Supporting Information for "***Vertical Ionization Energies and Electron Affinities of Native and Damaged DNA Bases, Nucleotides and Pairs from Density Functional Theory Calculations: Model Assessment and Implications for DNA Damage Recognition and Repair***"

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VIEs/VEAs of G and 8OG bases/nucleotides computed at different levels of theory

Functional/basis set	**System, gas phase**							
	G (base)		**G (nucleotide)**		**8OG (base)**		**8OG (nucleotide)**	
	VEA (eV)	**VIE (eV)**	**VEA (eV)**	**VIE (eV)**	**VEA (eV)**	**VIE (eV)**	**VEA (eV)**	**VIE (eV)**
M06/6-31++G*	-0.38	8.07	-2.06	5.05	-0.26	7.85	-1.81	5.06
M06/TZVP	-1.38	7.97	-3.53	4.94	-0.99	7.71	-2.78	4.93
BLYP/6-31+G(3df,2p)	-0.36	7.67	-2.23	4.20	-0.25	7.40	-1.82	4.10
BLYP/TZVP	-1.46	7.69	-3.03	4.16	-0.78	7.41	-2.49	4.05
B3LYP/6-31+G(3df,2p)	-0.38	7.95	-2.21	4.83	-0.25	7.69	-1.78	4.81
B3LYP/6-31++G*	-0.08	7.99	-1.79	4.90	0.01	7.74	-1.48	4.86
ωB97XD/6-31++G*	-	8.09	-	5.29	-	-	-	-
ωB97X/6-31++G*	-	8.14	-	5.34	-	-	-	-
Experimental Values	-	8.00 - 8.30	-	5.05 ± 0.10	-	-	-	-

Table S1. Computed VEAs and VAEs of G and 8OG and their nucleotides in vacuum. The geometries of the neutral species have been optimized at the corresponding level of theory. Experimental values (where available) are indicated in the last row.

Functional/basis set	System, PCM (water)							
	G (base)		G (nucleotide)		8OG (base)		8OG (nucleotide)	
	VEA (eV)	VIE (eV)	VEA (eV)	VIE (eV)	VEA (eV)	VIE (eV)	VEA (eV)	VIE (eV)
M06/TZVP	-0.49	7.17	-0.47	7.06	-0.29	6.86	-0.22	6.81
BLYP/6w-31+G(3df,2p)	-0.03	6.84	0.12	6.80	0.02	6.52	0.20	6.50
BLYP/TZVP	-0.34	6.87	-0.36	6.71	-0.21	6.53	-0.11	6.49
B3LYP/6-31+G(3df,2p)	-0.12	7.13	-0.07	7.02	-0.05	6.83	0.04	6.76
M06/6-31++G*	-0.29	7.28	-0.13	7.16	-0.04	7.01	0.07	6.95
B3LYP/6-31++G*	0.01	7.19	0.07	7.08	0.08	6.89	0.14	6.82
ωB97XD/6-31++G*	-	7.31	-	7.18	-	-	-	-
ωB97X/6-31++G*	-	7.36	-	7.23	-	-	-	-
Experimental Values	-	7.00 ± 0.20	-	7.00 ± 0.20	-	-	-	-

Table S2. Computed VEAs and VAEs of G and 8OG and their nucleotides under implicit solvation. The geometries of the neutral species have been optimized at the corresponding level of theory. Experimental values (where available) are indicated in the last row.

Sensitivity of VIEs and VEAs on the level of theory

Amongst the different combinations of DFT functionals and basis sets considered, M06/6-31++G*, B3LYP/6-31++G*, ωB97XD/6-31++G* and ωB97X/6-31++G* provide the best overall agreement with reported experimental and computed VIE and VEA values (**Table 2** in the manuscript, **Tables S1/S2** here). These include the single guanine base in vacuum (VIE: 8.07 eV/7.99 eV/8.09 eV/8.14 eV vs 8.0-8.3 eV (exp.)[1-5], VEA: -0.38 eV/-0.08 eV vs -0.19 eV/-0.23 eV (EOM-CC)[6]), the 8OG base in vacuum (VIE: 7.85 eV/7.74 eV vs 7.84 eV (MP2)[7]/7.54 eV (RHF)[8]/7.87 eV (DFT-Electron Propagator Theory)[9], VEA: -0.26 eV/0.01 eV vs -0.22 eV (DFT-Electron Propagator Theory)[9]), the G nucleotide in vacuum (VIE: 5.05 eV/4.90 eV/5.29 eV/5.34 eV vs 5.05 ± 0.10 eV (exp)[10]), the G base with the PCM (7.28 eV/7.19 eV/7.31 eV/7.36 eV vs 7.34 eV (MP2)[11]/7.00 ± 0.20 eV (exp)[12]), the G nucleotide with PCM (7.16 eV/7.08 eV/7.18 eV/7.23 eV vs 7.08 eV (MP2)[11]/7.00 ± 0.20 eV (exp)[12]), the 8OG base with the PCM (VIE: 7.01 eV/6.89 eV vs 6.94 eV (MP2)[7]) and the 8OG nucleotide with the PCM (VIE: 6.95 eV/6.82 eV vs 6.79 eV (MP2)[7]). However, both ωB97XD and

ωB97X functionals significantly overestimate the experimental averages of G base in vacuum and G nucleotide in gas phase and in aqueous solution. Under this scope, the choice had to be made between M06/6-31++G* and B3LYP/6-31++G*. Subsequent M06/6-31++G* calculations on larger systems under implicit solvation lead to very small and inconsistent VIE and VEA differences between native and defect fragments (**Table S4**). This can be attributed to numerical instabilities and a pronounced basis set dependence related to employing the M06 functional. Such issues were not observed with B3LYP/6-31++G* calculations.

Taking all the above into consideration, the VIEs and VEAs presented in the manuscript have been computed at the B3LYP/6-31++G* level of theory for all systems.

Test with Na^+ counter ions

In gas phase, the addition of a Na^+ counter ion has a profound effect on the VEAs of both the G nucleotide (0.72 eV with Na^+ vs -1.79 eV without Na^+) and the 8OG nucleotide (0.69 eV with Na^+ vs -1.48 eV without Na^+). In a similar vein, VIEs of G and 8OG nucleotides neutralized by Na^+ ions are 7.37 eV and 7.58 eV, respectively, while VIEs of the sole nucleotides are 4.90 eV and 4.86 eV, respectively. However, the computed B3LYP/6-31++G* VIE for the sole G nucleotide is in very good agreement with the experimental value (5.05 ± 0.10 eV[10]). In addition, calculations with the PCM model yielded VIE estimates of 7.11 eV and 6.84 eV, in excellent agreement with the respective Na^+-free estimates (G: 7.08 eV and 8OG: 6.82 eV). The difference for electron affinities was also much smaller compared to gas phase: 0.32 eV vs 0.07 eV for G, and 0.34 eV vs 0.14 eV for 8OG.

These findings, as well as the good agreement of the computed VIE and VEA of the G base (Na^+-free setup, **Table S1**) with the respective experimental range (8.00-8.30 eV) and

computed estimate (-0.08 eV), confirm that the counter ion – free setup for the nucleotide systems is sufficient for the B3LYP/6-31++G* calculations presented here.

G, 8OG bases and their nucleotides in gas phase

From all gas phase VEA values computed at different levels of theory (**Table S1** in the Supporting Information), it is evident that in agreement with other computational studies[13,14-23], the electron affinity strongly depends on the size of the selected basis set, especially on the inclusion of diffuse functions. With the exception of the 8OG base, all gas phase VEAs (**Table S1**) are – as expected – negative. The influence of the basis set is equally strong for both bases and nucleotides, and much more pronounced in gas phase with variations of up to ≈ 1.5 eV. The addition of the sugar moiety and the phosphate backbone strongly decrease the VEAs. However, given that only a single experimental VEA value is available for the enol form of G (-0.46 eV[24]), and that G is experimentally reported[24] to be highly unstable and prone to interchanges between its keto and enol forms in gas phase (with a relative energy difference calculated to be of the order of 0.08 kcal/mol[6]), it is not possible to draw definitive quantitative or even qualitative conclusions from the computed results for single bases and nucleotides.

What concerns VIEs, the factor having the strongest influence on gas phase values (**Table S1**) is the choice of the DFT functional. It is by now well established both experimentally[1-5] and computationally[1,13,25,26] that G possesses the lowest VIE of the for bases in gas phase. On the other hand, it has been stated[27,28] and shown computationally[29,30] that the VIE of the defect base 8OG is even lower than that of G. Our results for the bases (**Table S1**) are also in support of these findings, as 8OG VIEs are up to 0.35 eV lower than G, while the ionization energies at the nucleotide level are very similar. Moreover, similar to the results for VEAs,

addition of the sugar group and the phosphate backbone causes a large decrease in the absolute value of the VIE with respect to the one of the corresponding base.

Fragments with one or multiple base/nucleotide pairs in gas phase

Inclusion of sugar and phosphate groups to the base lead to large changes in VIE and VEA values in gas phase, indicating that even larger fragments are indeed necessary in order to obtain convergence. Gas phase VIEs and VEAs for the base pair stacks are displayed in **Table S3**.

System	EA (eV)	IE(eV)
G-C bases	-0.15	7.23
8OG-C bases	0.04	7.10
2 (G-C) bases	0.49	6.62
(G-C)-(8OG-C) bases	0.45	6.39
(8OG-C)-(G-C) bases	0.46	6.38
3 (G-C) bases	0.61	6.44
(G-C)-(8OG-C)-(G-C) bases	0.62	5.95

Table S3. Computed VEAs and VIEs of base pairs and small native and damaged base pair stacks in gas phase, in the B3LYP/6-31++G* level of theory.

The addition of the complementary cytosine base lowers the ionization energy and enhances the electron capturing ability of G-C/8OG-C base pairs with respect to single bases. When considering systems of multiple base pairs, the VIE and VEA are further decreased and increased respectively (by 1.28 eV and 0.77 eV respectively). The VIE drop observed from (G-C) to 3 (G-C) is in agreement with computational studies involving stacks of G bases[31].Gas phase VIEs of defect fragments are also consistently smaller than those of the respective wild type fragments, indicating that they are more easily oxidizable and can indeed act as hole traps. The relative difference increases from 0.13 eV for a single base pair to as much as 0.49 eV for three base pairs. The (G-C)-(8OG-C) and (8OG-C)-(G-C) base pairs

have very similar ionization energies (6.39 eV vs 6.38 eV), in contrast to the observation of Foote et al[32] for 8OG-G and G-8OG base stacks, indicating that the inclusion of the complementary C bases eliminates the effect of the base sequence in single stranded stacks. Gas phase VEAs are very close for native and 8OG-containing fragments, suggesting that replacement of G with its oxidized counterpart has practically no effects on the electron capturing ability of the fragments.

To display the aforementioned changes in VIE and VEA, all gas phase values are depicted in two graphs (**Figures S1, S2**). For defect systems composed of 2 pairs, the value of the *y*-axis corresponds to the averages of the two fragments.

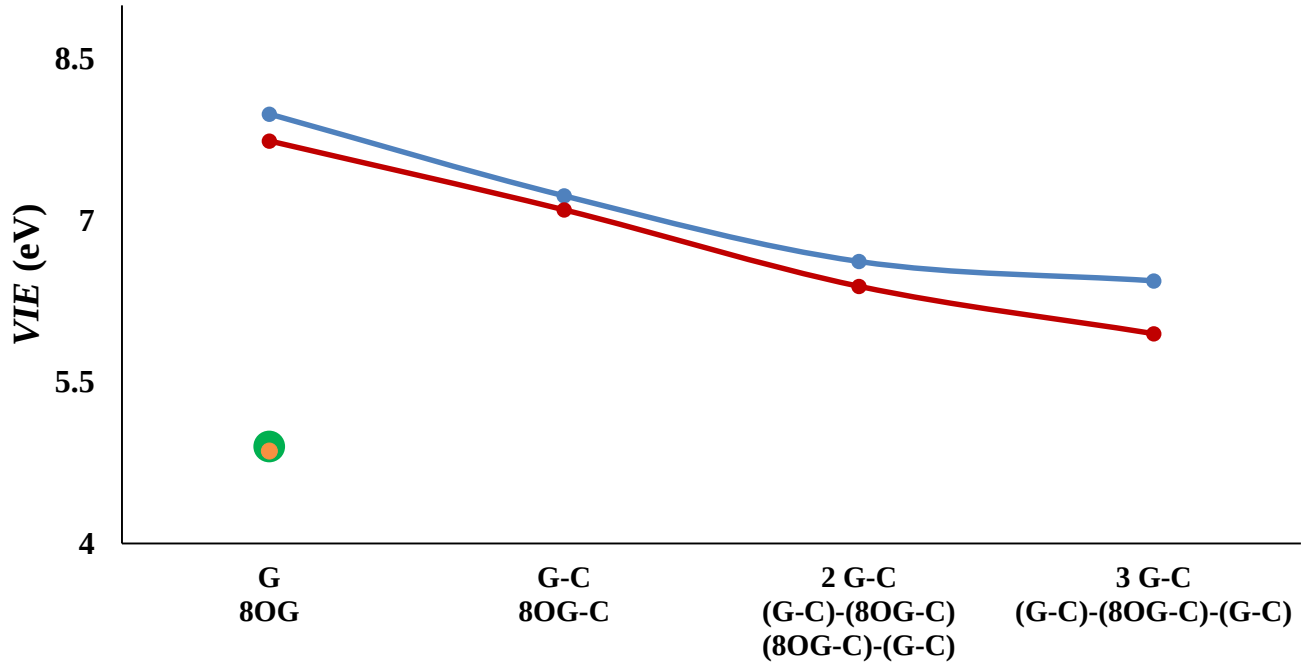

Figure S1. VIEs of native and defect fragments in gas phase. Color assignment: (i) native base systems in blue color, (ii) defect base systems in red color, (iii) native nucleotide systems in green color and (iv) defect nucleotide systems in orange color.

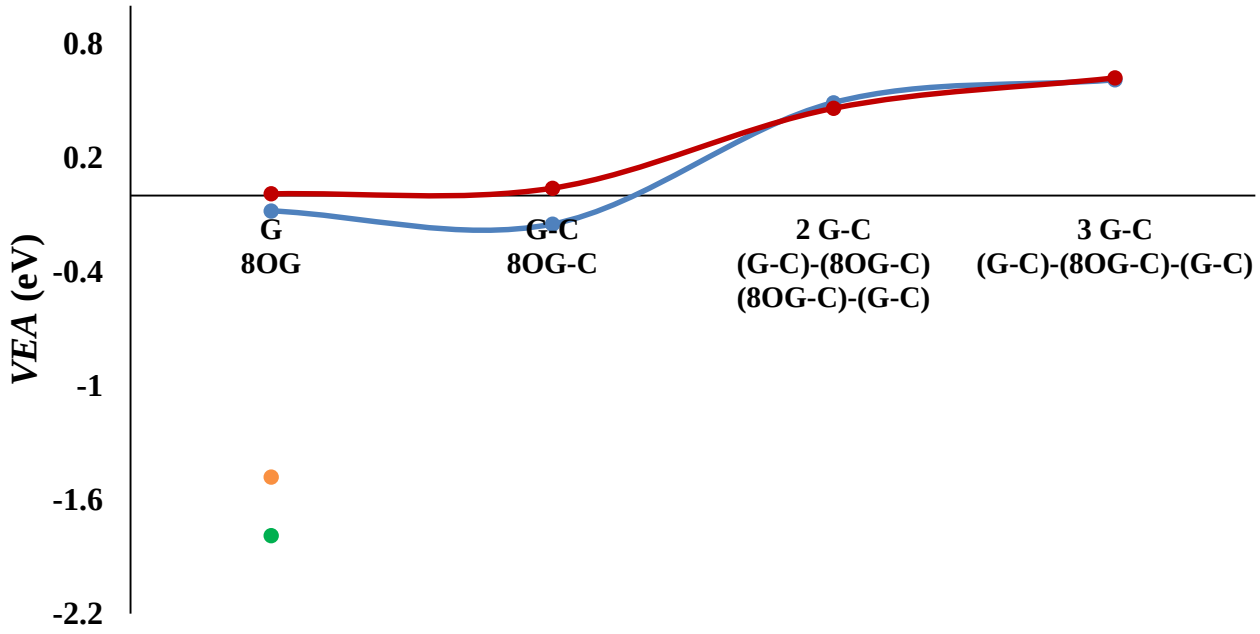

Figure S2. VEAs of native and defect fragments in gas phase. Color assignment: (i) native base systems in blue color, (ii) defect base systems in red color, (iii) native nucleotide systems in green color and (iv) defect nucleotide systems in orange color.

