Supporting Information

Novel Insights into a major DNA oxidative lesion: its effects on Z-DNA stabilization

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General information: All the oligonucleotides, including 6mer-3G, 6mer-1oxoG, 6mer-2oxoG, 6mer-3oxoG, 12mer-G, 12mer-1oxoG, 12mer-2oxoG, P0, P1, P2, P3, Template A, Template C, Template G and Template T, dNTPs, dATP, dCTP, dGTP and dTTP were purchased from Takara Co. (Dalian, China). Klenow Fragment(exo-) was purchased from New England Biolabs, Inc. Poly(dI-dC) was purchased from Sigma Inc. 8-Oxo-2'-deoxyguanosine-5'-Triphosphate (8-oxodGTP) and 2'-deoxycytidine-5'-Triphosphate (dCTP) were purchased from Trilink Biotechnologies Inc. The HhaI restriction enzyme and Klenow Fragment were purchased from Thermo Scientific Inc. CD experiments were performed on a Jasco-810 spectropolarimeter (Jasco, Easton, MD, USA).

Preparation of PolyC-oxoG The preparation of the modified polymer was conducted in a solution (1 mL) containing 50 mM Tris-HCl (pH 8.0 at 25°C), 1 mM DTT, 5 mM $MgCl_2$, 0.4 mM 8-oxo-2'-deoxyguanosine-5'-triphosphate and dCTP, 50 μg of poly(dI-dC), and 40 units of E. coli Klenow Fragment. After 20 hours incubation at 37°C, the reaction was quenched by EDTA at a final concentration of 10 mM. Low molecular weight species were removed by passage through a mini quick spin oligo column, and the polymers were precipitated with ethanol and redissolved in 0.8 ml buffer containing 33 mM Tris-acetate (pH 7.9 at 37°C), 10 mM Mg-acetate, 66 mM K-acetate, and 0.1 mg/mL BSA. The starting poly(dI-dC) was digested overnight by Hha I (final concentration at 60 units/ml) incubation at 37°C. EDTA at a final concentration of 10 mM was added to stop the digestion and the low molecular weight materials were removed by another passage through a mini quick spin oligo column. Protein was removed by digestion with proteinase K and the desired polymers were extracted with phenol and chloroform. The PolyC-oxoG product was analysed with the NanoDrop® ND-2000 spectrophotometer and the ratio of OD_{260}/OD_{280} was 1.76, suggesting DNA of high quality.

Circular Dichroic Studies CD experiments utilizing a Jasco-810 spectropolarimeter (Jasco, Easton, MD, USA) were measured at room temperature using a quartz cell with a 1 cm path length, CD spectra were collected from 200 to 350 nm at scanning speed of 200 nm/min. The bandwidth was 5 nm, and the response time was 2 s. All CD spectra were baseline-corrected for signal contributions due to the buffer and were the average of at least two runs.

CD Melting Studies For Z-DNA study, a solution of different oligomer (10 μM) was prepared in buffer (5 mM Na cacodylate buffer, pH 7.0 at 10 °C) containing different concentrations of NaCl. The mixture was first heated to 95 °C for 5 min, then slowly cooled to room temperature, and incubated at 4 °C for at least 16 h. The CD absorbance were recorded on a Jasco-810 spectropolarimeter equipped with a Jasco Pelter temperature controller and a 1 nm bandwidth. Melting curves were obtained by monitoring absorbance at the indicated nm, while the temperature was ramped from 4 to 90 °C at about 0.5‑1.5 °C/min. Melting profiles were analyzed by fitting them to a concerted two-state model.

Synthesis of zinc(II) porphyrin 1 Zinc(II) derivative (**1**) of H_2TMpyP4 was prepared and purified according to an previous protocol (*Biochemistry* **1983,** *22*, 2406-14).

Table S1 Sequences of oligomers used in the studies

Oligomer	Sequence(from 5'to 3')
6mer-3G	5'- CG CG CG -3'
6mer-1oxoG	5'- C(8-oxodG) CG CG -3'
6mer-2oxoG	5'- C(8-oxodG) C(8-oxodG) CG -3'
6mer-3oxoG	5'- C(8-oxodG) C(8-oxodG) C(8-oxodG) -3'
12mer-G	5'- CG CG CG CG CG CG -3'
12mer-1oxoG	5'- CG C(8-oxodG) CG CG CG CG -3'
12mer-2oxoG	5'- CG C(8-oxodG) CG CG C(8-oxodG) CG -3'

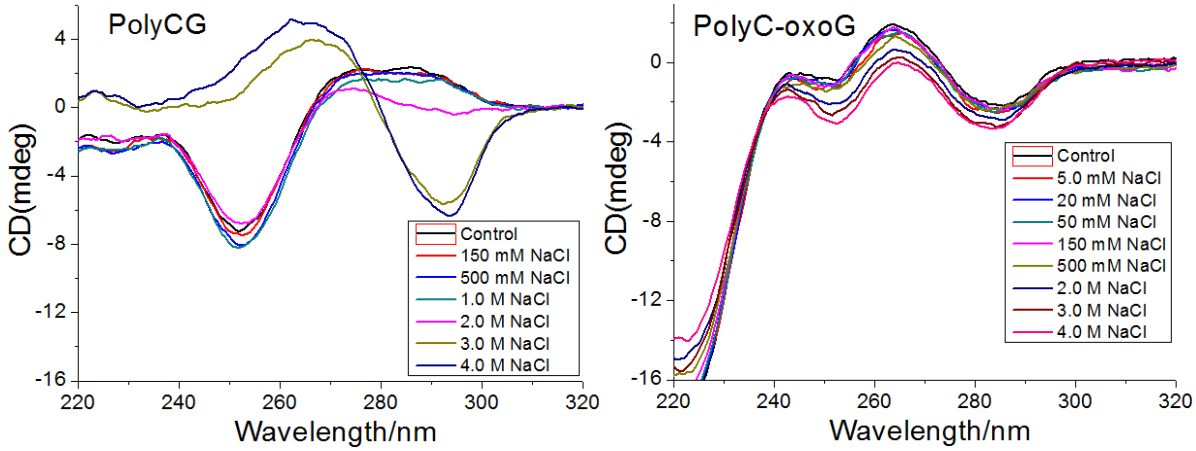


FIGURE S1. Circular dichroic (CD) spectra of polyCG and polyC-oxoG in 5 mM Na cacodylate buffer (pH 7.0 at 10 °C), at varied concentrations of NaCl ranging from 0 mM (control) to 4.0 M (each DNA concentration at 80 μg/mL).

