Electronic Supplementary Information (ESI)

B-DNA Model Systems in Non-Terran Bio-Solvents: Implications for Structure, Stability and Replication

Trevor A. Hamlin,[a] Jordi Poater,*[bc] Célia Fonseca Guerra[ad] and F. Matthias Bickelhaupt*[ae]

[a] *Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, VU University Amsterdam, De Boelelaan 1083, NL-1081 HV Amsterdam, The Netherlands. E-mails: f.m.bickelhaupt@vu.nl & j.poater@vu.nl*
[b] *Departament de Química Inorgànica i Orgánica & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Martí i Franqués 1-11, 08028 Barcelona, Catalonia, Spain.*
[c] *ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Spain.*
[d] *Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, P.O. Box 9502, 2300 RA Leiden, Netherlands*
[e] *Institute of Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands.*

Structures of DNA Base Pairs

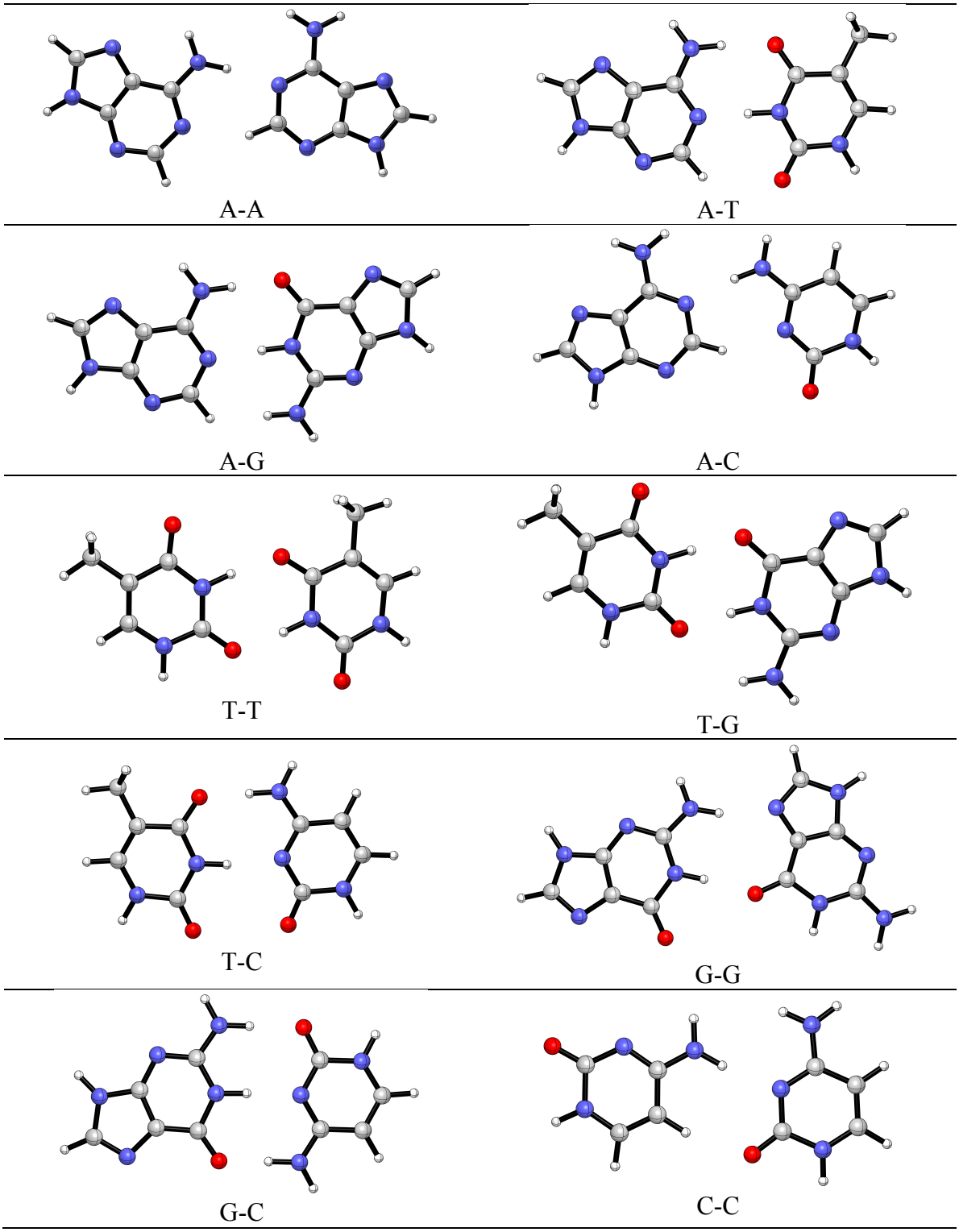

Figure S1: Structures of Watson-Crick pairs and mismatched DNA base pairs in the gas phase, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (atom color code: C-silver, H-white, N-blue, O-red).

Justification of Method

For the addition of a nucleotide base to a template primer complex study (Section 3.3 in the manuscript), the best method for optimizing the primer had to be determined. When embarking on a theoretical investigation on large biological systems with many heavy atoms, one must consider the balance between computational cost and accuracy of the calculation. The three general schemes tested here differed by their treatment of the key atoms involved in the intermolecular hydrogen bonding of the Y_1/Z-Y_2 template primer. In all of the methods, the dissociated X is completely optimized in the respective medium. It should be noted that the computational cost increases going from A to B to C. Method A uses a single point calculation, thereby allowing no relaxation of any of the atoms in the template primer. Method B uses a constrained geometry relaxation of only the Y_1 front atoms (i.e., hydrogen-bond donor groups ≥C–NH_2 and >NH, and hydrogen-bond acceptor groups =N– and >C=O) of the template and has been used previously in the literature. Method C relaxes the front atoms of Y_1, Z, and Y_2 because one might expect the hydrogen bond distances to be slightly affected upon stacking.

Table S1: Summary of affinity values (in kcal mol^{-1}) of model template-primer complexes Y_1/Z-Y_2 for model nucleotides X using three distinct methods. [a]

Medium		Gas Phase	Gas Phase	Gas Phase
Template-primer Complex Y_1/Z-Y_2	Incoming nucleotide X	**A**	**B**	**C**
[X]-A/T-A	A	–14.3	–12.7	–12.7
	T	–24.6	–22.9	–22.9
	G	–26.9	–25.3	–25.4
	C	–16.7	–15.0	–15.1
[X]-T/A-T	A	–27.5	–26.1	–25.9
	T	–25.0	–23.6	–23.4
	G	–29.5	–28.1	–28.1
	C	–23.8	–22.4	–22.3
[X]-G/C-G	A	–29.0	–22.3	–21.8
	T	–28.9	–22.2	–22.0
	G	–21.9	–15.2	–14.9
	C	–38.4	–31.8	–31.3
[X]-C/G-C	A	–17.3	–15.3	–15.2
	T	–25.1	–23.1	–23.3
	G	–40.3	–38.3	–38.0
	C	–15.9	–13.9	–13.9

[a] Computed at BLYP-D3(BJ)/TZ2P, in the gas phase (ΔE_{aff})

Previously, our group utilized Method B, but we felt a more comprehensive analysis of the various methods would be insightful.[1] The results of the comparison study are shown above in Table 1. When comparing the ΔE_{aff} values in Table 1, the most favorable affinity values were obtained through Method A. These are artificially more stable than Method B because the energetic stabilization associated with the relaxation of the front atoms of Y involved in hydrogen-bonding for [X]-A/T-A, [X]-T/A-T, [X]-G/C-G, [X]-C/G-C is 1.6, 1.4, 6.7, 2.0 kcal mol^{-1}, respectively. The differences between Method B and C are much smaller and are evidence that relaxation of the hydrogen-bonding atoms of Z, and Y_2 is not significantly important compared to optimizing those key atoms on Y only. Additionally, there is a significant increase in computational cost associated with optimizing the 9 and 15 front atoms involved in H-bonding of A-T and G-C, respectively associated with method C. The differences between Method B and C are within the intrinsic error of DFT calculations and as such we opted to continue with Method B as we have in previous studies.[1]

[1] J. Poater, M. Swart, C. Fonseca Guerra, F. M. Bickelhaupt, *Chem. Commun.*, 2011, **47**, 7326–7328.

Effect of Explicit Solvation

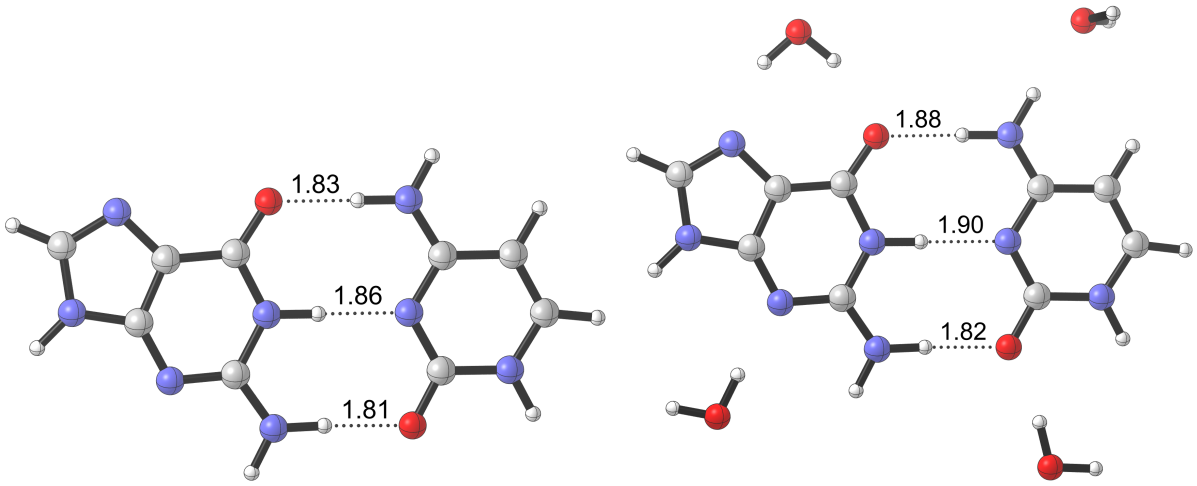

Figure S2: Structures of optimized base pairs, G-C (left) and G-C with four explicit water molecules (right), in water, optimized in C_s symmetry at COSMO-BLYP-D3(BJ)/TZ2P (atom color code: C-silver, H-white, N-blue, O-red).

Comparing the above structures, we find that the inclusion of four explicit water molecules as a first layer of solvation has a minimal effect on hydrogen bond lengths. Furthermore, the affinity of G-C in implicit water (COSMO)[2] is –12.3 kcal mol^{-1} and the affinity of G-C with four explicit waters (geometry is taken from X-ray crystal structures) in implicit aqueous solvation is –12.9 kcal mol^{-1}. These results are in agreement with previous findings.[3] Given the increase in computational cost associated with explicit solvent molecules and minimal differences in geometries and energies, we opted for simulating solvation using COSMO.

[2] (a) A. Klamt and G. Schüürmann, *J. Chem. Soc. Perkin Trans. 2*, 1993, **2**, 799–805; (b) A. Klamt, *J. Phys. Chem.*, 1995, **99**, 2224–2235; (c) A. Klamt and V. Jones, *J. Chem. Phys.*, 1996, **105**, 9972–9981.

[3] C. Fonseca Guerra, F. M. Bickelhaupt, J. G. Snijders and E. J. Baerends, *J. Am. Chem. Soc.*, 2000, **122**, 4117–4128.

Cartesian Coordinates of Systems in the Gas Phase

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in the gas phase, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2308.64 kcal mol^{-1}

N	-2.061188	0.754705	0.000000
C	-2.324885	-0.609092	0.000000
H	-3.337776	-0.988914	0.000000
N	-1.230920	-1.346496	0.000000
C	-0.190339	-0.418485	0.000000
C	1.216050	-0.557302	0.000000
N	1.824484	-1.772787	0.000000
N	1.979361	0.557646	0.000000
C	1.364693	1.758188	0.000000
H	2.026090	2.621719	0.000000
N	0.046599	2.026531	0.000000
C	-0.682660	0.898761	0.000000
H	-2.733902	1.511436	0.000000
H	2.833727	-1.818952	0.000000
H	1.270665	-2.616956	0.000000

T
Total Energy = -2169.10 kcal mol^{-1}

N	-1.582781	-0.876605	0.000000
C	-0.228916	-1.163875	0.000000
H	0.015968	-2.221937	0.000000
C	0.724410	-0.199356	0.000000
C	2.202047	-0.485775	0.000000
H	2.394844	-1.563646	0.000000
H	2.681850	-0.039480	-0.879157
H	2.681850	-0.039480	0.879157
C	0.295261	1.206734	0.000000
O	1.046124	2.179209	0.000000
N	-1.110576	1.391082	0.000000
H	-1.435299	2.355188	0.000000
C	-2.105351	0.419182	0.000000
O	-3.306456	0.656807	0.000000
H	-2.272974	-1.618048	0.000000

G
Total Energy = -2463.80 kcal mol^{-1}

N	1.886532	-1.288776	0.000000
C	2.895156	-0.325538	0.000000
H	3.940836	-0.600962	0.000000
N	2.419697	0.899889	0.000000
C	1.037093	0.747819	0.000000
C	-0.009560	1.736229	0.000000
O	0.023635	2.959975	0.000000
N	-1.302488	1.067763	0.000000
H	-2.084803	1.716978	0.000000

C	-1.522676	-0.290114	0.000000
N	-2.821419	-0.723403	0.000000
H	-3.605696	-0.090941	0.000000
H	-2.985300	-1.719593	0.000000
N	-0.548355	-1.181021	0.000000
C	0.686111	-0.612381	0.000000
H	1.991238	-2.295925	0.000000

C
Total Energy = -1905.95 kcal mol^{-1}

N	1.611315	-0.700210	0.000000
C	0.489581	-1.465949	0.000000
H	0.626458	-2.542729	0.000000
C	-0.737542	-0.872333	0.000000
H	-1.648770	-1.460102	0.000000
C	-0.750083	0.569868	0.000000
N	-1.949110	1.223235	0.000000
H	-1.942041	2.234746	0.000000
H	-2.826936	0.727317	0.000000
N	0.341762	1.322640	0.000000
C	1.588328	0.742398	0.000000
O	2.660473	1.337805	0.000000
H	2.536564	-1.116686	0.000000

A-A
Total Energy = -4625.43 kcal mol^{-1}

N	-0.008566	-0.015041	0.000000
C	1.347998	-0.027840	0.000000
N	2.178579	1.025978	0.000000
C	1.507351	2.189095	0.000000
C	0.111226	2.354718	0.000000
C	-0.657213	1.170511	0.000000
N	2.009584	3.480072	0.000000
C	0.918035	4.339046	0.000000
N	-0.238360	3.703793	0.000000
N	-2.016653	1.192767	0.000000
H	1.791603	-1.021501	0.000000
H	2.990867	3.730300	0.000000
H	1.043770	5.413420	0.000000
H	-2.503883	2.077305	0.000000
H	-2.536964	0.327711	0.000000
N	1.543243	-3.346480	0.000000
C	2.538836	-4.254870	0.000000
N	2.455856	-5.596956	0.000000
C	1.173849	-6.003169	0.000000
C	0.033200	-5.183405	0.000000
C	0.258522	-3.784725	0.000000
N	0.674491	-7.296365	0.000000
C	-0.710928	-7.194569	0.000000
N	-1.134993	-5.945022	0.000000
N	-0.754386	-2.888765	0.000000
H	3.545632	-3.841575	0.000000

H	1.229795	-8.142836	0.000000
H	-1.342797	-8.072550	0.000000
H	-1.700720	-3.243128	0.000000
H	-0.570671	-1.875921	0.000000

A-T

Total Energy = -4494.40 kcal mol^{-1}

N	3.536826	-1.754831	0.000000
C	4.249941	-0.572753	0.000000
H	5.330523	-0.682294	0.000000
C	3.641850	0.641205	0.000000
C	4.387211	1.949201	0.000000
H	5.470129	1.786190	0.000000
H	4.119484	2.547498	-0.879304
H	4.119484	2.547498	0.879304
C	2.175627	0.671621	0.000000
O	1.511918	1.724393	0.000000
N	1.536863	-0.569104	0.000000
H	0.474883	-0.571686	0.000000
C	2.137170	-1.815111	0.000000
O	1.525010	-2.879716	0.000000
H	4.008646	-2.651411	0.000000
N	-5.278676	-0.770489	0.000000
C	-5.539742	0.594053	0.000000
H	-6.551418	0.976864	0.000000
N	-4.442887	1.327176	0.000000
C	-3.406188	0.396983	0.000000
C	-1.998041	0.544111	0.000000
N	-1.375178	1.739168	0.000000
H	-0.348204	1.793533	0.000000
H	-1.937441	2.578545	0.000000
N	-1.255657	-0.594944	0.000000
C	-1.865830	-1.800877	0.000000
H	-1.191425	-2.654451	0.000000
N	-3.181304	-2.055498	0.000000
C	-3.901687	-0.918029	0.000000
H	-5.951889	-1.526846	0.000000

A-G

Total Energy = -4791.09 kcal mol^{-1}

N	-0.018140	0.002095	0.000000
C	1.354915	-0.011691	0.000000
N	2.110990	1.075895	0.000000
C	1.377205	2.214819	0.000000
C	-0.020833	2.359642	0.000000
C	-0.827906	1.174958	0.000000
N	1.867623	3.502710	0.000000
C	0.763430	4.356650	0.000000
N	-0.377825	3.705322	0.000000
O	-2.065684	1.071970	0.000000
N	1.957283	-1.238846	0.000000
H	-0.526171	-0.910207	0.000000

H	2.847843	3.756382	0.000000
H	0.880322	5.431752	0.000000
H	2.965461	-1.274577	0.000000
H	1.420554	-2.090852	0.000000
N	-1.400085	-2.578612	0.000000
C	-0.780784	-3.778789	0.000000
N	-1.312272	-5.005609	0.000000
C	-2.659404	-4.949872	0.000000
C	-3.447560	-3.789973	0.000000
C	-2.767492	-2.544210	0.000000
N	-3.568540	-5.992928	0.000000
C	-4.835556	-5.422116	0.000000
N	-4.803561	-4.103240	0.000000
N	-3.412968	-1.368647	0.000000
H	0.309139	-3.750212	0.000000
H	-3.337222	-6.978779	0.000000
H	-5.730368	-6.029665	0.000000
H	-4.424315	-1.385016	0.000000
H	-2.910275	-0.462154	0.000000

A-C

Total Energy = -4223.11 kcal mol^{-1}

N	-0.043677	-0.009571	0.000000
C	1.327335	-0.035998	0.000000
N	1.986403	1.244350	0.000000
C	1.313805	2.426514	0.000000
C	-0.048037	2.433307	0.000000
C	-0.705845	1.146292	0.000000
N	-2.062301	1.091215	0.000000
O	2.024743	-1.047872	0.000000
H	3.000142	1.210125	0.000000
H	1.910787	3.333086	0.000000
H	-0.606174	3.363340	0.000000
H	-2.545207	0.177636	0.000000
H	-2.598320	1.946139	0.000000
N	-3.262083	-1.616122	0.000000
C	-2.210689	-2.477962	0.000000
N	-2.254909	-3.818295	0.000000
C	-3.515019	-4.278841	0.000000
C	-4.691976	-3.510360	0.000000
C	-4.519521	-2.109861	0.000000
N	-3.958350	-5.591326	0.000000
C	-5.346312	-5.549929	0.000000
N	-5.826457	-4.320587	0.000000
N	-5.580074	-1.256040	0.000000
H	-1.231647	-2.003419	0.000000
H	-3.365249	-6.412258	0.000000
H	-5.939039	-6.454793	0.000000
H	-6.519874	-1.625424	0.000000
H	-5.427956	-0.258544	0.000000

T-T

Total Energy = -4351.49 kcal mol^{-1}

N	-0.001893	-0.000183	0.000000
C	1.388559	0.000133	0.000000
N	1.932867	1.292319	0.000000
C	1.178061	2.447226	0.000000
C	-0.179009	2.424978	0.000000
C	-0.841807	1.118888	0.000000
O	-2.077562	0.985678	0.000000
O	2.085651	-1.005295	0.000000
C	-1.038155	3.661279	0.000000
H	-0.465033	-0.929942	0.000000
H	2.945351	1.329073	0.000000
H	1.745218	3.373538	0.000000
H	-1.693789	3.677102	-0.878750
H	-0.423577	4.567615	0.000000
H	-1.693789	3.677102	0.878750
N	-3.511495	-1.435311	0.000000
C	-2.667142	-2.519411	0.000000
N	-3.316796	-3.748006	0.000000
C	-4.695737	-3.882967	0.000000
C	-5.524134	-2.811326	0.000000
C	-4.928983	-1.463247	0.000000
O	-5.574530	-0.418747	0.000000
O	-1.429192	-2.450513	0.000000
C	-7.025245	-2.915471	0.000000
H	-3.048487	-0.503548	0.000000
H	-2.709705	-4.558848	0.000000
H	-5.059055	-4.906310	0.000000
H	-7.445749	-2.411752	0.878658
H	-7.350095	-3.961303	0.000000
H	-7.445749	-2.411752	-0.878658

T-G

Total Energy = -4650.46 kcal mol^{-1}

N	-0.019422	0.008877	0.000000
C	1.352482	-0.003016	0.000000
N	2.099849	1.090670	0.000000
C	1.353484	2.223086	0.000000
C	-0.047523	2.359734	0.000000
C	-0.843754	1.167233	0.000000
N	1.834261	3.514657	0.000000
C	0.724484	4.361467	0.000000
N	-0.412274	3.702828	0.000000
O	-2.079732	1.036376	0.000000
N	1.945533	-1.233937	0.000000
H	-0.522102	-0.897139	0.000000
H	2.812683	3.775077	0.000000
H	0.834247	5.437365	0.000000
H	2.953300	-1.279710	0.000000
H	1.395483	-2.080645	0.000000
N	-3.351978	-1.452609	0.000000
C	-2.519273	-2.539249	0.000000

N	-3.165196	-3.765518	0.000000
C	-4.545752	-3.904235	0.000000
C	-5.371687	-2.832631	0.000000
C	-4.775163	-1.483838	0.000000
O	-5.420716	-0.442881	0.000000
O	-1.272443	-2.482670	0.000000
C	-6.872624	-2.932930	0.000000
H	-2.902761	-0.503008	0.000000
H	-2.558835	-4.576446	0.000000
H	-4.906238	-4.928397	0.000000
H	-7.290581	-2.426935	0.878440
H	-7.200772	-3.977643	0.000000
H	-7.290581	-2.426935	-0.878440

T-C

Total Energy = -4089.30 kcal mol^{-1}

N	-0.022349	-0.004654	0.000000
C	1.355384	-0.024676	0.000000
N	2.007319	1.257118	0.000000
C	1.334136	2.438204	0.000000
C	-0.026307	2.441397	0.000000
C	-0.689110	1.157568	0.000000
N	-2.037777	1.110260	0.000000
O	2.052432	-1.032039	0.000000
H	3.020847	1.221067	0.000000
H	1.929719	3.345721	0.000000
H	-0.588721	3.368392	0.000000
H	-2.525115	0.198801	0.000000
H	-2.571672	1.966451	0.000000
N	-1.421693	-2.639064	0.000000
C	-0.725069	-3.848492	0.000000
N	-1.575679	-4.969665	0.000000
C	-2.949530	-4.899855	0.000000
C	-3.608412	-3.713381	0.000000
C	-2.810396	-2.485494	0.000000
O	-3.332022	-1.353954	0.000000
O	0.488305	-3.963292	0.000000
C	-5.109288	-3.592106	0.000000
H	-0.845757	-1.765044	0.000000
H	-1.094847	-5.861416	0.000000
H	-3.467479	-5.854755	0.000000
H	-5.454622	-3.035330	0.879472
H	-5.582577	-4.579831	0.000000
H	-5.454622	-3.035330	-0.879472

G-G

Total Energy = -4942.80 kcal mol^{-1}

N	3.076176	1.783422	0.000000
C	4.417008	1.461206	0.000000
N	4.864104	0.215899	0.000000
C	3.869133	-0.703826	0.000000

C	2.483573	-0.492732	0.000000
C	1.983018	0.848841	0.000000
N	4.016391	-2.075775	0.000000
C	2.739484	-2.626400	0.000000
N	1.800190	-1.702717	0.000000
O	0.829179	1.273538	0.000000
N	5.312905	2.489561	0.000000
H	2.776125	2.755606	0.000000
H	4.899174	-2.572419	0.000000
H	2.578543	-3.695087	0.000000
H	6.296091	2.258479	0.000000
H	5.031530	3.457675	0.000000
N	-1.941248	0.330904	0.000000
C	-2.256797	-1.006439	0.000000
N	-3.505142	-1.464889	0.000000
C	-4.426909	-0.471472	0.000000
C	-4.231978	0.918625	0.000000
C	-2.883398	1.428832	0.000000
N	-5.797786	-0.638350	0.000000
C	-6.362115	0.637941	0.000000
N	-5.453589	1.588306	0.000000
O	-2.469040	2.584496	0.000000
N	-1.233283	-1.906484	0.000000
H	-0.956955	0.619726	0.000000
H	-6.277764	-1.529407	0.000000
H	-7.433888	0.783042	0.000000
H	-1.501212	-2.879825	0.000000
H	-0.241519	-1.670276	0.000000

G-C

Total Energy = -4400.21 kcal mol^{-1}

N	4.882008	-0.566744	0.000000
C	5.207910	0.791168	0.000000
H	6.236571	1.125121	0.000000
N	4.146332	1.565232	0.000000
C	3.064406	0.686898	0.000000
C	1.654584	0.929149	0.000000
O	1.048940	2.021983	0.000000
N	0.922198	-0.282661	0.000000
H	-0.114003	-0.181895	0.000000
C	1.461966	-1.551725	0.000000
N	0.588336	-2.587231	0.000000
H	-0.430983	-2.457461	0.000000
H	0.982682	-3.516496	0.000000
N	2.773508	-1.786060	0.000000
C	3.504829	-0.650514	0.000000
H	5.514999	-1.356750	0.000000
N	-4.124246	-0.894012	0.000000
C	-4.708357	0.339794	0.000000
H	-5.792817	0.365027	0.000000
C	-3.937862	1.459909	0.000000
H	-4.383784	2.448220	0.000000

C	-2.504285	1.278895	0.000000
N	-1.679111	2.336003	0.000000
H	-0.638976	2.207265	0.000000
H	-2.063582	3.270185	0.000000
N	-1.949489	0.052780	0.000000
C	-2.715708	-1.071318	0.000000
O	-2.268592	-2.230640	0.000000
H	-4.677472	-1.744119	0.000000

C-C

Total Energy = -3822.48 kcal mol^{-1}

N	3.532347	1.066353	0.000000
C	4.704901	0.351959	0.000000
N	4.573029	-1.079980	0.000000
C	3.370157	-1.721694	0.000000
C	2.214717	-1.003039	0.000000
C	2.360931	0.432450	0.000000
N	1.237794	1.201774	0.000000
O	5.839812	0.828561	0.000000
H	5.447628	-1.593279	0.000000
H	3.392708	-2.807270	0.000000
H	1.237395	-1.472826	0.000000
H	1.378922	2.203566	0.000000
H	0.297462	0.804107	0.000000
N	-1.680236	0.266129	0.000000
C	-1.880371	-1.095403	0.000000
N	-3.242898	-1.533756	0.000000
C	-4.300753	-0.680469	0.000000
C	-4.088195	0.665423	0.000000
C	-2.716423	1.101902	0.000000
N	-2.444819	2.435500	0.000000
O	-0.990996	-1.943070	0.000000
H	-3.373565	-2.540206	0.000000
H	-5.290942	-1.124078	0.000000
H	-4.914705	1.366875	0.000000
H	-1.482830	2.745628	0.000000
H	-3.181069	3.124845	0.000000

Cartesian Coordinates of Systems in Toluene

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in toluene, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2316.72 kcal mol^{-1}

N	-2.060654	-0.755673	0.000000
C	-2.329217	0.601572	0.000000
H	-3.343148	0.976569	0.000000
N	-1.234277	1.344380	0.000000
C	-0.189780	0.418908	0.000000
C	1.217139	0.562617	0.000000
N	1.825694	1.773363	0.000000
N	1.980920	-0.557666	0.000000
C	1.367312	-1.758862	0.000000
H	2.028471	-2.622133	0.000000
N	0.048759	-2.026398	0.000000
C	-0.684734	-0.896926	0.000000
H	-2.739329	-1.508002	0.000000
H	2.835415	1.826388	0.000000
H	1.277426	2.621862	0.000000

T
Total Energy = -2176.62 kcal mol^{-1}

N	-1.580816	0.874193	0.000000
C	-0.229800	1.160874	0.000000
H	0.013794	2.218127	0.000000
C	0.723709	0.193791	0.000000
C	2.200657	0.485734	0.000000
H	2.385641	1.564402	0.000000
H	2.683503	0.044755	0.880305
H	2.683503	0.044755	-0.880305
C	0.289922	-1.204415	0.000000
O	1.041306	-2.185598	0.000000
N	-1.109523	-1.390319	0.000000
H	-1.437340	-2.353838	0.000000
C	-2.096059	-0.415130	0.000000
O	-3.303159	-0.659371	0.000000
H	-2.265338	1.622040	0.000000

G
Total Energy = -2476.35 kcal mol^{-1}

N	1.889774	1.291143	0.000000
C	2.893726	0.330849	0.000000
H	3.938879	0.605741	0.000000
N	2.415845	-0.897866	0.000000
C	1.031148	-0.741295	0.000000
C	-0.017437	-1.719453	0.000000
O	0.034002	-2.953247	0.000000
N	-1.298945	-1.069663	0.000000

H	-2.087712	-1.711497	0.000000
C	-1.525885	0.289160	0.000000
N	-2.820602	0.708297	0.000000
H	-3.596198	0.063080	0.000000
H	-3.005024	1.701617	0.000000
N	-0.547831	1.184956	0.000000
C	0.687260	0.620808	0.000000
H	2.008999	2.297369	0.000000

C

Total Energy = -1916.14 kcal mol^{-1}

N	1.613265	0.696942	0.000000
C	0.489066	1.462286	0.000000
H	0.629941	2.537325	0.000000
C	-0.737281	0.867836	0.000000
H	-1.649779	1.453118	0.000000
C	-0.755001	-0.571535	0.000000
N	-1.946434	-1.223465	0.000000
H	-1.952421	-2.235456	0.000000
H	-2.823176	-0.723291	0.000000
N	0.350206	-1.321378	0.000000
C	1.584963	-0.727379	0.000000
O	2.662365	-1.338615	0.000000
H	2.534287	1.123612	0.000000

A-A

Total Energy = -4639.03 kcal mol^{-1}

N	1.534547	-0.416537	0.000000
C	1.555242	0.937053	0.000000
N	2.628250	1.744010	0.000000
C	3.779171	1.044425	0.000000
C	3.907643	-0.355608	0.000000
C	2.705858	-1.098971	0.000000
N	5.078217	1.516623	0.000000
C	5.912263	0.412722	0.000000
N	5.250528	-0.733238	0.000000
N	2.686823	-2.453785	0.000000
H	0.573381	1.405252	0.000000
H	5.358494	2.490255	0.000000
H	6.988183	0.516947	0.000000
H	3.552277	-2.975130	0.000000
H	1.807161	-2.951133	0.000000
N	-1.791203	1.123639	0.000000
C	-2.699357	2.118355	0.000000
N	-4.042596	2.032074	0.000000
C	-4.450526	0.747103	0.000000
C	-3.626493	-0.390794	0.000000
C	-2.227715	-0.164948	0.000000
N	-5.741126	0.248575	0.000000
C	-5.643264	-1.131664	0.000000
N	-4.390804	-1.558857	0.000000
N	-1.325555	-1.169768	0.000000