System	EA (eV)		IE(eV)	
G-C bases	0.45		7.06	
8OG-C bases	0.48		6.82	
2 (G-C) bases	0.67	0.68	6.66	6.59
(G-C)-(8OG-C) bases	0.75	0.67	6.64	6.62
(8OG-C)-(G-C) bases	0.76	0.75	6.63	6.64
3 (G-C) bases	0.79	0.80	6.44	6.49
(G-C)-(8OG-C)-(G-C) bases	0.82	0.86	6.53	6.49

Table S4. Computed VEAs and VIEs of base pairs and small native and damaged base pair stacks under implicit solvation (PCM water), at the M06/6-31++G* level of theory. For fragments composed of three base pairs, VIEs and VEAs are given for two optimization schemes: (i) optimization of each base pair individually (left) and (ii) optimization of the entire stack (right)

Hole/excess electron distributions

G-C pair		
fraction in C	0.087	**0.735**
fraction in G	**0.913**	0.265

Table S5. Hole distribution (2nd column) and excess electron distribution (3rd column) in the G-C base pair under implicit solvation (vertical IE/EA).

8OG-C pair		
fraction in C	0.031	**0.706**
fraction in 8OG	**0.969**	0.294

Table S6. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 8OG-C base pair under implicit solvation (vertical IE/EA).

2 G-C pairs		
fraction in 5' C	0.007	**0.422**
fraction in 3' G	**0.493**	0.070
fraction in 3' C	0.005	**0.425**
fraction in 5' G	**0.495**	0.083

Table S7. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 2 G-C base pairs under implicit solvation (vertical IE/EA).

(G-C)-(8OG-C) pairs		
fraction in 5' C	0.003	**0.424**
fraction in 3' 8OG	**0.594**	0.091
fraction in 3' C	0.003	**0.414**
fraction in 5' G	**0.400**	0.071

Table S8. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C) base pairs under implicit solvation (vertical IE/EA).

(8OG-C)-(G-C) pairs		
fraction in 5' C	0.003	**0.414**
fraction in 3' G	**0.397**	0.073
fraction in 3' C	0.003	**0.424**
fraction in 5' 8OG	**0.597**	0.089

Table S9. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (8OG-C)-(G-C) base pairs under implicit solvation (vertical IE/EA).

3 G-C pairs		
fraction in 5' C	0.003	**0.335**
fraction in 3' G	**0.365**	0.039
fraction in central C	0.002	**0.230**
fraction in central G	**0.268**	0.017
fraction in 3' C	0.001	**0.332**
fraction in 5' G	**0.361**	0.047

Table S10. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 3 G-C base pairs under implicit solvation (vertical IE/EA).

(G-C)-(8OG-C)-(G-C) pairs		
fraction in 5' C	0.002	**0.326**
fraction in 3' G	**0.287**	0.031
fraction in central C	0.002	**0.250**
fraction in central 8OG	**0.420**	0.024
fraction in 3' C	0.000	**0.327**
fraction in 5' G	**0.289**	0.042

Table S11. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C)-(G-C) base pairs under implicit solvation (vertical IE/EA).

G-C pair		
fraction in C phosphate	0.091	0.000
fraction in C sugar	0.003	0.025
fraction in C base	0.063	**0.734**
fraction in G phosphate	0.006	0.010
fraction in G sugar	-0.003	0.011
fraction in G base	**0.840**	**0.220**

Table S12. Hole distribution (2nd column) and excess electron distribution (3rd column) in the G-C nucleotide pair under implicit solvation (vertical IE/EA).

8OG-C pair		
fraction in C phosphate	0.004	0.000
fraction in C sugar	0.009	0.006
fraction in C base	0.080	**0.673**
fraction in 8OG phosphate	0.037	0.002
fraction in 8OG sugar	-0.008	0.006
fraction in 8OG base	**0.878**	**0.313**

Table S13. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 8OG-C nucleotide pair under implicit solvation (vertical IE/EA).

2 G-C pairs		
fraction in 5' C phosphate	0.000	0.004
fraction in 5' C sugar	0.000	0.004
fraction in 5' C base	0.010	**0.455**
fraction in 3' G phosphate	0.000	0.000
fraction in 3' G sugar	0.004	0.008
fraction in 3' G base	**0.454**	0.061
fraction in 3' C phosphate	0.000	-0.015
fraction in 3' C sugar	0.003	-0.025
fraction in 3' C base	0.024	**0.414**
fraction in 5' G phosphate	0.001	0.000
fraction in 5' G sugar	0.002	0.000
fraction in 5' G base	**0.502**	0.094

Table S14. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 2 G-C nucleotide pairs under implicit solvation (vertical IE/EA).

(G-C)-(8OG-C) pairs		
fraction in 5' C phosphate	0.000	0.003
fraction in 5' C sugar	0.001	-0.001
fraction in 5' C base	0.006	**0.375**
fraction in 3' 8OG phosphate	0.000	0.000
fraction in 3' 8OG sugar	-0.004	0.012
fraction in 3' 8OG base	**0.584**	0.086
fraction in 3' C phosphate	0.000	-0.012
fraction in 3' C sugar	-0.001	-0.026
fraction in 3' C base	0.006	**0.485**
fraction in 5' G phosphate	0.000	0.000
fraction in 5' G sugar	0.000	-0.002
fraction in 5' G base	**0.408**	0.080

Table S15. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C) nucleotide pairs under implicit solvation (vertical IE/EA).

(8OG-C)-(G-C) pairs		
fraction in 5' C phosphate	0.000	-0.003
fraction in 5' C sugar	0.001	-0.007
fraction in 5' C base	0.016	**0.330**
fraction in 3' G phosphate	0.000	0.000
fraction in 3' G sugar	-0.004	0.001
fraction in 3' G base	**0.395**	0.036
fraction in 3' C phosphate	0.000	0.003

fraction in 3' C sugar	-0.002	-0.025
fraction in 3' C base	0.005	**0.528**
fraction in 5' 8OG phosphate	0.005	0.000
fraction in 5' 8OG sugar	-0.001	0.001
fraction in 5' 8OG base	**0.583**	**0.136**

Table S16. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (8OG-C)-(G-C) nucleotide pairs under implicit solvation (vertical IE/EA).

G-C pair		
fraction in C	0.000	**0.985**
fraction in G	**1.000**	0.015

Table S17. Hole distribution (2nd column) and excess electron distribution (3rd column) in the G-C base pair under implicit solvation (adiabatic IE/EA).

8OG-C pair		
fraction in C	0.000	**0.984**
fraction in 8OG	**1.000**	0.016

Table S18. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 8OG-C base pair under implicit solvation (adiabatic IE/EA).

2 G-C pairs		
fraction in 5' C	0.000	**0.979**
fraction in 3' G	**0.655**	0.000
fraction in 3' C	0.000	0.021
fraction in 5' G	**0.345**	0.000

Table S19. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 2 G-C base pairs under implicit solvation (adiabatic IE/EA).

(G-C)-(8OG-C) pairs		
fraction in 5' C	0.000	**1.000**
fraction in 3' 8OG	**0.968**	0.000
fraction in 3' C	0.000	0.000
fraction in 5' G	0.032	0.000

Table S20. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C) base pairs under implicit solvation (adiabatic IE/EA).

(8OG-C)-(G-C) pairs		
fraction in 5' C	0.000	0.001

fraction in 3' G	0.038	0.000
fraction in 3' C	0.000	**0.999**
fraction in 5' 8OG	**0.962**	0.000

Table S21. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (8OG-C)-(G-C) base pairs under implicit solvation (adiabatic IE/EA).

2 G-C pairs		
fraction in 5' C	0.000	**0.470**
fraction in 3' G	**0.500**	0.011
fraction in 3' C	0.000	**0.509**
fraction in 5' G	**0.500**	0.010

Table S22. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 2 G-C base pairs under implicit solvation, determined with the ωB97XD functional (vertical IE/EA).

(G-C)-(8OG-C) pairs		
fraction in 5' C	0.000	**0.981**
fraction in 3' 8OG	**0.997**	0.010
fraction in 3' C	0.000	0.010
fraction in 5' G	0.003	-0.001

Table S23. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C) base pairs under implicit solvation, determined with the ωB97XD functional (vertical IE/EA).

(8OG-C)-(G-C) pairs		
fraction in 5' C	0.000	0.009
fraction in 3' G	0.003	-0.001
fraction in 3' C	-0.001	**0.981**
fraction in 5' 8OG	**0.998**	0.011

Table S24. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (8OG-C)-(G-C) base pairs under implicit solvation, determined with the ωB97XD functional (vertical IE/EA).

3 G-C pairs		
fraction in 5' C	-0.001	0.010
fraction in 3' G	**0.520**	0.000
fraction in central C	0.001	**0.986**

fraction in central G	**0.478**	-0.003
fraction in 3' C	0.000	0.008
fraction in 5' G	0.002	-0.001

Table S25. Hole distribution (2nd column) and excess electron distribution (3rd column) in the 3 G-C base pairs under implicit solvation, determined with the ωB97XD functional.

(G-C)-(8OG-C)-(G-C) pairs		
fraction in 5' C	0.000	0.005
fraction in 3' G	0.003	0.001
fraction in central C	-0.002	**0.992**
fraction in central 8OG	**0.994**	-0.007
fraction in 3' C	0.000	0.008
fraction in 5' G	0.005	0.001

Table S26. Hole distribution (2nd column) and excess electron distribution (3rd column) in the (G-C)-(8OG-C)-(G-C) base pairs under implicit solvation, determined with the ωB97XD functional (vertical IE/EA).

Optimized coordinates for all neutral species

Guanine base in gas phase

```
H   -1.858441   -2.511224   -0.012449
N   -1.732943   -1.507764   -0.004552
C   -2.717229   -0.532943    0.000645
H   -3.768797   -0.787370   -0.002233
N   -2.227322    0.680422    0.008523
C   -0.856559    0.504055    0.008733
C    0.210179    1.471241    0.003241
O    0.189877    2.692232   -0.003415
N    1.477855    0.792389   -0.004565
H    2.271470    1.420431   -0.081256
C    1.676100   -0.565262   -0.001996
N    2.981183   -1.005385   -0.068613
H    3.689815   -0.447939    0.392193
H    3.075578   -2.000443    0.096753
N    0.696995   -1.438872    0.008242
C   -0.528994   -0.853230   -0.000442
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Guanine base with PCM

