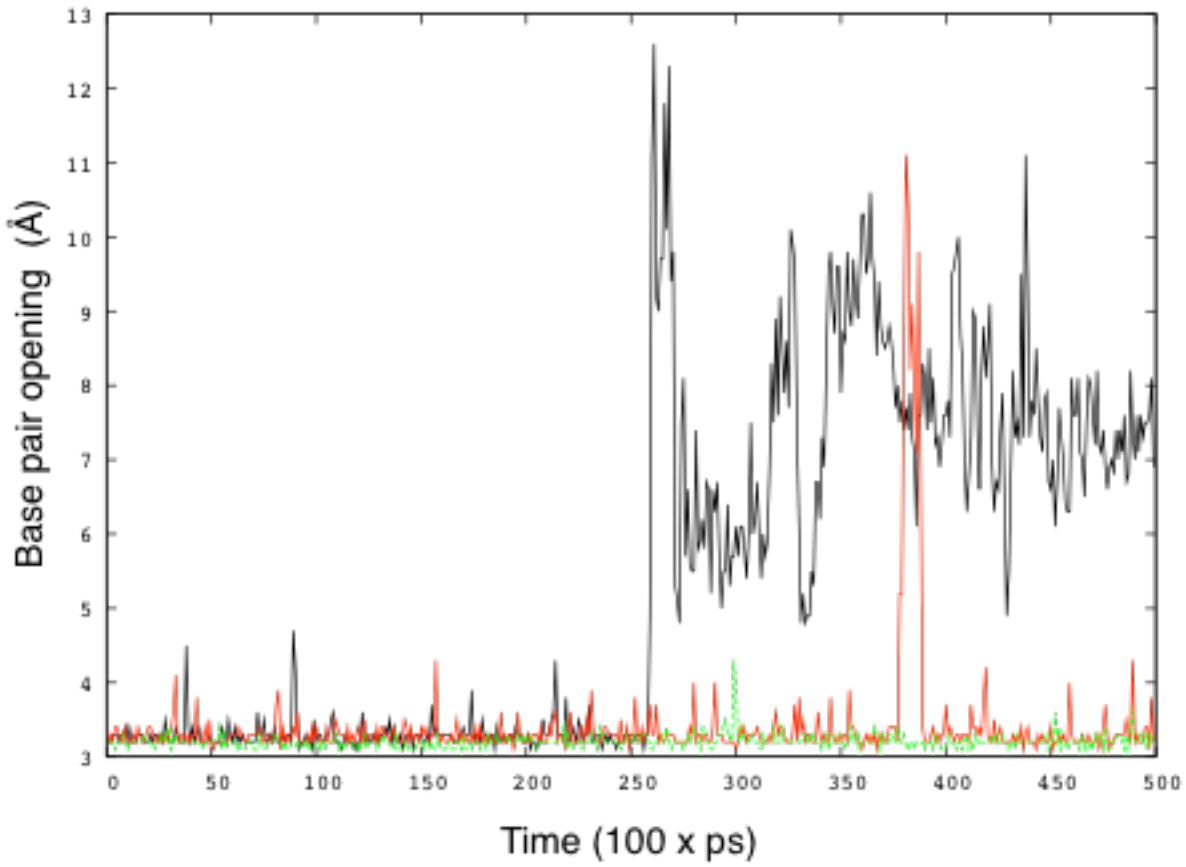


Figure S5. Percentage BII for each base pair step as a function of the nearest-neighbor sequence (in each graphic, the two letter code along the abscissa indicates the 5'- and 3'-flanking bases). Results are given for the Watson strand (red) and the Crick strand (green).