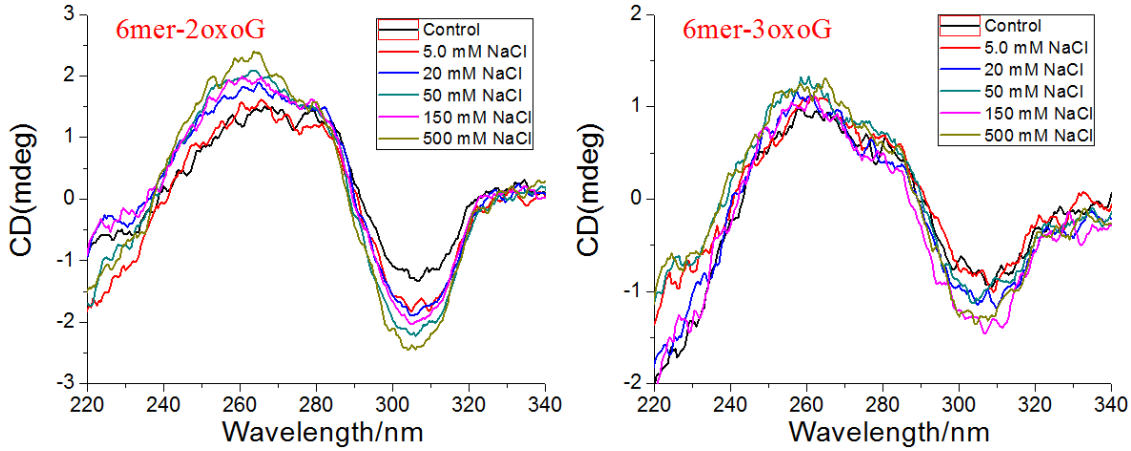
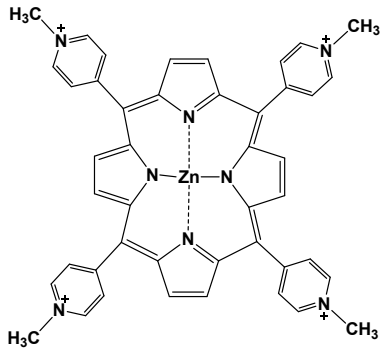


FIGURE S2. Circular dichroic (CD) spectra of 6mer-2oxoG and 6mer-3oxoG in 5 mM Na cacodylate buffer (pH 7.0 at 10 °C), at varied concentrations of NaCl ranging from 0 mM (control) to 4.0 M (each oligomer at 10 μM strand concentration). A concentration dependent manner could be observed in their circular dichroic spectra.

a)



b)

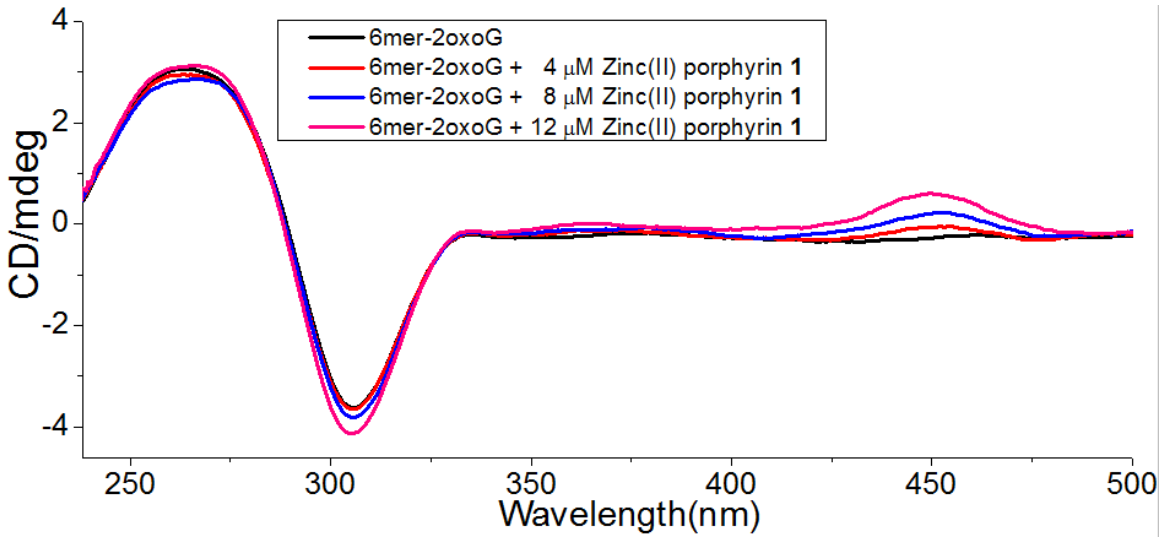


FIGURE S3. a) Chemical structure of Zinc(II) porphyrin **1;**

b) CD spectra of 6mer-2oxoG (8.0 μM) in the presence of different amounts of zinc(II) porphyrin (from 4.0 μM to 12 μM). This experiment was performed in Na cacodylate buffer (5 mM, pH 7.0) supplemented with 150 mM NaCl. A dose-dependent ICD signal was observed at around 450 nm, indicating a left-handed conformation of 6mer-2oxoG (*Angew Chem Int Ed Engl* **2005,** *44*, 4006-9).

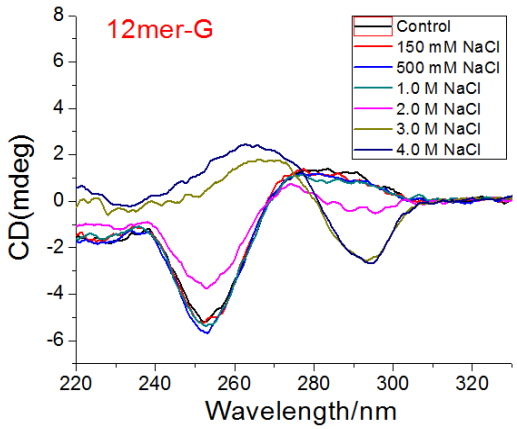


FIGURE S4. Circular dichroic (CD) spectra of 12mer-G in 5 mM Na cacodylate buffer (pH 7.0 at 10 °C), at varied concentrations of NaCl ranging from 0 mM (control) to 4.0 M (each oligomer at 10 μM strand concentration). A concentration dependent manner could be observed in their circular dichroic spectra.