```
H   -1.890291   -2.502956    0.000476
N   -1.741175   -1.501025    0.000503
```

C	-2.716559	-0.525847	0.001180
H	-3.767973	-0.778924	0.001382
N	-2.219512	0.689871	0.001579
C	-0.846125	0.502377	0.000767
C	0.223703	1.451882	0.001000
O	0.180265	2.688157	0.000745
N	1.478846	0.794007	-0.001043
H	2.282286	1.415156	-0.023943
C	1.680379	-0.567818	-0.000199
N	2.970093	-1.005826	-0.062192
H	3.716618	-0.402787	0.260562
H	3.104229	-1.989492	0.137539
N	0.690663	-1.441517	0.004479
C	-0.531298	-0.859732	-0.000291

8-oxoguanine base in gas phase

H	1.736820	-2.294776	-0.009934
N	1.508832	-1.310384	-0.002727
C	2.494197	-0.301411	0.000651
O	3.704554	-0.456310	-0.002175
N	1.766428	0.878701	0.008220
H	2.196540	1.792316	0.009035
C	0.397746	0.609262	0.007573
C	-0.735206	1.463805	0.002637
O	-0.800067	2.691637	-0.002969
N	-1.932190	0.675965	-0.004533
H	-2.783229	1.224006	-0.080262
C	-1.987509	-0.692557	-0.001141
N	-3.233387	-1.273877	-0.067524
H	-4.005935	-0.797706	0.381266
H	-3.219648	-2.274416	0.090146
N	-0.916953	-1.457915	0.008550
C	0.245847	-0.765678	-0.000220

8-oxoguanine base with PCM

H	1.741252	-2.293480	-0.000445
N	1.512870	-1.307521	-0.000278
C	2.482586	-0.297948	0.001022
O	3.705950	-0.450007	0.001487
N	1.767257	0.878925	0.001778
H	2.201939	1.791435	0.000559
C	0.395681	0.610440	-0.000575
C	-0.741694	1.451042	0.000650
O	-0.802660	2.690674	0.002096
N	-1.930090	0.675218	-0.002259
H	-2.789828	1.216155	-0.026048
C	-1.990498	-0.694955	-0.000223
N	-3.220204	-1.274715	-0.057731
H	-4.034716	-0.756300	0.246231
H	-3.246046	-2.267669	0.138530
N	-0.908764	-1.460603	0.003615

C	0.246190	-0.767679	-0.001436

Guanine nucleotide + Na^+ (gas phase)

Na	-6.010282	-1.556631	-0.946925
O	-2.493203	-1.707259	0.926483
H	-2.899619	-2.355218	1.523391
P	-3.620658	-0.887960	0.065344
O	-4.919822	-0.794310	0.866473
O	-3.823535	-1.448851	-1.331484
O	-2.856918	0.535671	-0.088351
C	-2.647039	1.402837	1.039652
H	-2.595468	0.828245	1.969699
H	-3.490478	2.101537	1.099731
C	-1.347420	2.174350	0.854956
H	-1.348675	3.024772	1.549126
O	-0.232157	1.323931	1.175661
C	0.731453	1.355363	0.126817
H	1.504614	2.102405	0.334746
N	1.410180	0.073843	0.084693
C	0.847266	-1.198078	0.121300
H	-0.220315	-1.340815	0.218308
N	1.742716	-2.153337	0.074806
C	2.956089	-1.497582	0.002606
C	4.295838	-2.016100	-0.057430
O	4.719861	-3.163177	-0.067755
N	5.236039	-0.927707	-0.100478
H	6.204684	-1.228266	-0.064784
C	4.932388	0.409233	-0.094620
N	5.997925	1.290816	-0.078541
H	6.821095	1.030497	-0.609011
H	5.712696	2.251308	-0.230089
N	3.706797	0.871195	-0.051484
C	2.770197	-0.114512	0.015285
C	-1.108050	2.700863	-0.577520
H	-2.031193	2.706677	-1.167310
C	-0.069994	1.719135	-1.130567
H	-0.571799	0.829641	-1.524411
H	0.557457	2.153297	-1.916059
O	-0.594688	4.034681	-0.446112
H	-0.436312	4.396050	-1.332500

8-oxoguanine nucleotide + Na^+ (gas phase)

Na	-3.838827	-2.601885	1.808755
O	-2.642206	-1.714198	0.171918
H	-1.864334	-1.639824	-0.427205
P	-3.914001	-0.677168	-0.247019
O	-4.793322	-0.854394	0.991944
O	-4.378433	-0.915236	-1.639285
O	-3.171365	0.788590	-0.212175
C	-2.762605	1.426402	0.993610

H	-2.680679	0.713122	1.820895
H	-3.514063	2.180186	1.264190
C	-1.418095	2.111688	0.782543
H	-1.274545	2.866375	1.566991
O	-0.350443	1.141522	0.883208
C	0.562607	1.354177	-0.189661
H	1.307338	2.105990	0.092746
N	1.327622	0.138938	-0.418317
C	0.833218	-1.095116	-0.894543
O	-0.303263	-1.352221	-1.284187
N	1.905630	-1.959359	-0.849286
H	1.855938	-2.913710	-1.177116
C	3.034102	-1.308691	-0.360340
C	4.360596	-1.760591	-0.132543
O	4.858945	-2.868364	-0.322058
N	5.149766	-0.688101	0.390001
H	6.130054	-0.920160	0.515046
C	4.698322	0.581059	0.644038
N	5.617630	1.498782	1.095792
H	6.378961	1.168977	1.676041
H	5.201015	2.365629	1.414238
N	3.458926	0.962657	0.426215
C	2.665867	-0.007488	-0.083768
C	-1.263664	2.796021	-0.596986
H	-2.225944	2.893903	-1.107164
C	-0.304595	1.859754	-1.344746
H	-0.860491	1.033619	-1.794556
H	0.277662	2.378038	-2.113787
O	-0.688188	4.091820	-0.357982
H	-0.699126	4.592246	-1.188855

Guanine nucleotide + Na^+ (PCM)

Na	-6.900364	0.034799	0.035331
O	-3.266476	-2.191125	1.267466
H	-3.960067	-1.960059	1.907817
P	-3.465822	-1.355974	-0.146775
O	-4.856037	-0.747268	-0.130458
O	-2.993473	-2.229300	-1.276104
O	-2.342995	-0.156021	-0.015282
C	-2.491447	0.869615	0.974935
H	-2.401996	0.434527	1.978188
H	-3.476665	1.343205	0.882959
C	-1.410931	1.925566	0.793208
H	-1.609176	2.728966	1.512218
O	-0.108863	1.374114	1.094699
C	0.750176	1.430720	-0.046258
H	1.504312	2.208130	0.100748
N	1.490369	0.180190	-0.143993
C	0.969754	-1.095912	-0.300406
H	-0.096814	-1.255500	-0.384624
N	1.891055	-2.030389	-0.306095
C	3.084573	-1.345176	-0.142743
C	4.430182	-1.823045	-0.074117

O	4.860942	-2.980536	-0.148644
N	5.336537	-0.748568	0.109150
H	6.310917	-1.024989	0.188313
C	5.002912	0.582730	0.207315
N	6.016050	1.464110	0.444142
H	6.961678	1.218459	0.178792
H	5.780201	2.440483	0.315368
N	3.759119	1.018846	0.135055
C	2.853739	0.027374	-0.031931
C	-1.306664	2.521936	-0.621070
H	-2.240963	2.410477	-1.181486
C	-0.156006	1.730601	-1.248320
H	-0.540116	0.801877	-1.678188
H	0.368086	2.287664	-2.030092
O	-0.992201	3.913881	-0.462336
H	-0.924866	4.317846	-1.343238

8-oxoguanine nucleotide + Na^+ (PCM)

Na	-7.188526	0.802029	0.741453
O	-3.778323	-1.912773	1.612108
H	-3.117997	-2.617747	1.499227
P	-4.097678	-1.166154	0.170538
O	-5.300010	-0.288867	0.448025
O	-4.088970	-2.168335	-0.954826
O	-2.767893	-0.220706	-0.057131
C	-2.518660	0.887433	0.816766
H	-2.379668	0.530361	1.844632
H	-3.371242	1.576978	0.798703
C	-1.275384	1.635514	0.369738
H	-1.202559	2.547497	0.978620
O	-0.106003	0.825553	0.602548
C	0.820332	1.058133	-0.464542
H	1.412757	1.953962	-0.250483
N	1.775341	-0.028424	-0.512665
C	1.523168	-1.359535	-0.923925
O	0.471711	-1.813858	-1.373587
N	2.704283	-2.033031	-0.719221
H	2.820628	-3.014434	-0.932325
C	3.666532	-1.178911	-0.181842
C	5.009650	-1.385526	0.211490
O	5.689160	-2.422946	0.166042
N	5.569552	-0.182774	0.713140
H	6.541494	-0.255090	0.999960
C	4.916561	1.019099	0.813673
N	5.622830	2.091052	1.264279
H	6.459859	1.950453	1.815751
H	5.075270	2.905814	1.512110
N	3.655090	1.180736	0.442738
C	3.080413	0.065861	-0.047171
C	-1.242516	2.055095	-1.122381
H	-2.179990	1.812716	-1.631697
C	-0.058353	1.267791	-1.700951

H	-0.394670	0.303278	-2.085897
H	0.458437	1.814899	-2.494828
O	-1.033612	3.477005	-1.148285
H	-1.091978	3.778083	-2.070001

Guanine nucleotide in gas phase

O	-4.600058	-2.202374	0.552543
H	-5.447707	-1.771902	0.745304
P	-3.720739	-1.117030	-0.358764
O	-4.634259	0.064006	-0.621683
O	-2.945379	-1.852630	-1.408543
O	-2.546644	-0.631382	0.744906
C	-2.715527	0.518184	1.556277
H	-2.412858	0.257789	2.579474
H	-3.762178	0.849879	1.562708
C	-1.842998	1.678184	1.072688
H	-2.042528	2.557894	1.698407
O	-0.440743	1.354331	1.222990
C	0.195208	1.240726	-0.044829
H	0.890130	2.076206	-0.170849
N	1.033564	0.043538	-0.068234
C	0.639168	-1.289213	0.001507
H	-0.409869	-1.560317	0.019948
N	1.654492	-2.120062	0.046285
C	2.774494	-1.313099	0.010787
C	4.169429	-1.649889	0.046794
O	4.748071	-2.729346	0.119075
N	4.962277	-0.450223	-0.002611
H	5.956592	-0.614439	0.111742
C	4.485024	0.832613	-0.079231
N	5.437499	1.850432	-0.059544
H	6.254774	1.692152	-0.640289
H	5.009773	2.750526	-0.250116
N	3.214773	1.130044	-0.117177
C	2.404862	0.033559	-0.050938
C	-2.038862	2.041015	-0.406279
H	-3.033636	1.749948	-0.757248
C	-0.919986	1.257281	-1.100691
H	-1.264862	0.244713	-1.329819
H	-0.590372	1.733969	-2.030357
O	-1.855942	3.471227	-0.530519
H	-2.159643	3.726105	-1.415135

Guanine nucleotide with PCM

O	-3.618927	-2.176079	1.297182
H	-4.322035	-1.960756	1.932269
P	-3.866322	-1.367327	-0.133083
O	-5.270393	-0.801657	-0.116226
O	-3.359035	-2.247416	-1.246992

O	-2.760640	-0.139036	-0.024775
C	-2.923264	0.887840	0.958797
H	-2.845135	0.457978	1.965677
H	-3.908566	1.359665	0.855633
C	-1.843474	1.946776	0.787721
H	-2.046870	2.748372	1.507282
O	-0.541130	1.398183	1.096652
C	0.321031	1.446995	-0.041552
H	1.081778	2.217501	0.108027
N	1.052584	0.190646	-0.139858
C	0.524170	-1.081048	-0.306549
H	-0.543465	-1.233253	-0.392308
N	1.440002	-2.021030	-0.319199
C	2.637653	-1.344428	-0.150467
C	3.980410	-1.830649	-0.087372
O	4.404600	-2.989936	-0.172707
N	4.893371	-0.763245	0.104409
H	5.866037	-1.046579	0.180479
C	4.567775	0.569170	0.213327
N	5.586395	1.442739	0.457307
H	6.529636	1.194895	0.185518
H	5.355204	2.421324	0.336865
N	3.326741	1.013228	0.145233
C	2.414953	0.028611	-0.028937
C	-1.730279	2.546268	-0.624247
H	-2.662023	2.437494	-1.189312
C	-0.578077	1.753963	-1.247137
H	-0.963100	0.827972	-1.681855
H	-0.047460	2.311439	-2.024281
O	-1.413969	3.937596	-0.461087
H	-1.342257	4.343265	-1.340856

8-oxoguanine nucleotide in gas phase

O	-5.487652	0.483533	1.797546
H	-5.645295	-0.075113	2.575270
P	-4.622696	-0.450331	0.710703
O	-4.851210	0.193720	-0.641241
O	-4.860708	-1.896066	1.026688
O	-3.050305	-0.112059	1.183495
C	-2.551444	1.199274	0.959919
H	-2.033388	1.520417	1.873930
H	-3.374295	1.899038	0.772844
C	-1.571944	1.311297	-0.207256
H	-1.549959	2.371379	-0.519909
O	-0.237292	0.929587	0.200011
C	0.532267	0.785219	-0.988876
H	1.084039	1.714589	-1.173588
N	1.577446	-0.208263	-0.745532
C	1.427327	-1.622510	-0.785403
O	0.475154	-2.265023	-1.186768
N	2.630386	-2.119403	-0.296684
H	2.795144	-3.106114	-0.162540

C	3.469447	-1.080322	0.084730
C	4.773347	-1.075271	0.636562
O	5.517250	-2.015116	0.932576
N	5.206823	0.272868	0.842803
H	6.162067	0.354913	1.174159
C	4.476950	1.392395	0.545675
N	5.089982	2.617888	0.764624
H	5.647477	2.693322	1.608605
H	4.431730	3.384020	0.670375
N	3.275375	1.354469	0.025788
C	2.804236	0.101529	-0.197202
C	-1.825346	0.442347	-1.452381
H	-2.041868	-0.578161	-1.116532
C	-0.453302	0.484101	-2.143845
H	-0.222401	-0.441576	-2.671602
H	-0.444380	1.313502	-2.860477
O	-2.845443	0.927623	-2.292866
H	-3.696091	0.683911	-1.835152

8-oxoguanine nucleotide with PCM

O	-4.165508	-1.804666	1.676973
H	-3.531614	-2.510930	1.465148
P	-4.567310	-0.947645	0.311767
O	-5.721424	-0.061512	0.717163
O	-4.641825	-1.883624	-0.872018
O	-3.211435	-0.032924	0.057890
C	-2.886876	1.022422	0.968077
H	-2.732232	0.617782	1.976311
H	-3.707692	1.748964	1.007412
C	-1.624676	1.735729	0.515171
H	-1.501146	2.625093	1.148586
O	-0.481190	0.874756	0.696755
C	0.424416	1.097227	-0.389653
H	1.058005	1.963465	-0.171680
N	1.334569	-0.023907	-0.491473
C	1.017105	-1.335776	-0.918621
O	-0.066273	-1.741091	-1.338100
N	2.178339	-2.057289	-0.770248
H	2.249489	-3.037702	-1.006465
C	3.191778	-1.250514	-0.254510
C	4.540585	-1.514047	0.080823
O	5.178363	-2.574687	-0.010708
N	5.164888	-0.342609	0.580791
H	6.144696	-0.456070	0.824205
C	4.561986	0.880186	0.729205
N	5.325468	1.916823	1.170143
H	6.172492	1.733941	1.693300
H	4.817474	2.745974	1.452324
N	3.294046	1.095428	0.411971
C	2.658839	0.012474	-0.075123
C	-1.608868	2.196751	-0.964706
H	-2.569436	2.014153	-1.455283

C	-0.478091	1.372058	-1.595445
H	-0.867248	0.431820	-1.990865
H	0.039716	1.913900	-2.392317
O	-1.330796	3.607391	-0.957695
H	-1.400513	3.936959	-1.868871

G-C base pair in gas phase

H	4.880416	1.786150	-0.002347
N	4.349902	0.923525	-0.001390
C	4.964433	-0.292245	-0.001678
H	6.049496	-0.287313	-0.002693
C	4.225826	-1.431789	-0.000702
H	4.696499	-2.407620	-0.000848
C	2.789187	-1.281892	0.000502
N	1.991161	-2.356691	0.001443
H	2.383516	-3.286788	0.000536
H	0.960491	-2.248956	0.001594
N	2.206480	-0.075364	0.000804
C	2.947049	1.062656	-0.000208