H	-2.288201	3.125635	0.000000
H	-6.593130	0.796667	0.000000
H	-6.522317	-1.760847	0.000000
H	-1.662533	-2.123017	0.000000
H	-0.313216	-0.975038	0.000000

A-T

Total Energy = -4505.67 kcal mol^{-1}

N	3.543752	1.750473	0.000000
C	4.256566	0.570546	0.000000
H	5.335790	0.682744	0.000000
C	3.648432	-0.645234	0.000000
C	4.400589	-1.949900	0.000000
H	5.481598	-1.778350	0.000000
H	4.139156	-2.549705	0.880298
H	4.139156	-2.549705	-0.880298
C	2.187537	-0.674211	0.000000
O	1.514875	-1.726487	0.000000
N	1.548235	0.565438	0.000000
H	0.489649	0.569620	0.000000
C	2.152846	1.807082	0.000000
O	1.530386	2.873161	0.000000
H	4.023974	2.643504	0.000000
N	-5.290885	0.772581	0.000000
C	-5.555644	-0.585604	0.000000
H	-6.568147	-0.964284	0.000000
N	-4.457585	-1.323786	0.000000
C	-3.417392	-0.395321	0.000000
C	-2.009424	-0.543250	0.000000
N	-1.383011	-1.735222	0.000000
H	-0.356788	-1.783354	0.000000
H	-1.933044	-2.583090	0.000000
N	-1.264634	0.596787	0.000000
C	-1.874534	1.800824	0.000000
H	-1.202853	2.656115	0.000000
N	-3.191147	2.056633	0.000000
C	-3.916265	0.918513	0.000000
H	-5.971185	1.523484	0.000000

A-G

Total Energy = -4806.28 kcal mol^{-1}

N	1.483386	0.289392	0.000000
C	2.165309	1.483755	0.000000
N	3.491125	1.580711	0.000000
C	4.102967	0.372272	0.000000
C	3.513266	-0.902650	0.000000
C	2.087093	-0.993169	0.000000
N	5.459521	0.136837	0.000000
C	5.635136	-1.241961	0.000000
N	4.491076	-1.896956	0.000000
O	1.375592	-2.018980	0.000000
N	1.417606	2.620528	0.000000

H	0.438429	0.309653	0.000000
H	6.185133	0.843940	0.000000
H	6.620485	-1.685973	0.000000
H	1.890749	3.512596	0.000000
H	0.410342	2.594688	0.000000
N	-1.448219	0.377270	0.000000
C	-2.157196	1.525862	0.000000
N	-3.485265	1.696500	0.000000
C	-4.132139	0.510662	0.000000
C	-3.538418	-0.760469	0.000000
C	-2.121200	-0.814314	0.000000
N	-5.491909	0.267323	0.000000
C	-5.656736	-1.106910	0.000000
N	-4.507216	-1.761899	0.000000
N	-1.436024	-1.967783	0.000000
H	-1.573462	2.444911	0.000000
H	-6.225349	0.966469	0.000000
H	-6.638585	-1.558938	0.000000
H	-1.952091	-2.837766	0.000000
H	-0.403407	-1.985605	0.000000

A-C

Total Energy = -4238.25 kcal mol^{-1}

N	0.957196	0.793709	0.000000
C	-0.035268	1.732833	0.000000
N	-1.377243	1.254354	0.000000
C	-1.689909	-0.070699	0.000000
C	-0.697199	-1.003268	0.000000
C	0.658684	-0.511994	0.000000
N	1.690021	-1.388512	0.000000
O	0.153109	2.958784	0.000000
H	-2.104023	1.962602	0.000000
H	-2.744461	-0.322926	0.000000
H	-0.919362	-2.064579	0.000000
H	2.664856	-1.046383	0.000000
H	1.504749	-2.381489	0.000000
N	4.414068	-0.228788	0.000000
C	4.256373	1.117764	0.000000
N	5.216255	2.055913	0.000000
C	6.448184	1.513916	0.000000
C	6.758980	0.142931	0.000000
C	5.664770	-0.750305	0.000000
N	7.674619	2.151920	0.000000
C	8.645445	1.166629	0.000000
N	8.139911	-0.056459	0.000000
N	5.826362	-2.097130	0.000000
H	3.222080	1.454459	0.000000
H	7.825478	3.153995	0.000000
H	9.698422	1.411214	0.000000
H	6.753685	-2.498072	0.000000
H	5.021172	-2.707091	0.000000

T-T

Total Energy = -4363.07 kcal mol^{-1}

N	2.137305	0.892742	0.000000
C	3.280605	1.676799	0.000000
N	4.458355	0.934739	0.000000
C	4.496023	-0.442666	0.000000
C	3.366807	-1.198776	0.000000
C	2.083145	-0.504188	0.000000
O	0.982763	-1.091726	0.000000
O	3.271724	2.908015	0.000000
C	3.373208	-2.704584	0.000000
H	1.230082	1.397177	0.000000
H	5.316857	1.474220	0.000000
H	5.489954	-0.877903	0.000000
H	2.848162	-3.095312	0.879889
H	4.397292	-3.090716	0.000000
H	2.848162	-3.095312	-0.879889
N	-1.547050	0.146105	0.000000
C	-1.475164	1.518360	0.000000
N	-2.703009	2.154705	0.000000
C	-3.909195	1.479338	0.000000
C	-3.977943	0.124315	0.000000
C	-2.722646	-0.634209	0.000000
O	-2.649074	-1.867621	0.000000
O	-0.408646	2.159674	0.000000
C	-5.274115	-0.641106	0.000000
H	-0.635706	-0.356336	0.000000
H	-2.678000	3.168198	0.000000
H	-4.790286	2.112315	0.000000
H	-5.338937	-1.292608	-0.879896
H	-6.131738	0.038969	0.000000
H	-5.338937	-1.292608	0.879896

T-G

Total Energy = -4665.46 kcal mol^{-1}

N	1.735658	0.726354	0.000000
C	2.775489	1.624599	0.000000
N	4.055840	1.266899	0.000000
C	4.219641	-0.078925	0.000000
C	3.232919	-1.081591	0.000000
C	1.860986	-0.681851	0.000000
N	5.416177	-0.760089	0.000000
C	5.115314	-2.117202	0.000000
N	3.817485	-2.347153	0.000000
O	0.833652	-1.393224	0.000000
N	2.438371	2.942288	0.000000
H	0.765563	1.093279	0.000000
H	6.338478	-0.340636	0.000000
H	5.892352	-2.868385	0.000000
H	3.174509	3.633515	0.000000
H	1.472891	3.239481	0.000000
N	-1.758910	-0.313035	0.000000

C	-1.834952	1.055285	0.000000
N	-3.118770	1.561999	0.000000
C	-4.251311	0.766381	0.000000
C	-4.179276	-0.587521	0.000000
C	-2.851070	-1.211952	0.000000
O	-2.649003	-2.428546	0.000000
O	-0.840498	1.813037	0.000000
C	-5.388504	-1.483486	0.000000
H	-0.801562	-0.735554	0.000000
H	-3.199174	2.572389	0.000000
H	-5.192000	1.306653	0.000000
H	-5.384002	-2.138209	-0.879788
H	-6.312290	-0.896590	0.000000
H	-5.384002	-2.138209	0.879788

T-C

Total Energy = -4102.37 kcal mol^{-1}

N	1.934001	0.342210	0.000000
C	2.733429	1.459073	0.000000
N	4.141140	1.242468	0.000000
C	4.704247	0.003898	0.000000
C	3.909328	-1.100498	0.000000
C	2.483954	-0.886058	0.000000
N	1.652919	-1.946501	0.000000
O	2.316087	2.621898	0.000000
H	4.715349	2.079047	0.000000
H	5.787728	-0.040554	0.000000
H	4.328540	-2.100074	0.000000
H	0.631475	-1.806721	0.000000
H	2.030549	-2.883222	0.000000
N	-1.046328	0.730384	0.000000
C	-1.613079	2.001212	0.000000
N	-3.009360	1.984915	0.000000
C	-3.766187	0.837416	0.000000
C	-3.200673	-0.397945	0.000000
C	-1.743472	-0.480809	0.000000
O	-1.128605	-1.568403	0.000000
O	-0.973883	3.048335	0.000000
C	-3.998565	-1.675393	0.000000
H	-0.002287	0.682292	0.000000
H	-3.452497	2.896840	0.000000
H	-4.840767	0.988650	0.000000
H	-3.760297	-2.284499	-0.880439
H	-5.072450	-1.463464	0.000000
H	-3.760297	-2.284499	0.880439

G-G

Total Energy = -4964.17 kcal mol^{-1}

N	3.031409	-1.840098	0.000000
C	4.374120	-1.520873	0.000000
N	4.820895	-0.269703	0.000000
C	3.826112	0.649296	0.000000

C	2.440855	0.429891	0.000000
C	1.951208	-0.910872	0.000000
N	3.967041	2.020513	0.000000
C	2.693734	2.567332	0.000000
N	1.753772	1.639973	0.000000
O	0.785467	-1.331971	0.000000
N	5.259879	-2.548881	0.000000
H	2.743905	-2.816108	0.000000
H	4.844002	2.528589	0.000000
H	2.531916	3.635390	0.000000
H	6.247161	-2.333295	0.000000
H	4.966781	-3.514688	0.000000
N	-1.892267	-0.263893	0.000000
C	-2.212774	1.075227	0.000000
N	-3.469171	1.526476	0.000000
C	-4.387704	0.531062	0.000000
C	-4.176021	-0.856173	0.000000
C	-2.827209	-1.348310	0.000000
N	-5.758972	0.682466	0.000000
C	-6.311316	-0.593051	0.000000
N	-5.392809	-1.539234	0.000000
O	-2.417498	-2.515920	0.000000
N	-1.195480	1.972205	0.000000
H	-0.902249	-0.551080	0.000000
H	-6.258627	1.563567	0.000000
H	-7.381178	-0.746533	0.000000
H	-1.456207	2.948714	0.000000
H	-0.198779	1.729984	0.000000

G-C

Total Energy = -4414.18 kcal mol^{-1}

N	4.892010	0.579336	0.000000
C	5.226326	-0.770612	0.000000
H	6.256320	-1.098210	0.000000
N	4.166083	-1.553635	0.000000
C	3.078474	-0.679140	0.000000
C	1.672671	-0.929482	0.000000
O	1.081084	-2.034400	0.000000
N	0.928859	0.269673	0.000000
H	-0.109321	0.163071	0.000000
C	1.459359	1.543895	0.000000
N	0.580993	2.570758	0.000000
H	-0.438601	2.430810	0.000000
H	0.960208	3.507320	0.000000
N	2.773028	1.787042	0.000000
C	3.515707	0.657742	0.000000
H	5.529600	1.366581	0.000000
N	-4.119678	0.900969	0.000000
C	-4.713371	-0.328016	0.000000
H	-5.797005	-0.341786	0.000000
C	-3.949847	-1.453533	0.000000
H	-4.398896	-2.440020	0.000000

C	-2.519340	-1.281968	0.000000
N	-1.703362	-2.346494	0.000000
H	-0.672188	-2.227422	0.000000
H	-2.093255	-3.278963	0.000000
N	-1.952692	-0.056829	0.000000
C	-2.720215	1.065683	0.000000
O	-2.257714	2.227457	0.000000
H	-4.675237	1.750174	0.000000

C-C

Total Energy = -3839.72 kcal mol^{-1}

N	3.512314	-1.073288	0.000000
C	4.671611	-0.345895	0.000000
N	4.545715	1.069835	0.000000
C	3.340604	1.709302	0.000000
C	2.186910	0.987747	0.000000
C	2.327812	-0.445750	0.000000
N	1.211805	-1.213776	0.000000
O	5.813374	-0.836137	0.000000
H	5.414519	1.593889	0.000000
H	3.365901	2.793551	0.000000
H	1.208091	1.455660	0.000000
H	1.338238	-2.218325	0.000000
H	0.268859	-0.810023	0.000000
N	-1.648348	-0.239963	0.000000
C	-1.870845	1.113867	0.000000
N	-3.223093	1.541588	0.000000
C	-4.275210	0.679328	0.000000
C	-4.051993	-0.664645	0.000000
C	-2.680376	-1.093497	0.000000
N	-2.399169	-2.419225	0.000000
O	-0.975977	1.970738	0.000000
H	-3.371577	2.545844	0.000000
H	-5.266026	1.118894	0.000000
H	-4.870905	-1.374608	0.000000
H	-1.438342	-2.733413	0.000000
H	-3.133893	-3.111699	0.000000

Cartesian Coordinates of Systems in Chloroform

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in chloroform, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2320.10 kcal mol^{-1}

N	-2.060735	-0.755387	0.000000
C	-2.331335	0.599124	0.000000
H	-3.345268	0.973156	0.000000
N	-1.235670	1.343986	0.000000
C	-0.189648	0.419425	0.000000
C	1.217695	0.564784	0.000000
N	1.827135	1.772815	0.000000
N	1.981232	-0.558419	0.000000
C	1.367481	-1.759583	0.000000
H	2.028246	-2.623122	0.000000
N	0.048714	-2.026252	0.000000
C	-0.686165	-0.895634	0.000000
H	-2.740961	-1.506811	0.000000
H	2.837105	1.828178	0.000000
H	1.282174	2.623740	0.000000

T
Total Energy = -2180.16 kcal mol^{-1}

N	-1.579598	0.873090	0.000000
C	-0.230237	1.159262	0.000000
H	0.013072	2.216008	0.000000
C	0.723360	0.190725	0.000000
C	2.199892	0.485680	0.000000
H	2.380701	1.564772	0.000000
H	2.684349	0.047588	0.880962
H	2.684349	0.047588	-0.880962
C	0.287394	-1.203323	0.000000
O	1.038969	-2.189315	0.000000
N	-1.109054	-1.389810	0.000000
H	-1.438445	-2.352927	0.000000
C	-2.091840	-0.413055	0.000000
O	-3.301894	-0.660606	0.000000
H	-2.261019	1.624324	0.000000

G
Total Energy = -2482.28 kcal mol^{-1}

N	1.892479	1.290080	0.000000
C	2.893072	0.330247	0.000000
H	3.938203	0.604254	0.000000
N	2.412954	-0.899772	0.000000
C	1.027198	-0.739384	0.000000
C	-0.022757	-1.711510	0.000000
O	0.037505	-2.950773	0.000000
N	-1.298637	-1.069590	0.000000
H	-2.091347	-1.706872	0.000000

C	-1.527370	0.290350	0.000000
N	-2.819110	0.704453	0.000000
H	-3.591806	0.054786	0.000000
H	-3.011676	1.696544	0.000000
N	-0.546227	1.187241	0.000000
C	0.688047	0.624189	0.000000
H	2.019470	2.295755	0.000000

C

Total Energy = -1921.13 kcal mol^{-1}

N	1.614406	0.695027	0.000000
C	0.488808	1.460557	0.000000
H	0.631650	2.534719	0.000000
C	-0.736958	0.865834	0.000000
H	-1.649970	1.449933	0.000000
C	-0.757726	-0.571948	0.000000
N	-1.945244	-1.222988	0.000000
H	-1.957554	-2.235064	0.000000
H	-2.821338	-0.720509	0.000000
N	0.354333	-1.320893	0.000000
C	1.582987	-0.720759	0.000000
O	2.663360	-1.340754	0.000000
H	2.533244	1.126845	0.000000

A-A

Total Energy = -4644.80 kcal mol^{-1}

N	1.530245	-0.385702	0.000000
C	1.568511	0.966127	0.000000
N	2.651326	1.760538	0.000000
C	3.795330	1.046193	0.000000
C	3.904212	-0.355487	0.000000
C	2.693566	-1.085486	0.000000
N	5.099058	1.501982	0.000000
C	5.919104	0.390367	0.000000
N	5.242974	-0.748954	0.000000
N	2.653789	-2.437547	0.000000
H	0.592901	1.447038	0.000000
H	5.395106	2.471414	0.000000
H	6.995932	0.481545	0.000000
H	3.509337	-2.975391	0.000000
H	1.767098	-2.923187	0.000000
N	-1.798001	1.130097	0.000000
C	-2.712095	2.118969	0.000000
N	-4.055309	2.023427	0.000000
C	-4.456631	0.734748	0.000000
C	-3.624016	-0.396970	0.000000
C	-2.226568	-0.162905	0.000000
N	-5.742950	0.228985	0.000000
C	-5.638607	-1.148413	0.000000
N	-4.382340	-1.569479	0.000000
N	-1.315909	-1.158712	0.000000
H	-2.307828	3.129005	0.000000

H	-6.600141	0.769685	0.000000
H	-6.513896	-1.782424	0.000000
H	-1.639227	-2.116973	0.000000
H	-0.304972	-0.952492	0.000000

A-T

Total Energy = -4510.56 kcal mol^{-1}

N	3.544671	1.749141	0.000000
C	4.258524	0.571124	0.000000
H	5.336956	0.685554	0.000000
C	3.651619	-0.646308	0.000000
C	4.408903	-1.948215	0.000000
H	5.488678	-1.770830	0.000000
H	4.151480	-2.549047	0.880871
H	4.151480	-2.549047	-0.880871
C	2.193541	-0.676278	0.000000
O	1.516938	-1.728844	0.000000
N	1.552828	0.562272	0.000000
H	0.496038	0.566022	0.000000
C	2.157867	1.802631	0.000000
O	1.528642	2.868543	0.000000
H	4.028153	2.640858	0.000000
N	-5.295683	0.774937	0.000000
C	-5.563723	-0.580249	0.000000
H	-6.576587	-0.956999	0.000000
N	-4.465811	-1.321770	0.000000
C	-3.423090	-0.395286	0.000000
C	-2.015262	-0.544793	0.000000
N	-1.387471	-1.735469	0.000000
H	-0.361455	-1.780616	0.000000
H	-1.932295	-2.586925	0.000000
N	-1.268689	0.595342	0.000000
C	-1.877294	1.799166	0.000000
H	-1.205695	2.654415	0.000000
N	-3.194130	2.056552	0.000000
C	-3.922217	0.918647	0.000000
H	-5.976915	1.525473	0.000000

A-G

Total Energy = -4812.98 kcal mol^{-1}

N	1.484953	0.287403	0.000000
C	2.163704	1.485141	0.000000
N	3.491824	1.582751	0.000000
C	4.106232	0.376364	0.000000
C	3.516175	-0.898292	0.000000
C	2.092085	-0.989052	0.000000
N	5.462300	0.141001	0.000000
C	5.640423	-1.234894	0.000000
N	4.495653	-1.892767	0.000000
O	1.384010	-2.021513	0.000000
N	1.415280	2.617091	0.000000
H	0.439576	0.305440	0.000000

H	6.189772	0.846814	0.000000
H	6.626149	-1.677505	0.000000
H	1.882202	3.512906	0.000000
H	0.407751	2.589532	0.000000
N	-1.448028	0.366399	0.000000
C	-2.150378	1.518805	0.000000
N	-3.478736	1.693457	0.000000
C	-4.132054	0.510219	0.000000
C	-3.542899	-0.763309	0.000000
C	-2.126469	-0.822011	0.000000
N	-5.491842	0.273796	0.000000
C	-5.665328	-1.096910	0.000000
N	-4.518166	-1.759750	0.000000
N	-1.442340	-1.977000	0.000000
H	-1.563126	2.434939	0.000000
H	-6.223336	0.975439	0.000000
H	-6.649596	-1.543072	0.000000
H	-1.954474	-2.849312	0.000000
H	-0.411318	-1.992111	0.000000

A-C

Total Energy = -4245.29 kcal mol^{-1}

N	0.950321	0.798969	0.000000
C	-0.048163	1.727832	0.000000
N	-1.382670	1.250249	0.000000
C	-1.691349	-0.076699	0.000000
C	-0.695607	-1.005836	0.000000
C	0.657529	-0.512368	0.000000
N	1.691258	-1.382481	0.000000
O	0.141449	2.960061	0.000000
H	-2.115534	1.952530	0.000000
H	-2.745061	-0.329989	0.000000
H	-0.913180	-2.067907	0.000000
H	2.665047	-1.038291	0.000000
H	1.510365	-2.376834	0.000000
N	4.414857	-0.221691	0.000000
C	4.262563	1.123344	0.000000
N	5.224161	2.060532	0.000000
C	6.456648	1.514589	0.000000
C	6.761733	0.142355	0.000000
C	5.665201	-0.749620	0.000000
N	7.683187	2.149254	0.000000
C	8.651566	1.164563	0.000000
N	8.142937	-0.059022	0.000000
N	5.817538	-2.094800	0.000000
H	3.229268	1.463104	0.000000
H	7.838854	3.150885	0.000000
H	9.704682	1.407260	0.000000
H	6.740667	-2.505856	0.000000
H	5.008686	-2.700806	0.000000

T-T

Total Energy = -4368.80 kcal mol^{-1}

N	2.127327	0.880959	0.000000
C	3.267763	1.665774	0.000000
N	4.445519	0.932583	0.000000
C	4.488376	-0.443587	0.000000
C	3.361227	-1.204504	0.000000
C	2.078000	-0.515242	0.000000
O	0.974905	-1.103502	0.000000
O	3.249357	2.900853	0.000000
C	3.377381	-2.710347	0.000000
H	1.219961	1.384477	0.000000
H	5.304769	1.471554	0.000000
H	5.483886	-0.873914	0.000000
H	2.856419	-3.105168	0.880583
H	4.404207	-3.088212	0.000000
H	2.856419	-3.105168	-0.880583
N	-1.541470	0.161381	0.000000
C	-1.477710	1.534068	0.000000
N	-2.705718	2.163047	0.000000
C	-3.906544	1.481915	0.000000
C	-3.968402	0.125209	0.000000
C	-2.710882	-0.622259	0.000000
O	-2.625986	-1.859285	0.000000
O	-0.409171	2.176453	0.000000
C	-5.262867	-0.643628	0.000000
H	-0.628224	-0.337921	0.000000
H	-2.691155	3.177128	0.000000
H	-4.790406	2.110219	0.000000
H	-5.328148	-1.294283	-0.880590
H	-6.120685	0.035683	0.000000
H	-5.328148	-1.294283	0.880590

T-G

Total Energy = -4672.79 kcal mol^{-1}

N	1.734980	0.726628	0.000000
C	2.775762	1.626138	0.000000
N	4.057521	1.264818	0.000000
C	4.221617	-0.080234	0.000000
C	3.231591	-1.079455	0.000000
C	1.863109	-0.677191	0.000000
N	5.415489	-0.764907	0.000000
C	5.113760	-2.118856	0.000000
N	3.813574	-2.347648	0.000000
O	0.835543	-1.395293	0.000000
N	2.441304	2.941056	0.000000
H	0.764751	1.094608	0.000000
H	6.341158	-0.351918	0.000000
H	5.889995	-2.870480	0.000000
H	3.176054	3.634428	0.000000
H	1.476572	3.241416	0.000000
N	-1.761782	-0.307416	0.000000
C	-1.841456	1.061861	0.000000

N	-3.124300	1.563438	0.000000
C	-4.251706	0.764620	0.000000
C	-4.175690	-0.590742	0.000000
C	-2.848025	-1.206485	0.000000
O	-2.636480	-2.426553	0.000000
O	-0.843732	1.816448	0.000000
C	-5.385031	-1.487200	0.000000
H	-0.804329	-0.724927	0.000000
H	-3.212971	2.573633	0.000000
H	-5.193885	1.301298	0.000000
H	-5.382903	-2.141108	-0.880537
H	-6.307586	-0.898869	0.000000
H	-5.382903	-2.141108	0.880537

T-C

Total Energy = -4108.83 kcal mol^{-1}

N	1.939979	0.346578	0.000000
C	2.741929	1.458452	0.000000
N	4.143470	1.246845	0.000000
C	4.708540	0.008231	0.000000
C	3.914822	-1.096892	0.000000
C	2.490984	-0.884952	0.000000
N	1.660227	-1.943744	0.000000
O	2.317963	2.625259	0.000000
H	4.721481	2.081079	0.000000
H	5.791508	-0.032588	0.000000
H	4.334071	-2.096256	0.000000
H	0.639749	-1.805623	0.000000
H	2.037091	-2.881344	0.000000
N	-1.050642	0.722108	0.000000
C	-1.615156	1.991363	0.000000
N	-3.006093	1.982343	0.000000
C	-3.766739	0.837911	0.000000
C	-3.205547	-0.400238	0.000000
C	-1.751227	-0.487603	0.000000
O	-1.133659	-1.575488	0.000000
O	-0.965339	3.037232	0.000000
C	-4.011011	-1.673023	0.000000
H	-0.007438	0.672157	0.000000
H	-3.450826	2.893915	0.000000
H	-4.839996	0.994260	0.000000
H	-3.777577	-2.283308	-0.880946
H	-5.082986	-1.453365	0.000000
H	-3.777577	-2.283308	0.880946

G-G

Total Energy = -4973.91 kcal mol^{-1}

N	3.020040	-1.851114	0.000000
C	4.362557	-1.527292	0.000000
N	4.803246	-0.271319	0.000000
C	3.804818	0.642636	0.000000

C	2.420436	0.413491	0.000000
C	1.942082	-0.928687	0.000000
N	3.936775	2.013999	0.000000
C	2.662504	2.553774	0.000000
N	1.726398	1.620764	0.000000
O	0.771598	-1.352868	0.000000
N	5.248210	-2.550737	0.000000
H	2.742982	-2.830139	0.000000
H	4.809865	2.529274	0.000000
H	2.494373	3.620641	0.000000
H	6.236216	-2.337399	0.000000
H	4.954747	-3.516959	0.000000
N	-1.869537	-0.242567	0.000000
C	-2.198948	1.096495	0.000000
N	-3.461173	1.537822	0.000000
C	-4.373319	0.537586	0.000000
C	-4.147090	-0.847435	0.000000
C	-2.796672	-1.324657	0.000000
N	-5.745350	0.674490	0.000000
C	-6.285846	-0.603040	0.000000
N	-5.358229	-1.543068	0.000000
O	-2.383999	-2.496984	0.000000
N	-1.188865	1.996481	0.000000
H	-0.875655	-0.525162	0.000000
H	-6.258592	1.548323	0.000000
H	-7.354200	-0.764931	0.000000
H	-1.450676	2.973273	0.000000
H	-0.188697	1.755306	0.000000

G-C

Total Energy = -4420.77 kcal mol^{-1}

N	1.669197	0.325183	0.000000
C	1.691041	1.708164	0.000000
N	2.970190	2.235867	0.000000
C	4.115092	1.465344	0.000000
C	4.081168	0.106616	0.000000
C	2.774691	-0.548066	0.000000
O	2.587898	-1.773391	0.000000
O	0.671225	2.408535	0.000000
C	5.319217	-0.750670	0.000000
H	0.747008	-0.110783	0.000000
H	3.035359	3.248002	0.000000
H	5.043576	2.025740	0.000000
H	5.340539	-1.403748	0.880905
H	6.221303	-0.131435	0.000000
H	5.340539	-1.403748	-0.880905
C	-2.348131	0.989737	0.000000
C	-3.618165	1.557834	0.000000
C	-4.784157	0.802280	0.000000
C	-4.667403	-0.594476	0.000000
C	-3.417942	-1.237547	0.000000
C	-2.301268	-0.398116	0.000000

F	-1.047971	-0.995348	0.000000
F	-3.713021	2.932600	0.000000
C	-3.268940	-2.742411	0.000000
H	-1.441793	1.589101	0.000000
H	-5.752723	1.291955	0.000000
H	-5.568380	-1.203004	0.000000
H	-2.713718	-3.085103	-0.881703
H	-4.250713	-3.224009	0.000000
H	-2.713718	-3.085103	0.881703

C-C

Total Energy = -3847.75 kcal mol^{-1}

N	3.503721	-1.076159	0.000000
C	4.657066	-0.343885	0.000000
N	4.535351	1.064649	0.000000
C	3.329592	1.703993	0.000000
C	2.176248	0.981851	0.000000
C	2.313117	-0.450783	0.000000
N	1.200233	-1.217640	0.000000
O	5.801960	-0.842402	0.000000
H	5.401636	1.593422	0.000000
H	3.357026	2.787633	0.000000
H	1.197188	1.449801	0.000000
H	1.319797	-2.223431	0.000000
H	0.255895	-0.810925	0.000000
N	-1.635036	-0.227545	0.000000
C	-1.868496	1.122160	0.000000
N	-3.216218	1.544592	0.000000
C	-4.265489	0.677569	0.000000
C	-4.036530	-0.665107	0.000000
C	-2.664964	-1.090030	0.000000
N	-2.378656	-2.411724	0.000000
O	-0.970975	1.984174	0.000000
H	-3.373596	2.547590	0.000000
H	-5.256900	1.114609	0.000000
H	-4.851708	-1.379040	0.000000
H	-1.418188	-2.727013	0.000000
H	-3.112073	-3.106358	0.000000

Cartesian Coordinates of Systems in Ammonia

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in ammonia, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2322.84 kcal mol^{-1}

N	-2.060622	-0.754494	0.000000
C	-2.331777	0.597797	0.000000
H	-3.345904	0.970718	0.000000
N	-1.235028	1.343878	0.000000
C	-0.188814	0.419208	0.000000
C	1.218655	0.565691	0.000000
N	1.827254	1.772345	0.000000
N	1.982182	-0.559725	0.000000
C	1.367800	-1.760811	0.000000
H	2.028189	-2.624683	0.000000
N	0.048917	-2.026633	0.000000
C	-0.687323	-0.895002	0.000000
H	-2.743297	-1.504031	0.000000
H	2.837230	1.832096	0.000000
H	1.282538	2.623646	0.000000

T
Total Energy = -2183.22 kcal mol^{-1}

N	-1.578287	0.872208	0.000000
C	-0.230561	1.157822	0.000000
H	0.012536	2.214189	0.000000
C	0.722991	0.187835	0.000000
C	2.199120	0.485561	0.000000
H	2.375741	1.565089	0.000000
H	2.685211	0.050173	0.881532
H	2.685211	0.050173	-0.881532
C	0.285138	-1.202322	0.000000
O	1.037088	-2.192756	0.000000
N	-1.108671	-1.389420	0.000000
H	-1.439382	-2.352124	0.000000
C	-2.088252	-0.411201	0.000000
O	-3.300915	-0.661559	0.000000
H	-2.256966	1.626334	0.000000

G
Total Energy = -2487.07 kcal mol^{-1}

N	1.894379	1.289150	0.000000
C	2.892772	0.329915	0.000000
H	3.938224	0.601918	0.000000
N	2.410778	-0.901273	0.000000
C	1.024045	-0.737902	0.000000
C	-0.026995	-1.704867	0.000000
O	0.041409	-2.949115	0.000000
N	-1.298293	-1.069714	0.000000
H	-2.094550	-1.702714	0.000000