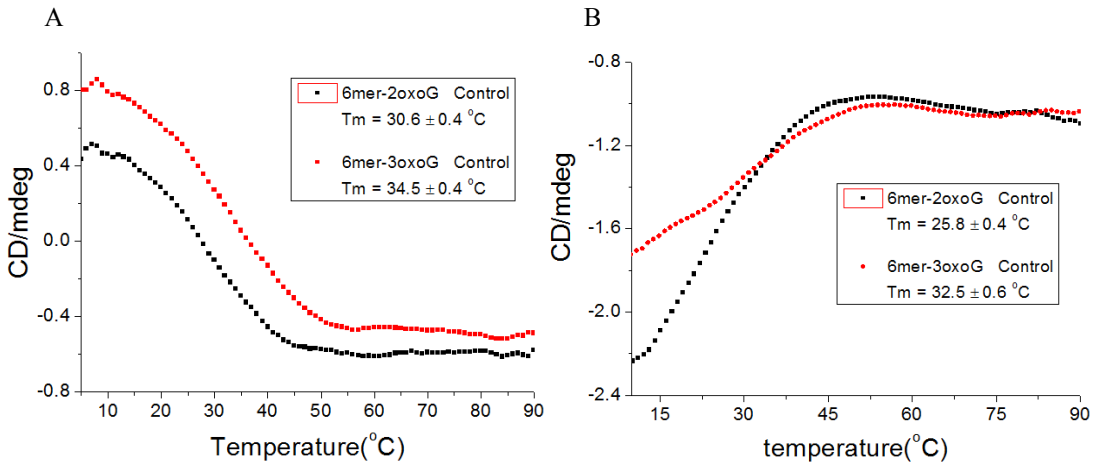


FIGURE S5. Normalized CD melting curves of 6mer-2oxoG or 6mer-3oxoG recorded in a quartz cuvette of 0.1 cm path length, at a scan rate of 0.5 °C/min. The experiments were performed in a buffer solution containing 5 mM Na cacodylate (pH 7.0 at 10 °C), 10 μM oligomer. 6mer-3oxoG was found to have a larger Tm than the one of 6mer-2oxoG, which indicated a more stable Z-DNA structure of 6mer-3oxoG. A: CD absorbance at 260 nm was recorded. B: CD absorbance at 305 nm was recorded.

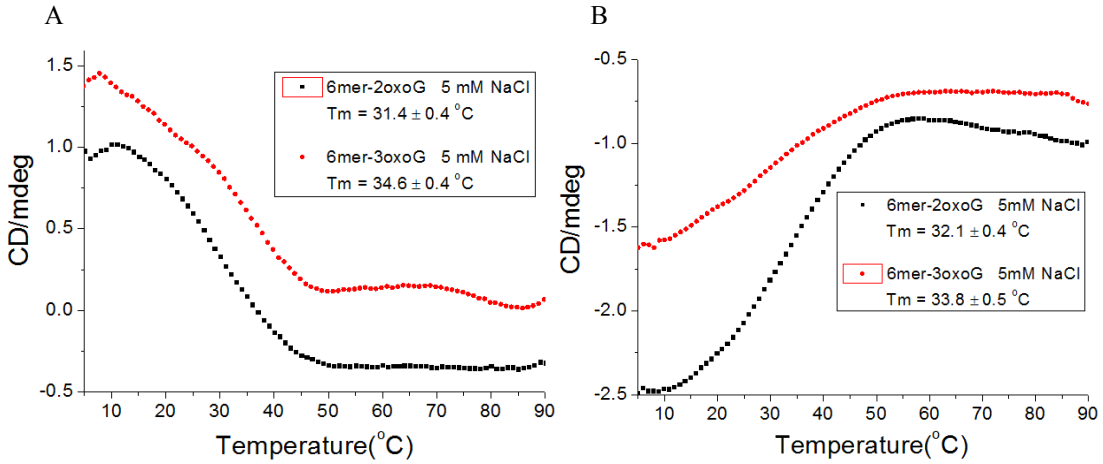


FIGURE S6. Normalized CD melting curves of 6mer-2oxoG or 6mer-3oxoG recorded in a quartz cuvette of 0.1 cm path length, at a scan rate of 0.5 °C/min. The experiments were performed in a buffer solution containing 5 mM Na cacodylate (pH 7.0 at 10 °C), 5 mM NaCl, 10 μM oligomer. 6mer-3oxoG was found to have a larger Tm than the one of 6mer-2oxoG, which indicated a more stable Z-DNA structure of 6mer-3oxoG. A: CD absorbance at 260 nm was recorded. B: CD absorbance at 305 nm was recorded.

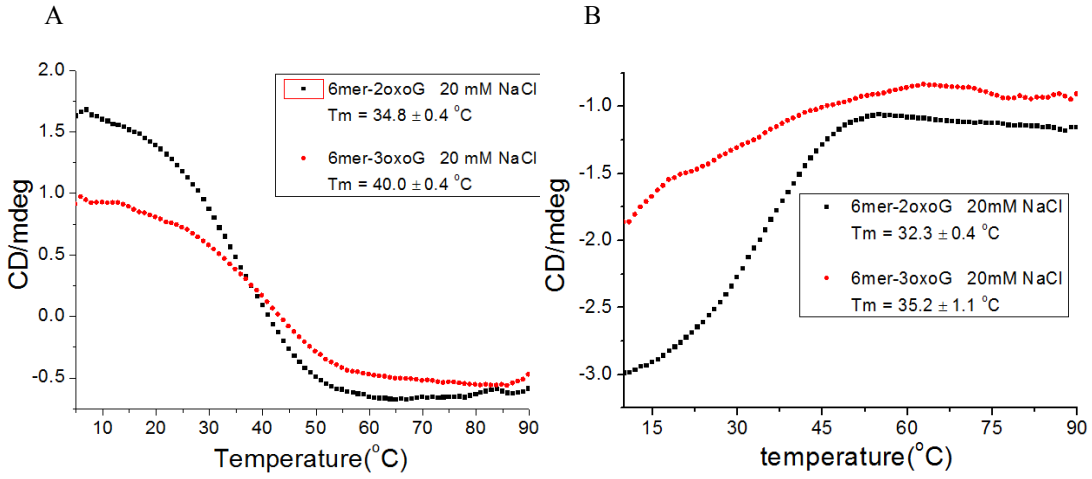


FIGURE S7. Normalized CD melting curves of 6mer-2oxoG or 6mer-3oxoG recorded in a quartz cuvette of 0.1 cm path length, at a scan rate of 0.5 °C/min. The experiments were performed in a buffer solution containing 5 mM Na cacodylate (pH 7.0 at 10 °C), 20 mM NaCl, 10 μM oligomer. 6mer-3oxoG was found to have a larger Tm than the one of 6mer-2oxoG, which indicated a more stable Z-DNA structure of 6mer-3oxoG. A: CD absorbance at 260 nm was recorded. B: CD absorbance at 305 nm was recorded.