O	2.468898	2.204849	-0.000199
H	-5.336969	1.247737	-0.001625
N	-4.686985	0.473440	-0.001355
C	-4.983578	-0.882197	-0.001405
H	-6.005301	-1.238602	-0.002212
N	-3.915251	-1.635210	-0.000627
C	-2.857342	-0.740278	-0.000027
C	-1.443005	-0.953507	0.000676
O	-0.812887	-2.023843	0.001129
N	-0.739851	0.268520	0.000742
H	0.289408	0.181914	0.001219
C	-1.302660	1.524060	0.000760
N	-0.450448	2.573175	0.002232
H	0.567731	2.466566	0.000758
H	-0.855861	3.497010	0.000602
N	-2.612520	1.731630	-0.000030
C	-3.319065	0.581971	-0.000443

G-C base pair with PCM

H	4.874233	1.805511	0.001729
N	4.341232	0.943161	0.001133
C	4.974322	-0.263243	0.000670
H	6.057861	-0.238569	0.001004
C	4.250617	-1.413522	-0.000149
H	4.732884	-2.383011	-0.000502
C	2.819076	-1.282847	-0.000450
N	2.034771	-2.370206	-0.001147
H	2.440274	-3.295849	-0.001688
H	1.012082	-2.276777	-0.001059
N	2.214243	-0.080865	-0.000033

C	2.949753	1.059548	0.000728
O	2.443441	2.201442	0.001080
H	-5.352452	1.263798	0.000744
N	-4.694509	0.493787	0.000641
C	-5.005074	-0.851547	0.001109
H	-6.031252	-1.193191	0.001569
N	-3.940415	-1.619164	0.000876
C	-2.873140	-0.731519	0.000231
C	-1.465174	-0.960352	-0.000244
O	-0.858873	-2.051816	-0.000140
N	-0.740904	0.241280	-0.000905
H	0.291599	0.143105	-0.000887
C	-1.289489	1.506230	-0.001001
N	-0.426400	2.541494	-0.001872
H	0.593057	2.417112	-0.000800
H	-0.811314	3.475578	-0.000681
N	-2.600336	1.729418	-0.000517
C	-3.327107	0.592746	0.000075

8OG-C base pair in gas phase

H	-5.290669	1.620554	0.006370
N	-4.721885	0.782529	0.004198
C	-5.281578	-0.459358	0.003266
H	-6.365740	-0.502733	0.004850
C	-4.493071	-1.565176	0.000526
H	-4.920169	-2.560812	-0.000185
C	-3.065062	-1.351765	-0.001263
N	-2.219541	-2.390334	-0.003810
H	-2.571259	-3.336547	-0.004069
H	-1.194979	-2.238244	-0.003869
N	-2.536860	-0.120551	-0.000478
C	-3.327397	0.984108	0.002420
O	-2.899071	2.145711	0.003534
H	4.939393	1.559621	0.002790
N	4.323092	0.759076	0.002081
C	4.799183	-0.567230	0.002959
O	5.967072	-0.928249	0.004721
N	3.651427	-1.339928	0.001393
H	3.667561	-2.348895	0.001087
C	2.513085	-0.526343	-0.000670
C	1.133816	-0.812099	-0.002174
O	0.576720	-1.932853	-0.002381
N	0.366662	0.369447	-0.003538
H	-0.658998	0.232263	-0.003633
C	0.877437	1.642246	-0.003360
N	-0.007249	2.662102	-0.006456
H	-1.021175	2.518557	-0.002122
H	0.367138	3.599043	-0.001344
N	2.183840	1.899450	-0.001422
C	2.946042	0.793581	-0.000144

8OG-C base pair with PCM

H	-5.284583	1.646935	0.006092
N	-4.714702	0.808551	0.003897
C	-5.295180	-0.424049	0.001585
H	-6.378782	-0.445872	0.002091
C	-4.522450	-1.542024	-0.001170
H	-4.962074	-2.531412	-0.003024
C	-3.097984	-1.350126	-0.001507
N	-2.267909	-2.402909	-0.004210
H	-2.634207	-3.344862	-0.004759
H	-1.249733	-2.267321	-0.003019
N	-2.545991	-0.122852	0.000616
C	-3.329829	0.985044	0.003521
O	-2.872864	2.147583	0.005909
H	4.935893	1.583262	0.001088
N	4.328399	0.774023	0.001033
C	4.808284	-0.540899	0.002561
O	5.990506	-0.893802	0.004123
N	3.681145	-1.329938	0.001880
H	3.712101	-2.340034	0.002454
C	2.531678	-0.530845	-0.000200
C	1.154035	-0.830920	-0.001043
O	0.609004	-1.959230	-0.000291
N	0.372606	0.337646	-0.002971
H	-0.655799	0.191327	-0.002536
C	0.867975	1.618124	-0.003772
N	-0.026159	2.624672	-0.007944
H	-1.040771	2.463551	-0.001248
H	0.327638	3.570985	-0.000742
N	2.175199	1.889634	-0.002344
C	2.949976	0.793236	-0.000642

2 G-C base pairs in gas phase

H	3.652920	4.478566	-1.047129
N	4.348259	3.773204	-0.837791
C	5.681890	4.057609	-0.883379
H	5.951390	5.079503	-1.128479
C	6.593942	3.086635	-0.627264
H	7.657232	3.292645	-0.654549
C	6.085034	1.768613	-0.326189
N	6.922283	0.760515	-0.068443
H	7.920836	0.910882	-0.090834
H	6.573485	-0.196242	0.144929
N	4.765807	1.512928	-0.294811
C	3.862192	2.488980	-0.536803
O	2.628542	2.319322	-0.511993
H	0.707178	2.332007	-0.106291
N	-0.232967	2.561985	0.216985
C	-0.448387	3.737862	0.863319
H	0.424198	4.366541	1.006942
C	-1.691667	4.077684	1.295906

H	-1.874961	5.011082	1.814761
C	-2.750484	3.136974	1.030111
N	-4.008667	3.396027	1.411475
H	-4.229199	4.253031	1.896978
H	-4.768815	2.716866	1.230026
N	-2.517708	1.977940	0.397455
C	-1.268736	1.645493	-0.017676
O	-1.005915	0.573204	-0.593031
H	-7.803721	-3.319711	-1.253896
N	-7.727778	-2.421337	-0.796604
C	-8.737720	-1.695132	-0.181536
H	-9.754889	-2.062044	-0.140159
N	-8.316539	-0.562850	0.317487
C	-6.963192	-0.532606	0.021258
C	-5.957932	0.444546	0.306829
O	-6.067427	1.527096	0.905114
N	-4.700407	0.047976	-0.192189
H	-3.925030	0.705851	-0.007496
C	-4.433512	-1.117686	-0.872725
N	-3.159596	-1.300980	-1.286087
H	-2.401065	-0.658132	-1.041716
H	-2.941883	-2.179981	-1.731220
N	-5.357661	-2.030894	-1.139010
C	-6.576374	-1.684614	-0.674573
H	1.855109	-5.549026	0.531264
N	2.747318	-5.076401	0.584644
C	3.978914	-5.624706	0.912751
H	4.085922	-6.674426	1.152658
N	4.946829	-4.746521	0.894430
C	4.331717	-3.557137	0.538190
C	4.857756	-2.240897	0.357838
O	6.028019	-1.835371	0.477574
N	3.845836	-1.332955	-0.003022
H	4.147209	-0.355397	-0.113104
C	2.510814	-1.627870	-0.183765
N	1.727184	-0.600918	-0.575660
H	2.084966	0.351576	-0.575298
H	0.717686	-0.695445	-0.572057
N	2.014027	-2.844595	-0.015778
C	2.956101	-3.742756	0.339675

2 G-C base pairs with PCM

H	-6.703176	0.887366	0.881060
N	-6.169840	0.330796	0.222654
C	-6.666959	0.057991	-1.016173
H	-7.644680	0.466742	-1.242995
C	-5.945167	-0.690712	-1.891095
H	-6.320636	-0.920664	-2.880363
C	-4.663634	-1.162742	-1.442072
N	-3.894406	-1.913713	-2.243464
H	-4.204531	-2.154186	-3.174704
H	-2.980880	-2.254977	-1.921288
N	-4.189591	-0.877193	-0.215874

C	-4.921504	-0.128883	0.647902
O	-4.532645	0.166160	1.797589
H	-1.579350	4.508688	1.772074
N	-1.357776	3.966978	0.944213
C	-2.255369	3.861868	-0.075356
H	-3.197761	4.381362	0.057096
C	-1.948256	3.135862	-1.182411
H	-2.646215	3.038534	-2.004351
C	-0.656752	2.505072	-1.211070
N	-0.279402	1.770972	-2.267297
H	-0.887316	1.675697	-3.068876
H	0.656622	1.350372	-2.303335
N	0.213953	2.620614	-0.191738
C	-0.106195	3.348949	0.907739
O	0.662149	3.492365	1.882097
H	7.269612	-0.393340	0.200909
N	6.479068	-0.332667	-0.429214
C	6.391058	-0.881859	-1.692928
H	7.208421	-1.446251	-2.120816
N	5.239977	-0.637132	-2.274066
C	4.533736	0.112418	-1.343509
C	3.224092	0.675785	-1.394574
O	2.393011	0.617414	-2.324265
N	2.906638	1.366269	-0.215250
H	1.966391	1.803793	-0.190074
C	3.734088	1.503740	0.878968
N	3.244183	2.197743	1.925666
H	2.326808	2.659359	1.904767
H	3.852874	2.344655	2.718550
N	4.956709	0.984119	0.934983
C	5.293643	0.311439	-0.185063
H	2.555143	-3.069044	2.737800
N	2.000763	-3.168393	1.896198
C	2.338191	-3.893501	0.770903
H	3.270841	-4.437757	0.708847
N	1.419904	-3.835811	-0.165108
C	0.426293	-3.029690	0.372896
C	-0.825714	-2.602955	-0.161760
O	-1.323743	-2.871724	-1.274962
N	-1.526251	-1.785709	0.738135
H	-2.454093	-1.453846	0.415016
C	-1.087868	-1.416970	1.991644
N	-1.894686	-0.600302	2.699972
H	-2.836382	-0.343008	2.380797
H	-1.625341	-0.387369	3.650033
N	0.073600	-1.814881	2.501524
C	0.773581	-2.604424	1.660431

(G-C)-(8OG-C) base pairs in gas phase

H	-7.621538	4.274940	-0.485923
N	-6.639154	4.035142	-0.540321
C	-5.704328	4.941227	-0.940987
H	-6.066145	5.933439	-1.190205

C	-4.395466	4.586640	-1.014923
H	-3.638338	5.293218	-1.333357
C	-4.061737	3.228689	-0.651096
N	-2.793754	2.801805	-0.694747
H	-2.061126	3.411486	-1.027223
H	-2.557924	1.815252	-0.470873
N	-4.998380	2.356089	-0.255837
C	-6.308247	2.708400	-0.194223
O	-7.220720	1.942798	0.142360
H	8.078354	3.722698	0.402182
N	7.081123	3.575690	0.499761
C	6.258325	4.553546	0.970749
H	6.725385	5.498930	1.226831
C	4.926449	4.322329	1.101644
H	4.256713	5.087350	1.475896
C	4.447376	3.013953	0.720035
N	3.146949	2.708692	0.815486
H	2.493396	3.372966	1.203439
H	2.808842	1.757422	0.577098
N	5.274866	2.068403	0.256195
C	6.608120	2.297391	0.137225
O	7.425745	1.459570	-0.264612
H	3.384576	-5.257870	-0.869218
N	2.947784	-4.368879	-0.666794
C	1.614539	-4.141887	-0.382843
H	0.872136	-4.930363	-0.337464
N	1.364242	-2.874287	-0.155239
C	2.588676	-2.235151	-0.289408
C	2.970286	-0.868866	-0.115196
O	2.267523	0.105430	0.200997
N	4.350414	-0.688252	-0.341309
H	4.695265	0.273610	-0.194572
C	5.249915	-1.674706	-0.672519
N	6.532479	-1.289696	-0.870447
H	6.862022	-0.342511	-0.666771
H	7.208519	-2.022577	-1.026430
N	4.908186	-2.946960	-0.815674
C	3.591093	-3.157636	-0.609848
H	-3.867750	-5.142742	0.732175
N	-3.340675	-4.294668	0.580076
C	-1.952647	-4.287409	0.355137
O	-1.226010	-5.280662	0.321719
N	-1.624858	-2.961816	0.182227
H	-0.652595	-2.648292	0.068830
C	-2.773417	-2.170237	0.296371
C	-3.009262	-0.786107	0.139388
O	-2.192906	0.119635	-0.128900
N	-4.374191	-0.474065	0.321793
H	-4.618483	0.519892	0.182595
C	-5.367939	-1.379328	0.583326
N	-6.621096	-0.892478	0.750935
H	-6.859821	0.080482	0.542473
H	-7.363106	-1.571826	0.832171
N	-5.143269	-2.683814	0.696436
C	-3.848750	-3.016850	0.541844

(G-C)-(8OG-C) base pairs with PCM

H	-6.841780	0.181631	0.342302
N	-6.161846	-0.257382	-0.268189
C	-6.465634	-0.517661	-1.570819
H	-7.456479	-0.227796	-1.901186
C	-5.548767	-1.111558	-2.379357
H	-5.768298	-1.329339	-3.417174
C	-4.277427	-1.438423	-1.793496
N	-3.321046	-2.028030	-2.524747
H	-3.486454	-2.258288	-3.494648
H	-2.417735	-2.276698	-2.103282
N	-3.997835	-1.169573	-0.504942
C	-4.923803	-0.578390	0.291771
O	-4.721696	-0.310699	1.494986
H	-1.638061	4.567495	2.542672
N	-1.532312	4.119093	1.639623
C	-2.548076	4.139375	0.732013
H	-3.453935	4.652105	1.033412
C	-2.394081	3.538293	-0.477423
H	-3.186816	3.543502	-1.214785
C	-1.131675	2.899165	-0.731741
N	-0.903126	2.282551	-1.900032
H	-1.608934	2.276088	-2.623129
H	0.009253	1.852301	-2.093923
N	-0.141825	2.891160	0.179376
C	-0.308670	3.497296	1.382043
O	0.576294	3.526455	2.263179
H	6.907141	-0.025346	-0.722686
N	6.032965	0.076472	-1.223683
C	5.766539	-0.355200	-2.507867
H	6.517714	-0.859589	-3.100497
N	4.541356	-0.082783	-2.891923
C	3.971859	0.562071	-1.802549
C	2.664927	1.100758	-1.611479
O	1.708116	1.111142	-2.413733
N	2.517614	1.675372	-0.340107
H	1.589200	2.092356	-0.139969
C	3.492273	1.723927	0.633568
N	3.152744	2.302422	1.803169
H	2.237197	2.739800	1.961275
H	3.869867	2.388242	2.509794
N	4.713817	1.227124	0.464252
C	4.890397	0.669307	-0.751548
H	2.511885	-2.750188	3.235152
N	2.102752	-2.860221	2.316130
C	2.768660	-3.481633	1.253216
O	3.901316	-3.970198	1.278207
N	1.886396	-3.423452	0.199067
H	2.094876	-3.791636	-0.718695
C	0.706306	-2.781034	0.591521
C	-0.490530	-2.473153	-0.087787
O	-0.788388	-2.722377	-1.279010
N	-1.402318	-1.809535	0.751511
H	-2.315940	-1.566040	0.321266

C	-1.176249	-1.492086	2.067365
N	-2.153609	-0.831560	2.719035
H	-3.072808	-0.655409	2.295460
H	-2.027755	-0.666292	3.707900
N	-0.041808	-1.795468	2.702107
C	0.852167	-2.430188	1.927098

(8OG-C)-(G-C) base pairs in gas phase

H	-7.622097	4.274620	-0.485711
N	-6.639702	4.034888	-0.540192
C	-5.704973	4.941021	-0.940980
H	-6.066880	5.933197	-1.190207
C	-4.396092	4.586521	-1.015017
H	-3.639040	5.293139	-1.333544
C	-4.062237	3.228610	-0.651158
N	-2.794227	2.801821	-0.694872
H	-2.061668	3.411543	-1.027426
H	-2.558304	1.815304	-0.470948
N	-4.998790	2.355957	-0.255798
C	-6.308671	2.708183	-0.194077
O	-7.221057	1.942523	0.142621
H	-3.867545	-5.142772	0.732236
N	-3.340534	-4.294655	0.580160
C	-1.952501	-4.287288	0.355265
O	-1.225790	-5.280498	0.321935
N	-1.624821	-2.961672	0.182337
H	-0.652615	-2.648081	0.068890
C	-2.773449	-2.170187	0.296431
C	-3.009407	-0.786084	0.139402
O	-2.193117	0.119720	-0.128880