C	-1.528535	0.291323	0.000000
N	-2.817528	0.701613	0.000000
H	-3.587986	0.048453	0.000000
H	-3.016150	1.692782	0.000000
N	-0.544624	1.188983	0.000000
C	0.688479	0.626755	0.000000
H	2.024575	2.294693	0.000000

C

Total Energy = -1925.33 kcal mol^{-1}

N	1.615483	0.693418	0.000000
C	0.488557	1.459124	0.000000
H	0.632522	2.532599	0.000000
C	-0.736457	0.864024	0.000000
H	-1.649693	1.447246	0.000000
C	-0.760013	-0.572320	0.000000
N	-1.944405	-1.222396	0.000000
H	-1.962407	-2.234485	0.000000
H	-2.819911	-0.717785	0.000000
N	0.357998	-1.320684	0.000000
C	1.581406	-0.715418	0.000000
O	2.664599	-1.343075	0.000000
H	2.532319	1.129751	0.000000

A-A

Total Energy = -4649.50 kcal mol^{-1}

N	1.528233	-0.365585	0.000000
C	1.578091	0.984736	0.000000
N	2.667100	1.771342	0.000000
C	3.807143	1.047554	0.000000
C	3.902822	-0.355140	0.000000
C	2.686534	-1.076531	0.000000
N	5.113415	1.492405	0.000000
C	5.924338	0.376619	0.000000
N	5.238849	-0.758898	0.000000
N	2.633829	-2.426343	0.000000
H	0.607047	1.474583	0.000000
H	5.420199	2.458729	0.000000
H	7.001530	0.460621	0.000000
H	3.482944	-2.974588	0.000000
H	1.743247	-2.905430	0.000000
N	-1.804153	1.135677	0.000000
C	-2.723107	2.119879	0.000000
N	-4.066091	2.017340	0.000000
C	-4.462467	0.725693	0.000000
C	-3.622864	-0.400959	0.000000
C	-2.226498	-0.160668	0.000000
N	-5.745304	0.213930	0.000000
C	-5.635752	-1.161072	0.000000
N	-4.376167	-1.577187	0.000000
N	-1.310075	-1.149909	0.000000
H	-2.324013	3.131982	0.000000

H	-6.606902	0.748069	0.000000
H	-6.508372	-1.798346	0.000000
H	-1.623577	-2.111619	0.000000
H	-0.299980	-0.936883	0.000000

A-T

Total Energy = -4514.96 kcal mol^{-1}

N	3.551859	1.746214	0.000000
C	4.263386	0.568057	0.000000
H	5.341540	0.681527	0.000000
C	3.653836	-0.648861	0.000000
C	4.411460	-1.950528	0.000000
H	5.490543	-1.770917	0.000000
H	4.155700	-2.551340	0.881468
H	4.155700	-2.551340	-0.881468
C	2.198482	-0.675410	0.000000
O	1.516086	-1.727017	0.000000
N	1.559621	0.563695	0.000000
H	0.504790	0.569797	0.000000
C	2.168997	1.800771	0.000000
O	1.537486	2.869176	0.000000
H	4.040437	2.635468	0.000000
N	-5.303338	0.770649	0.000000
C	-5.568896	-0.582871	0.000000
H	-6.581147	-0.960678	0.000000
N	-4.468382	-1.323403	0.000000
C	-3.427353	-0.394452	0.000000
C	-2.019413	-0.540752	0.000000
N	-1.388491	-1.729380	0.000000
H	-0.362458	-1.770994	0.000000
H	-1.928302	-2.584224	0.000000
N	-1.274081	0.601131	0.000000
C	-1.886075	1.802464	0.000000
H	-1.217907	2.660310	0.000000
N	-3.203859	2.057532	0.000000
C	-3.931387	0.917742	0.000000
H	-5.988832	1.517631	0.000000

A-G

Total Energy = -4818.55 kcal mol^{-1}

N	1.485715	0.288781	0.000000
C	2.163613	1.488405	0.000000
N	3.493861	1.584825	0.000000
C	4.109158	0.379719	0.000000
C	3.516769	-0.893844	0.000000
C	2.094610	-0.982839	0.000000
N	5.464377	0.142192	0.000000
C	5.642363	-1.231220	0.000000
N	4.496056	-1.890168	0.000000
O	1.389122	-2.021301	0.000000
N	1.417148	2.618240	0.000000
H	0.439967	0.305763	0.000000

H	6.195159	0.845037	0.000000
H	6.628048	-1.673398	0.000000
H	1.881338	3.515826	0.000000
H	0.409516	2.591698	0.000000
N	-1.448116	0.357659	0.000000
C	-2.146073	1.512377	0.000000
N	-3.474600	1.690114	0.000000
C	-4.132895	0.508800	0.000000
C	-3.546157	-0.766177	0.000000
C	-2.130597	-0.827998	0.000000
N	-5.492350	0.276395	0.000000
C	-5.671194	-1.091328	0.000000
N	-4.525312	-1.759737	0.000000
N	-1.447486	-1.984510	0.000000
H	-1.556122	2.426150	0.000000
H	-6.223664	0.978577	0.000000
H	-6.657223	-1.533028	0.000000
H	-1.957372	-2.858077	0.000000
H	-0.417659	-1.996933	0.000000

A-C

Total Energy = -4251.49 kcal mol^{-1}

N	0.942600	0.802984	0.000000
C	-0.062873	1.720371	0.000000
N	-1.389912	1.241730	0.000000
C	-1.692630	-0.087714	0.000000
C	-0.692578	-1.011747	0.000000
C	0.657428	-0.514180	0.000000
N	1.694590	-1.376426	0.000000
O	0.126120	2.959218	0.000000
H	-2.129499	1.937158	0.000000
H	-2.745105	-0.343954	0.000000
H	-0.904033	-2.074828	0.000000
H	2.666720	-1.028382	0.000000
H	1.519628	-2.372326	0.000000
N	4.413221	-0.206101	0.000000
C	4.270344	1.138167	0.000000
N	5.236708	2.071401	0.000000
C	6.468039	1.517805	0.000000
C	6.762864	0.143140	0.000000
C	5.661405	-0.743865	0.000000
N	7.697454	2.144256	0.000000
C	8.659355	1.155969	0.000000
N	8.143163	-0.065987	0.000000
N	5.801473	-2.087901	0.000000
H	3.239241	1.484235	0.000000
H	7.862674	3.144558	0.000000
H	9.713423	1.393406	0.000000
H	6.719746	-2.510054	0.000000
H	4.987386	-2.687603	0.000000

T-T

Total Energy = -4374.31 kcal mol^{-1}

N	2.116713	0.869361	0.000000
C	3.255119	1.654710	0.000000
N	4.432633	0.928677	0.000000
C	4.479528	-0.445890	0.000000
C	3.353791	-1.210725	0.000000
C	2.072278	-0.525319	0.000000
O	0.965627	-1.113995	0.000000
O	3.228094	2.893063	0.000000
C	3.378213	-2.716655	0.000000
H	1.209723	1.372622	0.000000
H	5.292918	1.466676	0.000000
H	5.476123	-0.872341	0.000000
H	2.861270	-3.115433	0.881351
H	4.407451	-3.086990	0.000000
H	2.861270	-3.115433	-0.881351
N	-1.534119	0.181428	0.000000
C	-1.480638	1.554654	0.000000
N	-2.710954	2.173440	0.000000
C	-3.904671	1.483432	0.000000
C	-3.956758	0.124987	0.000000
C	-2.695442	-0.608596	0.000000
O	-2.595873	-1.848952	0.000000
O	-0.411655	2.199911	0.000000
C	-5.247943	-0.649749	0.000000
H	-0.618505	-0.313290	0.000000
H	-2.709331	3.188029	0.000000
H	-4.792952	2.104407	0.000000
H	-5.312377	-1.299718	-0.881318
H	-6.107154	0.027407	0.000000
H	-5.312377	-1.299718	0.881318

T-G

Total Energy = -4679.20 kcal mol^{-1}

N	1.733219	0.726016	0.000000
C	2.775046	1.626409	0.000000
N	4.058010	1.261646	0.000000
C	4.221729	-0.082424	0.000000
C	3.228928	-1.078765	0.000000
C	1.863531	-0.673825	0.000000
N	5.413423	-0.769997	0.000000
C	5.111033	-2.121549	0.000000
N	3.808780	-2.349268	0.000000
O	0.835663	-1.398119	0.000000
N	2.443518	2.938917	0.000000
H	0.763564	1.096172	0.000000
H	6.340824	-0.360176	0.000000
H	5.885798	-2.874372	0.000000
H	3.177840	3.633260	0.000000
H	1.479522	3.242181	0.000000
N	-1.762960	-0.299054	0.000000
C	-1.847757	1.071140	0.000000

N	-3.130787	1.566312	0.000000
C	-4.251889	0.762971	0.000000
C	-4.170142	-0.593717	0.000000
C	-2.842389	-1.199190	0.000000
O	-2.620569	-2.422933	0.000000
O	-0.848161	1.823686	0.000000
C	-5.378678	-1.491928	0.000000
H	-0.804783	-0.711137	0.000000
H	-3.228584	2.576135	0.000000
H	-5.196292	1.294666	0.000000
H	-5.378525	-2.145107	-0.881283
H	-6.300389	-0.902845	0.000000
H	-5.378525	-2.145107	0.881283

T-C

Total Energy = -4114.63 kcal mol^{-1}

N	1.946132	0.353660	0.000000
C	2.751471	1.460021	0.000000
N	4.147445	1.251487	0.000000
C	4.712929	0.012056	0.000000
C	3.918980	-1.092630	0.000000
C	2.496721	-0.881416	0.000000
N	1.665372	-1.938127	0.000000
O	2.322961	2.631371	0.000000
H	4.729695	2.082975	0.000000
H	5.795480	-0.026805	0.000000
H	4.337117	-2.092227	0.000000
H	0.645521	-1.801403	0.000000
H	2.042253	-2.876207	0.000000
N	-1.054707	0.711237	0.000000
C	-1.615577	1.979446	0.000000
N	-3.001579	1.978752	0.000000
C	-3.766963	0.837895	0.000000
C	-3.210998	-0.403290	0.000000
C	-1.759488	-0.496250	0.000000
O	-1.140458	-1.585160	0.000000
O	-0.954419	3.023529	0.000000
C	-4.024401	-1.670889	0.000000
H	-0.012515	0.659100	0.000000
H	-3.446465	2.890566	0.000000
H	-4.838859	1.000122	0.000000
H	-3.795622	-2.282317	-0.881402
H	-5.094403	-1.443178	0.000000
H	-3.795622	-2.282317	0.881402

G-G

Total Energy = -4982.1 kcal mol^{-1}

N	3.014504	-1.860427	0.000000
C	4.356513	-1.531275	0.000000
N	4.790677	-0.270957	0.000000
C	3.788295	0.637631	0.000000

C	2.404703	0.398526	0.000000
C	1.937774	-0.945054	0.000000
N	3.910722	2.009187	0.000000
C	2.635133	2.541149	0.000000
N	1.703314	1.602460	0.000000
O	0.762789	-1.372925	0.000000
N	5.242867	-2.550453	0.000000
H	2.748211	-2.842234	0.000000
H	4.779180	2.532677	0.000000
H	2.461401	3.606955	0.000000
H	6.231249	-2.338090	0.000000
H	4.949728	-3.517288	0.000000
N	-1.853608	-0.227041	0.000000
C	-2.188602	1.112634	0.000000
N	-3.455192	1.546781	0.000000
C	-4.362801	0.543813	0.000000
C	-4.126526	-0.839807	0.000000
C	-2.775572	-1.305665	0.000000
N	-5.734968	0.670845	0.000000
C	-6.267800	-0.607624	0.000000
N	-5.334001	-1.543922	0.000000
O	-2.361217	-2.483045	0.000000
N	-1.183415	2.013376	0.000000
H	-0.857119	-0.506469	0.000000
H	-6.255671	1.540693	0.000000
H	-7.334874	-0.776256	0.000000
H	-1.445008	2.990696	0.000000
H	-0.180686	1.771110	0.000000

G-C

Total Energy = -4426.01 kcal mol^{-1}

N	4.900310	0.589398	0.000000
C	5.241822	-0.753223	0.000000
H	6.273428	-1.074256	0.000000
N	4.182987	-1.544775	0.000000
C	3.090396	-0.673250	0.000000
C	1.688811	-0.930410	0.000000
O	1.110949	-2.047769	0.000000
N	0.934321	0.256392	0.000000
H	-0.105803	0.145180	0.000000
C	1.457231	1.535385	0.000000
N	0.574798	2.554769	0.000000
H	-0.445237	2.406327	0.000000
H	0.942721	3.496677	0.000000
N	2.772315	1.786414	0.000000
C	3.525117	0.663559	0.000000
H	5.541750	1.374491	0.000000
N	-4.115250	0.908508	0.000000
C	-4.717741	-0.315872	0.000000
H	-5.800537	-0.319482	0.000000
C	-3.960625	-1.446103	0.000000
H	-4.413006	-2.430597	0.000000

C	-2.533305	-1.283435	0.000000
N	-1.725172	-2.354830	0.000000
H	-0.700070	-2.243257	0.000000
H	-2.122022	-3.284937	0.000000
N	-1.955412	-0.059576	0.000000
C	-2.723532	1.061745	0.000000
O	-2.246636	2.225939	0.000000
H	-4.672607	1.756987	0.000000

C-C

Total Energy = -3854.81 kcal mol^{-1}

N	3.494119	-1.081734	0.000000
C	4.644039	-0.348097	0.000000
N	4.529206	1.054947	0.000000
C	3.324237	1.697024	0.000000
C	2.169741	0.976974	0.000000
C	2.299458	-0.455472	0.000000
N	1.187348	-1.217898	0.000000
O	5.790593	-0.856632	0.000000
H	5.394328	1.586018	0.000000
H	3.355838	2.780115	0.000000
H	1.191863	1.447593	0.000000
H	1.295401	-2.225298	0.000000
H	0.243430	-0.805268	0.000000
N	-1.624309	-0.209114	0.000000
C	-1.872691	1.135659	0.000000
N	-3.218514	1.547862	0.000000
C	-4.261477	0.671876	0.000000
C	-4.021732	-0.668550	0.000000
C	-2.648295	-1.084042	0.000000
N	-2.351415	-2.400927	0.000000
O	-0.976260	2.006036	0.000000
H	-3.388405	2.548894	0.000000
H	-5.255271	1.102365	0.000000
H	-4.830421	-1.389591	0.000000
H	-1.389650	-2.712753	0.000000
H	-3.081161	-3.099986	0.000000

Cartesian Coordinates of Systems in Methanol

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in methanol, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2323.38 kcal mol^{-1}

N	-2.061396	0.752896	0.000000
C	-2.332077	-0.599167	0.000000
H	-3.346034	-0.972420	0.000000
N	-1.234814	-1.344820	0.000000
C	-0.188675	-0.419739	0.000000
C	1.219125	-0.565396	0.000000
N	1.829656	-1.770676	0.000000
N	1.981560	0.561303	0.000000
C	1.366252	1.761793	0.000000
H	2.025847	2.626244	0.000000
N	0.047095	2.026463	0.000000
C	-0.688322	0.894047	0.000000
H	-2.745164	1.501541	0.000000
H	2.839799	-1.828610	0.000000
H	1.287147	-2.623457	0.000000

T
Total Energy = -2183.69 kcal mol^{-1}

N	-1.578093	-0.872162	0.000000
C	-0.230525	-1.157567	0.000000
H	0.012592	-2.213794	0.000000
C	0.723039	-0.187279	0.000000
C	2.199107	-0.485453	0.000000
H	2.375311	-1.565018	0.000000
H	2.685312	-0.050486	-0.881687
H	2.685312	-0.050486	0.881687
C	0.284845	1.202227	0.000000
O	1.036529	2.193556	0.000000
N	-1.108728	1.389201	0.000000
H	-1.439681	2.351850	0.000000
C	-2.087902	0.410761	0.000000
O	-3.300933	0.661592	0.000000
H	-2.256182	-1.626942	0.000000

G
Total Energy = -2487.95 kcal mol^{-1}

N	1.897515	-1.284632	0.000000
C	2.893406	-0.323442	0.000000
H	3.939429	-0.593028	0.000000
N	2.408468	0.906982	0.000000
C	1.021858	0.740117	0.000000
C	-0.031550	1.703710	0.000000
O	0.035386	2.949046	0.000000
N	-1.300671	1.066920	0.000000
H	-2.098897	1.697559	0.000000

C	-1.528194	-0.294893	0.000000
N	-2.815561	-0.707562	0.000000
H	-3.587434	-0.055949	0.000000
H	-3.012882	-1.699047	0.000000
N	-0.541630	-1.190389	0.000000
C	0.689917	-0.625535	0.000000
H	2.030841	-2.289857	0.000000

C
Total Energy = -1926.15 kcal mol^{-1}

N	1.615868	-0.692460	0.000000
C	0.488902	-1.458732	0.000000
H	0.633750	-2.532023	0.000000
C	-0.736206	-0.863990	0.000000
H	-1.649706	-1.447017	0.000000
C	-0.760521	0.572162	0.000000
N	-1.944434	1.221515	0.000000
H	-1.964379	2.233577	0.000000
H	-2.819321	0.715826	0.000000
N	0.358349	1.320838	0.000000
C	1.580785	0.714968	0.000000
O	2.664388	1.344589	0.000000
H	2.532525	-1.129254	0.000000

A-A
Total Energy = -4650.60 kcal mol^{-1}

N	0.093636	-0.028543	0.000000
C	1.443674	0.016449	0.000000
N	2.234268	1.102716	0.000000
C	1.514274	2.245498	0.000000
C	0.111846	2.346130	0.000000
C	-0.614238	1.132234	0.000000
N	1.964202	3.549854	0.000000
C	0.852069	4.365252	0.000000
N	-0.286240	3.684057	0.000000
N	-1.963647	1.081505	0.000000
H	1.930056	-0.956399	0.000000
H	2.931532	3.853542	0.000000
H	0.939955	5.442092	0.000000
H	-2.511598	1.930839	0.000000
H	-2.442868	0.190774	0.000000
N	1.562474	-3.370097	0.000000
C	2.539035	-4.297094	0.000000
N	2.424921	-5.639330	0.000000
C	1.129820	-6.025117	0.000000
C	0.010308	-5.175960	0.000000
C	0.262123	-3.781584	0.000000
N	0.607751	-7.303453	0.000000
C	-0.765931	-7.182816	0.000000
N	-1.171939	-5.919728	0.000000
N	-0.718516	-2.856399	0.000000
H	3.554462	-3.906581	0.000000

H	1.134091	-8.169923	0.000000
H	-1.409985	-8.050445	0.000000
H	-1.683660	-3.159210	0.000000
H	-0.495571	-1.848264	0.000000

A-T

Total Energy = -4515.67 kcal mol^{-1}

N	3.550387	-1.747447	0.000000
C	4.262943	-0.570190	0.000000
H	5.340821	-0.685065	0.000000
C	3.654618	0.647607	0.000000
C	4.414303	1.948302	0.000000
H	5.493083	1.767048	0.000000
H	4.159737	2.549628	-0.881486
H	4.159737	2.549628	0.881486
C	2.199614	0.675537	0.000000
O	1.517402	1.727597	0.000000
N	1.559672	-0.563030	0.000000
H	0.504991	-0.568160	0.000000
C	2.167906	-1.800479	0.000000
O	1.534508	-2.868230	0.000000
H	4.038750	-2.636921	0.000000
N	-5.303783	-0.770371	0.000000
C	-5.570319	0.582614	0.000000
H	-6.582808	0.959623	0.000000
N	-4.470098	1.323918	0.000000
C	-3.428202	0.395740	0.000000
C	-2.020180	0.542669	0.000000
N	-1.388841	1.730917	0.000000
H	-0.362861	1.771544	0.000000
H	-1.927711	2.586436	0.000000
N	-1.274544	-0.599384	0.000000
C	-1.886078	-1.800869	0.000000
H	-1.217715	-2.658561	0.000000
N	-3.203829	-2.056278	0.000000
C	-3.931926	-0.916626	0.000000
H	-5.989580	-1.517198	0.000000

A-G

Total Energy = -4819.42 kcal mol^{-1}

N	-0.013742	0.008192	0.000000
C	1.364520	-0.017556	0.000000
N	2.123288	1.079591	0.000000
C	1.398158	2.222019	0.000000
C	0.000084	2.357877	0.000000
C	-0.798825	1.178531	0.000000
N	1.881459	3.510277	0.000000
C	0.788846	4.360700	0.000000
N	-0.361039	3.707500	0.000000
O	-2.052432	1.099281	0.000000
N	1.956427	-1.234839	0.000000
H	-0.529025	-0.901706	0.000000

H	2.857750	3.783931	0.000000
H	0.907733	5.434443	0.000000
H	2.965276	-1.293744	0.000000
H	1.419027	-2.087497	0.000000
N	-1.434071	-2.562206	0.000000
C	-0.793076	-3.749863	0.000000
N	-1.314736	-4.984743	0.000000
C	-2.666724	-4.952852	0.000000
C	-3.466883	-3.799819	0.000000
C	-2.801973	-2.548808	0.000000
N	-3.557413	-6.005954	0.000000
C	-4.826197	-5.465469	0.000000
N	-4.820076	-4.138667	0.000000
N	-3.452773	-1.373580	0.000000
H	0.293691	-3.706308	0.000000
H	-3.325289	-6.992961	0.000000
H	-5.707509	-6.090388	0.000000
H	-4.464261	-1.369783	0.000000
H	-2.942413	-0.479400	0.000000

A-C

Total Energy = -4252.84 kcal mol^{-1}

N	-0.009917	-0.001307	0.000000
C	1.350670	0.024281	0.000000
N	1.986017	1.282654	0.000000
C	1.292697	2.457012	0.000000
C	-0.068649	2.441017	0.000000
C	-0.708256	1.152521	0.000000
N	-2.053765	1.067394	0.000000
O	2.065181	-1.006481	0.000000
H	3.001207	1.285694	0.000000
H	1.881687	3.366081	0.000000
H	-0.645532	3.358506	0.000000
H	-2.521647	0.147062	0.000000
H	-2.611102	1.911313	0.000000
N	-3.223502	-1.652148	0.000000
C	-2.199521	-2.533930	0.000000
N	-2.264108	-3.875906	0.000000
C	-3.540833	-4.315975	0.000000
C	-4.697066	-3.516089	0.000000
C	-4.502061	-2.114935	0.000000
N	-4.007139	-5.614476	0.000000
C	-5.384631	-5.553777	0.000000
N	-5.845702	-4.309864	0.000000
N	-5.523182	-1.230857	0.000000
H	-1.211080	-2.079847	0.000000
H	-3.442890	-6.456890	0.000000
H	-5.990174	-6.448555	0.000000
H	-6.481638	-1.551595	0.000000
H	-5.340562	-0.236100	0.000000

T-T

Total Energy = -4374.93 kcal mol^{-1}

N	-0.062112	0.016039	0.000000
C	1.320479	0.008444	0.000000
N	1.884505	1.270864	0.000000
C	1.149187	2.433268	0.000000
C	-0.211924	2.431313	0.000000
C	-0.884857	1.143461	0.000000
O	-2.130859	1.005982	0.000000
O	1.994810	-1.031312	0.000000
C	-1.039477	3.689675	0.000000
H	-0.526918	-0.911307	0.000000
H	2.898407	1.311492	0.000000
H	1.732722	3.346702	0.000000
H	-1.691074	3.728181	-0.881435
H	-0.397306	4.575172	0.000000
H	-1.691074	3.728181	0.881435
N	-3.454902	-1.476180	0.000000
C	-2.638567	-2.581623	0.000000
N	-3.307395	-3.784932	0.000000
C	-4.682229	-3.885571	0.000000
C	-5.489426	-2.791368	0.000000
C	-4.858913	-1.476121	0.000000
O	-5.473419	-0.393352	0.000000
O	-1.391395	-2.513258	0.000000
C	-6.992838	-2.877052	0.000000
H	-2.977080	-0.551315	0.000000
H	-2.736075	-4.623489	0.000000
H	-5.067326	-4.898613	0.000000
H	-7.411797	-2.376069	0.881387
H	-7.322351	-3.920146	0.000000
H	-7.411797	-2.376069	-0.881387

T-G

Total Energy = -4680.20 kcal mol^{-1}

N	-0.014145	0.003221	0.000000
C	1.363618	-0.005688	0.000000
N	2.102741	1.105157	0.000000
C	1.355576	2.234161	0.000000
C	-0.046338	2.347148	0.000000
C	-0.822268	1.153419	0.000000
N	1.815730	3.530822	0.000000
C	0.708761	4.362527	0.000000
N	-0.429839	3.690206	0.000000
O	-2.075194	1.039852	0.000000
N	1.963103	-1.218805	0.000000
H	-0.511936	-0.907453	0.000000
H	2.787051	3.821671	0.000000
H	0.809372	5.438132	0.000000
H	2.972529	-1.269945	0.000000
H	1.427820	-2.076042	0.000000
N	-3.345626	-1.480739	0.000000
C	-2.524238	-2.581416	0.000000

N	-3.183444	-3.788283	0.000000
C	-4.557664	-3.899620	0.000000
C	-5.372255	-2.811311	0.000000
C	-4.750976	-1.491660	0.000000
O	-5.372753	-0.413809	0.000000
O	-1.275247	-2.509329	0.000000
C	-6.874941	-2.907603	0.000000
H	-2.880997	-0.547312	0.000000
H	-2.605869	-4.622543	0.000000
H	-4.934778	-4.915599	0.000000
H	-7.297252	-2.409559	0.881408
H	-7.196891	-3.953043	0.000000
H	-7.297252	-2.409559	-0.881408

T-C

Total Energy = -4115.53 kcal mol^{-1}

N	0.010787	0.003607	0.000000
C	1.378964	0.005679	0.000000
N	2.030712	1.256341	0.000000
C	1.360839	2.442851	0.000000
C	0.000527	2.449930	0.000000
C	-0.664832	1.175732	0.000000
N	-2.008115	1.124824	0.000000
O	2.075207	-1.030344	0.000000
H	3.045666	1.238778	0.000000
H	1.965836	3.341286	0.000000
H	-0.562687	3.375595	0.000000
H	-2.497277	0.219818	0.000000
H	-2.545381	1.981264	0.000000
N	-1.464743	-2.629838	0.000000
C	-0.765344	-3.826777	0.000000
N	-1.576594	-4.949750	0.000000
C	-2.949503	-4.902174	0.000000
C	-3.630628	-3.724684	0.000000
C	-2.856315	-2.493816	0.000000
O	-3.374765	-1.353455	0.000000
O	0.468838	-3.900117	0.000000
C	-5.134825	-3.643955	0.000000
H	-0.896039	-1.754672	0.000000
H	-1.099194	-5.845091	0.000000
H	-3.445491	-5.865959	0.000000
H	-5.497849	-3.101483	0.881530
H	-5.574850	-4.645506	0.000000
H	-5.497849	-3.101483	-0.881530

G-G

Total Energy = -4983.53 kcal mol^{-1}

N	3.030438	1.829726	0.000000
C	4.369253	1.486982	0.000000
N	4.790188	0.221737	0.000000
C	3.778703	-0.676380	0.000000

C	2.397606	-0.422437	0.000000
C	1.945437	0.925598	0.000000
N	3.886306	-2.049020	0.000000
C	2.605510	-2.567468	0.000000
N	1.683365	-1.619028	0.000000
O	0.773682	1.365073	0.000000
N	5.265365	2.496635	0.000000
H	2.775153	2.814520	0.000000
H	4.748955	-2.582175	0.000000
H	2.420704	-3.631409	0.000000
H	6.251808	2.275215	0.000000
H	4.981875	3.466397	0.000000
N	-1.847393	0.243836	0.000000
C	-2.197620	-1.092457	0.000000
N	-3.469498	-1.511764	0.000000
C	-4.365673	-0.498811	0.000000
C	-4.112970	0.881954	0.000000
C	-2.757217	1.331678	0.000000
N	-5.739147	-0.609364	0.000000
C	-6.256986	0.674752	0.000000
N	-5.312253	1.600458	0.000000
O	-2.330333	2.505440	0.000000
N	-1.202946	-2.004007	0.000000
H	-0.847403	0.512580	0.000000
H	-6.270771	-1.472723	0.000000
H	-7.322044	0.855636	0.000000
H	-1.474979	-2.978585	0.000000
H	-0.197114	-1.772587	0.000000

G-C

Total Energy = -4426.92 kcal mol^{-1}

N	4.901416	-0.588276	0.000000
C	5.242616	0.753998	0.000000
H	6.274059	1.075371	0.000000
N	4.183301	1.545475	0.000000
C	3.090930	0.673391	0.000000
C	1.689676	0.930415	0.000000
O	1.112499	2.048568	0.000000
N	0.934825	-0.255726	0.000000
H	-0.105516	-0.144519	0.000000
C	1.457952	-1.534880	0.000000
N	0.575769	-2.554118	0.000000
H	-0.444340	-2.405562	0.000000
H	0.943190	-3.496304	0.000000
N	2.773268	-1.785738	0.000000
C	3.526309	-0.663066	0.000000
H	5.543739	-1.372765	0.000000
N	-4.114635	-0.910278	0.000000
C	-4.718390	0.313595	0.000000
H	-5.801063	0.316241	0.000000
C	-3.962263	1.444500	0.000000
H	-4.415547	2.428589	0.000000

C	-2.535111	1.283314	0.000000
N	-1.727973	2.355396	0.000000
H	-0.703296	2.244732	0.000000
H	-2.125510	3.285268	0.000000
N	-1.955802	0.059595	0.000000
C	-2.723371	-1.062133	0.000000
O	-2.244760	-2.226214	0.000000
H	-4.671971	-1.758867	0.000000

C-C

Total Energy = -3855.81 kcal mol^{-1}

N	3.493374	1.080946	0.000000
C	4.642442	0.346750	0.000000
N	4.528415	-1.055228	0.000000
C	3.323417	-1.697442	0.000000
C	2.168846	-0.977410	0.000000
C	2.297894	0.454873	0.000000
N	1.186376	1.217463	0.000000
O	5.789424	0.856813	0.000000
H	5.393284	-1.586850	0.000000
H	3.355487	-2.780442	0.000000
H	1.190867	-1.448003	0.000000
H	1.295167	2.224884	0.000000
H	0.241869	0.804991	0.000000
N	-1.622912	0.209095	0.000000
C	-1.872166	-1.135196	0.000000
N	-3.217128	-1.547260	0.000000
C	-4.260326	-0.671197	0.000000
C	-4.020489	0.669125	0.000000
C	-2.647246	1.084534	0.000000
N	-2.350842	2.400974	0.000000
O	-0.974794	-2.005867	0.000000
H	-3.387687	-2.548192	0.000000
H	-5.253919	-1.101995	0.000000
H	-4.828698	1.390834	0.000000
H	-1.389704	2.714169	0.000000
H	-3.080952	3.099633	0.000000

Cartesian Coordinates of Systems in Water

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of Watson-Crick pairs and mismatched DNA base pairs in water, optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P.