DFT Calculation: The two conformations of guanosine residue were obtained from standard B-DNA (anti, and $C_{2'}$-endo) and Z-DNA (syn, and $C_{3'}$-endo). The phosphate group is removed. And the 5'-OH is capped with methyl group to avoid unnecessary hydrogen bond formation (between 5'-OH and 8-O of 8-oxo-guanine). The guanine groups of up prepared two structures were modified manually to generate their 8-oxo-guanine counterpart. The geometries of all above four structures were optimized at wb97xd/6-311+g(2d,p) level, using Gaussian 09 program. The energies were taken from SCF energy directly.

Model building: Since Amber is one of the most popular tools for intrinsic DNA dynamics, it was used in our assay. Eight structural models of 6 base paired $d(CGCGCG)_2$ repeats were built using the canonical B- and non-canonical Z-DNA settings. Corresponding Guanine was manually modified to 8-oxoGuanine, and the resulting 6mer-3G, 6mer-1oxoG, 6mer-2oxoG, or 6mer-3oxoG was made respectively. Then, the model structures (four Z- and four B-DNA) were prepared for the following simulation study.

Charge fitting of 8-oxoGuanine residue: Fitting the charge of non-standard nucleic acids 8-oxoguanine based on multiple orientation, multiple conformation charge derivation automatically carried out using the R.E.D. Tools [F.-Y. Dupradeau, C. Cézard, R. Lelong, E. Stanislawiak, J. Pecher, J. C. Delepine and P. Cieplak, R.E.DD.B.: A database for RESP and ESP atomic charges, and force field libraries, Nucl. Acids Res. (Database issue), 2008, 36, D360-D367]. Dimethylphosphate (gauche+, gauche+ conformation) and the four stable conformations of 8-oxoguanine (C2'-endo and C3'-endo combined with syn-2' and anti-2' conformations) were obtained by DFT calculations at B3LYP/6-31g(d) level using Gaussian09 program. [Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009]. An inter-molecular charge constraint between the methyl groups of dimethylphosphate and the

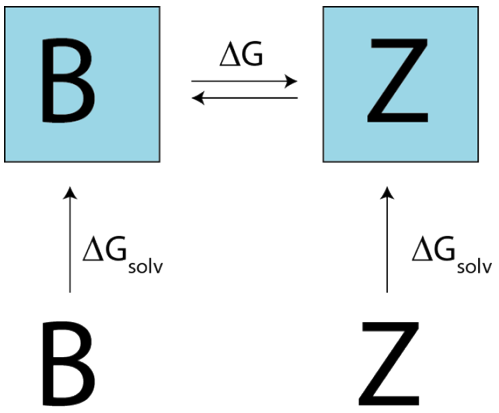
HO5' and HO3' hydroxyl groups of the nucleoside used during the fitting step. Additional intramolecular charge constrain were used when building 3' and 5' nucleoside. RESP charge derivation procedure with the Connolly surface algorithm and HF/6-31G* in MEP computation were used. Stretch, bend, and torsion force constants for 8-oxoguanine residue were assigned by analogy with the standard parm10.dat and gaff.dat Amber force field. The charges and RRMS (which represent the quanity of the fitting) of the 8-oxoguanine - central, 3', and 5' residue - are reported in Table S5, Table S6 and Table S7, respectively. The Stretch, bend and torsion force parameters are listed in Table S8.

MD Simulations: The AMBER 12 simulation suite [D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, R. Luo, R.C. Walker, W. Zhang, K.M. Merz, B. Roberts, S. Hayik, A. Roitberg, G. Seabra, J. Swails, A.W. Goetz, I. Kolossváry, K.F. Wong, F. Paesani, J. Vanicek, R.M. Wolf, J. Liu, X. Wu, S.R. Brozell, T. Steinbrecher, H. Gohlke, Q. Cai, X. Ye, J. Wang, M.-J. Hsieh, G. Cui, D.R. Roe, D.H. Mathews, M.G. Seetin, R. Salomon-Ferrer, C. Sagui, V. Babin, T. Luchko, S. Gusarov, A. Kovalenko, and P.A. Kollman (2012), AMBER 12, University of California, San Francisco] was used to carry out MD simulations in the study. The AMBER ff12SB force field was employed to set up the force field and to simulate molecular interactions. TIP3P model was used to perform the simulation of water molecules. 11 Sodium counterions were added for each 6-mer oligonucleotide. Then the models were solvated in a truncated octahedral box of TIP3P water with a distance of 8 Å to the edge using leap. For the simulations, a time step of 2 femtoseconds was used, and all bonds involving hydrogens were fixed with SHAKE algorithm. The systems were energy minimized and then heated to 300 K in 20 picoseconds (ps) at constant volume with 100 kcal/mol/Å^2 harmonic restraints on all solute atoms. The harmonic restraints were then reduced to 50, 10, 5 kcal/mol/ Å^2 in 20 ps intervals, followed by 200 ps of unrestrained equilibration at constant pressure and temperature. Then a 20 ns-long production runs were performed for each 6-mer system starting with different initial velocities.

MM/PBSA analysis: The MM/PBSA analysis was carried out to calculate the conformational free energies and the python scripts readily within the AMBER 12 simulation suite was used. Snapshots for the MM/PBSA analysis [Miller, Bill R.; McGee, T. Dwight; Swails, Jason M.; Homeyer, Nadine; Gohlke, Holger;Roitberg, Adrian E. MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. J. Chem. Theory Comput., 2012, 8(9), 3314–3321] were extracted from all eight 20 ns

simulations in 40 ps intervals, yielding 500 snapshots per independent trajectory. The ionic strength (istrng of &pb namelist variables) were set to 0, 0.005, 0.020, 0.050, 1.000 and 2.000 M for each trajectory. The results were averaged over the 500 snapshots for each system. The sum of total free energy was given in Table S2 - Table S3, and all the detailed free enenergy results were given in Table S9 – Table S32.