N	-4.374370	-0.474156	0.321753
H	-4.618738	0.519787	0.182606
C	-5.368054	-1.379497	0.583259
N	-6.621258	-0.892759	0.750721
H	-6.860051	0.080233	0.542478
H	-7.363197	-1.572146	0.832229
N	-5.143274	-2.683962	0.696416
C	-3.848720	-3.016890	0.541882
H	8.078720	3.722470	0.402752
N	7.081456	3.575560	0.500139
C	6.258663	4.553490	0.970985
H	6.725766	5.498821	1.227185
C	4.926740	4.322398	1.101612
H	4.257006	5.087474	1.475756
C	4.447610	3.014081	0.719871
N	3.147125	2.708978	0.815084
H	2.493622	3.373334	1.202983
H	2.808912	1.757740	0.576734
N	5.275088	2.068465	0.256150
C	6.608393	2.297322	0.137464
O	7.426016	1.459434	-0.264234
H	3.384765	-5.257797	-0.869004
N	2.947965	-4.368792	-0.666643

C	1.614739	-4.141754	-0.382640
H	0.872298	-4.930195	-0.337245
N	1.364449	-2.874130	-0.155175
C	2.588878	-2.235017	-0.289460
C	2.970512	-0.868718	-0.115397
O	2.267784	0.105615	0.200749
N	4.350626	-0.688136	-0.341614
H	4.695499	0.273715	-0.194864
C	5.250099	-1.674628	-0.672784
N	6.532633	-1.289613	-0.871000
H	6.862252	-0.342570	-0.666781
H	7.208701	-2.022607	-1.026356
N	4.908361	-2.946894	-0.815768
C	3.591276	-3.157545	-0.609853

(8OG-C)-(G-C) base pairs with PCM

H	-6.834021	0.132941	0.422542
N	-6.165228	-0.330010	-0.182799
C	-6.499600	-0.659355	-1.462206
H	-7.502492	-0.398152	-1.780036
C	-5.596858	-1.283021	-2.264219
H	-5.840807	-1.555434	-3.283693
C	-4.306850	-1.565814	-1.696533
N	-3.362595	-2.181766	-2.422241
H	-3.548727	-2.458646	-3.376032
H	-2.445420	-2.397252	-2.012835
N	-3.997271	-1.229614	-0.430761
C	-4.908931	-0.607829	0.359207
O	-4.677964	-0.275356	1.541093
H	2.641850	-2.504997	3.199583
N	2.207917	-2.672350	2.300745
C	2.855358	-3.336653	1.252017
O	3.998975	-3.798808	1.267085
N	1.939819	-3.354718	0.224971
H	2.127425	-3.770588	-0.676969
C	0.757155	-2.718619	0.620273
C	-0.464112	-2.467705	-0.038510
O	-0.790054	-2.781800	-1.206781
N	-1.365463	-1.779939	0.792779
H	-2.293011	-1.570199	0.374954
C	-1.107864	-1.389744	2.083450
N	-2.082070	-0.722530	2.731768
H	-3.010574	-0.567640	2.320638
H	-1.922849	-0.481653	3.700108
N	0.051765	-1.635461	2.697690
C	0.935889	-2.292248	1.929825
H	-1.741226	4.556860	2.404770
N	-1.612947	4.109062	1.504222
C	-2.607828	4.124752	0.573648
H	-3.522568	4.633746	0.854528
C	-2.424092	3.523438	-0.631378
H	-3.200973	3.524437	-1.385811
C	-1.153693	2.889641	-0.856995

N	-0.896472	2.271242	-2.018483
H	-1.588148	2.254318	-2.755146
H	0.017506	1.833916	-2.186671
N	-0.183538	2.888691	0.075385
C	-0.380948	3.492884	1.274631
O	0.482830	3.524747	2.176192
H	6.853885	-0.113494	-0.614918
N	5.992428	-0.011535	-1.137800
C	5.740794	-0.490946	-2.407927
H	6.490975	-1.037492	-2.963280
N	4.530231	-0.206535	-2.828216
C	3.955222	0.496868	-1.778525
C	2.656202	1.068885	-1.634762
O	1.714014	1.064020	-2.454087
N	2.497696	1.698032	-0.390661
H	1.567906	2.123927	-0.217507
C	3.456500	1.770847	0.597229
N	3.117689	2.429009	1.724124
H	2.176090	2.806330	1.884929
H	3.793562	2.452974	2.474757
N	4.669192	1.239781	0.473325
C	4.855511	0.626983	-0.714272

3 G-C base pairs in gas phase

H	-6.688603	-1.083819	1.271953
N	-5.886155	-0.678904	1.740487
C	-5.601186	-0.953893	3.039365
H	-6.277529	-1.632009	3.554097
C	-4.521417	-0.394508	3.632749
H	-4.274275	-0.599549	4.669983
C	-3.717631	0.484109	2.825429
N	-2.638064	1.072995	3.341461
H	-2.373740	0.910205	4.302188
H	-2.062222	1.707893	2.759883
N	-4.014854	0.740414	1.551038
C	-5.094755	0.181461	0.958620
O	-5.426283	0.375651	-0.210161
H	-0.142606	5.331085	-3.160933
N	-0.115838	4.994834	-2.207273
C	0.803862	5.304672	-1.220421
H	1.627763	5.984026	-1.410784
N	0.561540	4.704166	-0.092502
C	-0.573018	3.958366	-0.337981
C	-1.319984	3.090098	0.511463
O	-1.121188	2.796007	1.692561
N	-2.416596	2.535850	-0.170865
H	-3.001407	1.897117	0.394013
C	-2.756305	2.772514	-1.477022
N	-3.847772	2.134535	-1.939132
H	-4.421073	1.515613	-1.357301
H	-4.112402	2.313757	-2.896514
N	-2.071782	3.574996	-2.271269

C	-1.012325	4.124807	-1.650341
H	-4.508062	-2.154119	-2.377000
N	-4.032202	-2.187506	-1.482650
C	-4.495650	-2.941163	-0.452544
H	-5.404934	-3.509023	-0.634128
C	-3.834121	-2.961644	0.727660
H	-4.185789	-3.556964	1.564854
C	-2.643788	-2.158946	0.820327
N	-1.938231	-2.129325	1.951643
H	-2.231034	-2.667763	2.753957
H	-1.080474	-1.552260	2.016684
N	-2.205866	-1.425479	-0.203572
C	-2.867605	-1.405436	-1.383119
O	-2.519200	-0.752615	-2.366032
H	4.028646	2.978190	-0.269848
N	3.518053	2.363823	0.350574
C	3.822241	2.029852	1.658894
H	4.697160	2.435476	2.155450
N	2.963608	1.207997	2.186969
C	2.043339	0.982386	1.183989
C	0.870410	0.171778	1.159700
O	0.393247	-0.534228	2.051272
N	0.230720	0.245728	-0.089534
H	-0.628590	-0.323394	-0.171653
C	0.646533	0.985421	-1.165359
N	-0.115236	0.915941	-2.272883
H	-0.960853	0.340114	-2.334231
H	0.187487	1.453113	-3.071907
N	1.730702	1.738934	-1.152875
C	2.369974	1.692954	0.030117
H	-0.151092	-2.906770	-4.358659
N	-0.031719	-3.065073	-3.364617
C	-0.935722	-3.771603	-2.638303
H	-1.796784	-4.160507	-3.176422
C	-0.743797	-3.963050	-1.312609
H	-1.453104	-4.524294	-0.711909
C	0.443025	-3.388319	-0.737359
N	0.699581	-3.534571	0.563179
H	0.063927	-4.045972	1.157888
H	1.551633	-3.115530	0.977087
N	1.318890	-2.698539	-1.468906
C	1.126266	-2.507129	-2.794000
O	1.892204	-1.881418	-3.525741
H	7.736799	0.572299	1.057161
N	6.953944	0.030641	1.399201
C	6.712244	-0.392619	2.694630
H	7.396866	-0.156049	3.502043
N	5.611843	-1.076353	2.809481
C	5.094769	-1.111213	1.530741
C	3.906424	-1.712839	1.021477
O	3.042392	-2.358130	1.619846
N	3.780155	-1.491479	-0.360679
H	2.933802	-1.901423	-0.790430
C	4.659384	-0.796781	-1.149192
N	4.352067	-0.706695	-2.456618
H	3.496733	-1.103790	-2.857821

H	4.984916	-0.180393	-3.040778
N	5.761557	-0.235418	-0.687199
C	5.915676	-0.427269	0.635576

3 G-C base pairs with PCM

H	-6.915174	-2.661360	1.126336
N	-6.422758	-1.877535	1.539910
C	-6.340193	-1.746583	2.893718
H	-6.825486	-2.516406	3.482717
C	-5.675713	-0.693084	3.437892
H	-5.596596	-0.569342	4.510780
C	-5.083758	0.246098	2.524112
N	-4.410285	1.310483	2.982478
H	-4.314988	1.468477	3.976082
H	-3.989264	1.983542	2.330542
N	-5.178369	0.097692	1.189988
C	-5.842258	-0.960883	0.660495
O	-5.958101	-1.152430	-0.568499
H	-2.197193	4.716738	-4.172719
N	-2.262006	4.628401	-3.165649
C	-1.702351	5.473903	-2.228367
H	-1.120001	6.336130	-2.523040
N	-1.960720	5.107514	-0.994597
C	-2.730890	3.960263	-1.127603
C	-3.305977	3.099052	-0.146258
O	-3.241652	3.191139	1.096995
N	-4.015739	2.040382	-0.733256
H	-4.442690	1.364309	-0.072749
C	-4.163745	1.829401	-2.087181
N	-4.918178	0.773400	-2.457836
H	-5.261762	0.080450	-1.781940
H	-4.947343	0.547451	-3.442387
N	-3.623831	2.620351	-3.008868
C	-2.929880	3.648585	-2.477827
H	-2.763126	-4.356238	-2.147375
N	-2.477820	-4.050277	-1.223746
C	-2.750591	-4.810396	-0.126709
H	-3.278641	-5.740207	-0.304383
C	-2.365679	-4.390178	1.107072
H	-2.571173	-4.977836	1.993200
C	-1.677997	-3.129931	1.181450
N	-1.275816	-2.642134	2.363489
H	-1.440414	-3.160885	3.215056
H	-0.785276	-1.741236	2.417985
N	-1.414704	-2.397269	0.084301
C	-1.803243	-2.829968	-1.141881
O	-1.586208	-2.192729	-2.193858
H	2.291977	4.315273	-0.186727
N	1.961336	3.631635	0.483776
C	2.051119	3.718703	1.858465
H	2.509051	4.571577	2.341054
N	1.531554	2.678744	2.468427

C	1.074417	1.866184	1.440485
C	0.410266	0.603852	1.468973
O	0.085250	-0.076610	2.463999
N	0.119693	0.138437	0.177717
H	-0.395897	-0.760368	0.129221
C	0.427734	0.790879	-0.996029
N	0.100147	0.159864	-2.146010
H	-0.519637	-0.659192	-2.153251
H	0.189751	0.694640	-2.999369
N	1.043730	1.967671	-1.033317
C	1.335211	2.447231	0.193823
H	2.347518	-4.118385	-3.825048
N	2.468430	-4.035994	-2.821914
C	1.943385	-4.970638	-1.981107
H	1.400390	-5.785963	-2.445381
C	2.113670	-4.852294	-0.638070
H	1.705793	-5.583348	0.048987
C	2.858574	-3.713872	-0.173259
N	3.064636	-3.523145	1.137768
H	2.712099	-4.185970	1.813952
H	3.610643	-2.718866	1.469191
N	3.370959	-2.803856	-1.021550
C	3.193030	-2.934647	-2.360530
O	3.645385	-2.122228	-3.194552
H	7.491816	3.409677	0.837381
N	7.023207	2.623093	1.270643
C	6.946677	2.355365	2.622977
H	7.408757	3.004988	3.354019
N	6.271617	1.261341	2.887082
C	5.884758	0.783379	1.642500
C	5.127491	-0.368743	1.275848
O	4.627199	-1.235078	2.023305
N	4.969616	-0.469082	-0.114437
H	4.418404	-1.282622	-0.446913
C	5.473449	0.416763	-1.042852
N	5.232845	0.137893	-2.340069
H	4.652731	-0.655387	-2.638463
H	5.546280	0.806418	-3.029680
N	6.177171	1.495164	-0.711017
C	6.346073	1.622894	0.621633

(G-C)-(8OG-C)-(G-C) base pairs in gas phase

H	-7.202899	0.537028	-1.125310
N	-6.427749	-0.001472	-1.495143
C	-6.262830	-0.196452	-2.828794
H	-7.004256	0.255741	-3.483087
C	-5.216928	-0.922905	-3.286591
H	-5.064774	-1.091639	-4.348336
C	-4.316594	-1.459704	-2.301198
N	-3.262680	-2.185606	-2.676747
H	-3.091979	-2.376359	-3.653356
H	-2.621403	-2.580790	-1.965738

N	-4.495948	-1.255162	-0.995796
C	-5.542715	-0.530426	-0.538683
O	-5.768456	-0.306231	0.649813
H	-0.022740	-3.810535	4.635834
N	-0.100833	-3.847917	3.627999
C	0.735656	-4.490919	2.732146
H	1.602285	-5.048654	3.070571
N	0.364030	-4.344942	1.494403
C	-0.773927	-3.568071	1.567467
C	-1.631779	-3.072106	0.542095
O	-1.556242	-3.227630	-0.679026
N	-2.681196	-2.311088	1.085262
H	-3.339899	-1.921345	0.390076
C	-2.885261	-2.053513	2.415410
N	-3.947037	-1.285053	2.723018
H	-4.609748	-0.942274	2.020177
H	-4.127334	-1.125617	3.703185
N	-2.098920	-2.510811	3.372344
C	-1.081126	-3.245758	2.888303
H	-4.134499	3.536409	1.583062
N	-3.804815	3.134208	0.712891
C	-4.388960	3.426985	-0.477425
H	-5.230109	4.115404	-0.451566
C	-3.922495	2.871829	-1.620127
H	-4.374066	3.091100	-2.582888
C	-2.802130	1.978058	-1.498326
N	-2.286868	1.390918	-2.579962
H	-2.675921	1.568481	-3.494536
H	-1.481817	0.746169	-2.489884
N	-2.243008	1.704708	-0.319434
C	-2.709587	2.260096	0.822628
O	-2.239970	2.050081	1.940068
H	3.684830	-2.950609	0.934965
N	3.110784	-2.602022	0.179031
C	3.307645	-2.981486	-1.159465
O	4.151805	-3.745809	-1.583455
N	2.335458	-2.292314	-1.852813
H	2.217598	-2.363334	-2.853410
C	1.569069	-1.520937	-0.978382
C	0.480216	-0.657046	-1.180645
O	-0.083374	-0.367276	-2.248951
N	0.045914	-0.101391	0.033655
H	-0.758977	0.545564	-0.042677
C	0.596573	-0.354931	1.257811
N	0.049461	0.272274	2.313776
H	-0.754722	0.902396	2.229851
H	0.447689	0.077340	3.220612
N	1.623990	-1.172737	1.436171
C	2.064456	-1.721330	0.296852
H	0.681409	4.690897	3.409669
N	0.683743	4.421558	2.432537
C	-0.289165	4.825902	1.575907
H	-1.074455	5.453162	1.990740
C	-0.252886	4.448123	0.277118
H	-1.019997	4.758797	-0.425718
C	0.848672	3.616056	-0.127910

N	0.950586	3.202218	-1.391632
H	0.255869	3.464509	-2.075665
H	1.739571	2.596338	-1.680226
N	1.795578	3.232453	0.728992
C	1.758632	3.610277	2.027301
O	2.597613	3.292439	2.869109
H	7.808286	-1.192509	-0.858535
N	6.997197	-0.792304	-1.311463
C	6.600901	-0.934816	-2.629917
H	7.173660	-1.534656	-3.329062
N	5.506594	-0.287980	-2.904975
C	5.156251	0.315045	-1.714436
C	4.051304	1.153558	-1.383498
O	3.128492	1.545311	-2.101773
N	4.097607	1.541089	-0.033298
H	3.315414	2.144270	0.272337
C	5.058157	1.182572	0.875586
N	4.921758	1.676341	2.120707
H	4.113510	2.234923	2.412829
H	5.599446	1.378202	2.806727
N	6.083002	0.404496	0.579921
C	6.071933	0.013875	-0.707560

(G-C)-(8OG-C)-(G-C) base pairs with PCM

H	-7.909535	2.178867	-1.235120
N	-7.316171	1.465096	-1.642900
C	-7.229800	1.324362	-2.995325
H	-7.821852	2.010845	-3.589532
C	-6.434254	0.361787	-3.531515
H	-6.352186	0.230879	-4.603222
C	-5.710750	-0.473204	-2.611645