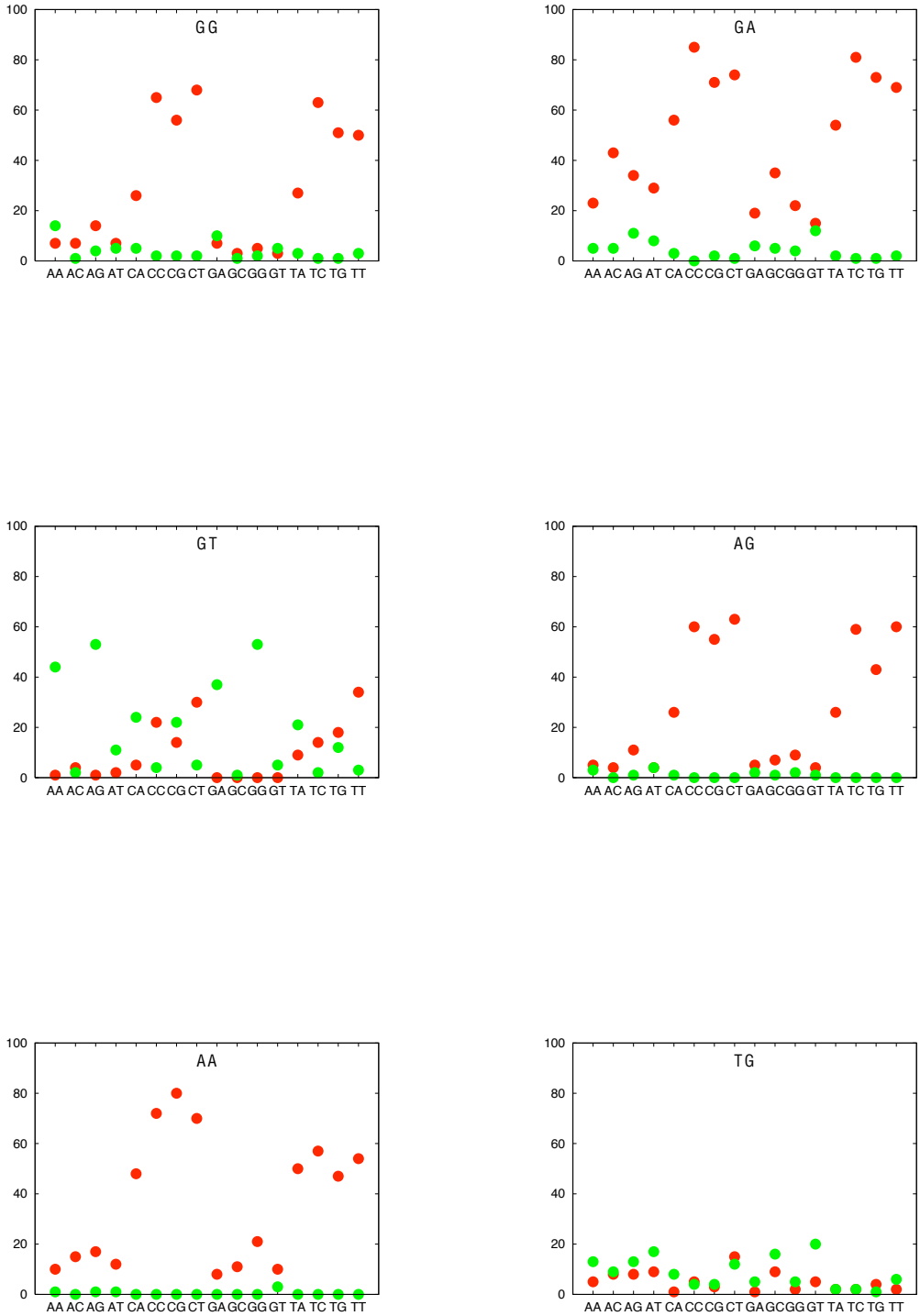
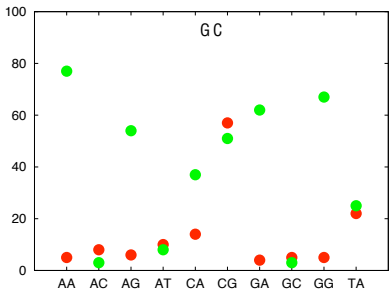
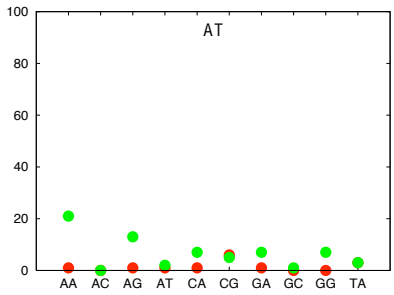
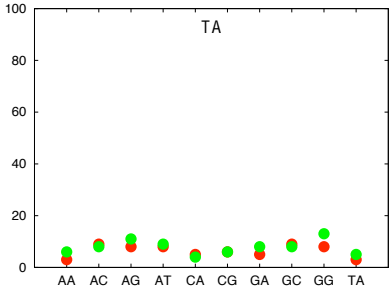


Figure S5 continued.