A
Total Energy = -2323.73 kcal mol^{-1}

N	-2.060789	-0.754679	0.000000
C	-2.332926	0.596623	0.000000
H	-3.347366	0.968552	0.000000
N	-1.236407	1.343761	0.000000
C	-0.189194	0.419805	0.000000
C	1.218494	0.566956	0.000000
N	1.828463	1.772267	0.000000
N	1.982003	-0.559468	0.000000
C	1.367778	-1.760546	0.000000
H	2.028272	-2.624344	0.000000
N	0.048936	-2.026366	0.000000
C	-0.687859	-0.894485	0.000000
H	-2.743888	-1.503899	0.000000
H	2.838599	1.830843	0.000000
H	1.285884	2.624980	0.000000

T
Total Energy = -2323.73 kcal mol^{-1}

N	-1.577765	0.871915	0.000000
C	-0.230596	1.157264	0.000000
H	0.012647	2.213403	0.000000
C	0.722830	0.186806	0.000000
C	2.198658	0.485461	0.000000
H	2.373806	1.565134	0.000000
H	2.685144	0.051057	0.881835
H	2.685144	0.051057	-0.881835
C	0.284287	-1.201741	0.000000
O	1.036509	-2.193923	0.000000
N	-1.108401	-1.389232	0.000000
H	-1.439547	-2.351789	0.000000
C	-2.086807	-0.410505	0.000000
O	-3.300481	-0.661983	0.000000
H	-2.255429	1.627076	0.000000

G
Total Energy = -2488.68 kcal mol^{-1}

N	1.615785	0.692777	0.000000
C	0.488514	1.458552	0.000000
H	0.633036	2.531810	0.000000
C	-0.736243	0.863455	0.000000
H	-1.649595	1.446351	0.000000
C	-0.760604	-0.572297	0.000000
N	-1.944058	-1.222158	0.000000
H	-1.964083	-2.234224	0.000000
H	-2.819348	-0.716874	0.000000

N	0.359232	-1.320600	0.000000
C	1.580577	-0.713407	0.000000
O	2.664882	-1.344044	0.000000
H	2.531904	1.130658	0.000000

C

Total Energy = -1926.74 kcal mol^{-1}

N	1.895177	1.288793	0.000000
C	2.892456	0.329681	0.000000
H	3.937955	0.601285	0.000000
N	2.409824	-0.901951	0.000000
C	1.022748	-0.737203	0.000000
C	-0.028473	-1.702405	0.000000
O	0.043174	-2.948514	0.000000
N	-1.298285	-1.069791	0.000000
H	-2.095801	-1.701252	0.000000
C	-1.528988	0.291689	0.000000
N	-2.817050	0.700523	0.000000
H	-3.586594	0.045990	0.000000
H	-3.017874	1.691328	0.000000
N	-0.544176	1.189682	0.000000
C	0.688639	0.627953	0.000000
H	2.027267	2.294192	0.000000

A-A

Total Energy = -4651.15 kcal mol^{-1}

N	1.527810	-0.353049	0.000000
C	1.584632	0.996465	0.000000
N	2.677621	1.777831	0.000000
C	3.814604	1.047952	0.000000
C	3.902753	-0.355403	0.000000
C	2.682628	-1.071142	0.000000
N	5.122527	1.486397	0.000000
C	5.928096	0.367714	0.000000
N	5.237240	-0.765056	0.000000
N	2.620557	-2.419765	0.000000
H	0.616326	1.491664	0.000000
H	5.434676	2.451046	0.000000
H	7.005560	0.447081	0.000000
H	3.465120	-2.975080	0.000000
H	1.726419	-2.892461	0.000000
N	-1.808195	1.138719	0.000000
C	-2.730033	2.120180	0.000000
N	-4.072734	2.013400	0.000000
C	-4.465692	0.720178	0.000000
C	-3.622466	-0.403894	0.000000
C	-2.226609	-0.159639	0.000000
N	-5.746776	0.205155	0.000000
C	-5.634123	-1.168856	0.000000
N	-4.373153	-1.582134	0.000000
N	-1.306166	-1.144536	0.000000
H	-2.334000	3.133494	0.000000

H	-6.610486	0.736061	0.000000
H	-6.505421	-1.807891	0.000000
H	-1.613689	-2.108225	0.000000
H	-0.297029	-0.926208	0.000000

A-T

Total Energy = -4516.43 kcal mol^{-1}

N	3.554274	1.744807	0.000000
C	4.265128	0.566791	0.000000
H	5.343065	0.679979	0.000000
C	3.654926	-0.650064	0.000000
C	4.413263	-1.951381	0.000000
H	5.492044	-1.770512	0.000000
H	4.158456	-2.552407	0.881642
H	4.158456	-2.552407	-0.881642
C	2.200569	-0.675645	0.000000
O	1.516413	-1.727156	0.000000
N	1.562087	0.563437	0.000000
H	0.508039	0.570465	0.000000
C	2.172750	1.799434	0.000000
O	1.540346	2.868687	0.000000
H	4.044588	2.633212	0.000000
N	-5.306702	0.769041	0.000000
C	-5.571416	-0.583814	0.000000
H	-6.583452	-0.961963	0.000000
N	-4.470147	-1.324017	0.000000
C	-3.429354	-0.394386	0.000000
C	-2.021062	-0.539188	0.000000
N	-1.387747	-1.726294	0.000000
H	-0.361636	-1.765268	0.000000
H	-1.925114	-2.582696	0.000000
N	-1.276652	0.603903	0.000000
C	-1.890144	1.804195	0.000000
H	-1.223651	2.663302	0.000000
N	-3.208368	2.057978	0.000000
C	-3.935308	0.917220	0.000000
H	-5.993650	1.514749	0.000000

A-G

Total Energy = -4820.39 kcal mol^{-1}

N	1.485720	0.289198	0.000000
C	2.163366	1.489539	0.000000
N	3.494338	1.585737	0.000000
C	4.110072	0.381199	0.000000
C	3.516863	-0.891987	0.000000
C	2.095454	-0.980440	0.000000
N	5.464983	0.142832	0.000000
C	5.642869	-1.229689	0.000000
N	4.496024	-1.889070	0.000000
O	1.391256	-2.021476	0.000000
N	1.417374	2.618469	0.000000
H	0.439880	0.305859	0.000000

H	6.196555	0.844972	0.000000
H	6.628475	-1.671877	0.000000
H	1.880635	3.516651	0.000000
H	0.409661	2.592081	0.000000
N	-1.447964	0.353938	0.000000
C	-2.143920	1.509760	0.000000
N	-3.472493	1.688875	0.000000
C	-4.132803	0.508453	0.000000
C	-3.547304	-0.767287	0.000000
C	-2.132068	-0.830535	0.000000
N	-5.492281	0.277740	0.000000
C	-5.673364	-1.088929	0.000000
N	-4.528154	-1.759539	0.000000
N	-1.449203	-1.987656	0.000000
H	-1.552631	2.422432	0.000000
H	-6.223328	0.980290	0.000000
H	-6.660094	-1.528817	0.000000
H	-1.958160	-2.861760	0.000000
H	-0.419757	-1.998960	0.000000

A-C

Total Energy = -4253.58 kcal mol^{-1}

N	-0.005696	0.007279	-0.143854
C	1.354115	0.039524	-0.137959
N	1.984622	1.291135	-0.000363
C	1.286352	2.456313	0.120594
C	-0.074862	2.435259	0.115200
C	-0.709070	1.151688	-0.019174
N	-2.054201	1.060749	-0.028456
O	2.072215	-0.984593	-0.248332
H	2.999788	1.298986	0.003255
H	1.871476	3.362450	0.218226
H	-0.655808	3.345272	0.210469
H	-2.516641	0.138598	-0.070920
H	-2.613591	1.894099	0.096222
N	-3.214408	-1.659607	-0.083545
C	-2.194680	-2.545689	-0.063568
N	-2.265800	-3.886346	-0.007566
C	-3.544461	-4.319311	0.034215
C	-4.696727	-3.512700	0.023757
C	-4.494726	-2.114628	-0.041198
N	-4.017219	-5.613736	0.091607
C	-5.393731	-5.545164	0.114163
N	-5.848996	-4.299577	0.075384
N	-5.511671	-1.222001	-0.040503
H	-1.204089	-2.098093	-0.098721
H	-3.457980	-6.459279	0.111109
H	-6.003428	-6.435990	0.158590
H	-6.465512	-1.545104	-0.134431
H	-5.320758	-0.244732	-0.221678

T-T

Total Energy = -4376.31 kcal mol^{-1}

N	2.111167	0.863623	0.000000
C	3.248151	1.649986	0.000000
N	4.426179	0.927631	0.000000
C	4.475715	-0.446561	0.000000
C	3.351142	-1.213552	0.000000
C	2.069535	-0.530700	0.000000
O	0.962174	-1.120534	0.000000
O	3.217042	2.889654	0.000000
C	3.379704	-2.719279	0.000000
H	1.203831	1.366350	0.000000
H	5.286308	1.466072	0.000000
H	5.473005	-0.870847	0.000000
H	2.864514	-3.119488	0.881750
H	4.410075	-3.086098	0.000000
H	2.864514	-3.119488	-0.881750
N	-1.531117	0.188417	0.000000
C	-1.481102	1.561586	0.000000
N	-2.711593	2.177353	0.000000
C	-3.902894	1.484836	0.000000
C	-3.951883	0.125892	0.000000
C	-2.689682	-0.602895	0.000000
O	-2.585417	-1.844849	0.000000
O	-0.411486	2.207677	0.000000
C	-5.242030	-0.650614	0.000000
H	-0.615025	-0.305028	0.000000
H	-2.714070	3.192071	0.000000
H	-4.792531	2.103508	0.000000
H	-5.306287	-1.300287	-0.881602
H	-6.101652	0.025850	0.000000
H	-5.306287	-1.300287	0.881602

T-G

Total Energy = -4681.33 kcal mol^{-1}

N	1.729710	0.722213	0.000000
C	2.770779	1.624009	0.000000
N	4.054652	1.259992	0.000000
C	4.220066	-0.083612	0.000000
C	3.227234	-1.079944	0.000000
C	1.862564	-0.675741	0.000000
N	5.411595	-0.771249	0.000000
C	5.110115	-2.122098	0.000000
N	3.807343	-2.350769	0.000000
O	0.835474	-1.403766	0.000000
N	2.437558	2.935156	0.000000
H	0.760116	1.092830	0.000000
H	6.339371	-0.362008	0.000000
H	5.885227	-2.874443	0.000000
H	3.169826	3.631818	0.000000
H	1.472972	3.236803	0.000000
N	-1.760798	-0.293397	0.000000
C	-1.847758	1.077023	0.000000

N	-3.131055	1.569337	0.000000
C	-4.249729	0.763943	0.000000
C	-4.165434	-0.593151	0.000000
C	-2.837562	-1.194444	0.000000
O	-2.611053	-2.419253	0.000000
O	-0.847804	1.829462	0.000000
C	-5.373005	-1.492530	0.000000
H	-0.802662	-0.704128	0.000000
H	-3.232249	2.578967	0.000000
H	-5.195168	1.293381	0.000000
H	-5.372746	-2.145289	-0.881622
H	-6.294831	-0.903825	0.000000
H	-5.372746	-2.145289	0.881622

T-C

Total Energy = -4116.85 kcal mol^{-1}

N	1.946815	0.358100	0.000000
C	2.752992	1.462682	0.000000
N	4.146656	1.256123	0.000000
C	4.712804	0.016812	0.000000
C	3.919450	-1.088142	0.000000
C	2.497880	-0.877854	0.000000
N	1.666947	-1.934600	0.000000
O	2.322134	2.635877	0.000000
H	4.730107	2.086820	0.000000
H	5.795176	-0.020988	0.000000
H	4.337707	-2.087614	0.000000
H	0.647165	-1.800282	0.000000
H	2.044822	-2.872428	0.000000
N	-1.053705	0.700690	0.000000
C	-1.610303	1.969491	0.000000
N	-2.994353	1.975871	0.000000
C	-3.764277	0.838237	0.000000
C	-3.213170	-0.405347	0.000000
C	-1.762937	-0.503971	0.000000
O	-1.145841	-1.594869	0.000000
O	-0.942080	3.011214	0.000000
C	-4.032953	-1.668792	0.000000
H	-0.011528	0.646423	0.000000
H	-3.437024	2.888839	0.000000
H	-4.835282	1.005053	0.000000
H	-3.807866	-2.281219	-0.881703
H	-5.101471	-1.434908	0.000000
H	-3.807866	-2.281219	0.881703

G-G

Total Energy = -4984.93 kcal mol^{-1}

N	3.010318	-1.864035	0.000000
C	4.352428	-1.533896	0.000000
N	4.785256	-0.272447	0.000000
C	3.782234	0.635085	0.000000

C	2.398755	0.393541	0.000000
C	1.934778	-0.950094	0.000000
N	3.902317	2.006586	0.000000
C	2.626661	2.536810	0.000000
N	1.695597	1.596826	0.000000
O	0.757806	-1.378230	0.000000
N	5.238179	-2.552286	0.000000
H	2.747126	-2.846661	0.000000
H	4.769726	2.531924	0.000000
H	2.451575	3.602339	0.000000
H	6.226888	-2.341248	0.000000
H	4.943961	-3.518908	0.000000
N	-1.846394	-0.218599	0.000000
C	-2.185178	1.120919	0.000000
N	-3.453877	1.550873	0.000000
C	-4.358679	0.545787	0.000000
C	-4.116758	-0.837021	0.000000
C	-2.765206	-1.297162	0.000000
N	-5.731131	0.666991	0.000000
C	-6.259085	-0.612580	0.000000
N	-5.321744	-1.546180	0.000000
O	-2.348951	-2.475964	0.000000
N	-1.182670	2.022997	0.000000
H	-0.848640	-0.496111	0.000000
H	-6.256222	1.534376	0.000000
H	-7.325497	-0.784911	0.000000
H	-1.444607	3.000377	0.000000
H	-0.178969	1.780901	0.000000

G-C

Total Energy = -4427.71 kcal mol^{-1}

N	4.901799	0.590695	0.000000
C	5.243841	-0.750864	0.000000
H	6.275571	-1.071169	0.000000
N	4.184992	-1.543464	0.000000
C	3.092040	-0.671844	0.000000
C	1.691237	-0.929879	0.000000
O	1.115945	-2.049614	0.000000
N	0.935052	0.254720	0.000000
H	-0.105354	0.142864	0.000000
C	1.457118	1.534372	0.000000
N	0.574150	2.552715	0.000000
H	-0.445892	2.402859	0.000000
H	0.940470	3.495377	0.000000
N	2.772396	1.786596	0.000000
C	3.526814	0.664796	0.000000
H	5.544207	1.375158	0.000000
N	-4.114687	0.909435	0.000000
C	-4.718501	-0.314221	0.000000
H	-5.801161	-0.316266	0.000000
C	-3.962316	-1.445130	0.000000
H	-4.415181	-2.429297	0.000000

C	-2.535564	-1.283827	0.000000
N	-1.728540	-2.356313	0.000000
H	-0.704261	-2.245862	0.000000
H	-2.126600	-3.286017	0.000000
N	-1.955941	-0.060160	0.000000
C	-2.724157	1.061020	0.000000
O	-2.245017	2.225605	0.000000
H	-4.672459	1.757716	0.000000

C-C

Total Energy = -3857.18 kcal mol^{-1}

N	3.490980	-1.085048	0.000000
C	4.638946	-0.349930	0.000000
N	4.525694	1.050994	0.000000
C	3.320619	1.693091	0.000000
C	2.166317	0.972969	0.000000
C	2.294744	-0.459194	0.000000
N	1.183080	-1.220775	0.000000
O	5.786595	-0.861248	0.000000
H	5.390000	1.583511	0.000000
H	3.352802	2.776007	0.000000
H	1.188669	1.444032	0.000000
H	1.287588	-2.228706	0.000000
H	0.239467	-0.805740	0.000000
N	-1.619905	-0.199494	0.000000
C	-1.875456	1.142961	0.000000
N	-3.220884	1.550125	0.000000
C	-4.260405	0.669706	0.000000
C	-4.015245	-0.669520	0.000000
C	-2.640685	-1.079666	0.000000
N	-2.338424	-2.394598	0.000000
O	-0.980401	2.017633	0.000000
H	-3.396463	2.550184	0.000000
H	-5.255594	1.096570	0.000000
H	-4.820528	-1.394280	0.000000
H	-1.375712	-2.703353	0.000000
H	-3.065800	-3.096232	0.000000

Cartesian Coordinates of Systems in the Gas Phase

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in the gas phase and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6811.31 kcal mol^{-1}

N	3.400000	-3.347540	3.658540
C	3.400000	-2.397030	4.671780
H	3.400000	-2.681960	5.715260
N	3.400000	-1.159220	4.215310
C	3.400000	-1.302430	2.829850
C	3.400000	-0.355730	1.777100
N	3.400000	0.977200	1.975600
H	3.400000	1.624810	1.176700
H	3.400000	1.325800	2.923850
N	3.400000	-0.840910	0.506980
C	3.400000	-2.175180	0.291820
H	3.400000	-2.469350	-0.755500
N	3.400000	-3.154370	1.206420
C	3.400000	-2.657550	2.457800
H	3.400000	-4.355150	3.758620
N	0.000000	-0.557870	4.927440
C	0.000000	0.806670	5.188510
H	0.000000	1.189480	6.200180
N	0.000000	1.539790	4.091650
C	0.000000	0.609600	3.054950
C	0.047417	0.732803	1.646661
N	0.095725	1.946530	1.017025
H	0.418513	1.935516	0.056358
H	0.364616	2.745770	1.577491
N	0.032046	-0.387376	0.895667
C	0.000000	-1.588260	1.514600
H	0.000000	-2.441830	0.840190
N	0.000000	-1.842880	2.830070
C	0.000000	-0.705410	3.550450
H	0.000000	-1.314230	5.600660
N	3.400000	1.037590	-4.052020
C	3.400000	2.413070	-3.934160
H	3.400000	2.959580	-4.872760
C	3.400000	3.037780	-2.728660
C	3.400000	4.534090	-2.562880
H	3.400000	5.038710	-3.534810
H	2.520700	4.860760	-1.994620
H	4.279300	4.860760	-1.994620
C	3.400000	2.200590	-1.524570
O	3.400000	2.662200	-0.368820
N	3.400000	0.821360	-1.737060
H	3.400000	0.195070	-0.879400

C	3.400000	0.166150	-2.955090
O	3.400000	-1.054960	-3.085570
H	3.400000	0.589550	-4.960710

[X]-T/A-T

Total Energy = -6668.66 kcal mol^{-1}

N	0.000000	1.533160	3.908900
C	0.000000	0.355140	4.619750
H	0.000000	0.468330	5.697690
C	0.000000	-0.861710	4.009550
C	0.000000	-2.163030	4.767890
H	0.000000	-1.982160	5.846670
H	-0.881640	-2.764050	4.513080
H	0.881640	-2.764050	4.513080
C	0.023980	-0.923697	2.544437
O	0.053801	-1.957486	1.879413
N	0.018240	0.340153	1.919648
H	0.070240	0.350026	0.903374
C	0.000000	1.587790	2.527370
O	0.000000	2.657040	1.894970
H	0.000000	2.421570	4.399210
N	3.400000	3.361630	-3.678750
C	3.400000	2.422730	-4.688080
H	3.400000	2.711640	-5.729110
N	3.400000	1.176590	-4.232190
C	3.400000	1.316940	-2.843750
C	3.400000	0.372040	-1.789510
N	3.400000	-0.960610	-1.974890
H	3.400000	-1.595260	-1.167650
H	3.400000	-1.337610	-2.913000
N	3.400000	0.859290	-0.515390
C	3.400000	2.190950	-0.306230
H	3.400000	2.494250	0.737940
N	3.400000	3.171080	-1.223540
C	3.400000	2.675450	-2.482160
H	3.400000	4.368700	-3.796210
N	3.400000	-1.057160	4.063550
C	3.400000	-2.428030	3.946250
H	3.400000	-2.970040	4.884860
C	3.400000	-3.053840	2.737350
C	3.400000	-4.552370	2.585990
H	3.400000	-5.040120	3.565060
H	2.518360	-4.888850	2.026580
H	4.281640	-4.888850	2.026580
C	3.400000	-2.219710	1.545700
O	3.400000	-2.668280	0.374150
N	3.400000	-0.841980	1.757440
H	3.400000	-0.216750	0.908820
C	3.400000	-0.200950	2.977970
O	3.400000	1.035810	3.094810
H	3.400000	-0.626610	4.982410

[X]-G/C-G

Total Energy = -6875.30 kcal mol^{-1}

N	0.000000	-0.540430	-4.633030
C	0.000000	0.817480	-4.958940
H	0.000000	1.151430	-5.987600
N	0.000000	1.591540	-3.897360
C	0.000000	0.713210	-2.815430
C	0.000000	0.955460	-1.405610
O	0.000000	2.048290	-0.799970
N	0.000000	-0.256350	-0.673220
H	0.000000	-0.155580	0.362980
C	0.000000	-1.525410	-1.212990
N	0.000000	-2.560920	-0.339360
H	0.000000	-2.431150	0.679960
H	0.000000	-3.490190	-0.733710
N	0.000000	-1.759750	-2.524530
C	0.000000	-0.624200	-3.255860
H	0.000000	-1.330440	-5.266030
N	0.000000	-0.867700	4.373220
C	0.000000	0.366100	4.957330
H	0.000000	0.391340	6.041790
C	0.000000	1.486220	4.186840
H	0.000000	2.474530	4.632760
C	0.000000	1.305210	2.753260
N	0.000000	2.362310	1.928080
H	0.000000	2.233580	0.887950
H	0.000000	3.296500	2.312560
N	0.000000	0.079090	2.198460
C	0.000000	-1.045010	2.964680
O	0.000000	-2.204330	2.517570
H	0.000000	-1.717810	4.926450
N	3.400000	2.285930	-4.065900
C	3.400000	3.576080	-3.531430
H	3.400000	4.450870	-4.167360
N	3.400000	3.578350	-2.217610
C	3.400000	2.231830	-1.858560
C	3.357253	1.619649	-0.556427
O	3.344748	2.102468	0.571372
N	3.325720	0.178888	-0.706194
H	3.300997	-0.320344	0.179115
C	3.297587	-0.521965	-1.888359
N	3.268994	-1.906597	-1.796646
H	2.726124	-2.277346	-1.020388
H	2.991338	-2.327164	-2.679047
N	3.336582	0.055041	-3.073074
C	3.387345	1.413495	-2.998952
H	3.317899	2.019720	-5.038423

[X]-C/G-C

Total Energy = -6310.86 kcal mol^{-1}

N	0.000000	-0.540430	-4.633030
C	0.000000	0.817480	-4.958940

H	0.000000	1.151430	-5.987600
N	0.000000	1.591540	-3.897360
C	0.000000	0.713210	-2.815430
C	0.000000	0.955460	-1.405610
O	0.000000	2.048290	-0.799970
N	0.000000	-0.256350	-0.673220
H	0.000000	-0.155580	0.362980
C	0.000000	-1.525410	-1.212990
N	0.000000	-2.560920	-0.339360
H	0.000000	-2.431150	0.679960
H	0.000000	-3.490190	-0.733710
N	0.000000	-1.759750	-2.524530
C	0.000000	-0.624200	-3.255860
H	0.000000	-1.330440	-5.266030
N	0.000000	-0.867700	4.373220
C	0.000000	0.366100	4.957330
H	0.000000	0.391340	6.041790
C	0.000000	1.486220	4.186840
H	0.000000	2.474530	4.632760
C	0.000000	1.305210	2.753260
N	0.000000	2.362310	1.928080
H	0.000000	2.233580	0.887950
H	0.000000	3.296500	2.312560
N	0.000000	0.079090	2.198460
C	0.000000	-1.045010	2.964680
O	0.000000	-2.204330	2.517570
H	0.000000	-1.717810	4.926450
C	3.348361	-2.593078	1.759564
O	3.317714	-3.271959	0.739898
H	3.400000	-4.285370	2.975960
N	3.400000	-3.272440	3.028050
C	3.400000	-2.617580	4.225800
H	3.400000	-3.234580	5.117990
C	3.400000	-1.258500	4.260820
H	3.400000	-0.721030	5.202490
C	3.359759	-0.589175	2.979931
N	3.368920	0.783132	2.942940
H	3.142831	1.194922	2.043267
H	3.079907	1.296785	3.764666
N	3.334136	-1.217615	1.815717

Cartesian Coordinates of Systems in Toluene

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in toluene that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in toluene and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6828.64 kcal mol^{-1}

N	4.057353	1.043013	0.000000
C	3.941419	2.416655	0.000000
H	4.880847	2.959600	0.000000
C	2.735236	3.043608	0.000000
C	2.577895	4.541318	0.000000
H	3.553621	5.037271	0.000000
H	2.014060	4.873287	-0.880298
H	2.014060	4.873287	0.880298
C	1.535749	2.209171	0.000000
O	0.373351	2.665887	0.000000
N	1.746255	0.830358	0.000000
H	0.891875	0.205333	0.000000
C	2.964775	0.180402	0.000000
O	3.086987	-1.048029	0.000000
H	4.970473	0.602185	0.000000
N	-3.667792	-3.353488	0.000000
C	-4.679668	-2.409629	0.000000
H	-5.721578	-2.697699	0.000000
N	-4.224369	-1.167312	0.000000
C	-2.837192	-1.307987	0.000000
C	-1.784431	-0.361440	0.000000
N	-1.977372	0.971213	0.000000
H	-1.174997	1.612807	0.000000
H	-2.920476	1.334490	0.000000
N	-0.512115	-0.846836	0.000000
C	-0.298722	-2.179557	0.000000
H	0.747205	-2.477407	0.000000
N	-1.214189	-3.159777	0.000000
C	-2.469457	-2.664381	0.000000
H	-3.777479	-4.360778	0.000000
N	-4.938437	-0.557155	-3.400000
C	-5.202275	0.801209	-3.400000
H	-6.214521	1.180575	-3.400000
N	-4.103715	1.538646	-3.400000
C	-3.064152	0.609476	-3.400000
C	-1.655916	0.736316	-3.358020
N	-1.025560	1.946611	-3.322121
H	-0.056107	1.944554	-3.025841
H	-1.576411	2.757378	-3.067878
N	-0.904226	-0.387210	-3.375301
C	-1.522783	-1.587714	-3.400000
H	-0.851682	-2.443460	-3.400000

N	-2.839570	-1.842631	-3.400000
C	-3.563916	-0.704019	-3.400000
H	-5.619246	-1.307597	-3.400000

[X]-T/A-T

Total Energy = -6687.78 kcal mol^{-1}

N	4.057353	1.043013	0.000000
C	3.941419	2.416655	0.000000
H	4.880847	2.959600	0.000000
C	2.735236	3.043608	0.000000
C	2.577895	4.541318	0.000000
H	3.553621	5.037271	0.000000
H	2.014060	4.873287	-0.880298
H	2.014060	4.873287	0.880298
C	1.535749	2.209171	0.000000
O	0.373351	2.665887	0.000000
N	1.746255	0.830358	0.000000
H	0.891875	0.205333	0.000000
C	2.964775	0.180402	0.000000
O	3.086987	-1.048029	0.000000
H	4.970473	0.602185	0.000000
N	-3.667792	-3.353488	0.000000
C	-4.679668	-2.409629	0.000000
H	-5.721578	-2.697699	0.000000
N	-4.224369	-1.167312	0.000000
C	-2.837192	-1.307987	0.000000
C	-1.784431	-0.361440	0.000000
N	-1.977372	0.971213	0.000000
H	-1.174997	1.612807	0.000000
H	-2.920476	1.334490	0.000000
N	-0.512115	-0.846836	0.000000
C	-0.298722	-2.179557	0.000000
H	0.747205	-2.477407	0.000000
N	-1.214189	-3.159777	0.000000
C	-2.469457	-2.664381	0.000000
H	-3.777479	-4.360778	0.000000
N	3.895535	-1.541037	-3.400000
C	4.609149	-0.361593	-3.400000
H	5.688297	-0.474523	-3.400000
C	4.001840	0.854599	-3.400000
C	4.754881	2.158755	-3.400000
H	5.835773	1.986472	-3.400000
H	4.493855	2.758737	-2.519702
H	4.493855	2.758737	-4.280298
C	2.539269	0.910048	-3.399235
O	1.865735	1.944905	-3.407141
N	1.904309	-0.348841	-3.384829
H	0.886688	-0.345780	-3.366222
C	2.504591	-1.596703	-3.400000
O	1.881409	-2.662359	-3.400000
H	4.375152	-2.434393	-3.400000

[X]-G/C-G

Total Energy = -6898.43 kcal mol^{-1}

N	4.076955	2.282074	0.000000
C	3.553157	3.570393	0.000000
H	4.193352	4.441230	0.000000
N	2.235147	3.579874	0.000000
C	1.870089	2.232889	0.000000
C	0.572428	1.623152	-0.027342
O	-0.555207	2.124621	-0.022556
N	0.706401	0.191885	-0.063897
H	-0.179784	-0.306674	-0.085244
C	1.884759	-0.517842	-0.052734
N	1.788908	-1.894332	-0.051834
H	0.972678	-2.290468	-0.508745
H	2.653073	-2.348517	-0.331630
N	3.073888	0.058902	0.000000
C	3.010119	1.409022	0.000000
H	5.055666	2.020542	0.000000
N	-4.371795	-0.877259	-3.400000
C	-4.966237	0.351364	-3.400000
H	-6.049879	0.364474	-3.400000
C	-4.203398	1.477346	-3.400000
H	-4.653048	2.463559	-3.400000
C	-2.772787	1.306652	-3.400000
N	-1.957458	2.371675	-3.400000
H	-0.926211	2.253231	-3.400000
H	-2.347919	3.303906	-3.400000
N	-2.205393	0.081859	-3.400000
C	-2.972232	-1.041121	-3.400000
O	-2.509023	-2.202613	-3.400000
H	-4.926837	-1.726802	-3.400000
N	4.639695	-0.550137	-3.400000
C	4.973189	0.800015	-3.400000
H	6.002983	1.128240	-3.400000
N	3.912469	1.582392	-3.400000
C	2.825393	0.707234	-3.400000
C	1.419438	0.956720	-3.400000
O	0.827178	2.061277	-3.400000
N	0.676356	-0.242888	-3.400000
H	-0.361888	-0.136918	-3.400000
C	1.207633	-1.516787	-3.400000
N	0.329892	-2.544184	-3.400000
H	-0.689787	-2.404858	-3.400000
H	0.709678	-3.480515	-3.400000
N	2.520192	-1.759909	-3.393628
C	3.264348	-0.628368	-3.398373
H	5.278985	-1.335785	-3.401025