Since no binding energy need to be calculated in this system, there is no typical thermodynamic cycle to calculate ΔG. The thermodynamic cycle can be simply drawn as follows:



the free energy of solvated B and Z DNA is calculated and compared directly using mmPBSA

Table S2. Free energies of B and Z DNA and their difference with ion strength.of 0 mM, 5mM and 20 mM NaCl (Kcal/mol)

	0 mM NaCl			5 mM NaCl			20 mM NaCl		
	B-DNA	Z-DNA	delta	B-DNA	Z-DNA	delta	B-DNA	Z-DNA	delta
6mer-3G	-2690.25	-2680.50	9.75	-2690.01	-2680.90	9.11	-2689.79	-2681.17	8.63
6mer-1oxoG	-2872.09	-2868.87	3.22	-2871.89	-2868.96	2.93	-2871.63	-2869.41	2.23
6mer-2oxoG	-3055.51	-3054.49	1.02	-3055.43	-3054.74	0.68	-3055.09	-3055.18	-0.09
6mer-3oxoG	-3196.52	-3203.45	-6.93	-3196.46	-3203.54	-7.09	-3196.11	-3203.92	-7.81

Table S3. Free energies of B and Z DNA and their difference with ion strength.of 50 mM, 1M and 2M NaCl (Kcal/mol)

	50 mM NaCl			1 M NaCl			2 M NaCl		
	B-DNA	Z-DNA	delta	B-DNA	Z-DNA	delta	B-DNA	Z-DNA	delta
6mer-3G	-2690.34	-2681.20	9.14	-2690.47	-2681.84	8.63	-2690.16	-2682.22	7.94
6mer-1oxoG	-2872.12	-2869.89	2.23	-2872.37	-2870.53	1.85	-2872.10	-2870.92	1.17
6mer-2oxoG	-3055.03	-3055.34	-0.31	-3055.55	-3055.90	-0.35	-3055.40	-3056.12	-0.72
6mer-3oxoG	-3195.86	-3204.4	-8.54	-3196.63	-3205.04	-8.42	-3196.41	-3205.15	-8.75

Table S4. Energies difference between B and Z DNA and for all 4 DNA, the ion strength is 0 mM NaCl

	Δ_{BZ} - 6mer-3G	Δ_{BZ} - 6mer-1oxoG	Δ_{BZ} - 6mer-2oxoG	Δ_{BZ} - 6mer-3oxoG
BOND	1.68	0.166	-0.3483	0.0567
ANGLE	-3.7698	-5.6176	-7.7014	-13.7595
DIHED	27.1165	19.6848	20.4526	16.3925
VDWAALS	-14.1841	-16.0953	-12.0045	-10.5475
EEL	**304.8423**	**261.4251**	**208.9591**	**170.4366**
1-4 VDW	-0.6948	-1.2141	-1.1204	-1.4421
1-4 EEL	13.6363	30.1998	40.5955	47.3081
EPB	**-324.804**	**-293.117**	**-253.913**	**-221.957**
ENPOLAR	-5.6618	-6.0455	-4.4046	-3.4903
EDISPER	11.5916	13.8362	10.507	10.0718
G gas	328.6265	288.5487	248.8327	208.4448
G solv	-318.875	-285.327	-247.81	-215.376
TOTAL	9.7518	3.2222	1.0225	-6.9309

It can be inferred from this table that the major force stabilizing B-DNA is the EEL term (correspond to Electrostatic energy in gas phase) and the one stabilizing Z-DNA is the EPB term (correspond to Polar solvation energy). The substitution of guanine by 8-oxo-guanine decreases the EEL term, indicating a more stabilized Z-DNA in gas phase. The EPB term is also decreased, suggesting a more destabilized Z-DNA by salvation with the substituted 8-oxodG. The driving force by the stabilization in gas phase exceeds the one by the solvation term, resulting in a more stabilized system.

Table S5 RESP result of central Fragment

	pdb atomic name	x	y	z	atom type	charge
1	O5'	3.100106	2.401573	0	OS	-0.4996
2	P	3.604511	3.980633	0.297511	P	1.1507
3	OP1	3.739753	4.703955	-1.00736	O2	-0.7613
4	OP2	4.664185	3.874225	1.351052	O2	-0.7613
5	O3'	0	0	0	OS	-0.5841
6	C3'	1.424912	0	0	CT	0.3429
7	H3'	1.821449	0.480162	0.898223	H1	-0.0127
8	C4'	1.909913	0.743601	-1.25434	CT	0.0976
9	H4'	1.143761	0.632933	-2.03652	H1	0.0902
10	C5'	2.171646	2.227915	-1.06105	CT	0.125
11	H5'	2.557837	2.645956	-2.00347	H1	0.0271
12	H5"	1.205313	2.71096	-0.84268	H1	0.0271
13	O4'	3.109982	0.084337	-1.68675	OS	-0.3675
14	C1'	3.361382	-1.08782	-0.92354	CT	0.2092
15	H1'	3.639416	-1.87599	-1.62617	H2	0.065
16	C2'	2.062829	-1.38843	-0.16877	CT	-0.0863
17	H2'	1.416449	-1.98875	-0.81872	HC	0.0351
18	H2"	2.219551	-1.91183	0.774788	HC	0.0351
19	N2	7.90762	-1.68651	-3.33346	N2	-0.8681
20	H21	7.162992	-1.75568	-4.01648	H	0.3854
21	H22	8.734237	-1.22119	-3.6876	H	0.3854
22	O6	9.027679	-0.29065	0.962017	O	-0.5581
23	C6	8.111456	-0.56783	0.196	C	0.4907
24	C5	6.708037	-0.59431	0.415391	CB	0.0598
25	N7	5.946435	-0.32581	1.547473	NA	-0.5864
26	H7	6.295411	-0.05617	2.454128	H	0.411
27	C8	4.600535	-0.50964	1.287303	CK	0.5451
28	N9	4.546634	-0.91432	-0.07366	N*	-0.05
29	C4	5.831469	-0.95358	-0.58739	CB	0.1714
30	N3	6.154038	-1.2982	-1.85703	NC	-0.5669
31	C2	7.445104	-1.28675	-2.09705	CA	0.7254
32	N1	8.384159	-0.94625	-1.15982	NA	-0.5114
33	H1	9.372467	-1.01618	-1.37504	H	0.3634
34	O8	3.674085	-0.38837	2.073324	O	-0.5289
RRMS (step 1)		0.05636				
RRMS (step 2)		0.05654				