N	-4.907343	-1.447531	-3.061504
H	-4.807639	-1.614298	-4.053275
H	-4.403495	-2.054377	-2.403701
N	-5.807432	-0.313664	-1.279064
C	-6.607906	0.649932	-0.757462
O	-6.740874	0.839990	0.469922
H	-2.234985	-4.444603	4.122097
N	-2.331078	-4.390137	3.115330
C	-1.740622	-5.224096	2.186765
H	-1.099538	-6.041027	2.489453
N	-2.047911	-4.907152	0.950641
C	-2.883721	-3.805703	1.072774
C	-3.544685	-3.017977	0.084086
O	-3.516382	-3.151633	-1.156975
N	-4.302627	-1.987013	0.659551
H	-4.822079	-1.385511	-0.006849
C	-4.417821	-1.736640	2.010041
N	-5.175150	-0.678784	2.368562
H	-5.743920	-0.155884	1.691937
H	-5.343503	-0.541713	3.355568
N	-3.811212	-2.468749	2.939078

C	-3.071129	-3.470012	2.418871
H	-3.419540	4.110023	2.095820
N	-3.100833	3.746682	1.204668
C	-3.578182	4.259636	0.036308
H	-4.302226	5.061626	0.123028
C	-3.144899	3.765663	-1.153354
H	-3.511262	4.158241	-2.093716
C	-2.184424	2.697088	-1.104750
N	-1.713695	2.151627	-2.235046
H	-2.038138	2.477593	-3.134934
H	-1.039162	1.377242	-2.202129
N	-1.722698	2.208816	0.061140
C	-2.162069	2.713655	1.241726
O	-1.768363	2.300672	2.352842
H	3.300694	-3.509680	0.996103
N	2.842206	-2.999554	0.252115
C	3.068249	-3.259551	-1.104587
O	3.825935	-4.111890	-1.575440
N	2.266500	-2.365287	-1.775758
H	2.220589	-2.311108	-2.783809
C	1.560977	-1.570526	-0.864706
C	0.629881	-0.523904	-1.023907
O	0.191695	-0.036033	-2.092033
N	0.194137	-0.029206	0.217212
H	-0.485780	0.754849	0.176758
C	0.610943	-0.490987	1.440732
N	0.084401	0.095219	2.532418
H	-0.570739	0.884267	2.474456
H	0.408239	-0.216702	3.437149
N	1.493636	-1.483126	1.579552
C	1.930388	-1.977922	0.410596
H	2.196365	4.284447	3.517766
N	2.314642	4.154240	2.519428
C	1.689017	4.978623	1.633356
H	1.071909	5.762372	2.057342
C	1.856334	4.795979	0.297048
H	1.369658	5.439567	-0.425187
C	2.708470	3.712538	-0.111357
N	2.922331	3.464873	-1.411415
H	2.498081	4.045702	-2.121228
H	3.548053	2.704004	-1.701962
N	3.317456	2.910822	0.781378
C	3.141812	3.105428	2.112781
O	3.683427	2.395660	2.986360
H	8.282959	-2.744749	-0.761397
N	7.697484	-2.067206	-1.234675
C	7.571606	-1.900609	-2.599511
H	8.123141	-2.517045	-3.296354
N	6.735450	-0.940785	-2.919570
C	6.287310	-0.450749	-1.700591
C	5.363857	0.592100	-1.393235
O	4.733097	1.324011	-2.184185
N	5.200950	0.754360	-0.009379
H	4.539835	1.498970	0.281207
C	5.838962	0.014618	0.963489
N	5.559723	0.328332	2.244382

H	4.882070	1.054947	2.504195
H	5.996279	-0.222963	2.969789
N	6.698957	-0.961219	0.687027
C	6.878688	-1.143791	-0.637692

G-C nucleotide pair with PCM

O	7.083055	-0.971689	-1.756162
H	6.439742	-0.335365	-1.383865
P	8.202400	-1.426137	-0.647519
O	9.441856	-1.774465	-1.419285
O	7.614496	-2.386582	0.349750
O	8.415355	-0.029549	0.206869
C	8.419324	1.231012	-0.435517
H	8.455494	1.124406	-1.528972
H	9.314738	1.788260	-0.124872
C	7.191315	2.015242	-0.021373
H	7.192507	2.981982	-0.549814
O	6.005538	1.289576	-0.392399
C	5.101764	1.289613	0.713571
H	4.467008	2.180226	0.673517
C	7.083794	2.270212	1.496524
H	8.042605	2.080348	2.000593
C	5.996611	1.311038	1.938449
H	6.430192	0.323619	2.137543
H	5.476643	1.661192	2.836019
O	6.627805	3.585432	1.776853
H	7.317121	4.220493	1.530361
O	-6.018221	-1.901347	1.618229
H	-5.371752	-2.029167	0.899768
P	-7.548772	-1.908408	1.018637
O	-8.459043	-2.042667	2.203480
O	-7.615595	-2.817692	-0.174625
O	-7.684277	-0.389591	0.392417
C	-7.732603	0.719604	1.271666
H	-7.133887	0.529157	2.175384
H	-8.772210	0.905350	1.585473
C	-7.183048	1.950766	0.585619
H	-7.324419	2.801402	1.270007
O	-5.778167	1.821323	0.350235
C	-5.508206	1.616766	-1.026460
H	-4.889191	2.452016	-1.379701
C	-7.785367	2.271187	-0.783495
H	-8.825064	1.920551	-0.865961
C	-6.852643	1.554742	-1.742225
H	-7.192684	0.525242	-1.879001
H	-6.822337	2.046830	-2.719409
O	-7.697613	3.659240	-1.073888
H	-8.281211	4.146018	-0.472489
N	4.205052	0.150752	0.580717
C	4.723116	-1.102239	0.659078
H	5.786023	-1.174920	0.868963

C	3.924415	-2.181349	0.479489
H	4.314760	-3.192733	0.537920
C	2.541104	-1.926714	0.210189
N	1.694210	-2.943070	0.022264
H	2.019549	-3.899473	0.069400
H	0.700167	-2.766259	-0.170278
N	2.045840	-0.684853	0.136172
C	2.853912	0.386054	0.317319
O	2.452023	1.557719	0.260471
N	-4.681522	0.426390	-1.169626
C	-5.072176	-0.890137	-1.273387
H	-6.102846	-1.153477	-1.482322
N	-4.088797	-1.731277	-1.095992
C	-2.989505	-0.925928	-0.862793
C	-1.631900	-1.265722	-0.601600
O	-1.120610	-2.391869	-0.523267
N	-0.840700	-0.126193	-0.422570
H	0.163123	-0.302983	-0.227789
C	-1.286137	1.171128	-0.484548
N	-0.363793	2.126647	-0.283347
H	0.624168	1.917685	-0.092609
H	-0.667347	3.089882	-0.324124
N	-2.546315	1.497023	-0.726680
C	-3.338097	0.422599	-0.904925

8OG-C nucleotide pair with PCM

O	10.163001	-1.940381	-0.745106
H	11.006969	-1.496870	-0.920403
P	9.466284	-1.312576	0.607918
O	10.498073	-0.480615	1.318496
O	8.695656	-2.404568	1.284291
O	8.317167	-0.332292	-0.039454
C	8.684255	0.796333	-0.811997
H	8.727895	0.513959	-1.874948
H	9.674078	1.174442	-0.510375
C	7.662671	1.890910	-0.613211
H	7.971737	2.766808	-1.202886
O	6.378454	1.460826	-1.084589
C	5.426704	1.480775	-0.037660
H	4.761492	2.342943	-0.146400
C	7.464019	2.311311	0.842173
H	8.343058	2.062608	1.456105
C	6.224529	1.536054	1.257576
H	6.505632	0.525996	1.582653
H	5.668456	2.020783	2.068268
O	7.235764	3.714614	0.837795
H	7.078341	4.005458	1.748801
O	-8.013851	-1.868236	1.337351
H	-7.287947	-1.821326	0.675371
P	-9.376818	-1.246767	0.690298
O	-10.366127	-1.125742	1.816504
O	-9.733409	-1.950860	-0.589955

O	-8.866316	0.245554	0.218906
C	-8.484319	1.196728	1.194710
H	-8.261664	0.715019	2.158380
H	-9.312123	1.905846	1.355072
C	-7.267249	1.962685	0.731369
H	-7.151350	2.846944	1.380060
O	-6.092099	1.150630	0.861018
C	-5.353558	1.224057	-0.345058
H	-4.657752	2.076621	-0.313279
C	-7.323226	2.414740	-0.740731
H	-8.348850	2.382094	-1.133605
C	-6.397727	1.430225	-1.427996
H	-6.923474	0.489955	-1.624273
H	-5.978557	1.831477	-2.356730
O	-6.766127	3.712524	-0.915635
H	-7.336411	4.361917	-0.477602
N	4.569330	0.296155	-0.159502
C	5.165844	-0.920024	-0.256611
H	6.251363	-0.930468	-0.223757
C	4.413052	-2.038762	-0.386493
H	4.866222	-3.021513	-0.465848
C	2.991505	-1.865674	-0.414258
N	2.187420	-2.925875	-0.540186
H	2.574257	-3.857079	-0.616412
H	1.166704	-2.810298	-0.560423
N	2.418202	-0.659813	-0.317404
C	3.180384	0.452004	-0.187912
O	2.703935	1.592689	-0.094226
N	-4.505444	0.059116	-0.465719
C	-4.941928	-1.259932	-0.603518
O	-6.104350	-1.640695	-0.675810
N	-3.795117	-2.011921	-0.638248
H	-3.796543	-3.019127	-0.733982
C	-2.674756	-1.186469	-0.525773
C	-1.292761	-1.454726	-0.507747
O	-0.719463	-2.554431	-0.593253
N	-0.548173	-0.274975	-0.373471
H	0.483613	-0.392964	-0.352377
C	-1.078038	0.981653	-0.271832
N	-0.206835	1.995187	-0.149429
H	0.810795	1.853545	-0.130209
H	-0.579369	2.931876	-0.072339
N	-2.385127	1.222055	-0.290026
C	-3.129544	0.114757	-0.417513

2 G-C nucleotide pairs with PCM

O	8.992557	3.949653	2.672121
H	8.045923	4.164898	2.666758
P	9.558207	3.771472	1.134385
O	11.047857	3.914531	1.219706
O	8.699805	4.568813	0.196414

O	9.176324	2.199773	0.815836
C	9.753682	1.172623	1.607030
H	9.748735	1.463211	2.669620
H	10.797098	1.002942	1.293309
C	8.960551	-0.098225	1.420067
H	9.475777	-0.904307	1.962274
O	7.649803	0.058429	1.979049
C	6.646287	-0.158256	1.006728
H	6.145515	-1.115938	1.180457
C	8.776559	-0.503961	-0.045981
H	9.484911	0.019789	-0.700541
C	7.341386	-0.101388	-0.348891
H	7.327276	0.919142	-0.754505
H	6.873714	-0.775015	-1.075385
O	8.987205	-1.909090	-0.146716
P	9.110587	-2.600422	-1.640835
O	9.763411	-3.931218	-1.414080
O	9.623965	-1.590731	-2.622900
O	7.527221	-2.836909	-2.034738
C	6.821134	-3.824457	-1.306507
H	6.967644	-3.686997	-0.221059
H	7.196543	-4.828114	-1.564270
C	5.352462	-3.759544	-1.607899
H	4.871988	-4.615252	-1.092386
O	4.794379	-2.542391	-1.118171
C	3.468944	-2.532855	-1.594881
H	2.821992	-3.098914	-0.913004
C	4.907532	-3.793481	-3.070296
H	5.569071	-3.160565	-3.676931
C	3.505010	-3.192976	-2.983711
H	3.306085	-2.461331	-3.776862
H	2.752631	-3.988323	-3.058577
O	4.858026	-5.104171	-3.601047
H	5.717431	-5.328580	-3.985773
O	-8.012164	2.615654	-3.514940
H	-7.613492	1.822635	-3.098043
P	-9.057756	3.376757	-2.507004
O	-10.099196	4.014831	-3.381557
O	-8.323520	4.182513	-1.470018
O	-9.704605	2.113028	-1.661585
C	-9.990291	0.876319	-2.285581
H	-9.944701	0.953894	-3.383206
H	-11.010698	0.565624	-2.015046
C	-9.025578	-0.173350	-1.780379
H	-9.258172	-1.143046	-2.247323
O	-7.679466	0.199081	-2.134604
C	-6.834049	0.035757	-0.995774
H	-6.425447	-0.985505	-0.982153
C	-9.047277	-0.331537	-0.250756
H	-9.913403	0.175953	0.193071
C	-7.739875	0.304173	0.189863
H	-7.893234	1.386381	0.307568
H	-7.349472	-0.112966	1.126515
O	-9.113959	-1.722849	0.039279
P	-9.340116	-2.217122	1.598756
O	-9.833843	-3.629889	1.501999

O	-10.057593	-1.153843	2.374177
O	-7.792326	-2.214288	2.163784
C	-6.913837	-3.203842	1.657671
H	-6.844064	-3.128878	0.557449
H	-7.296474	-4.207207	1.904205
C	-5.546721	-3.044066	2.259154
H	-4.958342	-3.948804	2.019832
O	-4.883643	-1.909825	1.694047
C	-3.947336	-1.515201	2.674357
H	-3.123102	-2.247241	2.720375
C	-5.505242	-2.856229	3.801149
H	-6.515067	-2.818227	4.230071
C	-4.758500	-1.541068	3.959389
H	-5.465156	-0.699218	3.964548
H	-4.154709	-1.512327	4.873059
O	-4.746292	-3.877442	4.435452
H	-5.261807	-4.697676	4.425906
N	5.604309	0.870344	1.162425
N	-3.325801	-0.263783	2.322127
C	5.990528	2.164690	1.025850
H	7.057009	2.335908	0.885769
C	5.070314	3.157752	1.069877
H	5.361197	4.196608	0.961809
C	3.705436	2.769596	1.263671
N	2.742852	3.695851	1.318079
H	2.975322	4.676971	1.219850
H	1.768158	3.424356	1.455269
N	3.339908	1.488389	1.396294
C	4.268889	0.503937	1.350813
O	3.988658	-0.697725	1.467255
C	-3.854959	1.008689	2.308444
H	-4.917536	1.183293	2.424631
N	-2.952724	1.936487	2.139931
C	-1.762265	1.241490	2.035153
C	-0.430965	1.708561	1.841777
O	-0.034833	2.875065	1.721605
N	0.484334	0.651404	1.793993
H	1.478835	0.925022	1.655213
C	0.171048	-0.679422	1.914412
N	1.197935	-1.542671	1.835214
H	2.173599	-1.242637	1.719949
H	0.990766	-2.523959	1.942144
N	-1.063351	-1.123749	2.095042
C	-1.973328	-0.131428	2.146258
N	2.970519	-1.154631	-1.602432
N	-5.708654	0.930236	-1.105001
C	3.827879	-0.104320	-1.685125
H	4.888437	-0.351470	-1.736912
C	3.349917	1.162604	-1.693609
H	4.017961	2.015312	-1.756910
C	1.929143	1.316326	-1.609635
N	1.380170	2.534183	-1.601704
H	1.969911	3.358038	-1.632323
H	0.370717	2.637732	-1.497280
N	1.101675	0.265379	-1.538630
C	1.592202	-0.994265	-1.529520

O	0.880843	-2.008016	-1.461426
C	-5.745337	2.300109	-0.961511
H	-6.678697	2.833485	-0.842432
N	-4.561169	2.847452	-0.996301
C	-3.699197	1.781681	-1.174506
C	-2.282978	1.741364	-1.282509
O	-1.484911	2.687138	-1.241940
N	-1.818018	0.433016	-1.450771
H	-0.780709	0.338640	-1.512776
C	-2.600430	-0.691826	-1.515102
N	-1.964071	-1.858969	-1.723762
H	-0.943046	-1.935572	-1.614341
H	-2.520441	-2.695839	-1.633246
N	-3.918863	-0.666667	-1.411704
C	-4.397959	0.578844	-1.245081

(G-C)-(8OG-C) nucleotide pairs with PCM

O	-11.004210	-4.221911	0.686113
H	-11.871441	-3.829698	0.500185
P	-9.836115	-3.368148	-0.103172
O	-10.520552	-2.413604	-1.042418
O	-8.772748	-4.324980	-0.549187
O	-9.138350	-2.536006	1.131900
C	-9.801082	-1.488545	1.821683
H	-9.869109	-1.775480	2.881383
H	-10.820410	-1.338936	1.431753
C	-9.023570	-0.198388	1.681920
H	-9.574266	0.592996	2.210822
O	-7.733308	-0.331621	2.298431
C	-6.695424	-0.121817	1.364120
H	-6.206440	0.844126	1.538752