[X]-C/G-C

Total Energy = -6333.81 kcal mol^{-1}

N	2.521449	-1.759133	-3.400000
C	3.263440	-0.629381	-3.400000

H	5.277765	-1.336993	-3.400000
N	-4.371795	-0.877259	-3.400000
C	-4.966237	0.351364	-3.400000
H	-6.049879	0.364474	-3.400000
C	-4.203398	1.477346	-3.400000
H	-4.653048	2.463559	-3.400000
C	-2.772787	1.306652	-3.400000
N	-1.957458	2.371675	-3.400000
H	-0.926211	2.253231	-3.400000
H	-2.347919	3.303906	-3.400000
N	-2.205393	0.081859	-3.400000
C	-2.972232	-1.041121	-3.400000
O	-2.509023	-2.202613	-3.400000
H	-4.926837	-1.726802	-3.400000
N	-3.021217	-3.279394	0.000000
C	-4.224297	-2.634821	0.000000
H	-5.108687	-3.261164	0.000000
C	-4.268983	-1.275497	0.000000
H	-5.212439	-0.741932	0.000000
C	-2.998490	-0.593809	-0.015574
N	-2.971706	0.771372	-0.016145
H	-2.078336	1.211789	-0.206265
H	-3.805571	1.288319	-0.260224
N	-1.824826	-1.221855	-0.000070
C	-1.773577	-2.592293	0.017411
O	-0.734414	-3.261602	0.051955
H	-2.970906	-4.292934	0.000000
N	4.639695	-0.550137	-3.400000
C	4.973189	0.800015	-3.400000
H	6.002983	1.128240	-3.400000
N	3.912469	1.582392	-3.400000
C	2.825393	0.707234	-3.400000
C	1.419438	0.956720	-3.400000
O	0.827178	2.061277	-3.400000
N	0.676356	-0.242888	-3.400000
H	-0.361888	-0.136918	-3.400000
C	1.207633	-1.516787	-3.400000
N	0.329892	-2.544184	-3.400000
H	-0.689787	-2.404858	-3.400000
H	0.709678	-3.480515	-3.400000

Cartesian Coordinates of Systems in Chloroform

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in chloroform that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in chloroform and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6836.49 kcal mol^{-1}

N	4.059093	1.042702	0.000000
C	3.945820	2.415466	0.000000
H	4.886193	2.955660	0.000000
C	2.739982	3.045090	0.000000
C	2.589175	4.543656	0.000000
H	3.567577	5.033664	0.000000
H	2.028152	4.879095	-0.880871
H	2.028152	4.879095	0.880871
C	1.541768	2.213722	0.000000
O	0.376242	2.668952	0.000000
N	1.749786	0.834864	0.000000
H	0.896288	0.211678	0.000000
C	2.967567	0.185580	0.000000
O	3.083577	-1.046749	0.000000
H	4.973857	0.604385	0.000000
N	-3.670754	-3.356208	0.000000
C	-4.683046	-2.416187	0.000000
H	-5.724262	-2.705501	0.000000
N	-4.229193	-1.171485	0.000000
C	-2.841204	-1.309778	0.000000
C	-1.789000	-0.362572	0.000000
N	-1.979387	0.969938	0.000000
H	-1.175101	1.608585	0.000000
H	-2.920194	1.339658	0.000000
N	-0.515430	-0.847649	0.000000
C	-0.301793	-2.179546	0.000000
H	0.743892	-2.477942	0.000000
N	-1.217013	-3.160707	0.000000
C	-2.474306	-2.666588	0.000000
H	-3.781924	-4.363691	0.000000
N	-4.942432	-0.557614	-3.400000
C	-5.208863	0.797889	-3.400000
H	-6.221279	1.175841	-3.400000
N	-4.110071	1.538106	-3.400000
C	-3.068451	0.610385	-3.400000
C	-1.660397	0.739490	-3.359204
N	-1.031189	1.949259	-3.326538
H	-0.059916	1.952515	-3.035725
H	-1.580957	2.762610	-3.077735
N	-0.907517	-0.385045	-3.377882
C	-1.525261	-1.585900	-3.400000
H	-0.854677	-2.441946	-3.400000

N	-2.842401	-1.841723	-3.400000
C	-3.569137	-0.702954	-3.400000
H	-5.624554	-1.307341	-3.400000

[X]-T/A-T

Total Energy = -6695.69 kcal mol^{-1}

N	4.059093	1.042702	0.000000
C	3.945820	2.415466	0.000000
H	4.886193	2.955660	0.000000
C	2.739982	3.045090	0.000000
C	2.589175	4.543656	0.000000
H	3.567577	5.033664	0.000000
H	2.028152	4.879095	-0.880871
H	2.028152	4.879095	0.880871
C	1.541768	2.213722	0.000000
O	0.376242	2.668952	0.000000
N	1.749786	0.834864	0.000000
H	0.896288	0.211678	0.000000
C	2.967567	0.185580	0.000000
O	3.083577	-1.046749	0.000000
H	4.973857	0.604385	0.000000
N	-3.670754	-3.356208	0.000000
C	-4.683046	-2.416187	0.000000
H	-5.724262	-2.705501	0.000000
N	-4.229193	-1.171485	0.000000
C	-2.841204	-1.309778	0.000000
C	-1.789000	-0.362572	0.000000
N	-1.979387	0.969938	0.000000
H	-1.175101	1.608585	0.000000
H	-2.920194	1.339658	0.000000
N	-0.515430	-0.847649	0.000000
C	-0.301793	-2.179546	0.000000
H	0.743892	-2.477942	0.000000
N	-1.217013	-3.160707	0.000000
C	-2.474306	-2.666588	0.000000
H	-3.781924	-4.363691	0.000000
N	3.896760	-1.542311	-3.400000
C	4.612011	-0.365142	-3.400000
H	5.690306	-0.480853	-3.400000
C	4.006551	0.853009	-3.400000
C	4.765380	2.154016	-3.400000
H	5.844944	1.975350	-3.400000
H	4.508670	2.755153	-2.519129
H	4.508670	2.755153	-4.280871
C	2.546724	0.908841	-3.409102
O	1.869996	1.944483	-3.433076
N	1.909961	-0.347689	-3.386369
H	0.892156	-0.344012	-3.381519
C	2.509893	-1.594155	-3.400000
O	1.879403	-2.659319	-3.400000
H	4.379183	-2.434602	-3.400000

[X]-G/C-G

Total Energy = -6909.27 kcal mol^{-1}

N	4.080907	2.282536	0.000000
C	3.560413	3.568694	0.000000
H	4.203004	4.437477	0.000000
N	2.240337	3.580636	0.000000
C	1.874410	2.232811	0.000000
C	0.578788	1.624048	-0.017876
O	-0.547737	2.137300	-0.000489
N	0.703700	0.198317	-0.058527
H	-0.182507	-0.300914	-0.071204
C	1.881170	-0.515825	-0.048989
N	1.782080	-1.887199	-0.045464
H	0.946521	-2.291747	-0.456240
H	2.636990	-2.357417	-0.325901
N	3.073152	0.059165	0.000000
C	3.014616	1.409864	0.000000
H	5.061841	2.027709	0.000000
N	-4.370385	-0.882571	-3.400000
C	-4.970202	0.343339	-3.400000
H	-6.053435	0.350440	-3.400000
C	-4.211416	1.472265	-3.400000
H	-4.663331	2.457246	-3.400000
C	-2.782397	1.307081	-3.400000
N	-1.971861	2.376033	-3.400000
H	-0.944008	2.262184	-3.400000
H	-2.366151	3.306952	-3.400000
N	-2.208384	0.083090	-3.400000
C	-2.974974	-1.039662	-3.400000
O	-2.503388	-2.202130	-3.400000
H	-4.926090	-1.731952	-3.400000
N	4.643164	-0.552087	-3.400000
C	4.978060	0.794376	-3.400000
H	6.008585	1.119531	-3.400000
N	3.917116	1.579958	-3.400000
C	2.828843	0.704631	-3.400000
C	1.425088	0.956359	-3.400000
O	0.839142	2.066991	-3.400000
N	0.677344	-0.237459	-3.400000
H	-0.362095	-0.129455	-3.400000
C	1.206118	-1.513385	-3.400000
N	0.327071	-2.537595	-3.400000
H	-0.692909	-2.394388	-3.400000
H	0.701181	-3.476676	-3.400000
N	2.519825	-1.758778	-3.395969
C	3.267884	-0.630426	-3.398830
H	5.284749	-1.336404	-3.397046

[X]-C/G-C

Total Energy = -6345.01 kcal mol^{-1}

N	2.521009	-1.758488	-3.400000
C	3.267573	-0.631343	-3.400000

H	5.286973	-1.334825	-3.400000
N	-4.370385	-0.882571	-3.400000
C	-4.970202	0.343339	-3.400000
H	-6.053435	0.350440	-3.400000
C	-4.211416	1.472265	-3.400000
H	-4.663331	2.457246	-3.400000
C	-2.782397	1.307081	-3.400000
N	-1.971861	2.376033	-3.400000
H	-0.944008	2.262184	-3.400000
H	-2.366151	3.306952	-3.400000
N	-2.208384	0.083090	-3.400000
C	-2.974974	-1.039662	-3.400000
O	-2.503388	-2.202130	-3.400000
H	-4.926090	-1.731952	-3.400000
N	-3.016954	-3.282863	0.000000
C	-4.222787	-2.643644	0.000000
H	-5.103315	-3.274608	0.000000
C	-4.272483	-1.284321	0.000000
H	-5.217047	-0.753083	0.000000
C	-3.007662	-0.595901	-0.008158
N	-2.985467	0.764455	-0.016103
H	-2.096043	1.221146	-0.181276
H	-3.826783	1.285682	-0.221872
N	-1.828926	-1.224474	0.022044
C	-1.780231	-2.591711	0.037808
O	-0.731664	-3.256869	0.092361
H	-2.967275	-4.296662	0.000000
N	4.643164	-0.552087	-3.400000
C	4.978060	0.794376	-3.400000
H	6.008585	1.119531	-3.400000
N	3.917116	1.579958	-3.400000
C	2.828843	0.704631	-3.400000
C	1.425088	0.956359	-3.400000
O	0.839142	2.066991	-3.400000
N	0.677344	-0.237459	-3.400000
H	-0.362095	-0.129455	-3.400000
C	1.206118	-1.513385	-3.400000
N	0.327071	-2.537595	-3.400000
H	-0.692909	-2.394388	-3.400000
H	0.701181	-3.476676	-3.400000

Cartesian Coordinates of Systems in Ammonia

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in ammonia that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in ammonia and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6843.70 kcal mol^{-1}

N	4.063397	-1.049671	0.000000
C	3.948173	-2.421185	0.000000
H	4.887762	-2.961984	0.000000
C	2.740501	-3.048855	0.000000
C	2.590126	-4.547427	0.000000
H	3.569279	-5.035215	0.000000
H	2.030465	-4.883831	0.881468
H	2.030465	-4.883831	-0.881468
C	1.546492	-2.216326	0.000000
O	0.376842	-2.667393	0.000000
N	1.756320	-0.838104	0.000000
H	0.905784	-0.214171	0.000000
C	2.975680	-0.194010	0.000000
O	3.091291	1.041680	0.000000
H	4.980837	-0.616330	0.000000
N	-3.679313	3.356766	0.000000
C	-4.688608	2.416627	0.000000
H	-5.729951	2.704714	0.000000
N	-4.232055	1.171204	0.000000
C	-2.843990	1.312502	0.000000
C	-1.789803	0.367838	0.000000
N	-1.976439	-0.964854	0.000000
H	-1.170059	-1.600642	0.000000
H	-2.915171	-1.340268	0.000000
N	-0.516218	0.855071	0.000000
C	-0.306800	2.186942	0.000000
H	0.737628	2.489466	0.000000
N	-1.224158	3.166773	0.000000
C	-2.482099	2.670787	0.000000
H	-3.796030	4.363872	0.000000
N	-4.949684	0.553035	3.400000
C	-5.213621	-0.800802	3.400000
H	-6.225419	-1.179821	3.400000
N	-4.112221	-1.540016	3.400000
C	-3.072305	-0.609819	3.400000
C	-1.663771	-0.737937	3.362011
N	-1.030742	-1.943664	3.335521
H	-0.054113	-1.949237	3.063313
H	-1.572778	-2.766319	3.101458
N	-0.912959	0.389887	3.380175
C	-1.533659	1.588941	3.400000
H	-0.866518	2.447587	3.400000

N	-2.851747	1.842431	3.400000
C	-3.577910	0.701771	3.400000
H	-5.636072	1.299196	3.400000

[X]-T/A-T

Total Energy = -6701.67 kcal mol^{-1}

N	4.063397	-1.049671	0.000000
C	3.948173	-2.421185	0.000000
H	4.887762	-2.961984	0.000000
C	2.740501	-3.048855	0.000000
C	2.590126	-4.547427	0.000000
H	3.569279	-5.035215	0.000000
H	2.030465	-4.883831	0.881468
H	2.030465	-4.883831	-0.881468
C	1.546492	-2.216326	0.000000
O	0.376842	-2.667393	0.000000
N	1.756320	-0.838104	0.000000
H	0.905784	-0.214171	0.000000
C	2.975680	-0.194010	0.000000
O	3.091291	1.041680	0.000000
H	4.980837	-0.616330	0.000000
N	-4.949684	0.553035	3.400000
C	-5.213621	-0.800802	3.400000
H	-6.225419	-1.179821	3.400000
N	-4.112221	-1.540016	3.400000
C	-3.072305	-0.609819	3.400000
C	-1.664191	-0.754433	3.400000
N	-1.031846	-1.942305	3.400000
H	-0.005764	-1.982690	3.400000
H	-1.570633	-2.797794	3.400000
N	-0.920227	0.388342	3.400000
C	-1.533659	1.588941	3.400000
H	-0.866518	2.447587	3.400000
N	-2.851747	1.842431	3.400000
C	-3.577910	0.701771	3.400000
H	-5.636072	1.299196	3.400000
N	3.904339	1.539203	3.400000
C	4.617276	0.361898	3.400000
H	5.695293	0.476659	3.400000
C	4.009184	-0.855749	3.400000
C	4.768366	-2.156508	3.400000
H	5.847233	-1.975605	3.400000
H	4.513325	-2.757625	4.281468
H	4.513325	-2.757625	2.518532
C	2.552124	-0.886823	3.419642
O	1.872821	-1.935987	3.452496
N	1.912853	0.354469	3.397397
H	0.857641	0.359583	3.403010
C	2.521412	1.592104	3.400000
O	1.888623	2.659752	3.400000
H	4.391852	2.429041	3.400000

[X]-G/C-G

Total Energy = -6919.05 kcal mol^{-1}

N	4.086031	2.278519	0.000000
C	3.571809	3.564924	0.000000
H	4.216797	4.431679	0.000000
N	2.249913	3.581561	0.000000
C	1.879658	2.233888	0.000000
C	0.585471	1.628433	-0.014159
O	-0.539442	2.155440	0.005942
N	0.699026	0.207927	-0.054664
H	-0.188280	-0.289611	-0.063824
C	1.873876	-0.513669	-0.040540
N	1.768931	-1.878028	-0.025252
H	0.910411	-2.297597	-0.365166
H	2.612238	-2.372727	-0.295753
N	3.070342	0.058252	0.000000
C	3.017970	1.409093	0.000000
H	5.066700	2.021414	0.000000
N	-4.370275	-0.886830	-3.400000
C	-4.974039	0.336923	-3.400000
H	-6.056838	0.339407	-3.400000
C	-4.218098	1.467940	-3.400000
H	-4.671503	2.451963	-3.400000
C	-2.790610	1.306756	-3.400000
N	-1.983591	2.378991	-3.400000
H	-0.958374	2.268483	-3.400000
H	-2.381408	3.308685	-3.400000
N	-2.211445	0.083499	-3.400000
C	-2.978399	-1.038620	-3.400000
O	-2.500293	-2.202318	-3.400000
H	-4.926750	-1.735888	-3.400000
N	4.644948	-0.558348	-3.400000
C	4.985064	0.784628	-3.400000
H	6.016336	1.106733	-3.400000
N	3.925407	1.575078	-3.400000
C	2.833722	0.702418	-3.400000
C	1.431871	0.958121	-3.400000
O	0.852847	2.074878	-3.400000
N	0.678615	-0.229465	-3.400000
H	-0.361624	-0.119334	-3.400000
C	1.202854	-1.507914	-3.400000
N	0.321482	-2.528215	-3.400000
H	-0.698707	-2.380833	-3.400000
H	0.690384	-3.469740	-3.400000
N	2.517098	-1.757554	-3.398480
C	3.270151	-0.633459	-3.399343
H	5.286657	-1.343012	-3.399692

[X]-C/G-C

Total Energy = -6354.68 kcal mol^{-1}

N	2.518199	-1.757575	-3.400000
C	3.269833	-0.633938	-3.400000

H	5.287204	-1.342773	-3.400000
N	-4.370275	-0.886830	-3.400000
C	-4.974039	0.336923	-3.400000
H	-6.056838	0.339407	-3.400000
C	-4.218098	1.467940	-3.400000
H	-4.671503	2.451963	-3.400000
C	-2.790610	1.306756	-3.400000
N	-1.983591	2.378991	-3.400000
H	-0.958374	2.268483	-3.400000
H	-2.381408	3.308685	-3.400000
N	-2.211445	0.083499	-3.400000
C	-2.978399	-1.038620	-3.400000
O	-2.500293	-2.202318	-3.400000
H	-4.926750	-1.735888	-3.400000
N	-3.014361	-3.286244	0.000000
C	-4.222120	-2.651090	0.000000
H	-5.099583	-3.285534	0.000000
C	-4.275346	-1.291747	0.000000
H	-5.220553	-0.762161	0.000000
C	-3.015877	-0.597326	-0.003965
N	-2.999965	0.758246	-0.018724
H	-2.115947	1.233270	-0.155325
H	-3.850226	1.279281	-0.184120
N	-1.832494	-1.227351	0.033866
C	-1.787253	-2.591733	0.046207
O	-0.729221	-3.253426	0.107371
H	-2.965495	-4.300234	0.000000
N	4.644948	-0.558348	-3.400000
C	4.985064	0.784628	-3.400000
H	6.016336	1.106733	-3.400000
N	3.925407	1.575078	-3.400000
C	2.833722	0.702418	-3.400000
C	1.431871	0.958121	-3.400000
O	0.852847	2.074878	-3.400000
N	0.678615	-0.229465	-3.400000
H	-0.361624	-0.119334	-3.400000
C	1.202854	-1.507914	-3.400000
N	0.321482	-2.528215	-3.400000
H	-0.698707	-2.380833	-3.400000
H	0.690384	-3.469740	-3.400000

Cartesian Coordinates of Systems in Methanol

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in methanol that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in methanol and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6844.87 kcal mol^{-1}

N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000
H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000
N	-3.67882300	3.35748600	0.00000000
C	-4.68874900	2.41851800	0.00000000
H	-5.72977000	2.70756000	0.00000000
N	-4.23308900	1.17256800	0.00000000
C	-2.84475200	1.31250500	0.00000000
C	-1.79102200	0.36711300	0.00000000
N	-1.97731400	-0.96548500	0.00000000
H	-1.17050100	-1.60057400	0.00000000
H	-2.91574100	-1.34184600	0.00000000
N	-0.51701100	0.85409800	0.00000000
C	-0.30691600	2.18578900	0.00000000
H	0.73762700	2.48790400	0.00000000
N	-1.22388800	3.16602500	0.00000000
C	-2.48228900	2.67068900	0.00000000
H	-3.79571300	4.36466300	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000

C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000

[X]-T/A-T

Total Energy = -6703.82 kcal mol^{-1}

N	4.06322600	-1.04838400	0.00000000
C	3.94914000	-2.41975300	0.00000000
H	4.88924300	-2.95940500	0.00000000
C	2.74184300	-3.04865700	0.00000000
C	2.59346200	-4.54762700	0.00000000
H	3.57325600	-5.03406600	0.00000000
H	2.03441300	-4.88505900	0.88148600
H	2.03441300	-4.88505900	-0.88148600
C	1.54744200	-2.21725800	0.00000000
O	0.37760100	-2.66860900	0.00000000
N	1.75630300	-0.83887100	0.00000000
H	0.90541800	-0.21567500	0.00000000
C	2.97506200	-0.19400400	0.00000000
O	3.08896100	1.04224600	0.00000000
H	4.98069100	-0.61488700	0.00000000
N	-3.67882300	3.35748600	0.00000000
C	-4.68874900	2.41851800	0.00000000
H	-5.72977000	2.70756000	0.00000000
N	-4.23308900	1.17256800	0.00000000
C	-2.84475200	1.31250500	0.00000000
C	-1.79102200	0.36711300	0.00000000
N	-1.97731400	-0.96548500	0.00000000
H	-1.17050100	-1.60057400	0.00000000
H	-2.91574100	-1.34184600	0.00000000
N	-0.51701100	0.85409800	0.00000000
C	-0.30691600	2.18578900	0.00000000
H	0.73762700	2.48790400	0.00000000
N	-1.22388800	3.16602500	0.00000000
C	-2.48228900	2.67068900	0.00000000
H	-3.79571300	4.36466300	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000

[X]-G/C-G

Total Energy = -6920.26 kcal mol^{-1}

N	4.086488	-2.279147	0.000000
C	3.572448	-3.565179	0.000000
H	4.217258	-4.431999	0.000000
N	2.250211	-3.581708	0.000000
C	1.880223	-2.233779	0.000000
C	0.596041	-1.616972	0.000000
O	-0.528626	-2.181353	0.000000
N	0.683758	-0.213750	0.000000
H	-0.222811	0.308561	0.000000
C	1.859471	0.512609	0.000000
N	1.746020	1.855823	0.000000
H	0.833830	2.336029	0.000000
H	2.597544	2.401369	0.000000
N	3.070544	-0.058610	0.000000
C	3.018713	-1.409452	0.000000
H	5.067471	-2.022874	0.000000
N	-4.370083	0.887878	3.400000
C	-4.974892	-0.335474	3.400000
H	-6.057567	-0.337188	3.400000
C	-4.219740	-1.467030	3.400000
H	-4.673871	-2.450728	3.400000
C	-2.792449	-1.307074	3.400000
N	-1.986235	-2.379851	3.400000
H	-0.961463	-2.270069	3.400000
H	-2.384573	-3.309380	3.400000
N	-2.212086	-0.083854	3.400000
C	-2.978689	1.038535	3.400000
O	-2.499075	2.202203	3.400000
H	-4.926688	1.736947	3.400000
N	4.645352	0.558795	3.376313
C	4.985401	-0.786017	3.386316
H	6.016897	-1.106720	3.400000
N	3.925734	-1.575022	3.400000
C	2.834115	-0.701998	3.400000
C	1.432640	-0.957814	3.400000
O	0.854500	-2.075470	3.400000
N	0.678811	0.228976	3.400000
H	-0.361603	0.116941	3.395649
C	1.203863	1.507581	3.380701
N	0.320333	2.526825	3.345023
H	-0.699317	2.379037	3.380933
H	0.687936	3.468623	3.363347
N	2.517837	1.757143	3.381767
C	3.270767	0.633847	3.386774
H	5.288196	1.342499	3.365519

[X]-C/G-C

Total Energy = -6356.52 kcal mol^{-1}

N	4.086488	-2.279147	0.000000
C	3.572448	-3.565179	0.000000

H	4.217258	-4.431999	0.000000
N	2.250211	-3.581708	0.000000
C	1.880223	-2.233779	0.000000
C	0.596041	-1.616972	0.000000
O	-0.528626	-2.181353	0.000000
N	0.683758	-0.213750	0.000000
H	-0.222811	0.308561	0.000000
C	1.859471	0.512609	0.000000
N	1.746020	1.855823	0.000000
H	0.833830	2.336029	0.000000
H	2.597544	2.401369	0.000000
N	3.070544	-0.058610	0.000000
C	3.018713	-1.409452	0.000000
H	5.067471	-2.022874	0.000000
N	-3.013590	3.286979	0.000000
C	-4.221959	2.652764	0.000000
H	-5.098869	3.287758	0.000000
C	-4.276140	1.293449	0.000000
H	-5.221743	0.764552	0.000000
C	-3.027418	0.583915	0.000000
N	-3.005739	-0.757860	0.000000
H	-2.112153	-1.271391	0.000000
H	-3.874365	-1.275728	0.000000
N	-1.838903	1.232392	0.000000
C	-1.799374	2.591022	0.000000
O	-0.727372	3.250539	0.000000
H	-2.964822	4.301054	0.000000
C	-2.968410	1.047123	3.438913
O	-2.499423	2.202903	3.518269
H	-4.926688	1.736947	3.400000
N	-4.370083	0.887878	3.400000
C	-4.974892	-0.335474	3.400000
H	-6.057567	-0.337188	3.400000
C	-4.219740	-1.467030	3.400000
H	-4.673871	-2.450728	3.400000
C	-2.793363	-1.287757	3.343475
N	-1.983998	-2.372028	3.256682
H	-1.007702	-2.226443	3.027585
H	-2.376716	-3.286475	3.077213
N	-2.205177	-0.082917	3.388284

Cartesian Coordinates of Systems in Water

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in water that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in water and at BLYP-D3(BJ)/TZ2P (see above section for description).

[X]-A/T-A
Total Energy = -6846.38 kcal mol^{-1}

N	3.400000	3.361630	-3.678750
C	3.400000	2.422730	-4.688080
H	3.400000	2.711640	-5.729110
N	3.400000	1.176590	-4.232190
C	3.400000	1.316940	-2.843750
C	3.400000	0.372040	-1.789510
N	3.400000	-0.960610	-1.974890
H	3.400000	-1.595260	-1.167650
H	3.400000	-1.337610	-2.913000
N	3.400000	0.859290	-0.515390
C	3.400000	2.190950	-0.306230
H	3.400000	2.494250	0.737940
N	3.400000	3.171080	-1.223540
C	3.400000	2.675450	-2.482160
H	3.400000	4.368700	-3.796210
N	0.000000	0.557390	-4.952080
C	0.000000	-0.795460	-5.216790
H	0.000000	-1.173610	-6.228830
N	0.000000	-1.535660	-4.115520
C	0.000000	-0.606030	-3.074730
C	0.037444	-0.734896	-1.666253
N	0.063492	-1.939832	-1.033078
H	0.334331	-1.946607	-0.056030
H	0.295488	-2.763831	-1.574021
N	0.018669	0.393614	-0.915127
C	0.000000	1.592550	-1.535520
H	0.000000	2.451660	-0.869030
N	0.000000	1.846330	-2.853750
C	0.000000	0.705570	-3.580690
H	0.000000	1.303100	-5.639030
N	3.400000	-1.057160	4.063550
C	3.400000	-2.428030	3.946250
H	3.400000	-2.970040	4.884860
C	3.400000	-3.053840	2.737350
C	3.400000	-4.552370	2.585990
H	3.400000	-5.040120	3.565060
H	2.518360	-4.888850	2.026580
H	4.281640	-4.888850	2.026580
C	3.400000	-2.219710	1.545700
O	3.400000	-2.668280	0.374150
N	3.400000	-0.841980	1.757440
H	3.400000	-0.216750	0.908820

C	3.400000	-0.200950	2.977970
O	3.400000	1.035810	3.094810
H	3.400000	-0.626610	4.982410

[X]-T/A-T

Total Energy = -6705.58 kcal mol^{-1}

N	0.000000	1.533160	3.908900
C	0.000000	0.355140	4.619750
H	0.000000	0.468330	5.697690
C	0.000000	-0.861710	4.009550
C	0.000000	-2.163030	4.767890
H	0.000000	-1.982160	5.846670
H	-0.881640	-2.764050	4.513080
H	0.881640	-2.764050	4.513080
C	-0.016057	-0.909342	2.553251
O	-0.050703	-1.943075	1.866413
N	0.013288	0.346928	1.920237
H	0.010621	0.348065	0.902300
C	0.000000	1.587790	2.527370
O	0.000000	2.657040	1.894970
H	0.000000	2.421570	4.399210
N	3.400000	3.361630	-3.678750
C	3.400000	2.422730	-4.688080
H	3.400000	2.711640	-5.729110
N	3.400000	1.176590	-4.232190
C	3.400000	1.316940	-2.843750
C	3.400000	0.372040	-1.789510
N	3.400000	-0.960610	-1.974890
H	3.400000	-1.595260	-1.167650
H	3.400000	-1.337610	-2.913000
N	3.400000	0.859290	-0.515390
C	3.400000	2.190950	-0.306230
H	3.400000	2.494250	0.737940
N	3.400000	3.171080	-1.223540
C	3.400000	2.675450	-2.482160
H	3.400000	4.368700	-3.796210
N	3.400000	-1.057160	4.063550
C	3.400000	-2.428030	3.946250
H	3.400000	-2.970040	4.884860
C	3.400000	-3.053840	2.737350
C	3.400000	-4.552370	2.585990
H	3.400000	-5.040120	3.565060
H	2.518360	-4.888850	2.026580
H	4.281640	-4.888850	2.026580
C	3.400000	-2.219710	1.545700
O	3.400000	-2.668280	0.374150
N	3.400000	-0.841980	1.757440
H	3.400000	-0.216750	0.908820
C	3.400000	-0.200950	2.977970
O	3.400000	1.035810	3.094810
H	3.400000	-0.626610	4.982410

[X]-G/C-G

Total Energy = -6921.81 kcal mol^{-1}

N	0.000000	0.542030	4.632850
C	0.000000	-0.815770	4.959220
H	0.000000	-1.149360	5.987990
N	0.000000	-1.590190	3.897910
C	0.000000	-0.712240	2.815680
C	0.000000	-0.954970	1.405940
O	0.000000	-2.048010	0.800670
N	0.000000	0.256580	0.673140
H	0.000000	0.155470	-0.363030
C	0.000000	1.525840	1.212470
N	0.000000	2.561040	0.338480
H	0.000000	2.430920	-0.680790
H	0.000000	3.490440	0.732500
N	0.000000	1.760620	2.523930
C	0.000000	0.625320	3.255640
H	0.000000	1.332260	5.265570
N	0.000000	0.866190	-4.373520
C	0.000000	-0.367810	-4.957210
H	0.000000	-0.393420	-6.041660
C	0.000000	-1.487660	-4.186320
H	0.000000	-2.476130	-4.631900
C	0.000000	-1.306150	-2.752800
N	0.000000	-2.362970	-1.927270
H	0.000000	-2.233890	-0.887180
H	0.000000	-3.297300	-2.311420
N	0.000000	-0.079850	-2.198440
C	0.000000	1.043990	-2.965040
O	0.000000	2.203460	-2.518320
H	0.000000	1.716110	-4.927040
N	3.400000	-2.284540	4.066690
C	3.400000	-3.574860	3.532660
H	3.400000	-4.449430	4.168890
N	3.400000	-3.577580	2.218850
C	3.400000	-2.231200	1.859330
C	3.388570	-1.620703	0.568904
O	3.413822	-2.151186	-0.556800
N	3.344425	-0.203728	0.683083
H	3.331576	0.297706	-0.201934
C	3.346792	0.515498	1.860859
N	3.358849	1.877265	1.757838
H	3.048838	2.303654	0.891901
H	3.093185	2.377948	2.598720
N	3.378958	-0.058174	3.057707
C	3.394012	-1.413311	3.002664
H	3.384890	-2.035152	5.048593