Table S6 RESP result of 3’ fragment

	pdb atomic name	x	y	z	atom type	charge
1	P	-0.74492	1.500277	0.175031	P	1.1454
2	OP1	-2.21141	1.21304	0.280378	O2	-0.7641
3	OP2	0.052898	2.332857	1.131315	O2	-0.7641
4	O5'	0	0	0	OS	-0.4918
5	O3'	2.188723	-3.18129	-1.60948	OH	-0.6994
6	HO3'	1.736427	-3.80035	-2.20376	HO	0.4151
7	C3'	1.183784	-2.36707	-0.99496	CT	0.3926
8	H3'	0.629579	-1.79566	-1.74887	H1	-0.0288
9	C4'	1.916835	-1.43834	-0.00036	CT	0.0954
10	H4'	2.986195	-1.43823	-0.25135	H1	0.089
11	C5'	1.419183	0	0	CT	0.1129
12	H5'	1.827513	0.507266	0.887067	H1	0.0301
13	H5"	1.821842	0.503439	-0.89544	H1	0.0301
14	O4'	1.741478	-2.00969	1.306041	OS	-0.37
15	C1'	1.114078	-3.28561	1.180645	CT	0.2097
16	H1'	1.877906	-4.06255	1.065946	H2	0.0647
17	C2'	0.255006	-3.17248	-0.08153	CT	-0.0962
18	H2'	-0.01305	-4.14884	-0.49969	HC	0.034
19	H2"	-0.64842	-2.60255	0.14013	HC	0.034
20	N2	3.597527	-6.46703	4.472175	N2	-0.8684
21	H21	4.211193	-6.27401	3.689909	H	0.3856
22	H22	4.084586	-6.53834	5.356932	H	0.3856
23	O6	-0.2296	-5.11664	6.748282	O	-0.5582
24	C6	0.41035	-5.02847	5.706577	C	0.4917
25	C5	0.121659	-4.31988	4.50926	CB	0.0587
26	N7	-0.95613	-3.51638	4.151402	NA	-0.587
27	H7	-1.75325	-3.29352	4.727103	H	0.4114
28	C8	-0.8065	-3.03785	2.859957	CK	0.5443
29	N9	0.421217	-3.60411	2.410331	N*	-0.0461
30	C4	0.977534	-4.36111	3.428403	CB	0.1705
31	N3	2.155946	-5.0246	3.35543	NC	-0.5674
32	C2	2.456055	-5.69391	4.445066	CA	0.7262
33	N1	1.661418	-5.71424	5.559984	NA	-0.512
34	H1	1.902954	-6.29996	6.351553	H	0.3634
35	O8	-1.56815	-2.31605	2.243278	O	-0.529
RRMS (step 1)		0.05590				
RRMS (step 2)		0.05607				

Table S7 RESP result of 5’ fragment

	pdb atomic name	x	y	z	atom type	charge
1	O3'	0	0	0	OS	-0.5767
2	O5'	4.03565	1.102311	0	OH	-0.5892
3	HO5'	4.773468	1.661176	0.283998	HO	0.4034
4	C3'	1.431954	0	0	CT	0.3373
5	H3'	1.822261	0.219791	1.000696	H1	-0.011
6	C4'	1.872419	1.064453	-1.03057	CT	0.0979
7	H4'	1.014299	1.716657	-1.2422	H1	0.0902
8	C5'	3.039673	1.930763	-0.57947	CT	0.1277
9	H5'	3.422228	2.478612	-1.4538	H1	0.0265
10	H5"	2.659073	2.670173	0.145665	H1	0.0265
11	O4'	2.231246	0.357471	-2.22861	OS	-0.3674
12	C1'	1.892239	-1.02108	-2.08023	CT	0.2092
13	H1'	0.865194	-1.18734	-2.42338	H2	0.065
14	C2'	2.0178	-1.29141	-0.57855	CT	-0.0853
15	H2'	1.471305	-2.18674	-0.26277	HC	0.0352
16	H2"	3.071008	-1.385	-0.31001	HC	0.0352
17	N2	-0.24706	-2.4957	-6.59376	N2	-0.868
18	H21	-0.90368	-1.89535	-6.10981	H	0.3854
19	H22	-0.24973	-2.36699	-7.59802	H	0.3854
20	O6	4.183427	-3.89644	-6.83832	O	-0.5581
21	C6	3.337403	-3.33627	-6.15064	C	0.4906
22	C5	3.429092	-2.80191	-4.83722	CB	0.0599
23	N7	4.488782	-2.74508	-3.9377	NA	-0.5863
24	H7	5.421972	-3.09508	-4.08982	H	0.4109
25	C8	4.101647	-2.12943	-2.75859	CK	0.5451
26	N9	2.725102	-1.81826	-2.95456	N*	-0.0505
27	C4	2.341146	-2.21543	-4.22494	CB	0.1715
28	N3	1.105565	-2.05306	-4.75519	NC	-0.5668
29	C2	0.981987	-2.53721	-5.96997	CA	0.7253
30	N1	2.006562	-3.14125	-6.64841	NA	-0.5114
31	H1	1.843713	-3.55924	-7.55766	H	0.3634
32	O8	4.78194	-1.92502	-1.77025	O	-0.5288
RRMS (step 1)		0.05643				
RRMS (step 2)		0.05662				