C	-8.779489	0.221845	0.230806
H	-9.467957	-0.295259	-0.448335
C	-7.336608	-0.195979	-0.016096
H	-7.316500	-1.224733	-0.402283
H	-6.830869	0.457078	-0.737328
O	-8.970299	1.632102	0.152648
P	-8.934020	2.382939	-1.313679
O	-9.688749	3.666477	-1.128760
O	-9.249563	1.405748	-2.405398
O	-7.325665	2.717849	-1.460666
C	-6.781433	3.679778	-0.569296
H	-6.714912	3.249938	0.444390
H	-7.436828	4.564184	-0.529882
C	-5.414713	4.108401	-1.036977
H	-5.129785	5.012872	-0.473267
O	-4.452683	3.083020	-0.761995
C	-3.666845	2.874707	-1.924621
H	-2.805772	3.551502	-1.939007
C	-5.326468	4.398172	-2.549276
H	-6.323595	4.526733	-2.994569
C	-4.607695	3.170869	-3.077969
H	-5.328643	2.354052	-3.212968

H	-4.086609	3.357377	-4.023135
O	-4.502369	5.523035	-2.825157
H	-4.945225	6.320480	-2.498288
O	8.283590	-3.499974	-3.491374
H	8.867856	-3.508823	-4.264045
P	9.165331	-3.696451	-2.110950
O	10.562833	-4.084664	-2.506671
O	8.331155	-4.491278	-1.152862
O	9.154193	-2.173298	-1.495408
C	9.810053	-1.125156	-2.185813
H	9.792133	-1.296826	-3.274978
H	10.861671	-1.067619	-1.860794
C	9.109260	0.182618	-1.891861
H	9.661557	0.988174	-2.397097
O	7.778746	0.138556	-2.428636
C	6.828172	0.259067	-1.387064
H	6.390082	1.267639	-1.406041
C	8.964226	0.498493	-0.401498
H	9.740989	0.006627	0.199662
C	7.575152	-0.023377	-0.094995
H	7.635401	-1.106307	0.073094
H	7.095540	0.446361	0.769651
O	9.047082	1.911862	-0.229986
P	9.236496	2.516489	1.293090
O	9.546619	3.971979	1.106257
O	10.102346	1.592316	2.096014
O	7.722277	2.353685	1.924069
C	6.709565	3.232233	1.463611
H	6.596475	3.151974	0.367789
H	6.989466	4.272413	1.696423
C	5.395571	2.928044	2.132430
H	4.716503	3.781151	1.947079
O	4.794396	1.752073	1.582241
C	3.919907	1.297865	2.599717
H	3.065880	1.992605	2.681425
C	5.455433	2.714684	3.669779
H	6.489259	2.713077	4.038494
C	4.778447	1.365147	3.852816
H	5.514575	0.551768	3.826095
H	4.205751	1.316993	4.785873
O	4.699143	3.699481	4.365229
H	5.191928	4.533531	4.351230
N	-5.655989	-1.145982	1.567175
C	-6.051725	-2.444890	1.544272
H	-7.114008	-2.626658	1.471298
C	-5.133750	-3.437970	1.623410
H	-5.417509	-4.483742	1.622337
C	-3.760190	-3.046079	1.729644
N	-2.801966	-3.973549	1.810593
H	-3.026501	-4.954062	1.811629
H	-1.805484	-3.695993	1.891987
N	-3.385857	-1.761450	1.751213
C	-4.311257	-0.776420	1.671398
O	-4.022132	0.428555	1.689028
N	3.323703	0.022757	2.275164
C	3.962148	-1.216325	2.329396

O	5.165926	-1.417685	2.431214
N	2.949598	-2.141291	2.255745
H	3.118434	-3.127229	2.264909
C	1.716491	-1.494629	2.153118
C	0.396909	-1.974747	2.051184
O	0.003227	-3.156075	2.026952
N	-0.523289	-0.920809	1.974125
H	-1.515712	-1.192122	1.887884
C	-0.198400	0.408448	1.991208
N	-1.216854	1.278040	1.908670
H	-2.194408	0.984355	1.813683
H	-0.995581	2.270863	1.893679
N	1.051319	0.848208	2.090702
C	1.959710	-0.133596	2.164958
N	-3.105272	1.528736	-1.868588
N	5.719076	-0.652556	-1.588012
C	-3.943077	0.467423	-1.726182
H	-5.011373	0.668490	-1.762291
C	-3.440889	-0.779459	-1.558322
H	-4.091687	-1.653774	-1.440758
C	-2.014538	-0.908487	-1.543194
N	-1.449633	-2.107791	-1.380905
H	-2.021472	-2.945154	-1.268170
H	-0.427967	-2.218812	-1.375206
N	-1.200902	0.146699	-1.685225
C	-1.714568	1.387484	-1.854249
O	-1.008144	2.401150	-1.985558
C	5.749196	-2.017323	-1.406520
H	6.689423	-2.552862	-1.353262
N	4.559462	-2.550798	-1.330740
C	3.695708	-1.481300	-1.476462
C	2.271970	-1.435757	-1.480960
O	1.469521	-2.369383	-1.351046
N	1.799067	-0.130233	-1.654731
H	0.763381	-0.032768	-1.687041
C	2.581547	0.986338	-1.809805
N	1.929422	2.151272	-1.963633
H	0.897147	2.210081	-2.000217
H	2.473569	2.980592	-2.112613
N	3.905856	0.954630	-1.803089
C	4.398130	-0.288714	-1.639033

(8OG-C)-(G-C) nucleotide pairs with PCM

O	8.006007	-4.835752	-2.525878
H	7.054477	-4.982021	-2.651551
P	8.321769	-4.362491	-0.978894
O	9.766580	-4.679323	-0.733813
O	7.208758	-4.823361	-0.083532
O	8.134201	-2.728854	-1.080617
C	9.032053	-1.975078	-1.878782
H	9.044144	-2.368472	-2.907453
H	10.051925	-2.034094	-1.466480
C	8.575431	-0.536212	-1.881088

H	9.303917	0.066218	-2.440858
O	7.310971	-0.425556	-2.549772
C	6.322693	0.090097	-1.689512
H	6.076653	1.123604	-1.966222
C	8.383318	0.045787	-0.476512
H	8.937670	-0.541146	0.267264
C	6.878572	-0.012997	-0.274018
H	6.589909	-0.978225	0.165782
H	6.520258	0.794932	0.377281
O	8.862872	1.388117	-0.470041
P	9.288560	2.077881	0.968030
O	10.031059	3.328767	0.602727
O	9.849918	1.031462	1.883914
O	7.823620	2.475738	1.611155
C	7.115695	3.555708	1.027718
H	6.958651	3.370364	-0.050232
H	7.685225	4.491281	1.131403
C	5.778336	3.717581	1.698921
H	5.305434	4.631329	1.299207
O	4.959548	2.590957	1.386245
C	4.167053	2.288206	2.520477
H	3.263390	2.908936	2.550306
C	5.803869	3.835734	3.234111
H	6.830926	3.886600	3.621898
C	5.084531	2.572599	3.698187
H	5.813496	1.760428	3.825972
H	4.547454	2.708445	4.643440
O	5.088406	5.017607	3.568373
H	5.178522	5.176216	4.520858
O	-7.996766	-4.207548	2.158414
H	-7.221967	-4.084772	1.566060
P	-9.383252	-4.089831	1.306888
O	-10.500967	-4.173393	2.310002
O	-9.343883	-4.984074	0.097084
O	-9.284076	-2.566042	0.692115
C	-9.255864	-1.431779	1.543928
H	-9.204136	-1.736218	2.600344
H	-10.183654	-0.856273	1.399905
C	-8.081026	-0.549188	1.197289
H	-8.217438	0.439834	1.663278
O	-6.866466	-1.133238	1.698951
C	-5.896395	-1.034407	0.673681
H	-5.443624	-0.029867	0.680715
C	-7.877519	-0.367095	-0.323951
H	-8.773433	-0.658422	-0.892926
C	-6.682619	-1.252001	-0.606061
H	-7.002913	-2.297483	-0.674933
H	-6.131441	-0.961808	-1.508191
O	-7.506968	0.970343	-0.640289
P	-8.702777	2.036008	-1.031654
O	-9.651511	2.166252	0.127668
O	-9.214772	1.734626	-2.410836
O	-7.740308	3.349696	-1.159428
C	-7.261424	3.979916	0.018585
H	-7.138162	3.247310	0.831930
H	-7.985714	4.741112	0.347533

C	-5.929009	4.638409	-0.255904
H	-5.722129	5.341061	0.568009
O	-4.890956	3.648314	-0.279301
C	-4.154027	3.729822	-1.487166
H	-3.231677	4.314922	-1.337530
C	-5.845826	5.382318	-1.599744
H	-6.840477	5.609802	-1.998409
C	-5.085154	4.401819	-2.483113
H	-5.770331	3.666420	-2.921208
H	-4.544953	4.910842	-3.288296
O	-5.193915	6.639492	-1.487957
H	-4.340420	6.531054	-1.039708
N	5.079924	-0.680733	-1.878191
N	-3.699692	2.402190	-1.835426
C	5.144540	-2.026574	-2.039501
H	6.156564	-2.463083	-2.052173
C	4.006584	-2.751408	-2.170956
H	4.053665	-3.821371	-2.309895
C	2.766149	-2.034538	-2.131067
N	1.606023	-2.697813	-2.253664
H	1.623218	-3.690829	-2.395471
H	0.728367	-2.196394	-2.246753
N	2.708332	-0.709003	-1.971208
C	3.855878	0.010932	-1.840753
O	3.853206	1.238461	-1.692714
C	-4.465812	1.273961	-2.004566
H	-5.524611	1.349374	-2.068034
N	-3.762718	0.178096	-2.106615
C	-2.448370	0.606280	-2.008330
C	-1.230050	-0.137774	-2.051793
O	-1.073715	-1.359715	-2.187820
N	-0.115852	0.693304	-1.906749
H	0.830945	0.235874	-1.939102
C	-0.153338	2.057312	-1.744607
N	1.038356	2.666017	-1.624751
H	1.953617	2.168371	-1.651882
H	1.078458	3.677981	-1.501358
N	-1.281629	2.752196	-1.701880
C	-2.383469	1.988409	-1.838277
N	3.705498	0.911791	2.373364
C	4.647249	-0.064386	2.286374
H	5.681451	0.231428	2.463578
C	4.283047	-1.337783	2.001481
H	5.021340	-2.140230	1.925555
C	2.886061	-1.585436	1.804328
N	2.454369	-2.818113	1.521859
H	3.115430	-3.588261	1.430656
H	1.461364	-3.005657	1.361612
N	1.969281	-0.612735	1.895075
C	2.345431	0.656470	2.179222
O	1.539431	1.596257	2.275226
N	-4.796474	-1.937167	0.918907
C	-4.798534	-3.307504	0.650301
O	-5.781357	-4.005121	0.423347
N	-3.482827	-3.686434	0.724171
H	-3.162104	-4.631136	0.531079

C	-2.678989	-2.582701	1.017009
C	-1.289906	-2.436349	1.194334
O	-0.409027	-3.308878	1.127979
N	-0.953310	-1.107691	1.488450
H	0.066808	-0.921281	1.614779
C	-1.842678	-0.074746	1.588468
N	-1.334929	1.133770	1.877005
H	-0.320403	1.292755	2.003983
H	-1.967646	1.910286	1.940847
N	-3.153574	-0.226132	1.422342
C	-3.512330	-1.486051	1.138186

Optimized coordinates for cationic and anionic species (AIE and AEA calculations)

G-C base pair with PCM, cation

H	4.760165	1.889654	0.003432
N	4.263767	1.005211	0.002262
C	4.946517	-0.173845	0.001340
H	6.027824	-0.104017	0.002047
C	4.270409	-1.352555	-0.000400
H	4.791598	-2.301557	-0.001169
C	2.836686	-1.282736	-0.001099
N	2.102603	-2.403558	-0.002335
H	2.545696	-3.311788	-0.003183
H	1.083671	-2.359754	-0.002517
N	2.182395	-0.104723	-0.000466
C	2.874125	1.062168	0.001088
O	2.321984	2.185917	0.001522
H	-5.350075	1.287627	0.000108
N	-4.685826	0.519813	0.000441
C	-4.986366	-0.805287	0.001710
H	-6.007483	-1.161291	0.002457
N	-3.901907	-1.596820	0.001915
C	-2.866042	-0.743098	0.000828
C	-1.429955	-0.991216	0.000088
O	-0.881921	-2.090721	0.000066
N	-0.694590	0.195071	-0.000718
H	0.351897	0.087861	-0.001027
C	-1.232919	1.454790	-0.001523
N	-0.417543	2.490218	-0.002396
H	0.622879	2.386717	-0.001607
H	-0.830254	3.416955	-0.003197
N	-2.578659	1.705992	-0.001441
C	-3.313807	0.620044	-0.000179

G-C base pair with PCM, anion

H	4.728574	1.833804	0.518951
N	4.245772	0.951892	0.409094
C	4.985547	-0.227622	0.141316
H	6.019221	-0.232244	0.464150
C	4.220262	-1.380853	-0.117377
H	4.713621	-2.340713	-0.246137
C	2.845648	-1.270009	-0.244707
N	2.020011	-2.339729	-0.641228
H	2.432780	-3.251024	-0.466792
H	1.076962	-2.288778	-0.248441
N	2.166033	-0.057125	-0.106461
C	2.876914	1.041643	0.206880
O	2.339547	2.186589	0.345399
H	-5.301025	1.302132	-0.137085
N	-4.657912	0.528152	-0.023770
C	-4.992422	-0.792560	0.197658
H	-6.024177	-1.108984	0.269709
N	-3.940918	-1.571943	0.302985
C	-2.857600	-0.718183	0.142601
C	-1.450994	-0.975867	0.152634
O	-0.872613	-2.069058	0.313475
N	-0.702624	0.192783	-0.052912
H	0.346665	0.081114	-0.075812
C	-1.231922	1.449455	-0.242146
N	-0.346423	2.450958	-0.459734
H	0.645076	2.342886	-0.175177
H	-0.733717	3.385666	-0.441128
N	-2.538869	1.702442	-0.253448
C	-3.287924	0.596310	-0.062678

8OG-C base pair with PCM, cation

H	-5.184944	1.727853	-0.000574
N	-4.647678	0.867828	-0.000356
C	-5.274149	-0.341756	0.000065
H	-6.357568	-0.323129	0.000225
C	-4.543458	-1.487434	0.000284
H	-5.019662	-2.459683	0.000664
C	-3.114555	-1.350477	-0.000038
N	-2.329744	-2.436704	-0.000197
H	-2.730759	-3.364343	0.000391
H	-1.313934	-2.347505	-0.000084
N	-2.516006	-0.143250	-0.000263
C	-3.261888	0.990795	-0.000376
O	-2.763293	2.138373	-0.000503
H	4.929977	1.613017	-0.000276
N	4.319445	0.803049	0.000020
C	4.796974	-0.510494	-0.000330
O	5.945876	-0.894848	-0.000770
N	3.634149	-1.316302	-0.000049
H	3.666097	-2.331497	-0.000344

C	2.532314	-0.542570	0.000280
C	1.121740	-0.856880	0.000348
O	0.640396	-1.990996	0.000262
N	0.339494	0.293356	0.000568
H	-0.702542	0.141610	0.000367
C	0.834491	1.574253	0.000412
N	-0.026138	2.574428	0.000082
H	-1.057550	2.425462	-0.000036
H	0.344614	3.518045	0.000326
N	2.164540	1.869380	0.000446
C	2.954531	0.824138	0.000299

8OG-C base pair with PCM, anion

H	-5.134419	1.684137	0.551917
N	-4.616118	0.824315	0.429468
C	-5.306872	-0.383313	0.157603
H	-6.339709	-0.431665	0.479075
C	-4.496338	-1.501492	-0.114717
H	-4.950354	-2.479583	-0.250451
C	-3.127793	-1.333719	-0.245299
N	-2.260672	-2.364512	-0.655606
H	-2.636389	-3.293521	-0.491312
H	-1.318692	-2.281232	-0.265577
N	-2.498333	-0.094939	-0.096341
C	-3.252787	0.971526	0.227586
O	-2.761950	2.135901	0.375853
H	4.886377	1.602552	-0.195420
N	4.292194	0.792349	-0.076278
C	4.792396	-0.497009	0.131491
O	5.981083	-0.825274	0.201300
N	3.678499	-1.297154	0.237821
H	3.725785	-2.294474	0.393446
C	2.515451	-0.528730	0.100010
C	1.140446	-0.855557	0.124369
O	0.625744	-1.984917	0.285748
N	0.336218	0.280845	-0.065360