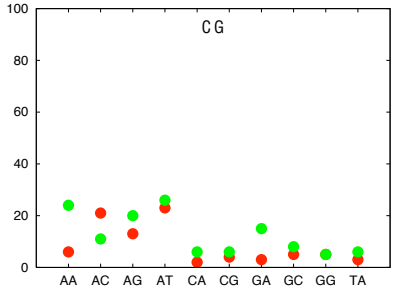
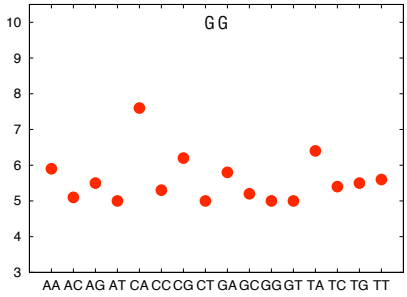
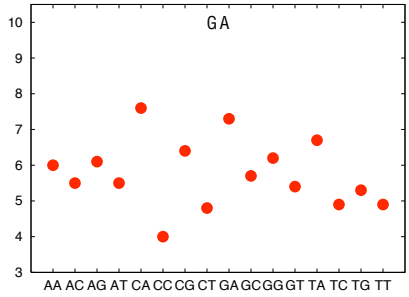
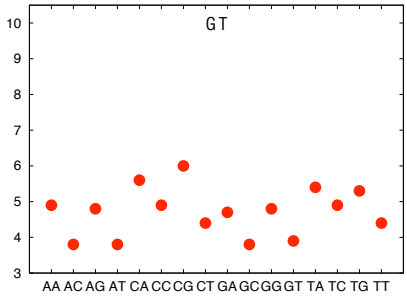
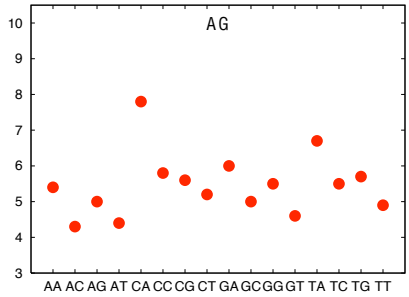


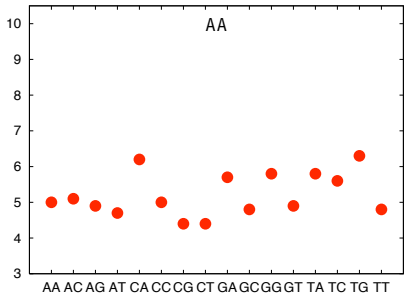
Figure S6. Standard deviations of twist for all base pair steps as a function of the nearest-neighbor sequence (in each graphic, the two letter code along the abscissa indicates the 5'- and 3'-flanking bases).











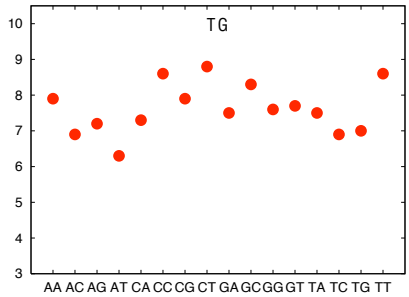
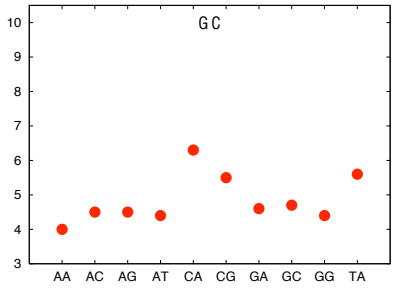
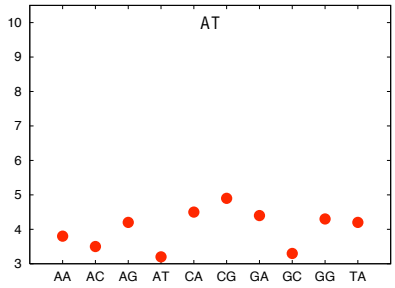
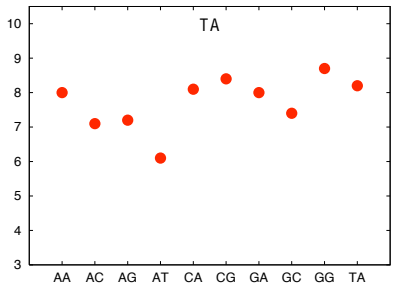
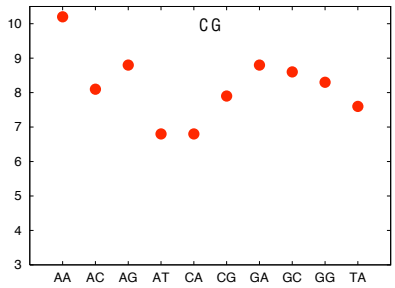


Figure S6. continued.









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3. Horn, H.W., Swope, W.C., Pitera, J.W., Madura, J.D., Dick, T.J., Hura, G.L. and Head-Gordon, T. (2004) Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. *J Chem Phys,* **120**, 9665-9678.