Figure S8 Parm file for 8-oxoGuanine

MASS
BOND
CB-NA 411.1 1.3910
NA-CK 420.5 1.3840
CK-O 648.0 1.2140
CK-N* 440.0 1.4228
ANGLE
C -CB-NA 70.0 131.00
CB-NA-H 47.630 126.350
CB-NA-CK 70.0 110.78
NA-CB-CB 70.0 107.21
NA-CK-N* 70.0 104.52
NA-CK-O 70.0 127.6
H -NA-CK 50.0 122.87
N*-CK-O 70.0 127.83
CB-N*-CK 70.0 109.41
CB-N*-CT 70.0 124.10
CK-N*-CT 70.0 125.83
C -CB-CB 70.0 121.30
CB-CB-N* 70.0 108.04
CB-CB-NC 70.0 126.63
N*-CB-NC 70.0 125.33
DIHE
X -CB-NA-X 4 6.60 180.0 2. same as parm10 x-cb-n*-x
X -NA-CK-X 4 5.40 180.0 2. same as parm10 x-c-na-x
IMPROPER
NONBON

Table S9. Detailed energy term of 6mer-3G in B and Z form with ion strength of 0 mM NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1941.91	18.7519	0.8386	-2266.72	31.001	1.3864
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1930.24	19.1451	0.8562	-2249.11	30.5337	1.3655
TOTAL	-2690.25	14.6804	0.6565	-2680.5	14.59	0.6525

Table S10. Detailed energy term of 6mer-1oxoG in B and Z form with ion strength of 0 mM NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1952.16	15.1088	0.6757	-2245.28	30.3421	1.3569
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943.46	14.7521	0.6597	-2228.78	29.9577	1.3397
TOTAL	-2872.09	14.9048	0.6666	-2868.87	14.9196	0.6672

Table S11. Detailed energy term of 6mer-2oxoG in B and Z form with ion strength of 0 mM NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1953.16	15.3302	0.6856	-2207.07	33.1197	1.4812
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1943.98	15.2084	0.6801	-2191.79	32.6104	1.4584
TOTAL	-3055.51	14.7278	0.6586	-3054.49	14.584	0.6522

Table S12. Detailed energy term of 6mer-3oxoG in B and Z form with ion strength of 0 mM NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.87	16.308	0.7293	-2180.83	30.1276	1.3473
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.82	15.9647	0.714	-2166.2	29.7223	1.3292
TOTAL	-3196.52	13.8036	0.6173	-3203.45	14.5675	0.6515

Table S13. Detailed energy term of 6mer-3G in B and Z form with ion strength of 5 mM NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1941.68	18.7714	0.8395	-2267.12	31.0046	1.3866
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1930	19.1686	0.8572	-2249.52	30.5392	1.3658
TOTAL	-2690.01	14.6756	0.6563	-2680.9	14.571	0.6516

Table S14. Detailed energy term of 6mer-1oxoG in B and Z form with ion strength of 5 mM NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1951.96	15.1121	0.6758	-2245.37	30.3472	1.3572
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943.26	14.7563	0.6599	-2228.88	29.962	1.3399
TOTAL	-2871.89	14.9093	0.6668	-2868.96	14.9151	0.667

Table S15. Detailed energy term of 6mer-2oxoG in B and Z form with ion strength of 5 mM NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1953.08	15.3433	0.6862	-2207.33	33.1286	1.4816
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1943.9	15.2236	0.6808	-2192.04	32.6187	1.4588
TOTAL	-3055.43	14.7254	0.6585	-3054.74	14.5869	0.6523

Table S16. Detailed energy term of 6mer-3oxoG in B and Z form with ion strength of 5 mM NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.8	16.3076	0.7293	-2180.91	30.1114	1.3466
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.76	15.9665	0.714	-2166.28	29.7038	1.3284
TOTAL	-3196.46	13.8044	0.6174	-3203.54	14.5488	0.6506

Table S17. Detailed energy term of 6mer-3G in B and Z form with ion strength of 20 mM NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1941.46	18.7975	0.8407	-2267.39	30.9995	1.3863
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1929.78	19.186	0.858	-2249.78	30.5355	1.3656
TOTAL	-2689.79	14.6512	0.6552	-2681.17	14.568	0.6515

Table S18. Detailed energy term of 6mer-1oxoG in B and Z form with 20 mM NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1951.7	15.2061	0.68	-2245.81	30.3597	1.3577
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943	14.8451	0.6639	-2229.32	29.9741	1.3405
TOTAL	-2871.63	14.8954	0.6661	-2869.41	14.9148	0.667

Table S19. Detailed energy term of 6mer-2oxoG in B and Z form with 20 mM NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1952.74	15.3404	0.686	-2207.77	33.113	1.4809
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1943.56	15.2185	0.6806	-2192.48	32.6043	1.4581
TOTAL	-3055.09	14.7118	0.6579	-3055.18	14.5768	0.6519

Table S20. Detailed energy term of 6mer-3oxoG in B and Z form with 20 mM NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.45	16.3112	0.7295	-2181.29	30.1051	1.3463
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.41	15.9711	0.7142	-2166.67	29.6965	1.3281
TOTAL	-3196.11	13.7813	0.6163	-3203.92	14.5516	0.6508

Table S21. Detailed energy term of 6mer-3G in B and Z form with 50 mM NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1942	18.7358	0.8379	-2267.42	31.0253	1.3875
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1930.33	19.1071	0.8545	-2249.82	30.5623	1.3668
TOTAL	-2690.34	14.6912	0.657	-2681.2	14.5746	0.6518

Table S22. Detailed energy term of 6mer-1oxoG in B and Z form with 50 mM NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1952.18	15.3281	0.6855	-2246.29	30.3366	1.3567
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943.48	14.9623	0.6691	-2229.8	29.9528	1.3395
TOTAL	-2872.12	14.9158	0.6671	-2869.89	14.912	0.6669

Table S23. Detailed energy term of 6mer-2oxoG in B and Z form with 50 mM NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1952.68	15.362	0.687	-2207.93	33.09	1.4798
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1943.5	15.2333	0.6813	-2192.64	32.583	1.4572
TOTAL	-3055.03	14.7212	0.6584	-3055.34	14.551	0.6507

Table S24. Detailed energy term of 6mer-3oxoG in B and Z form with 50 mM NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.21	16.3316	0.7304	-2181.77	30.1201	1.347
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.16	15.9844	0.7148	-2167.15	29.7134	1.3288
TOTAL	-3195.86	13.8044	0.6174	-3204.4	14.5691	0.6516

Table S25. Detailed energy term of 6mer-3G in B and Z form with 1.0 M NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1942.14	18.8033	0.8409	-2268.06	31.0752	1.3897
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1930.46	19.1869	0.8581	-2250.45	30.6136	1.3691
TOTAL	-2690.47	14.6789	0.6565	-2681.84	14.576	0.6519