[X]-C/G-C

Total Energy = -6357.29 kcal mol^{-1}

N	0.000000	0.542030	4.632850
C	0.000000	-0.815770	4.959220

H	0.000000	-1.149360	5.987990
N	0.000000	-1.590190	3.897910
C	0.000000	-0.712240	2.815680
C	0.000000	-0.954970	1.405940
O	0.000000	-2.048010	0.800670
N	0.000000	0.256580	0.673140
H	0.000000	0.155470	-0.363030
C	0.000000	1.525840	1.212470
N	0.000000	2.561040	0.338480
H	0.000000	2.430920	-0.680790
H	0.000000	3.490440	0.732500
N	0.000000	1.760620	2.523930
C	0.000000	0.625320	3.255640
H	0.000000	1.332260	5.265570
N	0.000000	0.866190	-4.373520
C	0.000000	-0.367810	-4.957210
H	0.000000	-0.393420	-6.041660
C	0.000000	-1.487660	-4.186320
H	0.000000	-2.476130	-4.631900
C	0.000000	-1.306150	-2.752800
N	0.000000	-2.362970	-1.927270
H	0.000000	-2.233890	-0.887180
H	0.000000	-3.297300	-2.311420
N	0.000000	-0.079850	-2.198440
C	0.000000	1.043990	-2.965040
O	0.000000	2.203460	-2.518320
H	0.000000	1.716110	-4.927040
C	3.442396	2.590024	-1.796163
O	3.498567	3.265535	-0.743114
H	3.400000	4.284350	-2.977440
N	3.400000	3.271400	-3.029180
C	3.400000	2.616130	-4.226710
H	3.400000	3.232820	-5.119110
C	3.400000	1.257030	-4.261250
H	3.400000	0.719230	-5.202730
C	3.393756	0.577703	-2.995017
N	3.377353	-0.776051	-2.960779
H	3.236973	-1.240496	-2.071785
H	3.211179	-1.307464	-3.804788
N	3.430692	1.226449	-1.819695

Cartesian Coordinates of Systems in the Gas Phase

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9132.65 kcal mol^{-1}

N	0.96672000	1.38097400	3.40000000
C	1.76753300	0.29079200	3.40000000
N	3.10339700	0.25039900	3.40000000
C	3.63001800	1.48210000	3.40000000
C	2.93479200	2.69897800	3.40000000
C	1.52762400	2.60671400	3.40000000
N	4.95937400	1.84887200	3.40000000
C	4.99478500	3.22884800	3.40000000
N	3.80039500	3.78051900	3.40000000
N	0.73803300	3.70712500	3.40000000
H	1.23442000	-0.66265000	3.40000000
H	5.74729600	1.21204100	3.40000000
H	5.93416700	3.77110900	3.40000000
H	1.15931000	4.62531900	3.40000000
H	-0.26705700	3.61056000	3.40000000
N	-0.82728100	-1.88477700	3.40000000
C	-0.99046500	-3.21902000	3.40000000
N	-2.12536600	-3.93108400	3.40000000
C	-3.19541100	-3.12217700	3.40000000
C	-3.19477600	-1.72171300	3.40000000
C	-1.92580300	-1.09554900	3.40000000
N	-4.53223000	-3.46527300	3.40000000
C	-5.24866300	-2.28506700	3.40000000
N	-4.48450800	-1.21389600	3.40000000
N	-1.78555900	0.24492300	3.40000000
H	-0.06641700	-3.79978300	3.40000000
H	-4.90007600	-4.40874000	3.40000000
H	-6.33331400	-2.28075400	3.40000000
H	-2.62570400	0.80740900	3.40000000
H	-0.85423200	0.68919800	3.40000000
N	3.88853200	-1.54101700	0.00000000
C	4.60128300	-0.35871900	0.00000000
H	5.68189800	-0.46792600	0.00000000
C	3.99281700	0.85505200	0.00000000
C	4.73777500	2.16327800	0.00000000
H	5.82074300	2.00060100	0.00000000
H	4.46986300	2.76149200	-0.87930400
H	4.46986300	2.76149200	0.87930400
C	2.52658500	0.88501500	0.00000000
O	1.86255100	1.93758300	0.00000000
N	1.88820400	-0.35590600	0.00000000
H	0.82622500	-0.35881600	0.00000000
C	2.48889500	-1.60172800	0.00000000

O	1.87706300	-2.66652200	0.00000000
H	4.36062900	-2.43745100	0.00000000
N	-4.92727300	-0.55939400	0.00000000
C	-5.18876000	0.80506800	0.00000000
H	-6.20055400	1.18756600	0.00000000
N	-4.09213100	1.53852900	0.00000000
C	-3.05514500	0.60865600	0.00000000
C	-1.64704300	0.75621800	0.00000000
N	-1.02454900	1.95146700	0.00000000
H	0.00240800	2.00614900	0.00000000
H	-1.58707100	2.79067100	0.00000000
N	-0.90430800	-0.38260800	0.00000000
C	-1.51410900	-1.58872900	0.00000000
H	-0.83944100	-2.44209500	0.00000000
N	-2.82950500	-1.84375600	0.00000000
C	-3.55023800	-0.70650900	0.00000000
H	-5.60025200	-1.31595900	0.00000000

[T]-A/T-A
Total Energy = -9003.35 kcal mol^{-1}

N	0.00000000	-1.54221000	-3.88806000
C	0.00000000	-0.36014000	-4.60117000
H	0.00000000	-0.46968000	-5.68176000
C	0.00000000	0.85382000	-3.99308000
C	0.00000000	2.16182000	-4.73844000
H	0.00000000	1.99881000	-5.82136000
H	-0.87930000	2.76011000	-4.47072000
H	0.87930000	2.76011000	-4.47072000
C	0.00000000	0.88424000	-2.52686000
O	0.00000000	1.93701000	-1.86315000
N	0.00000000	-0.35649000	-1.88810000
H	0.00000000	-0.35907000	-0.82612000
C	0.00000000	-1.60249000	-2.48840000
O	0.00000000	-2.66710000	-1.87624000
H	0.00000000	-2.43879000	-4.35988000
N	0.00000000	-0.55787000	4.92744000
C	0.00000000	0.80667000	5.18851000
H	0.00000000	1.18948000	6.20018000
N	0.00000000	1.53979000	4.09165000
C	0.00000000	0.60960000	3.05495000
C	0.00000000	0.75673000	1.64681000
N	0.00000000	1.95178000	1.02394000
H	0.00000000	2.00615000	-0.00303000
H	0.00000000	2.79116000	1.58621000
N	0.00000000	-0.38233000	0.90442000
C	0.00000000	-1.58826000	1.51460000
H	0.00000000	-2.44183000	0.84019000
N	0.00000000	-1.84288000	2.83007000
C	0.00000000	-0.70541000	3.55045000
H	0.00000000	-1.31423000	5.60066000
N	3.40000000	1.03759000	-4.05202000
C	3.40000000	2.41307000	-3.93416000

H	3.40000000	2.95958000	-4.87276000
C	3.40000000	3.03778000	-2.72866000
C	3.40000000	4.53409000	-2.56288000
H	3.40000000	5.03871000	-3.53481000
H	2.52070000	4.86076000	-1.99462000
H	4.27930000	4.86076000	-1.99462000
C	3.40000000	2.20059000	-1.52457000
O	3.40000000	2.66220000	-0.36882000
N	3.40000000	0.82136000	-1.73706000
H	3.40000000	0.19507000	-0.87940000
C	3.40000000	0.16615000	-2.95509000
O	3.40000000	-1.05496000	-3.08557000
H	3.40000000	0.58955000	-4.96071000
N	3.40000000	-3.34754000	3.65854000
C	3.40000000	-2.39703000	4.67178000
H	3.40000000	-2.68196000	5.71526000
N	3.40000000	-1.15922000	4.21531000
C	3.40000000	-1.30243000	2.82985000
C	3.40000000	-0.35573000	1.77710000
N	3.40000000	0.97720000	1.97560000
H	3.40000000	1.62481000	1.17670000
H	3.40000000	1.32580000	2.92385000
N	3.40000000	-0.84091000	0.50698000
C	3.40000000	-2.17518000	0.29182000
H	3.40000000	-2.46935000	-0.75550000
N	3.40000000	-3.15437000	1.20642000
C	3.40000000	-2.65755000	2.45780000
H	3.40000000	-4.35515000	3.75862000

[G]-A/T-A

Total Energy = -9300.38 kcal mol^{-1}

N	1.37903200	0.50465300	3.40000000
C	2.63220800	-0.05661400	3.40000000
N	3.75986900	0.63827700	3.40000000
C	3.54228300	1.97552900	3.40000000
C	2.31856300	2.66690100	3.40000000
C	1.10535500	1.90337700	3.40000000
N	4.50645100	2.96018900	3.40000000
C	3.83544000	4.18419900	3.40000000
N	2.52899800	4.04313200	3.40000000
O	-0.07047200	2.30354300	3.40000000
N	2.69406900	-1.42223800	3.40000000
H	0.54879100	-0.12866500	3.40000000
H	5.50638100	2.80106700	3.40000000
H	4.37217200	5.12304200	3.40000000
H	3.60399300	-1.85782900	3.40000000
H	1.86161400	-1.98881600	3.40000000
N	-0.91896900	-1.30891000	3.40000000
C	-0.83080700	-2.65656900	3.40000000
N	-1.80822100	-3.56883500	3.40000000
C	-3.02087100	-2.97946900	3.40000000
C	-3.27991800	-1.60126400	3.40000000

C	-2.15873100	-0.73100200	3.40000000
N	-4.27105100	-3.57238200	3.40000000
C	-5.20445100	-2.54285700	3.40000000
N	-4.64814100	-1.34662300	3.40000000
N	-2.28072400	0.60455300	3.40000000
H	0.17974900	-3.06587200	3.40000000
H	-4.45291600	-4.56854200	3.40000000
H	-6.26748500	-2.74226200	3.40000000
H	-3.21437000	0.99364900	3.40000000
H	-1.45769800	1.23467700	3.40000000
N	3.88853200	-1.54101700	0.00000000
C	4.60128300	-0.35871900	0.00000000
H	5.68189800	-0.46792600	0.00000000
C	3.99281700	0.85505200	0.00000000
C	4.73777500	2.16327800	0.00000000
H	5.82074300	2.00060100	0.00000000
H	4.46986300	2.76149200	-0.87930400
H	4.46986300	2.76149200	0.87930400
C	2.52658500	0.88501500	0.00000000
O	1.86255100	1.93758300	0.00000000
N	1.88820400	-0.35590600	0.00000000
H	0.82622500	-0.35881600	0.00000000
C	2.48889500	-1.60172800	0.00000000
O	1.87706300	-2.66652200	0.00000000
H	4.36062900	-2.43745100	0.00000000
N	-4.92727300	-0.55939400	0.00000000
C	-5.18876000	0.80506800	0.00000000
H	-6.20055400	1.18756600	0.00000000
N	-4.09213100	1.53852900	0.00000000
C	-3.05514500	0.60865600	0.00000000
C	-1.64704300	0.75621800	0.00000000
N	-1.02454900	1.95146700	0.00000000
H	0.00240800	2.00614900	0.00000000
H	-1.58707100	2.79067100	0.00000000
N	-0.90430800	-0.38260800	0.00000000
C	-1.51410900	-1.58872900	0.00000000
H	-0.83944100	-2.44209500	0.00000000
N	-2.82950500	-1.84375600	0.00000000
C	-3.55023800	-0.70650900	0.00000000
H	-5.60025200	-1.31595900	0.00000000

[C]-A/T-A
Total Energy = -8732.29 kcal mol^{-1}

N	2.18577200	-1.21079800	-3.40000000
C	3.54204500	-1.00857800	-3.40000000
N	4.36003300	-2.19371900	-3.40000000
C	3.84476800	-3.45244900	-3.40000000
C	2.49506700	-3.63402100	-3.40000000
C	1.67747400	-2.44210600	-3.40000000
N	0.32517200	-2.56162900	-3.40000000
O	4.10377700	0.08445600	-3.40000000
H	5.36098900	-2.02963200	-3.40000000

H	4.55319700	-4.27487800	-3.40000000
H	2.06094800	-4.62801200	-3.40000000
H	-0.27102400	-1.71760500	-3.40000000
H	-0.09665500	-3.47829300	-3.40000000
N	-1.21225300	-0.03072400	-3.40000000
C	-0.28020300	0.95896300	-3.40000000
N	-0.49613100	2.28252700	-3.40000000
C	-1.80493900	2.57748800	-3.40000000
C	-2.87349800	1.66426600	-3.40000000
C	-2.52267200	0.29749700	-3.40000000
N	-2.41310000	3.82219600	-3.40000000
C	-3.78426100	3.60295400	-3.40000000
N	-4.10260900	2.32214300	-3.40000000
N	-3.46483500	-0.68541400	-3.40000000
H	0.75165900	0.61403700	-3.40000000
H	-1.93029900	4.71247900	-3.40000000
H	-4.48825200	4.42423500	-3.40000000
H	-4.44428000	-0.43973900	-3.40000000
H	-3.18591500	-1.65512600	-3.40000000
N	3.88853200	1.54101700	0.00000000
C	4.60128300	0.35871900	0.00000000
H	5.68189800	0.46792600	0.00000000
C	3.99281700	-0.85505200	0.00000000
C	4.73777500	-2.16327800	0.00000000
H	5.82074300	-2.00060100	0.00000000
H	4.46986300	-2.76149200	-0.87930400
H	4.46986300	-2.76149200	0.87930400
C	2.52658500	-0.88501500	0.00000000
O	1.86255100	-1.93758300	0.00000000
N	1.88820400	0.35590600	0.00000000
H	0.82622500	0.35881600	0.00000000
C	2.48889500	1.60172800	0.00000000
O	1.87706300	2.66652200	0.00000000
H	4.36062900	2.43745100	0.00000000
N	-4.92727300	0.55939400	0.00000000
C	-5.18876000	-0.80506800	0.00000000
H	-6.20055400	-1.18756600	0.00000000
N	-4.09213100	-1.53852900	0.00000000
C	-3.05514500	-0.60865600	0.00000000
C	-1.64704300	-0.75621800	0.00000000
N	-1.02454900	-1.95146700	0.00000000
H	0.00240800	-2.00614900	0.00000000
H	-1.58707100	-2.79067100	0.00000000
N	-0.90430800	0.38260800	0.00000000
C	-1.51410900	1.58872900	0.00000000
H	-0.83944100	2.44209500	0.00000000
N	-2.82950500	1.84375600	0.00000000
C	-3.55023800	0.70650900	0.00000000
H	-5.60025200	1.31595900	0.00000000

[A]-T/A-T
Total Energy = -9003.35 kcal mol^{-1}

N	0.00000000	-1.54221000	-3.88806000
C	0.00000000	-0.36014000	-4.60117000
H	0.00000000	-0.46968000	-5.68176000
C	0.00000000	0.85382000	-3.99308000
C	0.00000000	2.16182000	-4.73844000
H	0.00000000	1.99881000	-5.82136000
H	-0.87930000	2.76011000	-4.47072000
H	0.87930000	2.76011000	-4.47072000
C	0.00000000	0.88424000	-2.52686000
O	0.00000000	1.93701000	-1.86315000
N	0.00000000	-0.35649000	-1.88810000
H	0.00000000	-0.35907000	-0.82612000
C	0.00000000	-1.60249000	-2.48840000
O	0.00000000	-2.66710000	-1.87624000
H	0.00000000	-2.43879000	-4.35988000
N	0.00000000	-0.55787000	4.92744000
C	0.00000000	0.80667000	5.18851000
H	0.00000000	1.18948000	6.20018000
N	0.00000000	1.53979000	4.09165000
C	0.00000000	0.60960000	3.05495000
C	0.00000000	0.75673000	1.64681000
N	0.00000000	1.95178000	1.02394000
H	0.00000000	2.00615000	-0.00303000
H	0.00000000	2.79116000	1.58621000
N	0.00000000	-0.38233000	0.90442000
C	0.00000000	-1.58826000	1.51460000
H	0.00000000	-2.44183000	0.84019000
N	0.00000000	-1.84288000	2.83007000
C	0.00000000	-0.70541000	3.55045000
H	0.00000000	-1.31423000	5.60066000
N	3.40000000	1.03759000	-4.05202000
C	3.40000000	2.41307000	-3.93416000
H	3.40000000	2.95958000	-4.87276000
C	3.40000000	3.03778000	-2.72866000
C	3.40000000	4.53409000	-2.56288000
H	3.40000000	5.03871000	-3.53481000
H	2.52070000	4.86076000	-1.99462000
H	4.27930000	4.86076000	-1.99462000
C	3.40000000	2.20059000	-1.52457000
O	3.40000000	2.66220000	-0.36882000
N	3.40000000	0.82136000	-1.73706000
H	3.40000000	0.19507000	-0.87940000
C	3.40000000	0.16615000	-2.95509000
O	3.40000000	-1.05496000	-3.08557000
H	3.40000000	0.58955000	-4.96071000
N	3.40000000	-3.34754000	3.65854000
C	3.40000000	-2.39703000	4.67178000
H	3.40000000	-2.68196000	5.71526000
N	3.40000000	-1.15922000	4.21531000
C	3.40000000	-1.30243000	2.82985000
C	3.40000000	-0.35573000	1.77710000
N	3.40000000	0.97720000	1.97560000

H	3.40000000	1.62481000	1.17670000
H	3.40000000	1.32580000	2.92385000
N	3.40000000	-0.84091000	0.50698000
C	3.40000000	-2.17518000	0.29182000
H	3.40000000	-2.46935000	-0.75550000
N	3.40000000	-3.15437000	1.20642000
C	3.40000000	-2.65755000	2.45780000
H	3.40000000	-4.35515000	3.75862000

[T]-T/A-T

Total Energy = -8861.37 kcal mol^{-1}

N	-1.98457600	0.65748100	0.00000000
C	-3.37442100	0.69858100	0.00000000
N	-3.88059300	2.00617600	0.00000000
C	-3.09223700	3.13844600	0.00000000
C	-1.73640400	3.07640300	0.00000000
C	-1.11220000	1.75143500	0.00000000
O	0.11911700	1.58203600	0.00000000
O	-4.10070300	-0.28596900	0.00000000
C	-0.84136500	4.28697300	0.00000000
H	-1.54890600	-0.28546200	0.00000000
H	-4.89156300	2.07261100	0.00000000
H	-3.63198100	4.08099500	0.00000000
H	-0.18554900	4.28355900	-0.87875000
H	-1.42909500	5.21094500	0.00000000
H	-0.18554900	4.28355900	0.87875000
N	1.48142200	-0.87997000	0.00000000
C	0.60563400	-1.93883800	0.00000000
N	1.21897300	-3.18596000	0.00000000
C	2.59336100	-3.36130800	0.00000000
C	3.45283500	-2.31442700	0.00000000
C	2.89748000	-0.94947100	0.00000000
O	3.57338600	0.07564500	0.00000000
O	-0.62976200	-1.83365900	0.00000000
C	4.95024600	-2.46255600	0.00000000
H	1.04594300	0.06497300	0.00000000
H	0.58836000	-3.97864600	0.00000000
H	2.92650800	-4.39486700	0.00000000
H	5.38534200	-1.97138700	0.87865800
H	5.24428000	-3.51746600	0.00000000
H	5.38534200	-1.97138700	-0.87865800
N	3.88853200	-1.54101700	3.40000000
C	4.60128300	-0.35871900	3.40000000
H	5.68189800	-0.46792600	3.40000000
C	3.99281700	0.85505200	3.40000000
C	4.73777500	2.16327800	3.40000000
H	5.82074300	2.00060100	3.40000000
H	4.46986300	2.76149200	2.52069600
H	4.46986300	2.76149200	4.27930400
C	2.52658500	0.88501500	3.40000000
O	1.86255100	1.93758300	3.40000000

N	1.88820400	-0.35590600	3.40000000
H	0.82622500	-0.35881600	3.40000000
C	2.48889500	-1.60172800	3.40000000
O	1.87706300	-2.66652200	3.40000000
H	4.36062900	-2.43745100	3.40000000
N	-4.92727300	-0.55939400	3.40000000
C	-5.18876000	0.80506800	3.40000000
H	-6.20055400	1.18756600	3.40000000
N	-4.09213100	1.53852900	3.40000000
C	-3.05514500	0.60865600	3.40000000
C	-1.64704300	0.75621800	3.40000000
N	-1.02454900	1.95146700	3.40000000
H	0.00240800	2.00614900	3.40000000
H	-1.58707100	2.79067100	3.40000000
N	-0.90430800	-0.38260800	3.40000000
C	-1.51410900	-1.58872900	3.40000000
H	-0.83944100	-2.44209500	3.40000000
N	-2.82950500	-1.84375600	3.40000000
C	-3.55023800	-0.70650900	3.40000000
H	-5.60025200	-1.31595900	3.40000000

[G]-T/A-T
Total Energy = -9160.58 kcal mol^{-1}

N	-1.57691300	0.10984600	0.00000000
C	-2.94394000	-0.00633700	0.00000000
N	-3.77231100	1.02735000	0.00000000
C	-3.11421900	2.21324400	0.00000000
C	-1.72766000	2.45603300	0.00000000
C	-0.84305200	1.32753300	0.00000000
N	-3.69181900	3.46451500	0.00000000
C	-2.64964900	4.39326400	0.00000000
N	-1.46609800	3.82297500	0.00000000
O	0.39929700	1.29104200	0.00000000
N	-3.44167000	-1.27879100	0.00000000
H	-1.00679200	-0.75532100	0.00000000
H	-4.68721200	3.64977900	0.00000000
H	-2.84091000	5.45770000	0.00000000
H	-4.44303800	-1.40106500	0.00000000
H	-2.82882700	-2.08122000	0.00000000
N	1.85713000	-1.09399000	0.00000000
C	1.10946800	-2.24080600	0.00000000
N	1.84677000	-3.41440600	0.00000000
C	3.23387700	-3.44773900	0.00000000
C	3.97593200	-2.31643100	0.00000000
C	3.27856900	-1.01690500	0.00000000
O	3.84309500	0.07012800	0.00000000
O	-0.13805400	-2.27920300	0.00000000
C	5.48015100	-2.30230400	0.00000000
H	1.33700300	-0.18129900	0.00000000
H	1.30383000	-4.26909500	0.00000000
H	3.67120000	-4.44152400	0.00000000
H	5.85842000	-1.76599100	-0.87844000

H	5.88679100	-3.31903800	0.00000000
H	5.85842000	-1.76599100	0.87844000
N	3.88853200	-1.54101700	3.40000000
C	4.60128300	-0.35871900	3.40000000
H	5.68189800	-0.46792600	3.40000000
C	3.99281700	0.85505200	3.40000000
C	4.73777500	2.16327800	3.40000000
H	5.82074300	2.00060100	3.40000000
H	4.46986300	2.76149200	2.52069600
H	4.46986300	2.76149200	4.27930400
C	2.52658500	0.88501500	3.40000000
O	1.86255100	1.93758300	3.40000000
N	1.88820400	-0.35590600	3.40000000
H	0.82622500	-0.35881600	3.40000000
C	2.48889500	-1.60172800	3.40000000
O	1.87706300	-2.66652200	3.40000000
H	4.36062900	-2.43745100	3.40000000
N	-4.92727300	-0.55939400	3.40000000
C	-5.18876000	0.80506800	3.40000000
H	-6.20055400	1.18756600	3.40000000
N	-4.09213100	1.53852900	3.40000000
C	-3.05514500	0.60865600	3.40000000
C	-1.64704300	0.75621800	3.40000000
N	-1.02454900	1.95146700	3.40000000
H	0.00240800	2.00614900	3.40000000
H	-1.58707100	2.79067100	3.40000000
N	-0.90430800	-0.38260800	3.40000000
C	-1.51410900	-1.58872900	3.40000000
H	-0.83944100	-2.44209500	3.40000000
N	-2.82950500	-1.84375600	3.40000000
C	-3.55023800	-0.70650900	3.40000000
H	-5.60025200	-1.31595900	3.40000000

[C]-T/A-T

Total Energy = -8597.01 kcal mol^{-1}

N	-1.37124700	1.05420600	0.00000000
C	-2.67496400	0.60825900	0.00000000
N	-3.69199500	1.62495100	0.00000000
C	-3.41792300	2.95650100	0.00000000
C	-2.12543000	3.38109000	0.00000000
C	-1.09743700	2.36583000	0.00000000
N	0.19950900	2.73875600	0.00000000
O	-3.02555700	-0.56551300	0.00000000
H	-4.64446700	1.27661800	0.00000000
H	-4.26540000	3.63480000	0.00000000
H	-1.87794100	4.43673200	0.00000000
H	0.94529100	2.02316800	0.00000000
H	0.44182300	3.71824100	0.00000000
N	0.77553400	-1.01693100	0.00000000
C	0.48795700	-2.38269100	0.00000000
N	1.64411200	-3.18510600	0.00000000
C	2.92871100	-2.69302400	0.00000000

C	3.18751700	-1.36078300	0.00000000
C	2.04830000	-0.44060900	0.00000000
O	2.19362600	0.79687100	0.00000000
O	-0.63012300	-2.86782300	0.00000000
C	4.57694200	-0.78040800	0.00000000
H	-0.04288400	-0.36439200	0.00000000
H	1.46327000	-4.18195900	0.00000000
H	3.71705800	-3.44043000	0.00000000
H	4.73275300	-0.14403000	-0.87947200
H	5.33299700	-1.57286200	0.00000000
H	4.73275300	-0.14403000	0.87947200
N	3.88853200	-1.54101700	3.40000000
C	4.60128300	-0.35871900	3.40000000
H	5.68189800	-0.46792600	3.40000000
C	3.99281700	0.85505200	3.40000000
C	4.73777500	2.16327800	3.40000000
H	5.82074300	2.00060100	3.40000000
H	4.46986300	2.76149200	2.52069600
H	4.46986300	2.76149200	4.27930400
C	2.52658500	0.88501500	3.40000000
O	1.86255100	1.93758300	3.40000000
N	1.88820400	-0.35590600	3.40000000
H	0.82622500	-0.35881600	3.40000000
C	2.48889500	-1.60172800	3.40000000
O	1.87706300	-2.66652200	3.40000000
H	4.36062900	-2.43745100	3.40000000
N	-4.92727300	-0.55939400	3.40000000
C	-5.18876000	0.80506800	3.40000000
H	-6.20055400	1.18756600	3.40000000
N	-4.09213100	1.53852900	3.40000000
C	-3.05514500	0.60865600	3.40000000
C	-1.64704300	0.75621800	3.40000000
N	-1.02454900	1.95146700	3.40000000
H	0.00240800	2.00614900	3.40000000
H	-1.58707100	2.79067100	3.40000000
N	-0.90430800	-0.38260800	3.40000000
C	-1.51410900	-1.58872900	3.40000000
H	-0.83944100	-2.44209500	3.40000000
N	-2.82950500	-1.84375600	3.40000000
C	-3.55023800	-0.70650900	3.40000000
H	-5.60025200	-1.31595900	3.40000000

[A]-G/C-G

Total Energy = -9206.20 kcal mol^{-1}

N	1.37903200	0.50465300	0.00000000
C	2.63220800	-0.05661400	0.00000000
N	3.75986900	0.63827700	0.00000000
C	3.54228300	1.97552900	0.00000000
C	2.31856300	2.66690100	0.00000000
C	1.10535500	1.90337700	0.00000000
N	4.50645100	2.96018900	0.00000000
C	3.83544000	4.18419900	0.00000000

N	2.52899800	4.04313200	0.00000000
O	-0.07047200	2.30354300	0.00000000
N	2.69406900	-1.42223800	0.00000000
H	0.54879100	-0.12866500	0.00000000
H	5.50638100	2.80106700	0.00000000
H	4.37217200	5.12304200	0.00000000
H	3.60399300	-1.85782900	0.00000000
H	1.86161400	-1.98881600	0.00000000
N	-0.91896900	-1.30891000	0.00000000
C	-0.83080700	-2.65656900	0.00000000
N	-1.80822100	-3.56883500	0.00000000
C	-3.02087100	-2.97946900	0.00000000
C	-3.27991800	-1.60126400	0.00000000
C	-2.15873100	-0.73100200	0.00000000
N	-4.27105100	-3.57238200	0.00000000
C	-5.20445100	-2.54285700	0.00000000
N	-4.64814100	-1.34662300	0.00000000
N	-2.28072400	0.60455300	0.00000000
H	0.17974900	-3.06587200	0.00000000
H	-4.45291600	-4.56854200	0.00000000
H	-6.26748500	-2.74226200	0.00000000
H	-3.21437000	0.99364900	0.00000000
H	-1.45769800	1.23467700	0.00000000
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000
O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000
H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

[T]-G/C-G

Total Energy = -9066.57 kcal mol^{-1}

N	1.57691300	0.10984600	0.00000000
C	2.94394000	-0.00633700	0.00000000
N	3.77231100	1.02735000	0.00000000
C	3.11421900	2.21324400	0.00000000
C	1.72766000	2.45603300	0.00000000
C	0.84305200	1.32753300	0.00000000
N	3.69181900	3.46451500	0.00000000
C	2.64964900	4.39326400	0.00000000
N	1.46609800	3.82297500	0.00000000
O	-0.39929700	1.29104200	0.00000000
N	3.44167000	-1.27879100	0.00000000
H	1.00679200	-0.75532100	0.00000000
H	4.68721200	3.64977900	0.00000000
H	2.84091000	5.45770000	0.00000000
H	4.44303800	-1.40106500	0.00000000
H	2.82882700	-2.08122000	0.00000000
N	-1.85713000	-1.09399000	0.00000000
C	-1.10946800	-2.24080600	0.00000000
N	-1.84677000	-3.41440600	0.00000000
C	-3.23387700	-3.44773900	0.00000000
C	-3.97593200	-2.31643100	0.00000000
C	-3.27856900	-1.01690500	0.00000000
O	-3.84309500	0.07012800	0.00000000
O	0.13805400	-2.27920300	0.00000000
C	-5.48015100	-2.30230400	0.00000000
H	-1.33700300	-0.18129900	0.00000000
H	-1.30383000	-4.26909500	0.00000000
H	-3.67120000	-4.44152400	0.00000000
H	-5.85842000	-1.76599100	-0.87844000
H	-5.88679100	-3.31903800	0.00000000
H	-5.85842000	-1.76599100	0.87844000
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000
O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000

H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

[G]-G/C-G

Total Energy = -9354.26 kcal mol^{-1}

N	-3.62911800	-0.55312800	0.00000000
C	-4.53534800	-1.59255200	0.00000000
N	-4.17832400	-2.86660800	0.00000000
C	-2.83450500	-3.03984700	0.00000000
C	-1.82744100	-2.06508600	0.00000000
C	-2.19666100	-0.68159400	0.00000000
N	-2.15971800	-4.24342200	0.00000000
C	-0.79992700	-3.95247700	0.00000000
N	-0.56943700	-2.65542700	0.00000000
O	-1.50221800	0.33303000	0.00000000
N	-5.86134500	-1.27337200	0.00000000
H	-3.94776800	0.41311900	0.00000000
H	-2.59154300	-5.15965800	0.00000000
H	-0.04961900	-4.73031500	0.00000000
H	-6.52885800	-2.03131700	0.00000000
H	-6.19285900	-0.32126200	0.00000000
N	1.30203000	1.16969900	0.00000000
C	2.33399900	0.26245000	0.00000000
N	3.61710900	0.61198000	0.00000000
C	3.79291200	1.95571500	0.00000000
C	2.82869700	2.97584000	0.00000000
C	1.43390200	2.61042800	0.00000000
N	5.00698000	2.61388900	0.00000000
C	4.72756100	3.98111600	0.00000000
N	3.43645200	4.22941200	0.00000000
O	0.42664800	3.31234700	0.00000000
N	2.02116800	-1.06412400	0.00000000
H	0.33241800	0.83488000	0.00000000
H	5.91442500	2.16566300	0.00000000
H	5.51709200	4.72030000	0.00000000
H	2.80344300	-1.70226500	0.00000000
H	1.07594700	-1.44615400	0.00000000
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000

O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000
H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