H	-0.710715	0.122243	-0.079493
C	0.813486	1.552959	-0.250246
N	-0.102639	2.528175	-0.451087
H	-1.088491	2.383040	-0.162063
H	0.254756	3.474613	-0.430056
N	2.115901	1.852477	-0.272780
C	2.911593	0.784890	-0.097822

2 G-C base pairs with PCM, cation

H	-6.863083	0.196726	1.186480
N	-6.279336	-0.248522	0.487090
C	-6.791828	-0.589640	-0.728205
H	-7.837726	-0.358020	-0.891603
C	-6.001380	-1.188025	-1.657708
H	-6.387723	-1.468977	-2.629319

C	-4.633939	-1.430901	-1.292342
N	-3.792517	-2.014722	-2.156954
H	-4.108552	-2.297005	-3.074452
H	-2.821874	-2.198948	-1.895713
N	-4.148811	-1.086365	-0.084257
C	-4.951975	-0.490506	0.832701
O	-4.557756	-0.150116	1.970041
H	-1.594934	4.660164	1.376716
N	-1.380220	4.069297	0.581309
C	-2.249699	3.968911	-0.462714
H	-3.163096	4.547314	-0.386315
C	-1.950263	3.176362	-1.525343
H	-2.625141	3.081682	-2.366683
C	-0.698935	2.471896	-1.481553
N	-0.333009	1.671548	-2.492580
H	-0.929601	1.557412	-3.300343
H	0.560802	1.172469	-2.465615
N	0.144833	2.584512	-0.438796
C	-0.168260	3.380341	0.614809
O	0.575970	3.524917	1.608704
H	7.023286	-0.694791	0.422170
N	6.240667	-0.671351	-0.221430
C	6.162317	-1.305767	-1.439218
H	6.971337	-1.920208	-1.809890
N	5.023346	-1.080448	-2.066627
C	4.319691	-0.261471	-1.216997
C	3.039480	0.373798	-1.366662
O	2.251327	0.276589	-2.320289
N	2.724772	1.179848	-0.265051
H	1.811163	1.677892	-0.315162
C	3.529695	1.378242	0.833138
N	3.069216	2.183860	1.795529
H	2.161762	2.672100	1.728961
H	3.665206	2.349027	2.596258
N	4.734442	0.804313	0.976876
C	5.069557	0.021888	-0.052001
H	2.917813	-2.093173	2.711142
N	2.371123	-2.255443	1.872417
C	2.811215	-2.833795	0.714935
H	3.822859	-3.199024	0.607632
N	1.862862	-2.919346	-0.218809
C	0.766956	-2.370340	0.359050
C	-0.573513	-2.177500	-0.149276
O	-1.001244	-2.499997	-1.261780
N	-1.402395	-1.555889	0.789964
H	-2.388076	-1.384930	0.484921
C	-1.020604	-1.168077	2.050280
N	-1.928176	-0.584058	2.823258
H	-2.904924	-0.418860	2.513073
H	-1.644917	-0.303632	3.754502
N	0.228270	-1.350416	2.542761
C	1.048747	-1.934765	1.684925

2 G-C base pairs with PCM, anion

H	-6.306783	1.992171	1.155252
N	-5.958407	1.435143	0.386174
C	-6.680930	1.389072	-0.832599
H	-7.318970	2.237185	-1.047809
C	-6.191627	0.487469	-1.796648
H	-6.636878	0.459707	-2.787748
C	-5.170445	-0.384416	-1.455727
N	-4.717116	-1.408804	-2.308897
H	-4.915143	-1.230558	-3.288857
H	-3.728724	-1.636608	-2.176430
N	-4.580977	-0.404879	-0.189284
C	-4.991379	0.498075	0.720050
O	-4.513982	0.548340	1.898182
H	1.588890	-4.142718	2.202060
N	1.119884	-3.899081	1.338281
C	1.528802	-4.224872	0.060822
H	2.430061	-4.796452	-0.114931
N	0.715613	-3.769776	-0.864175
C	-0.280408	-3.109034	-0.157446
C	-1.443176	-2.408982	-0.608013
O	-1.828641	-2.238279	-1.781780
N	-2.186759	-1.885533	0.460467
H	-3.065712	-1.360937	0.207717
C	-1.859448	-2.014438	1.791638
N	-2.723916	-1.471965	2.681771
H	-3.394046	-0.739467	2.380688
H	-2.395012	-1.432765	3.637983
N	-0.779647	-2.662235	2.223443
C	-0.043064	-3.180651	1.218719
H	-1.415857	3.840752	1.927743
N	-1.083270	3.425759	1.064709
C	-1.888453	3.370322	-0.032979
H	-2.881791	3.789992	0.075651
C	-1.433372	2.810173	-1.184482
H	-2.055086	2.755023	-2.069260
C	-0.092220	2.293555	-1.172735
N	0.429965	1.728082	-2.270339
H	-0.116152	1.651996	-3.117207
H	1.391072	1.366862	-2.265404
N	0.684832	2.355528	-0.075946
C	0.217409	2.918062	1.067045
O	0.892893	3.003403	2.114501
H	7.813047	-0.404171	0.678871
N	7.088031	-0.292061	-0.019303
C	7.157221	-0.672117	-1.344848
H	8.042126	-1.142665	-1.751425
N	6.059384	-0.398375	-2.010104
C	5.223956	0.193111	-1.072484
C	3.898147	0.706809	-1.191059
O	3.168674	0.738897	-2.203608
N	3.428368	1.224117	0.025640
H	2.470281	1.621484	0.005139
C	4.131428	1.244991	1.211051

N	3.498431	1.764785	2.282636
H	2.578332	2.216298	2.215386
H	4.025524	1.850664	3.140474
N	5.367754	0.770830	1.330973
C	5.851570	0.266963	0.176601

(G-C)-(8OG-C) base pairs with PCM, cation

H	-5.172175	-2.217084	1.273296
N	-4.462577	-2.537703	0.623699
C	-4.806607	-3.259939	-0.479066
H	-5.863048	-3.461255	-0.612443
C	-3.846282	-3.686669	-1.340573
H	-4.095755	-4.260770	-2.223910
C	-2.488384	-3.341175	-1.027991
N	-1.488420	-3.727955	-1.831824
H	-1.674547	-4.270661	-2.663846
H	-0.521850	-3.480502	-1.619637
N	-2.171159	-2.625577	0.068512
C	-3.143114	-2.208466	0.919055
O	-2.909293	-1.544614	1.953452
H	-4.598843	3.816365	1.785485
N	-4.274409	3.261689	1.001332
C	-5.163814	2.684250	0.146020
H	-6.213464	2.852252	0.357832
C	-4.718735	1.946661	-0.905161
H	-5.407546	1.479377	-1.597787
C	-3.294849	1.817679	-1.054401
N	-2.776354	1.109505	-2.067926
H	-3.379259	0.680465	-2.756103
H	-1.759263	1.042371	-2.190152
N	-2.434019	2.391742	-0.194144
C	-2.892943	3.126693	0.850321
O	-2.141849	3.685666	1.677127
H	5.232228	2.408708	-0.661938
N	4.419327	2.036695	-1.138177
C	4.417959	1.287341	-2.297463
H	5.338399	1.027465	-2.802440
N	3.209103	0.951219	-2.685114
C	2.371980	1.507805	-1.730270
C	0.948829	1.503982	-1.616201
O	0.115780	0.971492	-2.377157
N	0.514367	2.210155	-0.484613
H	-0.513915	2.265475	-0.357106
C	1.332707	2.845641	0.424358
N	0.727947	3.453794	1.464262
H	-0.293363	3.544684	1.530865
H	1.309074	3.995569	2.088938
N	2.659307	2.863558	0.321218
C	3.111841	2.192623	-0.756580
H	4.697948	-0.450348	2.632556
N	4.276614	-0.931558	1.845396
C	5.023196	-1.469730	0.793605
O	6.225800	-1.458756	0.641557

N	4.064111	-2.042491	-0.072517
H	4.312409	-2.518321	-0.934630
C	2.823508	-1.865017	0.424545
C	1.520003	-2.275008	-0.042072
O	1.292539	-2.909955	-1.073757
N	0.512326	-1.867646	0.827031
H	-0.467503	-2.137990	0.555379
C	0.719142	-1.171883	1.992069
N	-0.333968	-0.847983	2.719533
H	-1.305373	-1.101077	2.442150
H	-0.175022	-0.337314	3.580632
N	1.950098	-0.799458	2.438965
C	2.942396	-1.153783	1.658744

(G-C)-(8OG-C) base pairs with PCM, anion

H	-7.951250	-0.108704	0.346339
N	-7.198267	0.084483	-0.300650
C	-7.383493	1.034784	-1.335678
H	-8.404756	1.221756	-1.642981
C	-6.245083	1.319705	-2.112616
H	-6.328750	1.973948	-2.976429
C	-5.019472	0.790420	-1.743439
N	-3.809794	1.134266	-2.376580
H	-3.937744	1.486399	-3.320475
H	-3.118082	0.380607	-2.363800
N	-4.857012	-0.042277	-0.632957
C	-5.947814	-0.375166	0.082025
O	-5.889455	-1.123182	1.109524
H	-1.171941	2.124445	3.554087
N	-0.830155	2.358064	2.628730
C	-1.581586	3.118504	1.784323
H	-2.543083	3.448546	2.160344
C	-1.116419	3.423207	0.544362
H	-1.698907	4.022229	-0.144225
C	0.176378	2.905470	0.187811
N	0.701990	3.153765	-1.020350
H	0.191109	3.698626	-1.701004
H	1.613920	2.761516	-1.282677
N	0.904155	2.160310	1.039667
C	0.427054	1.864303	2.275027
O	1.056349	1.175833	3.105969
H	7.746826	-1.050447	-0.313962
N	7.044609	-0.482477	-0.772215
C	7.078174	-0.027457	-2.075189
H	7.904800	-0.260269	-2.732672
N	6.024810	0.689333	-2.390666
C	5.257930	0.706350	-1.233870
C	3.998761	1.315942	-0.954235
O	3.283216	1.997330	-1.717321
N	3.582436	1.072539	0.363438
H	2.658822	1.467350	0.622963
C	4.280068	0.340935	1.300260
N	3.730305	0.247077	2.530067

H	2.771539	0.560938	2.724181
H	4.175072	-0.379865	3.186433
N	5.451556	-0.233956	1.048216
C	5.880914	-0.021325	-0.213213
H	1.236844	-3.951020	1.627987
N	0.904703	-3.464910	0.805150
C	1.646810	-3.370103	-0.376482
O	2.767979	-3.844835	-0.583886
N	0.855609	-2.643004	-1.235404
H	1.134761	-2.403797	-2.176678
C	-0.345375	-2.291108	-0.606382
C	-1.474871	-1.557784	-1.035867
O	-1.660461	-1.024700	-2.152851
N	-2.447535	-1.468584	-0.025577
H	-3.326487	-0.928822	-0.262105
C	-2.327497	-2.020059	1.224215
N	-3.346085	-1.806780	2.089166
H	-4.281550	-1.533752	1.732511
H	-3.314782	-2.351340	2.941506
N	-1.255676	-2.712708	1.621220
C	-0.305637	-2.812936	0.677346

(8OG-C)-(G-C) base pairs with PCM, cation

H	-4.412871	-2.748267	1.687434
N	-3.793736	-2.846494	0.890437
C	-4.259673	-3.329955	-0.294811
H	-5.310262	-3.593574	-0.327490
C	-3.419354	-3.459522	-1.354899
H	-3.766845	-3.841979	-2.306286
C	-2.052525	-3.068130	-1.156504
N	-1.167186	-3.167052	-2.157533
H	-1.448777	-3.513982	-3.063989
H	-0.194735	-2.889325	-2.024431
N	-1.613319	-2.593650	0.025439
C	-2.466026	-2.472496	1.074392
O	-2.115405	-2.042012	2.195561
H	5.443787	-0.509195	2.113353
N	4.934435	-0.828238	1.296274
C	5.542515	-1.050870	0.057564
O	6.707645	-0.908906	-0.246073
N	4.494670	-1.486815	-0.784688
H	4.636032	-1.731634	-1.760060
C	3.334039	-1.529623	-0.099891
C	1.996053	-1.919200	-0.477105
O	1.650266	-2.315923	-1.591871
N	1.107492	-1.799875	0.587282
H	0.112541	-2.079062	0.389236
C	1.450741	-1.376135	1.847163
N	0.500988	-1.312108	2.762363
H	-0.485814	-1.578471	2.562559
H	0.759807	-1.003595	3.692565
N	2.715357	-1.020668	2.204484
C	3.598905	-1.108847	1.239591

H	-5.568288	2.354759	1.867378
N	-5.099721	2.094349	1.006855
C	-5.817131	1.680794	-0.074995
H	-6.893768	1.647347	0.045121
C	-5.180082	1.339141	-1.225917
H	-5.730598	1.010242	-2.098456
C	-3.746206	1.439742	-1.231895
N	-3.044566	1.123889	-2.329830
H	-3.516821	0.832146	-3.174312
H	-2.023391	1.228708	-2.344504
N	-3.056993	1.846800	-0.150242
C	-3.706690	2.187711	0.991455
O	-3.120253	2.579726	2.022341
H	4.501375	3.110757	0.291481
N	3.800201	2.778951	-0.359918
C	4.006271	2.423712	-1.677511
H	4.988265	2.472071	-2.128121
N	2.904077	2.039008	-2.279623
C	1.922409	2.147557	-1.306982
C	0.518300	1.893102	-1.360416
O	-0.155687	1.489054	-2.329228
N	-0.107157	2.158627	-0.133309
H	-1.136292	2.025653	-0.115338
C	0.524434	2.610269	1.005186
N	-0.243992	2.780304	2.100095
H	-1.269489	2.719872	2.063929
H	0.188634	3.210350	2.906167
N	1.831319	2.853919	1.064172
C	2.464336	2.611928	-0.100739

(8OG-C)-(G-C) base pairs with PCM, anion

H	-7.372846	0.167424	1.080655
N	-6.750677	0.026117	0.295819
C	-7.100170	0.532937	-0.980891
H	-8.155487	0.688086	-1.166858
C	-6.119608	0.395117	-1.981054
H	-6.346155	0.680828	-3.004894
C	-4.860405	-0.070459	-1.639607
N	-3.783553	-0.112399	-2.545422
H	-4.077302	-0.136891	-3.517155
H	-3.118082	-0.864386	-2.350131
N	-4.514112	-0.431398	-0.334756
C	-5.460889	-0.365865	0.619684
O	-5.229815	-0.668515	1.833547
H	1.825445	-3.688379	2.257460
N	1.354396	-3.530930	1.375937
C	1.865976	-3.965949	0.149141
O	2.920922	-4.581668	-0.034065
N	0.941914	-3.559365	-0.785233
H	1.043771	-3.731438	-1.775757
C	-0.116842	-2.889173	-0.159217
C	-1.295767	-2.284583	-0.652034

O	-1.677426	-2.210853	-1.841698
N	-2.063278	-1.728303	0.385113
H	-2.960060	-1.243827	0.100966
C	-1.723236	-1.763073	1.713038
N	-2.562877	-1.148137	2.577541
H	-3.543512	-0.953175	2.300018
H	-2.382039	-1.319921	3.558195
N	-0.606725	-2.338272	2.170035
C	0.151320	-2.876329	1.200870
H	-1.502149	4.044106	2.328693
N	-1.188122	3.730477	1.417267
C	-1.983518	3.879626	0.321216
H	-2.949287	4.343095	0.486227
C	-1.553424	3.455661	-0.896083
H	-2.169083	3.561386	-1.780381
C	-0.248643	2.855574	-0.953933
N	0.243678	2.408418	-2.117833
H	-0.303289	2.476087	-2.964943
H	1.171181	1.969736	-2.159611
N	0.522091	2.720981	0.140819
C	0.079135	3.147950	1.350395
O	0.748695	3.046637	2.400102
H	7.494652	-0.479886	0.493115
N	6.762721	-0.271412	-0.175122
C	6.767547	-0.578338	-1.521224
H	7.602263	-1.090847	-1.979865
N	5.677588	-0.183383	-2.136682
C	4.915736	0.415025	-1.142639
C	3.628646	1.028335	-1.191190
O	2.876371	1.168910	-2.177538
N	3.231268	1.507663	0.066084
H	2.293296	1.949319	0.103148
C	3.968327	1.414877	1.227220
N	3.425535	1.959925	2.335505
H	2.466978	2.328598	2.355969
H	3.916931	1.826965	3.208472
N	5.166527	0.841447	1.283394
C	5.579179	0.368172	0.089082

Explicit presentation of shortened references from the manuscript

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