Table S26. Detailed energy term of 6mer-1oxoG in B and Z form with 1.0 M NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1952.44	15.2305	0.6811	-2246.93	30.4058	1.3598
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943.74	14.8681	0.6649	-2230.44	30.024	1.3427
TOTAL	-2872.37	14.8895	0.6659	-2870.53	14.9347	0.6679

Table S27. Detailed energy term of 6mer-2oxoG in B and Z form with 1.0 M NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1953.21	15.4026	0.6888	-2208.49	33.2169	1.4855
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1944.02	15.2753	0.6831	-2193.21	32.7107	1.4629
TOTAL	-3055.55	14.7267	0.6586	-3055.9	14.5474	0.6506

Table S28. Detailed energy term of 6mer-3oxoG in B and Z form with 1.0 M NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.97	16.4134	0.734	-2182.42	30.2714	1.3538
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.93	16.0658	0.7185	-2167.79	29.8684	1.3358
TOTAL	-3196.63	13.8255	0.6183	-3205.04	14.5731	0.6517

Table S29. Detailed energy term of 6mer-3G in B and Z form with 2.0 M NaCl

6mer-3G						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.7189	8.9819	0.4017	104.3989	8.7434	0.391
ANGLE	205.3394	11.0223	0.4929	201.5696	10.9788	0.491
DIHED	247.5086	7.5233	0.3365	274.6251	7.3166	0.3272
VDWAALS	-187.691	6.6961	0.2995	-201.875	5.2431	0.2345
EEL	1068.667	18.9974	0.8496	1373.509	32.3462	1.4466
1-4 VDW	98.0088	3.5838	0.1603	97.314	3.6855	0.1648
1-4 EEL	-2294.56	13.1173	0.5866	-2280.93	13.7032	0.6128
EPB	-1941.83	18.8398	0.8425	-2268.44	31.1355	1.3924
ENPOLAR	242.4894	2.3348	0.1044	236.8276	1.4371	0.0643
EDISPER	-230.813	3.6818	0.1647	-219.222	1.7654	0.079
G gas	-760.012	24.6513	1.1024	-431.386	34.9444	1.5628
G solv	-1930.15	19.2137	0.8593	-2250.84	30.6737	1.3718
TOTAL	-2690.16	14.6607	0.6556	-2682.22	14.5723	0.6517

Table S30. Detailed energy term of 6mer-1oxoG in B and Z form with 2.0 M NaCl

6mer-1oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.1987	8.8418	0.3954	103.3647	8.5812	0.3838
ANGLE	206.3408	11.4703	0.513	200.7232	10.8764	0.4864
DIHED	252.6016	7.0169	0.3138	272.2864	6.856	0.3066
VDWAALS	-187.826	5.7635	0.2578	-203.921	5.3468	0.2391
EEL	1264.068	17.7462	0.7936	1525.493	31.5765	1.4121
1-4 VDW	100.0171	3.6924	0.1651	98.803	3.8556	0.1724
1-4 EEL	-2667.04	12.9431	0.5788	-2636.84	11.659	0.5214
EPB	-1952.16	15.2961	0.6841	-2247.33	30.4685	1.3626
ENPOLAR	244.1011	1.4543	0.065	238.0556	1.364	0.061
EDISPER	-235.398	1.9381	0.0867	-221.562	1.5312	0.0685
G gas	-928.636	21.2136	0.9487	-640.087	34.0006	1.5206
G solv	-1943.46	14.9236	0.6674	-2230.84	30.0861	1.3455
TOTAL	-2872.1	14.888	0.6658	-2870.92	14.9139	0.667

Table S31. Detailed energy term of 6mer-2oxoG in B and Z form with 2.0 M NaCl

6mer-2oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	103.3746	9.2147	0.4121	103.0263	9.015	0.4032
ANGLE	207.5846	11.7643	0.5261	199.8832	11.3122	0.5059
DIHED	248.1983	8.1933	0.3664	268.6509	7.712	0.3449
VDWAALS	-191.688	6.189	0.2768	-203.692	5.8882	0.2633
EEL	1459.464	18.7203	0.8372	1668.423	33.5632	1.501
1-4 VDW	100.9821	3.8706	0.1731	99.8617	3.8235	0.171
1-4 EEL	-3039.45	12.7868	0.5718	-2998.85	12.881	0.5761
EPB	-1953.05	15.4263	0.6899	-2208.71	33.2469	1.4868
ENPOLAR	244.0067	1.6125	0.0721	239.6021	1.6165	0.0723
EDISPER	-234.824	2.2432	0.1003	-224.317	2.0307	0.0908
G gas	-1111.53	21.2854	0.9519	-862.698	35.7952	1.6008
G solv	-1943.87	15.2913	0.6838	-2193.42	32.7408	1.4642
TOTAL	-3055.4	14.7385	0.6591	-3056.12	14.5484	0.6506

Table S32. Detailed energy term of 6mer-3oxoG in B and Z form with 2.0 M NaCl

6mer-3oxoG						
	B-DNA			Z-DNA		
Energy Component	Average	Std. Dev.	Std. Err. of Mean	Average	Std. Dev.	Std. Err. of Mean
BOND	102.0986	8.7241	0.3902	102.1553	8.6441	0.3866
ANGLE	211.0459	11.4594	0.5125	197.2864	11.5553	0.5168
DIHED	250.4703	7.3237	0.3275	266.8628	7.4162	0.3317
VDWAALS	-194.789	6.3598	0.2844	-205.337	5.3817	0.2407
EEL	1580.975	19.6165	0.8773	1751.412	32.9767	1.4748
1-4 VDW	101.5511	3.995	0.1787	100.109	3.5375	0.1582
1-4 EEL	-3297.05	14.2683	0.6381	-3249.74	12.7946	0.5722
EPB	-1958.75	16.4813	0.7371	-2182.53	30.2937	1.3548
ENPOLAR	244.3656	1.6205	0.0725	240.8753	1.4976	0.067
EDISPER	-236.321	2.0281	0.0907	-226.25	1.8423	0.0824
G gas	-1245.7	20.9007	0.9347	-1037.25	34.1625	1.5278
G solv	-1950.71	16.1291	0.7213	-2167.9	29.8898	1.3367
TOTAL	-3196.41	13.8242	0.6182	-3205.15	14.5487	0.6506