[C]-G/C-G

Total Energy = -8813.00 kcal mol^{-1}

N	0.00000000	-0.54043000	-4.63303000
C	0.00000000	0.81748000	-4.95894000
H	0.00000000	1.15143000	-5.98760000
N	0.00000000	1.59154000	-3.89736000
C	0.00000000	0.71321000	-2.81543000
C	0.00000000	0.95546000	-1.40561000
O	0.00000000	2.04829000	-0.79997000
N	0.00000000	-0.25635000	-0.67322000
H	0.00000000	-0.15558000	0.36298000
C	0.00000000	-1.52541000	-1.21299000
N	0.00000000	-2.56092000	-0.33936000
H	0.00000000	-2.43115000	0.67996000
H	0.00000000	-3.49019000	-0.73371000
N	0.00000000	-1.75975000	-2.52453000
C	0.00000000	-0.62420000	-3.25586000
H	0.00000000	-1.33044000	-5.26603000
N	0.00000000	-0.86770000	4.37322000
C	0.00000000	0.36610000	4.95733000
H	-0.00000000	0.39134000	6.04179000
C	0.00000000	1.48622000	4.18684000
H	0.00000000	2.47453000	4.63276000
C	0.00000000	1.30521000	2.75326000
N	0.00000000	2.36231000	1.92808000
H	0.00000000	2.23358000	0.88795000
H	0.00000000	3.29650000	2.31256000
N	0.00000000	0.07909000	2.19846000

C	0.00000000	-1.04501000	2.96468000
O	0.00000000	-2.20433000	2.51757000
H	0.00000000	-1.71781000	4.92645000
N	3.40000000	2.28593000	-4.06590000
C	3.40000000	3.57608000	-3.53143000
H	3.40000000	4.45087000	-4.16736000
N	3.40000000	3.57835000	-2.21761000
C	3.40000000	2.23183000	-1.85856000
C	3.40000000	1.59917000	-0.57559000
O	3.40000000	2.12732000	0.55673000
N	3.40000000	0.18831000	-0.69533000
H	3.40000000	-0.33922000	0.20221000
C	3.40000000	-0.52114000	-1.87794000
N	3.40000000	-1.87239000	-1.77979000
H	3.40000000	-2.36653000	-0.87885000
H	3.40000000	-2.39241000	-2.64502000
N	3.40000000	0.06016000	-3.07675000
C	3.40000000	1.40870000	-3.00097000
H	3.40000000	2.01885000	-5.04235000
N	3.40000000	-3.27244000	3.02805000
C	3.40000000	-2.61758000	4.22580000
H	3.40000000	-3.23458000	5.11799000
C	3.40000000	-1.25850000	4.26082000
H	3.40000000	-0.72103000	5.20249000
C	3.40000000	-0.56234000	2.99462000
N	3.40000000	0.77791000	2.94837000
H	3.40000000	1.28511000	2.03121000
H	3.40000000	1.30771000	3.80850000
N	3.40000000	-1.22820000	1.82510000
C	3.40000000	-2.58799000	1.78429000
O	3.40000000	-3.26311000	0.74114000
H	3.40000000	-4.28537000	2.97596000

[A]-C/G-C

Total Energy = -8634.79 kcal mol^{-1}

N	-1.82697800	-1.70463500	0.00000000
C	-2.05376700	-3.05701700	0.00000000
N	-3.43367500	-3.46874100	0.00000000
C	-4.47157300	-2.58972600	0.00000000
C	-4.22717800	-1.24997600	0.00000000
C	-2.84094900	-0.84072000	0.00000000
N	-2.53673700	0.48233000	0.00000000
O	-1.18781400	-3.92902200	0.00000000
H	-3.58693200	-4.47141200	0.00000000
H	-5.47266600	-3.00933800	0.00000000
H	-5.03836900	-0.52994300	0.00000000
H	-1.54978900	0.78852900	0.00000000
H	-3.27818500	1.16677500	0.00000000
N	0.34538600	1.16241600	0.00000000
C	0.99861500	-0.02984700	0.00000000
N	2.32412500	-0.23349100	0.00000000
C	3.00909400	0.92011200	0.00000000

C	2.47077100	2.21857200	0.00000000
C	1.06248500	2.30727200	0.00000000
N	4.38081300	1.11387100	0.00000000
C	4.59601400	2.48567200	0.00000000
N	3.47626500	3.18423200	0.00000000
N	0.41882600	3.50705800	0.00000000
H	0.35170900	-0.90461900	0.00000000
H	5.07832900	0.37958700	0.00000000
H	5.59464400	2.90141700	0.00000000
H	0.95514200	4.36264800	0.00000000
H	-0.58961600	3.54144800	0.00000000
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000
O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000
H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

[T]-C/G-C

Total Energy = -8503.09 kcal mol^{-1}

N	-1.42634800	-0.97836600	0.00000000
C	-1.40509800	-2.35608000	0.00000000
N	-2.68631000	-3.00915800	0.00000000
C	-3.86799600	-2.33702900	0.00000000
C	-3.87240200	-0.97659000	0.00000000
C	-2.58916500	-0.31264200	0.00000000
N	-2.54306000	1.03606700	0.00000000
O	-0.39711300	-3.05222900	0.00000000
H	-2.64935500	-4.02265400	0.00000000

H	-4.77498200	-2.93342100	0.00000000
H	-4.79989800	-0.41500300	0.00000000
H	-1.63203600	1.52421800	0.00000000
H	-3.39972600	1.56919800	0.00000000
N	1.20681200	0.42332800	0.00000000
C	2.41686100	-0.27221800	0.00000000
N	3.53727400	0.57939200	0.00000000
C	3.46624000	1.95318000	0.00000000
C	2.27917800	2.61100300	0.00000000
C	1.05200400	1.81189300	0.00000000
O	-0.08000100	2.33250900	0.00000000
O	2.53274300	-1.48548900	0.00000000
C	2.15656500	4.11177100	0.00000000
H	0.33330600	-0.15338800	0.00000000
H	4.42945500	0.09935500	0.00000000
H	4.42067700	2.47198100	0.00000000
H	1.59948100	4.45660800	-0.87947200
H	3.14386700	4.58594000	0.00000000
H	1.59948100	4.45660800	0.87947200
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000
O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000
H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

[G]-C/G-C
Total Energy = -8813.00 kcal mol^{-1}

N	0.00000000	-0.54043000	-4.63303000

C	0.00000000	0.81748000	-4.95894000
H	0.00000000	1.15143000	-5.98760000
N	0.00000000	1.59154000	-3.89736000
C	0.00000000	0.71321000	-2.81543000
C	0.00000000	0.95546000	-1.40561000
O	0.00000000	2.04829000	-0.79997000
N	0.00000000	-0.25635000	-0.67322000
H	0.00000000	-0.15558000	0.36298000
C	0.00000000	-1.52541000	-1.21299000
N	0.00000000	-2.56092000	-0.33936000
H	0.00000000	-2.43115000	0.67996000
H	0.00000000	-3.49019000	-0.73371000
N	0.00000000	-1.75975000	-2.52453000
C	0.00000000	-0.62420000	-3.25586000
H	0.00000000	-1.33044000	-5.26603000
N	0.00000000	-0.86770000	4.37322000
C	0.00000000	0.36610000	4.95733000
H	-0.00000000	0.39134000	6.04179000
C	0.00000000	1.48622000	4.18684000
H	0.00000000	2.47453000	4.63276000
C	0.00000000	1.30521000	2.75326000
N	0.00000000	2.36231000	1.92808000
H	0.00000000	2.23358000	0.88795000
H	0.00000000	3.29650000	2.31256000
N	0.00000000	0.07909000	2.19846000
C	0.00000000	-1.04501000	2.96468000
O	0.00000000	-2.20433000	2.51757000
H	0.00000000	-1.71781000	4.92645000
N	3.40000000	2.28593000	-4.06590000
C	3.40000000	3.57608000	-3.53143000
H	3.40000000	4.45087000	-4.16736000
N	3.40000000	3.57835000	-2.21761000
C	3.40000000	2.23183000	-1.85856000
C	3.40000000	1.59917000	-0.57559000
O	3.40000000	2.12732000	0.55673000
N	3.40000000	0.18831000	-0.69533000
H	3.40000000	-0.33922000	0.20221000
C	3.40000000	-0.52114000	-1.87794000
N	3.40000000	-1.87239000	-1.77979000
H	3.40000000	-2.36653000	-0.87885000
H	3.40000000	-2.39241000	-2.64502000
N	3.40000000	0.06016000	-3.07675000
C	3.40000000	1.40870000	-3.00097000
H	3.40000000	2.01885000	-5.04235000
N	3.40000000	-3.27244000	3.02805000
C	3.40000000	-2.61758000	4.22580000
H	3.40000000	-3.23458000	5.11799000
C	3.40000000	-1.25850000	4.26082000
H	3.40000000	-0.72103000	5.20249000
C	3.40000000	-0.56234000	2.99462000
N	3.40000000	0.77791000	2.94837000
H	3.40000000	1.28511000	2.03121000

H	3.40000000	1.30771000	3.80850000
N	3.40000000	-1.22820000	1.82510000
C	3.40000000	-2.58799000	1.78429000
O	3.40000000	-3.26311000	0.74114000
H	3.40000000	-4.28537000	2.97596000

[C]-C/G-C

Total Energy = -8230.73 kcal mol^{-1}

N	1.86599800	2.71613100	0.00000000
C	3.23451100	2.82754500	0.00000000
N	3.96964300	1.59165600	0.00000000
C	3.37383300	0.36539800	0.00000000
C	2.01666000	0.26749200	0.00000000
C	1.29104300	1.51468400	0.00000000
N	-0.06978700	1.47675700	0.00000000
O	3.87241100	3.88028300	0.00000000
H	4.97890600	1.69058400	0.00000000
H	4.03026500	-0.49951900	0.00000000
H	1.50223600	-0.68709000	0.00000000
H	-0.54455500	2.37012000	0.00000000
H	-0.59668500	0.60226200	0.00000000
N	-1.88027300	-0.99558500	0.00000000
C	-1.24175400	-2.21464800	0.00000000
N	-2.08626800	-3.37025600	0.00000000
C	-3.44364800	-3.30188300	0.00000000
C	-4.06292400	-2.08816800	0.00000000
C	-3.20982900	-0.92864200	0.00000000
N	-3.77411200	0.30984000	0.00000000
O	-0.02396900	-2.37752100	0.00000000
H	-1.60029800	-4.26123800	0.00000000
H	-3.98387000	-4.24285300	0.00000000
H	-5.14389600	-2.00662000	0.00000000
H	-3.17823000	1.12625200	0.00000000
H	-4.77495200	0.43465800	0.00000000
N	4.63284800	-0.54203500	-3.40000000
C	4.95921900	0.81576400	-3.40000000
H	5.98799500	1.14936200	-3.40000000
N	3.89790800	1.59019500	-3.40000000
C	2.81567900	0.71223400	-3.40000000
C	1.40594000	0.95497200	-3.40000000
O	0.80067400	2.04801500	-3.40000000
N	0.67313600	-0.25658500	-3.40000000
H	-0.36303000	-0.15546100	-3.40000000
C	1.21246600	-1.52583500	-3.40000000
N	0.33847900	-2.56104000	-3.40000000
H	-0.68079600	-2.43091800	-3.40000000
H	0.73250400	-3.49044100	-3.40000000
N	2.52392700	-1.76062300	-3.40000000
C	3.25564000	-0.62533000	-3.40000000
H	5.26556600	-1.33225900	-3.40000000
N	-4.37351900	-0.86619400	-3.40000000
C	-4.95720400	0.36781300	-3.40000000

H	-6.04165500	0.39342100	-3.40000000
C	-4.18632200	1.48766200	-3.40000000
H	-4.63190300	2.47612700	-3.40000000
C	-2.75280800	1.30615400	-3.40000000
N	-1.92726900	2.36297700	-3.40000000
H	-0.88717800	2.23388000	-3.40000000
H	-2.31141700	3.29729100	-3.40000000
N	-2.19843500	0.07984700	-3.40000000
C	-2.96504200	-1.04398600	-3.40000000
O	-2.51832600	-2.20346300	-3.40000000
H	-4.92703800	-1.71611000	-3.40000000

Cartesian Coordinates of Systems in Toluene

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in toluene that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9156.11 kcal mol^{-1}

N	0.96370300	1.34597800	0.00000000
C	1.77861900	0.26498600	0.00000000
N	3.12106800	0.24601200	0.00000000
C	3.63804200	1.48970600	0.00000000
C	2.91620900	2.69616900	0.00000000
C	1.50725900	2.58784500	0.00000000
N	4.96563900	1.87438500	0.00000000
C	4.98827300	3.25775700	0.00000000
N	3.77807300	3.79304500	0.00000000
N	0.69296000	3.67080400	0.00000000
H	1.26173700	-0.69214100	0.00000000
H	5.76614200	1.25333200	0.00000000
H	5.91867700	3.80804500	0.00000000
H	1.08449100	4.60220900	0.00000000
H	-0.31076100	3.55374500	0.00000000
N	-0.81403200	-1.85908300	0.00000000
C	-0.96090400	-3.19797500	0.00000000
N	-2.09661900	-3.92039200	0.00000000
C	-3.18381300	-3.12316800	0.00000000
C	-3.18931300	-1.71824500	0.00000000
C	-1.92644200	-1.07579400	0.00000000
N	-4.52011600	-3.48160200	0.00000000
C	-5.25499800	-2.30917400	0.00000000
N	-4.49539000	-1.22559400	0.00000000
N	-1.79036900	0.26772500	0.00000000
H	-0.03485600	-3.76902600	0.00000000
H	-4.88501100	-4.42667600	0.00000000
H	-6.33597000	-2.31940100	0.00000000
H	-2.62464600	0.83888000	0.00000000
H	-0.85794500	0.70742500	0.00000000
N	3.89553500	-1.54103700	-3.40000000
C	4.60914900	-0.36159300	-3.40000000
H	5.68829700	-0.47452300	-3.40000000
C	4.00184000	0.85459900	-3.40000000
C	4.75488100	2.15875500	-3.40000000
H	5.83577300	1.98647200	-3.40000000
H	4.49385500	2.75873700	-2.51970200
H	4.49385500	2.75873700	-4.28029800
C	2.54096500	0.88456600	-3.40000000
O	1.86901600	1.93729800	-3.40000000
N	1.90082200	-0.35464900	-3.40000000
H	0.84223400	-0.35811300	-3.40000000
C	2.50459100	-1.59670300	-3.40000000

O	1.88140900	-2.66235900	-3.40000000
H	4.37515200	-2.43439300	-3.40000000
N	-4.93843700	-0.55715500	-3.40000000
C	-5.20227500	0.80120900	-3.40000000
H	-6.21452100	1.18057500	-3.40000000
N	-4.10371500	1.53864600	-3.40000000
C	-3.06415200	0.60947600	-3.40000000
C	-1.65608400	0.75645100	-3.40000000
N	-1.02886300	1.94799800	-3.40000000
H	-0.00260800	1.99543400	-3.40000000
H	-1.57832100	2.79623800	-3.40000000
N	-0.91206700	-0.38409100	-3.40000000
C	-1.52278300	-1.58771400	-3.40000000
H	-0.85168200	-2.44346000	-3.40000000
N	-2.83957000	-1.84263100	-3.40000000
C	-3.56391600	-0.70401900	-3.40000000
H	-5.61924600	-1.30759700	-3.40000000

[T]-A/T-A
Total Energy = -9023.63 kcal mol^{-1}

N	4.05735300	1.04301300	0.00000000
C	3.94141900	2.41665500	0.00000000
H	4.88084700	2.95960000	0.00000000
C	2.73523600	3.04360800	0.00000000
C	2.57789500	4.54131800	0.00000000
H	3.55362100	5.03727100	0.00000000
H	2.01406000	4.87328700	-0.88029800
H	2.01406000	4.87328700	0.88029800
C	1.53574900	2.20917100	0.00000000
O	0.37335100	2.66588700	0.00000000
N	1.74625500	0.83035800	0.00000000
H	0.89187500	0.20533300	0.00000000
C	2.96477500	0.18040200	0.00000000
O	3.08698700	-1.04802900	0.00000000
H	4.97047300	0.60218500	0.00000000
N	-3.66779200	-3.35348800	0.00000000
C	-4.67966800	-2.40962900	0.00000000
H	-5.72157800	-2.69769900	0.00000000
N	-4.22436900	-1.16731200	0.00000000
C	-2.83719200	-1.30798700	0.00000000
C	-1.78443100	-0.36144000	0.00000000
N	-1.97737200	0.97121300	0.00000000
H	-1.17499700	1.61280700	0.00000000
H	-2.92047600	1.33449000	0.00000000
N	-0.51211500	-0.84683600	0.00000000
C	-0.29872200	-2.17955700	0.00000000
H	0.74720500	-2.47740700	0.00000000
N	-1.21418900	-3.15977700	0.00000000
C	-2.46945700	-2.66438100	0.00000000
H	-3.77747900	-4.36077800	0.00000000
N	3.89553500	-1.54103700	-3.40000000
C	4.60914900	-0.36159300	-3.40000000

H	5.68829700	-0.47452300	-3.40000000
C	4.00184000	0.85459900	-3.40000000
C	4.75488100	2.15875500	-3.40000000
H	5.83577300	1.98647200	-3.40000000
H	4.49385500	2.75873700	-2.51970200
H	4.49385500	2.75873700	-4.28029800
C	2.54096500	0.88456600	-3.40000000
O	1.86901600	1.93729800	-3.40000000
N	1.90082200	-0.35464900	-3.40000000
H	0.84223400	-0.35811300	-3.40000000
C	2.50459100	-1.59670300	-3.40000000
O	1.88140900	-2.66235900	-3.40000000
H	4.37515200	-2.43439300	-3.40000000
N	-4.93843700	-0.55715500	-3.40000000
C	-5.20227500	0.80120900	-3.40000000
H	-6.21452100	1.18057500	-3.40000000
N	-4.10371500	1.53864600	-3.40000000
C	-3.06415200	0.60947600	-3.40000000
C	-1.65608400	0.75645100	-3.40000000
N	-1.02886300	1.94799800	-3.40000000
H	-0.00260800	1.99543400	-3.40000000
H	-1.57832100	2.79623800	-3.40000000
N	-0.91206700	-0.38409100	-3.40000000
C	-1.52278300	-1.58771400	-3.40000000
H	-0.85168200	-2.44346000	-3.40000000
N	-2.83957000	-1.84263100	-3.40000000
C	-3.56391600	-0.70401900	-3.40000000
H	-5.61924600	-1.30759700	-3.40000000

[G]-A/T-A

Total Energy = -9324.41 kcal mol^{-1}

N	1.38492200	0.50494400	0.00000000
C	2.63972500	-0.05807400	0.00000000
N	3.76796900	0.64495800	0.00000000
C	3.55008000	1.98181900	0.00000000
C	2.32230400	2.66427000	0.00000000
C	1.11677700	1.89689300	0.00000000
N	4.50726400	2.97149900	0.00000000
C	3.83655500	4.18890400	0.00000000
N	2.52627200	4.04381900	0.00000000
O	-0.06258700	2.30631000	0.00000000
N	2.70561900	-1.41710700	0.00000000
H	0.55266000	-0.12726300	0.00000000
H	5.51020100	2.82787800	0.00000000
H	4.37092600	5.12832300	0.00000000
H	3.61359700	-1.85895000	0.00000000
H	1.87663900	-1.98985600	0.00000000
N	-0.93168100	-1.29377300	0.00000000
C	-0.82753600	-2.63953200	0.00000000
N	-1.79989500	-3.56007600	0.00000000
C	-3.02136000	-2.98328900	0.00000000
C	-3.29083600	-1.60645900	0.00000000

C	-2.17762300	-0.72773100	0.00000000
N	-4.26330400	-3.58807100	0.00000000
C	-5.20636000	-2.57499200	0.00000000
N	-4.66369700	-1.36837600	0.00000000
N	-2.30387100	0.60794100	0.00000000
H	0.18568800	-3.03799600	0.00000000
H	-4.44380000	-4.58514800	0.00000000
H	-6.26597900	-2.78845300	0.00000000
H	-3.23351100	1.00664500	0.00000000
H	-1.48014100	1.23090500	0.00000000
N	3.89553500	-1.54103700	-3.40000000
C	4.60914900	-0.36159300	-3.40000000
H	5.68829700	-0.47452300	-3.40000000
C	4.00184000	0.85459900	-3.40000000
C	4.75488100	2.15875500	-3.40000000
H	5.83577300	1.98647200	-3.40000000
H	4.49385500	2.75873700	-2.51970200
H	4.49385500	2.75873700	-4.28029800
C	2.54096500	0.88456600	-3.40000000
O	1.86901600	1.93729800	-3.40000000
N	1.90082200	-0.35464900	-3.40000000
H	0.84223400	-0.35811300	-3.40000000
C	2.50459100	-1.59670300	-3.40000000
O	1.88140900	-2.66235900	-3.40000000
H	4.37515200	-2.43439300	-3.40000000
N	-4.93843700	-0.55715500	-3.40000000
C	-5.20227500	0.80120900	-3.40000000
H	-6.21452100	1.18057500	-3.40000000
N	-4.10371500	1.53864600	-3.40000000
C	-3.06415200	0.60947600	-3.40000000
C	-1.65608400	0.75645100	-3.40000000
N	-1.02886300	1.94799800	-3.40000000
H	-0.00260800	1.99543400	-3.40000000
H	-1.57832100	2.79623800	-3.40000000
N	-0.91206700	-0.38409100	-3.40000000
C	-1.52278300	-1.58771400	-3.40000000
H	-0.85168200	-2.44346000	-3.40000000
N	-2.83957000	-1.84263100	-3.40000000
C	-3.56391600	-0.70401900	-3.40000000
H	-5.61924600	-1.30759700	-3.40000000

[C]-A/T-A

Total Energy = -8756.06 kcal mol^{-1}

N	2.20268100	1.21061400	0.00000000
C	3.55720700	1.03117300	0.00000000
N	4.36427300	2.20526200	0.00000000
C	3.84118700	3.46220600	0.00000000
C	2.49030400	3.63619200	0.00000000
C	1.67946600	2.44358400	0.00000000
N	0.33012500	2.54951600	0.00000000
O	4.12293500	-0.07263600	0.00000000
H	5.36821900	2.05722100	0.00000000

H	4.54792400	4.28453300	0.00000000
H	2.04842800	4.62638500	0.00000000
H	-0.25933300	1.70105100	0.00000000
H	-0.10160200	3.46272000	0.00000000
N	-1.19768200	0.01353500	0.00000000
C	-0.28085200	-0.98521000	0.00000000
N	-0.50894200	-2.30788600	0.00000000
C	-1.82480600	-2.59056900	0.00000000
C	-2.88001500	-1.66173700	0.00000000
C	-2.51675800	-0.29674300	0.00000000
N	-2.44476900	-3.82622100	0.00000000
C	-3.80881300	-3.59669000	0.00000000
N	-4.11586200	-2.30935600	0.00000000
N	-3.43690500	0.69994100	0.00000000
H	0.75456100	-0.65197400	0.00000000
H	-1.97982400	-4.72663200	0.00000000
H	-4.51875000	-4.41190200	0.00000000
H	-4.42328400	0.48144800	0.00000000
H	-3.14185800	1.66603100	0.00000000
N	3.89553500	-1.54103700	-3.40000000
C	4.60914900	-0.36159300	-3.40000000
H	5.68829700	-0.47452300	-3.40000000
C	4.00184000	0.85459900	-3.40000000
C	4.75488100	2.15875500	-3.40000000
H	5.83577300	1.98647200	-3.40000000
H	4.49385500	2.75873700	-2.51970200
H	4.49385500	2.75873700	-4.28029800
C	2.54096500	0.88456600	-3.40000000
O	1.86901600	1.93729800	-3.40000000
N	1.90082200	-0.35464900	-3.40000000
H	0.84223400	-0.35811300	-3.40000000
C	2.50459100	-1.59670300	-3.40000000
O	1.88140900	-2.66235900	-3.40000000
H	4.37515200	-2.43439300	-3.40000000
N	-4.93843700	-0.55715500	-3.40000000
C	-5.20227500	0.80120900	-3.40000000
H	-6.21452100	1.18057500	-3.40000000
N	-4.10371500	1.53864600	-3.40000000
C	-3.06415200	0.60947600	-3.40000000
C	-1.65608400	0.75645100	-3.40000000
N	-1.02886300	1.94799800	-3.40000000
H	-0.00260800	1.99543400	-3.40000000
H	-1.57832100	2.79623800	-3.40000000
N	-0.91206700	-0.38409100	-3.40000000
C	-1.52278300	-1.58771400	-3.40000000
H	-0.85168200	-2.44346000	-3.40000000
N	-2.83957000	-1.84263100	-3.40000000
C	-3.56391600	-0.70401900	-3.40000000
H	-5.61924600	-1.30759700	-3.40000000

[A]-T/A-T
Total Energy = -9023.63 kcal mol^{-1}

N	4.05735300	1.04301300	0.00000000
C	3.94141900	2.41665500	0.00000000
H	4.88084700	2.95960000	0.00000000
C	2.73523600	3.04360800	0.00000000
C	2.57789500	4.54131800	0.00000000
H	3.55362100	5.03727100	0.00000000
H	2.01406000	4.87328700	-0.88029800
H	2.01406000	4.87328700	0.88029800
C	1.53574900	2.20917100	0.00000000
O	0.37335100	2.66588700	0.00000000
N	1.74625500	0.83035800	0.00000000
H	0.89187500	0.20533300	0.00000000
C	2.96477500	0.18040200	0.00000000
O	3.08698700	-1.04802900	0.00000000
H	4.97047300	0.60218500	0.00000000
N	-3.66779200	-3.35348800	0.00000000
C	-4.67966800	-2.40962900	0.00000000
H	-5.72157800	-2.69769900	0.00000000
N	-4.22436900	-1.16731200	0.00000000
C	-2.83719200	-1.30798700	0.00000000
C	-1.78443100	-0.36144000	0.00000000
N	-1.97737200	0.97121300	0.00000000
H	-1.17499700	1.61280700	0.00000000
H	-2.92047600	1.33449000	0.00000000
N	-0.51211500	-0.84683600	0.00000000
C	-0.29872200	-2.17955700	0.00000000
H	0.74720500	-2.47740700	0.00000000
N	-1.21418900	-3.15977700	0.00000000
C	-2.46945700	-2.66438100	0.00000000
H	-3.77747900	-4.36077800	0.00000000
N	3.89553500	-1.54103700	-3.40000000
C	4.60914900	-0.36159300	-3.40000000
H	5.68829700	-0.47452300	-3.40000000
C	4.00184000	0.85459900	-3.40000000
C	4.75488100	2.15875500	-3.40000000
H	5.83577300	1.98647200	-3.40000000
H	4.49385500	2.75873700	-2.51970200
H	4.49385500	2.75873700	-4.28029800
C	2.54096500	0.88456600	-3.40000000
O	1.86901600	1.93729800	-3.40000000
N	1.90082200	-0.35464900	-3.40000000
H	0.84223400	-0.35811300	-3.40000000
C	2.50459100	-1.59670300	-3.40000000
O	1.88140900	-2.66235900	-3.40000000
H	4.37515200	-2.43439300	-3.40000000
N	-4.93843700	-0.55715500	-3.40000000
C	-5.20227500	0.80120900	-3.40000000
H	-6.21452100	1.18057500	-3.40000000
N	-4.10371500	1.53864600	-3.40000000
C	-3.06415200	0.60947600	-3.40000000
C	-1.65608400	0.75645100	-3.40000000
N	-1.02886300	1.94799800	-3.40000000

H	-0.00260800	1.99543400	-3.40000000
H	-1.57832100	2.79623800	-3.40000000
N	-0.91206700	-0.38409100	-3.40000000
C	-1.52278300	-1.58771400	-3.40000000
H	-0.85168200	-2.44346000	-3.40000000
N	-2.83957000	-1.84263100	-3.40000000
C	-3.56391600	-0.70401900	-3.40000000
H	-5.61924600	-1.30759700	-3.40000000

[T]-T/A-T

Total Energy = -8881.49 kcal mol^{-1}

N	-1.96471500	0.65515900	0.00000000
C	-3.35072900	0.68427300	0.00000000
N	-3.87537500	1.97365100	0.00000000
C	-3.10328600	3.11494000	0.00000000
C	-1.74500400	3.07132300	0.00000000
C	-1.10662500	1.75880100	0.00000000
O	0.12998700	1.59499900	0.00000000
O	-4.06101800	-0.32144100	0.00000000
C	-0.87267800	4.29873700	0.00000000
H	-1.52143400	-0.28346200	0.00000000
H	-4.88741900	2.03554800	0.00000000
H	-3.65735700	4.04785800	0.00000000
H	-0.21830200	4.31028200	-0.87988900
H	-1.47986900	5.20932200	0.00000000
H	-0.21830200	4.31028200	0.87988900
N	1.46446000	-0.88519500	0.00000000
C	0.60634400	-1.95845600	0.00000000
N	1.23330500	-3.19111800	0.00000000
C	2.60708200	-3.34520600	0.00000000
C	3.45260600	-2.28412000	0.00000000
C	2.87453700	-0.93617100	0.00000000
O	3.53353500	0.10902600	0.00000000
O	-0.63408800	-1.85808800	0.00000000
C	4.95198900	-2.41746600	0.00000000
H	1.01666700	0.05420700	0.00000000
H	0.62235600	-4.00015200	0.00000000
H	2.95421900	-4.37305700	0.00000000
H	5.38433700	-1.92580400	0.87989600
H	5.25260800	-3.46991400	0.00000000
H	5.38433700	-1.92580400	-0.87989600
N	3.89553500	-1.54103700	3.40000000
C	4.60914900	-0.36159300	3.40000000
H	5.68829700	-0.47452300	3.40000000
C	4.00184000	0.85459900	3.40000000
C	4.75488100	2.15875500	3.40000000
H	5.83577300	1.98647200	3.40000000
H	4.49385500	2.75873700	2.51970200
H	4.49385500	2.75873700	4.28029800
C	2.54096500	0.88456600	3.40000000
O	1.86901600	1.93729800	3.40000000

N	1.90082200	-0.35464900	3.40000000
H	0.84223400	-0.35811300	3.40000000
C	2.50459100	-1.59670300	3.40000000
O	1.88140900	-2.66235900	3.40000000
H	4.37515200	-2.43439300	3.40000000
N	-4.93843700	-0.55715500	3.40000000
C	-5.20227500	0.80120900	3.40000000
H	-6.21452100	1.18057500	3.40000000
N	-4.10371500	1.53864600	3.40000000
C	-3.06415200	0.60947600	3.40000000
C	-1.65608400	0.75645100	3.40000000
N	-1.02886300	1.94799800	3.40000000
H	-0.00260800	1.99543400	3.40000000
H	-1.57832100	2.79623800	3.40000000
N	-0.91206700	-0.38409100	3.40000000
C	-1.52278300	-1.58771400	3.40000000
H	-0.85168200	-2.44346000	3.40000000
N	-2.83957000	-1.84263100	3.40000000
C	-3.56391600	-0.70401900	3.40000000
H	-5.61924600	-1.30759700	3.40000000

[G]-T/A-T
Total Energy = -9183.77 kcal mol^{-1}

N	-1.57930900	0.10671600	0.00000000
C	-2.94847400	-0.00939700	0.00000000
N	-3.77451600	1.03218800	0.00000000
C	-3.11651200	2.21755900	0.00000000
C	-1.72898800	2.44937500	0.00000000
C	-0.85352500	1.31997000	0.00000000
N	-3.68471500	3.47168300	0.00000000
C	-2.64403400	4.39323500	0.00000000
N	-1.45864800	3.81695800	0.00000000
O	0.39575300	1.29219200	0.00000000
N	-3.44969000	-1.27380800	0.00000000
H	-1.00976900	-0.76008500	0.00000000
H	-4.67751100	3.67400700	0.00000000
H	-2.83161500	5.45760300	0.00000000
H	-4.45147400	-1.40078200	0.00000000
H	-2.84292300	-2.08146600	0.00000000
N	1.85933800	-1.10491200	0.00000000
C	1.11709600	-2.25693600	0.00000000
N	1.85841100	-3.42115300	0.00000000
C	3.24231700	-3.44255400	0.00000000
C	3.97933300	-2.30455100	0.00000000
C	3.27124500	-1.01899400	0.00000000
O	3.82237000	0.08427100	0.00000000
O	-0.13281700	-2.28600700	0.00000000
C	5.48424700	-2.28979000	0.00000000
H	1.33277100	-0.20060800	0.00000000
H	1.32995500	-4.28607300	0.00000000
H	3.68623200	-4.43236600	0.00000000
H	5.86520200	-1.75729100	0.87978800

H	5.88709400	-3.30740700	0.00000000
H	5.86520200	-1.75729100	-0.87978800
N	3.89553500	-1.54103700	3.40000000
C	4.60914900	-0.36159300	3.40000000
H	5.68829700	-0.47452300	3.40000000
C	4.00184000	0.85459900	3.40000000
C	4.75488100	2.15875500	3.40000000
H	5.83577300	1.98647200	3.40000000
H	4.49385500	2.75873700	2.51970200
H	4.49385500	2.75873700	4.28029800
C	2.54096500	0.88456600	3.40000000
O	1.86901600	1.93729800	3.40000000
N	1.90082200	-0.35464900	3.40000000
H	0.84223400	-0.35811300	3.40000000
C	2.50459100	-1.59670300	3.40000000
O	1.88140900	-2.66235900	3.40000000
H	4.37515200	-2.43439300	3.40000000
N	-4.93843700	-0.55715500	3.40000000
C	-5.20227500	0.80120900	3.40000000
H	-6.21452100	1.18057500	3.40000000
N	-4.10371500	1.53864600	3.40000000
C	-3.06415200	0.60947600	3.40000000
C	-1.65608400	0.75645100	3.40000000
N	-1.02886300	1.94799800	3.40000000
H	-0.00260800	1.99543400	3.40000000
H	-1.57832100	2.79623800	3.40000000
N	-0.91206700	-0.38409100	3.40000000
C	-1.52278300	-1.58771400	3.40000000
H	-0.85168200	-2.44346000	3.40000000
N	-2.83957000	-1.84263100	3.40000000
C	-3.56391600	-0.70401900	3.40000000
H	-5.61924600	-1.30759700	3.40000000

[C]-T/A-T

Total Energy = -8619.30 kcal mol^{-1}

N	-1.38469400	1.05761500	0.00000000
C	-2.68961400	0.62906600	0.00000000
N	-3.69721400	1.63570000	0.00000000
C	-3.41953300	2.96763000	0.00000000
C	-2.12561900	3.38878600	0.00000000
C	-1.10249000	2.37346200	0.00000000
N	0.19458500	2.73781900	0.00000000
O	-3.04012200	-0.55561900	0.00000000
H	-4.65481300	1.30016100	0.00000000
H	-4.26731100	3.64377900	0.00000000
H	-1.87309100	4.44288400	0.00000000
H	0.93598300	2.02142900	0.00000000
H	0.44351200	3.71663700	0.00000000
N	0.79015200	-1.01677200	0.00000000
C	0.49634700	-2.37687800	0.00000000
N	1.63236200	-3.18887300	0.00000000
C	2.92102000	-2.71043400	0.00000000

C	3.19486200	-1.37967100	0.00000000
C	2.06830400	-0.45168100	0.00000000
O	2.21500900	0.78904500	0.00000000
O	-0.63809900	-2.84385800	0.00000000
C	4.59344100	-0.82066900	0.00000000
H	-0.02365800	-0.36099200	0.00000000
H	1.45093300	-4.18640000	0.00000000
H	3.69851300	-3.46746500	0.00000000
H	4.76118500	-0.18849500	0.88043900
H	5.33450700	-1.62625300	0.00000000
H	4.76118500	-0.18849500	-0.88043900
N	3.89553500	-1.54103700	3.40000000
C	4.60914900	-0.36159300	3.40000000
H	5.68829700	-0.47452300	3.40000000
C	4.00184000	0.85459900	3.40000000
C	4.75488100	2.15875500	3.40000000
H	5.83577300	1.98647200	3.40000000
H	4.49385500	2.75873700	2.51970200
H	4.49385500	2.75873700	4.28029800
C	2.54096500	0.88456600	3.40000000
O	1.86901600	1.93729800	3.40000000
N	1.90082200	-0.35464900	3.40000000
H	0.84223400	-0.35811300	3.40000000
C	2.50459100	-1.59670300	3.40000000
O	1.88140900	-2.66235900	3.40000000
H	4.37515200	-2.43439300	3.40000000
N	-4.93843700	-0.55715500	3.40000000
C	-5.20227500	0.80120900	3.40000000
H	-6.21452100	1.18057500	3.40000000
N	-4.10371500	1.53864600	3.40000000
C	-3.06415200	0.60947600	3.40000000
C	-1.65608400	0.75645100	3.40000000
N	-1.02886300	1.94799800	3.40000000
H	-0.00260800	1.99543400	3.40000000
H	-1.57832100	2.79623800	3.40000000
N	-0.91206700	-0.38409100	3.40000000
C	-1.52278300	-1.58771400	3.40000000
H	-0.85168200	-2.44346000	3.40000000
N	-2.83957000	-1.84263100	3.40000000
C	-3.56391600	-0.70401900	3.40000000
H	-5.61924600	-1.30759700	3.40000000

[A]-G/C-G

Total Energy = -9233.28 kcal mol^{-1}

N	1.38492200	0.50494400	0.00000000
C	2.63972500	-0.05807400	0.00000000
N	3.76796900	0.64495800	0.00000000
C	3.55008000	1.98181900	0.00000000
C	2.32230400	2.66427000	0.00000000
C	1.11677700	1.89689300	0.00000000
N	4.50726400	2.97149900	0.00000000
C	3.83655500	4.18890400	0.00000000

N	2.52627200	4.04381900	0.00000000
O	-0.06258700	2.30631000	0.00000000
N	2.70561900	-1.41710700	0.00000000
H	0.55266000	-0.12726300	0.00000000
H	5.51020100	2.82787800	0.00000000
H	4.37092600	5.12832300	0.00000000
H	3.61359700	-1.85895000	0.00000000
H	1.87663900	-1.98985600	0.00000000
N	-0.93168100	-1.29377300	0.00000000
C	-0.82753600	-2.63953200	0.00000000
N	-1.79989500	-3.56007600	0.00000000
C	-3.02136000	-2.98328900	0.00000000
C	-3.29083600	-1.60645900	0.00000000
C	-2.17762300	-0.72773100	0.00000000
N	-4.26330400	-3.58807100	0.00000000
C	-5.20636000	-2.57499200	0.00000000
N	-4.66369700	-1.36837600	0.00000000
N	-2.30387100	0.60794100	0.00000000
H	0.18568800	-3.03799600	0.00000000
H	-4.44380000	-4.58514800	0.00000000
H	-6.26597900	-2.78845300	0.00000000
H	-3.23351100	1.00664500	0.00000000
H	-1.48014100	1.23090500	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[T]-G/C-G

Total Energy = -9092.92 kcal mol^{-1}

N	1.57930900	0.10671600	0.00000000
C	2.94847400	-0.00939700	0.00000000
N	3.77451600	1.03218800	0.00000000
C	3.11651200	2.21755900	0.00000000
C	1.72898800	2.44937500	0.00000000
C	0.85352500	1.31997000	0.00000000
N	3.68471500	3.47168300	0.00000000
C	2.64403400	4.39323500	0.00000000
N	1.45864800	3.81695800	0.00000000
O	-0.39575300	1.29219200	0.00000000
N	3.44969000	-1.27380800	0.00000000
H	1.00976900	-0.76008500	0.00000000
H	4.67751100	3.67400700	0.00000000
H	2.83161500	5.45760300	0.00000000
H	4.45147400	-1.40078200	0.00000000
H	2.84292300	-2.08146600	0.00000000
N	-1.85933800	-1.10491200	0.00000000
C	-1.11709600	-2.25693600	0.00000000
N	-1.85841100	-3.42115300	0.00000000
C	-3.24231700	-3.44255400	0.00000000
C	-3.97933300	-2.30455100	0.00000000
C	-3.27124500	-1.01899400	0.00000000
O	-3.82237000	0.08427100	0.00000000
O	0.13281700	-2.28600700	0.00000000
C	-5.48424700	-2.28979000	0.00000000
H	-1.33277100	-0.20060800	0.00000000
H	-1.32995500	-4.28607300	0.00000000
H	-3.68623200	-4.43236600	0.00000000
H	-5.86520200	-1.75729100	0.87978800
H	-5.88709400	-3.30740700	0.00000000
H	-5.86520200	-1.75729100	-0.87978800
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000

H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[G]-G/C-G

Total Energy = -9388.44 kcal mol^{-1}

N	-3.61636000	-0.54156500	0.00000000
C	-4.50788400	-1.59511300	0.00000000
N	-4.12528600	-2.86737600	0.00000000
C	-2.77927100	-3.01702900	0.00000000
C	-1.79427900	-2.01859800	0.00000000
C	-2.19551500	-0.64877600	0.00000000
N	-2.07924400	-4.20448800	0.00000000
C	-0.72980900	-3.88929400	0.00000000
N	-0.52328100	-2.58512000	0.00000000
O	-1.50689300	0.38179400	0.00000000
N	-5.83080200	-1.29302800	0.00000000
H	-3.96393500	0.41470200	0.00000000
H	-2.48379500	-5.13375700	0.00000000
H	0.03408500	-4.65309900	0.00000000
H	-6.49768400	-2.05228600	0.00000000
H	-6.16782200	-0.34165600	0.00000000
N	1.28236800	1.11054400	0.00000000
C	2.33481700	0.22267200	0.00000000
N	3.61394200	0.60476900	0.00000000
C	3.76284500	1.95101600	0.00000000
C	2.76945700	2.94218200	0.00000000
C	1.39167900	2.53817500	0.00000000
N	4.95655900	2.64264100	0.00000000
C	4.64450300	3.99713200	0.00000000
N	3.34376400	4.21391900	0.00000000
O	0.36916800	3.23505900	0.00000000
N	2.04801300	-1.10292200	0.00000000
H	0.31501200	0.75440400	0.00000000
H	5.88150500	2.22976100	0.00000000
H	5.41470600	4.75538600	0.00000000
H	2.83721900	-1.73435100	0.00000000
H	1.10195400	-1.49922500	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000

O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[C]-G/C-G
Total Energy = -8839.79 kcal mol^{-1}

N	4.07695500	2.28207400	0.00000000
C	3.55315700	3.57039300	0.00000000
H	4.19335200	4.44123000	0.00000000
N	2.23514700	3.57987400	0.00000000
C	1.87008900	2.23288900	0.00000000
C	0.58600400	1.60832700	0.00000000
O	-0.54238700	2.15381100	0.00000000
N	0.68994900	0.20105200	0.00000000
H	-0.21229500	-0.32348100	0.00000000
C	1.86854100	-0.51727800	0.00000000
N	1.76232200	-1.86438200	0.00000000
H	0.85549100	-2.35101800	0.00000000
H	2.61993700	-2.39865800	0.00000000
N	3.07388800	0.05890200	0.00000000
C	3.01011900	1.40902200	0.00000000
H	5.05566600	2.02054200	0.00000000
N	-3.02121700	-3.27939400	0.00000000
C	-4.22429700	-2.63482100	0.00000000
H	-5.10868700	-3.26116400	0.00000000
C	-4.26898300	-1.27549700	0.00000000
H	-5.21243900	-0.74193200	0.00000000
C	-3.01126300	-0.57270000	0.00000000
N	-2.97765200	0.76816000	0.00000000
H	-2.07373600	1.27848900	0.00000000
H	-3.84149400	1.29284400	0.00000000
N	-1.83231600	-1.23007200	0.00000000

C	-1.79263100	-2.58931900	0.00000000
O	-0.73517900	-3.25671800	0.00000000
H	-2.97090600	-4.29293400	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[A]-C/G-C

Total Energy = -8662.82 kcal mol^{-1}

N	-1.83202900	-1.72077400	0.00000000
C	-2.07994100	-3.06445500	0.00000000
N	-3.44596300	-3.46920700	0.00000000
C	-4.47974500	-2.58330600	0.00000000
C	-4.22777000	-1.24477500	0.00000000
C	-2.84297000	-0.84215800	0.00000000
N	-2.52674800	0.47387600	0.00000000
O	-1.20497600	-3.94359000	0.00000000
H	-3.61540500	-4.46976300	0.00000000
H	-5.48021900	-3.00133900	0.00000000
H	-5.03295300	-0.51854000	0.00000000
H	-1.53765700	0.77229400	0.00000000
H	-3.26184500	1.16666800	0.00000000
N	0.35723100	1.14324600	0.00000000
C	1.02377800	-0.03734100	0.00000000
N	2.35220200	-0.22914400	0.00000000
C	3.02767300	0.93496400	0.00000000

C	2.47038000	2.22555200	0.00000000
C	1.05994000	2.30188000	0.00000000
N	4.39442800	1.14274600	0.00000000
C	4.59764300	2.51095800	0.00000000
N	3.46819900	3.20078800	0.00000000
N	0.39637900	3.48498500	0.00000000
H	0.38689200	-0.91910100	0.00000000
H	5.10709300	0.42231500	0.00000000
H	5.59233900	2.93423400	0.00000000
H	0.90898600	4.35556900	0.00000000
H	-0.61360200	3.50291600	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[T]-C/G-C

Total Energy = -8527.94 kcal mol^{-1}

N	-1.43374600	-0.99010100	0.00000000
C	-1.42941400	-2.36358200	0.00000000
N	-2.69814500	-3.01080000	0.00000000
C	-3.87907700	-2.33512100	0.00000000
C	-3.87977900	-0.97439100	0.00000000
C	-2.59798500	-0.31509000	0.00000000
N	-2.54369000	1.03109400	0.00000000
O	-0.41102500	-3.06302400	0.00000000
H	-2.67494300	-4.02521800	0.00000000

H	-4.78411200	-2.93246400	0.00000000
H	-4.80425000	-0.40848900	0.00000000
H	-1.63325800	1.51482800	0.00000000
H	-3.39767900	1.57030900	0.00000000
N	1.21117800	0.43728000	0.00000000
C	2.41392500	-0.26244100	0.00000000
N	3.53722600	0.56705300	0.00000000
C	3.48042100	1.94048500	0.00000000
C	2.29941200	2.61215300	0.00000000
C	1.06871500	1.82749700	0.00000000
O	-0.06595100	2.35042700	0.00000000
O	2.50748700	-1.48566900	0.00000000
C	2.19995400	4.11502200	0.00000000
H	0.33601300	-0.13405300	0.00000000
H	4.42986600	0.08625100	0.00000000
H	4.44065900	2.44598900	0.00000000
H	1.65055600	4.46990800	0.88043900
H	3.19511200	4.57087700	0.00000000
H	1.65055600	4.46990800	-0.88043900
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[G]-C/G-C
Total Energy = -8839.79 kcal mol^{-1}

N	4.07695500	2.28207400	0.00000000

C	3.55315700	3.57039300	0.00000000
H	4.19335200	4.44123000	0.00000000
N	2.23514700	3.57987400	0.00000000
C	1.87008900	2.23288900	0.00000000
C	0.58600400	1.60832700	0.00000000
O	-0.54238700	2.15381100	0.00000000
N	0.68994900	0.20105200	0.00000000
H	-0.21229500	-0.32348100	0.00000000
C	1.86854100	-0.51727800	0.00000000
N	1.76232200	-1.86438200	0.00000000
H	0.85549100	-2.35101800	0.00000000
H	2.61993700	-2.39865800	0.00000000
N	3.07388800	0.05890200	0.00000000
C	3.01011900	1.40902200	0.00000000
H	5.05566600	2.02054200	0.00000000
N	-3.02121700	-3.27939400	0.00000000
C	-4.22429700	-2.63482100	0.00000000
H	-5.10868700	-3.26116400	0.00000000
C	-4.26898300	-1.27549700	0.00000000
H	-5.21243900	-0.74193200	0.00000000
C	-3.01126300	-0.57270000	0.00000000
N	-2.97765200	0.76816000	0.00000000
H	-2.07373600	1.27848900	0.00000000
H	-3.84149400	1.29284400	0.00000000
N	-1.83231600	-1.23007200	0.00000000
C	-1.79263100	-2.58931900	0.00000000
O	-0.73517900	-3.25671800	0.00000000
H	-2.97090600	-4.29293400	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000
H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000

H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

[C]-C/G-C

Total Energy = -8262.23 kcal mol^{-1}

N	1.85408900	2.70534100	0.00000000
C	3.21983800	2.79365400	0.00000000
N	3.94599100	1.57183400	0.00000000
C	3.34274900	0.34818700	0.00000000
C	1.98496000	0.25841800	0.00000000
C	1.26058300	1.50342600	0.00000000
N	-0.09382900	1.47339400	0.00000000
O	3.85900500	3.85921700	0.00000000
H	4.95718700	1.65510500	0.00000000
H	3.99759200	-0.51634700	0.00000000
H	1.46487900	-0.69370900	0.00000000
H	-0.57899000	2.36205800	0.00000000
H	-0.62235400	0.59428800	0.00000000
N	-1.84371400	-0.98967100	0.00000000
C	-1.23212000	-2.21780500	0.00000000
N	-2.07856900	-3.35580500	0.00000000
C	-3.43629700	-3.27203400	0.00000000
C	-4.04154100	-2.05147400	0.00000000
C	-3.18004500	-0.90122400	0.00000000
N	-3.72758500	0.33846600	0.00000000
O	-0.00507500	-2.38920200	0.00000000
H	-1.61146300	-4.25713200	0.00000000
H	-3.98269200	-4.20818900	0.00000000
H	-5.12103900	-1.95478300	0.00000000
H	-3.13216000	1.15539400	0.00000000
H	-4.72857400	0.47022500	0.00000000
N	4.63969500	-0.55013700	-3.40000000
C	4.97318900	0.80001500	-3.40000000
H	6.00298300	1.12824000	-3.40000000
N	3.91246900	1.58239200	-3.40000000
C	2.82539300	0.70723400	-3.40000000
C	1.41943800	0.95672000	-3.40000000
O	0.82717800	2.06127700	-3.40000000
N	0.67635600	-0.24288800	-3.40000000
H	-0.36188800	-0.13691800	-3.40000000
C	1.20763300	-1.51678700	-3.40000000
N	0.32989200	-2.54418400	-3.40000000
H	-0.68978700	-2.40485800	-3.40000000
H	0.70967800	-3.48051500	-3.40000000
N	2.52144900	-1.75913300	-3.40000000
C	3.26344000	-0.62938100	-3.40000000
H	5.27776500	-1.33699300	-3.40000000
N	-4.37179500	-0.87725900	-3.40000000
C	-4.96623700	0.35136400	-3.40000000

H	-6.04987900	0.36447400	-3.40000000
C	-4.20339800	1.47734600	-3.40000000
H	-4.65304800	2.46355900	-3.40000000
C	-2.77278700	1.30665200	-3.40000000
N	-1.95745800	2.37167500	-3.40000000
H	-0.92621100	2.25323100	-3.40000000
H	-2.34791900	3.30390600	-3.40000000
N	-2.20539300	0.08185900	-3.40000000
C	-2.97223200	-1.04112100	-3.40000000
O	-2.50902300	-2.20261300	-3.40000000
H	-4.92683700	-1.72680200	-3.40000000

Cartesian Coordinates of Systems in Chloroform

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in chloroform that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9166.24 kcal mol^{-1}

N	0.97620900	1.31998000	0.00000000
C	1.80586000	0.25199800	0.00000000
N	3.14883300	0.25092800	0.00000000
C	3.64966400	1.50320700	0.00000000
C	2.90926800	2.69835400	0.00000000
C	1.50122800	2.57192600	0.00000000
N	4.97077100	1.90585500	0.00000000
C	4.97550500	3.28721000	0.00000000
N	3.75682300	3.80684300	0.00000000
N	0.67021900	3.63920200	0.00000000
H	1.30294800	-0.71245500	0.00000000
H	5.78243400	1.29869400	0.00000000
H	5.89811600	3.84993700	0.00000000
H	1.04263000	4.57864200	0.00000000
H	-0.33208000	3.50705800	0.00000000
N	-0.81319700	-1.86951800	0.00000000
C	-0.96633200	-3.20742200	0.00000000
N	-2.10642900	-3.92403200	0.00000000
C	-3.19166200	-3.12152300	0.00000000
C	-3.18866600	-1.71652300	0.00000000
C	-1.92296400	-1.07962000	0.00000000
N	-4.52825300	-3.47356800	0.00000000
C	-5.25796300	-2.30069300	0.00000000
N	-4.49326800	-1.21868200	0.00000000
N	-1.77669800	0.26184900	0.00000000
H	-0.04337000	-3.78339400	0.00000000
H	-4.90030200	-4.41628300	0.00000000
H	-6.33873500	-2.30640000	0.00000000
H	-2.60376100	0.84388400	0.00000000
H	-0.83926800	0.69283200	0.00000000
N	3.89676000	-1.54231100	-3.40000000
C	4.61201100	-0.36514200	-3.40000000
H	5.69030600	-0.48085300	-3.40000000
C	4.00655100	0.85300900	-3.40000000
C	4.76538000	2.15401600	-3.40000000
H	5.84494400	1.97535000	-3.40000000
H	4.50867000	2.75515300	-2.51912900
H	4.50867000	2.75515300	-4.28087100
C	2.54851000	0.88471000	-3.40000000
O	1.87315700	1.93807800	-3.40000000
N	1.90632700	-0.35307900	-3.40000000
H	0.84953300	-0.35557400	-3.40000000
C	2.50989300	-1.59415500	-3.40000000

O	1.87940300	-2.65931900	-3.40000000
H	4.37918300	-2.43460200	-3.40000000
N	-4.94243200	-0.55761400	-3.40000000
C	-5.20886300	0.79788900	-3.40000000
H	-6.22127900	1.17584100	-3.40000000
N	-4.11007100	1.53810600	-3.40000000
C	-3.06845100	0.61038500	-3.40000000
C	-1.66044600	0.75822100	-3.40000000
N	-1.03124200	1.94815100	-3.40000000
H	-0.00517400	1.99208000	-3.40000000
H	-1.57505500	2.80025300	-3.40000000
N	-0.91522700	-0.38280000	-3.40000000
C	-1.52526100	-1.58590000	-3.40000000
H	-0.85467700	-2.44194600	-3.40000000
N	-2.84240100	-1.84172300	-3.40000000
C	-3.56913700	-0.70295400	-3.40000000
H	-5.62455400	-1.30734100	-3.40000000

[T]-A/T-A
Total Energy = -9033.19 kcal mol^{-1}

N	4.05909300	1.04270200	0.00000000
C	3.94582000	2.41546600	0.00000000
H	4.88619300	2.95566000	0.00000000
C	2.73998200	3.04509000	0.00000000
C	2.58917500	4.54365600	0.00000000
H	3.56757700	5.03366400	0.00000000
H	2.02815200	4.87909500	-0.88087100
H	2.02815200	4.87909500	0.88087100
C	1.54176800	2.21372200	0.00000000
O	0.37624200	2.66895200	0.00000000
N	1.74978600	0.83486400	0.00000000
H	0.89628800	0.21167800	0.00000000
C	2.96756700	0.18558000	0.00000000
O	3.08357700	-1.04674900	0.00000000
H	4.97385700	0.60438500	0.00000000
N	-3.67075400	-3.35620800	0.00000000
C	-4.68304600	-2.41618700	0.00000000
H	-5.72426200	-2.70550100	0.00000000
N	-4.22919300	-1.17148500	0.00000000
C	-2.84120400	-1.30977800	0.00000000
C	-1.78900000	-0.36257200	0.00000000
N	-1.97938700	0.96993800	0.00000000
H	-1.17510100	1.60858500	0.00000000
H	-2.92019400	1.33965800	0.00000000
N	-0.51543000	-0.84764900	0.00000000
C	-0.30179300	-2.17954600	0.00000000
H	0.74389200	-2.47794200	0.00000000
N	-1.21701300	-3.16070700	0.00000000
C	-2.47430600	-2.66658800	0.00000000
H	-3.78192400	-4.36369100	0.00000000
N	3.89676000	-1.54231100	-3.40000000
C	4.61201100	-0.36514200	-3.40000000

H	5.69030600	-0.48085300	-3.40000000
C	4.00655100	0.85300900	-3.40000000
C	4.76538000	2.15401600	-3.40000000
H	5.84494400	1.97535000	-3.40000000
H	4.50867000	2.75515300	-2.51912900
H	4.50867000	2.75515300	-4.28087100
C	2.54851000	0.88471000	-3.40000000
O	1.87315700	1.93807800	-3.40000000
N	1.90632700	-0.35307900	-3.40000000
H	0.84953300	-0.35557400	-3.40000000
C	2.50989300	-1.59415500	-3.40000000
O	1.87940300	-2.65931900	-3.40000000
H	4.37918300	-2.43460200	-3.40000000
N	-4.94243200	-0.55761400	-3.40000000
C	-5.20886300	0.79788900	-3.40000000
H	-6.22127900	1.17584100	-3.40000000
N	-4.11007100	1.53810600	-3.40000000
C	-3.06845100	0.61038500	-3.40000000
C	-1.66044600	0.75822100	-3.40000000
N	-1.03124200	1.94815100	-3.40000000
H	-0.00517400	1.99208000	-3.40000000
H	-1.57505500	2.80025300	-3.40000000
N	-0.91522700	-0.38280000	-3.40000000
C	-1.52526100	-1.58590000	-3.40000000
H	-0.85467700	-2.44194600	-3.40000000
N	-2.84240100	-1.84172300	-3.40000000
C	-3.56913700	-0.70295400	-3.40000000
H	-5.62455400	-1.30734100	-3.40000000

[G]-A/T-A

Total Energy = -9335.38 kcal mol^{-1}

N	1.38446300	0.50784100	0.00000000
C	2.63896900	-0.05916300	0.00000000
N	3.76911700	0.64524600	0.00000000
C	3.55386100	1.98185800	0.00000000
C	2.32562300	2.66328900	0.00000000
C	1.12200900	1.89674900	0.00000000
N	4.51021400	2.97165900	0.00000000
C	3.84265200	4.18787200	0.00000000
N	2.53016800	4.04405500	0.00000000
O	-0.05870900	2.31298300	0.00000000
N	2.70209600	-1.41469400	0.00000000
H	0.55085700	-0.12322200	0.00000000
H	5.51396200	2.83066300	0.00000000
H	4.37769700	5.12664100	0.00000000
H	3.60747400	-1.86279100	0.00000000
H	1.87216600	-1.98661400	0.00000000
N	-0.93761500	-1.28563900	0.00000000
C	-0.82521400	-2.63051900	0.00000000
N	-1.79499300	-3.55494800	0.00000000
C	-3.02040900	-2.98465500	0.00000000
C	-3.29565400	-1.60871300	0.00000000

C	-2.18636900	-0.72598500	0.00000000
N	-4.25799500	-3.59563600	0.00000000
C	-5.20645600	-2.59097000	0.00000000
N	-4.67091300	-1.37914000	0.00000000
N	-2.31500800	0.61023500	0.00000000
H	0.18932500	-3.02406200	0.00000000
H	-4.43496300	-4.59366800	0.00000000
H	-6.26446500	-2.81110900	0.00000000
H	-3.24303900	1.01268700	0.00000000
H	-1.49127000	1.23046900	0.00000000
N	3.89676000	-1.54231100	-3.40000000
C	4.61201100	-0.36514200	-3.40000000
H	5.69030600	-0.48085300	-3.40000000
C	4.00655100	0.85300900	-3.40000000
C	4.76538000	2.15401600	-3.40000000
H	5.84494400	1.97535000	-3.40000000
H	4.50867000	2.75515300	-2.51912900
H	4.50867000	2.75515300	-4.28087100
C	2.54851000	0.88471000	-3.40000000
O	1.87315700	1.93807800	-3.40000000
N	1.90632700	-0.35307900	-3.40000000
H	0.84953300	-0.35557400	-3.40000000
C	2.50989300	-1.59415500	-3.40000000
O	1.87940300	-2.65931900	-3.40000000
H	4.37918300	-2.43460200	-3.40000000
N	-4.94243200	-0.55761400	-3.40000000
C	-5.20886300	0.79788900	-3.40000000
H	-6.22127900	1.17584100	-3.40000000
N	-4.11007100	1.53810600	-3.40000000
C	-3.06845100	0.61038500	-3.40000000
C	-1.66044600	0.75822100	-3.40000000
N	-1.03124200	1.94815100	-3.40000000
H	-0.00517400	1.99208000	-3.40000000
H	-1.57505500	2.80025300	-3.40000000
N	-0.91522700	-0.38280000	-3.40000000
C	-1.52526100	-1.58590000	-3.40000000
H	-0.85467700	-2.44194600	-3.40000000
N	-2.84240100	-1.84172300	-3.40000000
C	-3.56913700	-0.70295400	-3.40000000
H	-5.62455400	-1.30734100	-3.40000000

[C]-A/T-A

Total Energy = -8766.81 kcal mol^{-1}

N	2.21119400	1.21001700	0.00000000
C	3.56453700	1.04203500	0.00000000
N	4.36640600	2.21079600	0.00000000
C	3.83933300	3.46708800	0.00000000
C	2.48805100	3.63689600	0.00000000
C	1.68038900	2.44434900	0.00000000
N	0.33289200	2.54406900	0.00000000
O	4.13263100	-0.06774300	0.00000000
H	5.37174600	2.07087400	0.00000000

H	4.54499800	4.28958600	0.00000000
H	2.04228900	4.62514200	0.00000000
H	-0.25475000	1.69471200	0.00000000
H	-0.10293300	3.45594400	0.00000000
N	-1.19464200	0.00791700	0.00000000
C	-0.28336000	-0.99302100	0.00000000
N	-0.51377500	-2.31585900	0.00000000
C	-1.83248300	-2.59530000	0.00000000
C	-2.88353300	-1.66181400	0.00000000
C	-2.51727200	-0.29658400	0.00000000
N	-2.45483400	-3.82813200	0.00000000
C	-3.81648000	-3.59727000	0.00000000
N	-4.12094800	-2.30763300	0.00000000
N	-3.42867400	0.70444600	0.00000000
H	0.75313300	-0.66314600	0.00000000
H	-1.99430000	-4.73113000	0.00000000
H	-4.52786400	-4.41083300	0.00000000
H	-4.41764000	0.49688600	0.00000000
H	-3.12806900	1.66939400	0.00000000
N	3.89676000	-1.54231100	-3.40000000
C	4.61201100	-0.36514200	-3.40000000
H	5.69030600	-0.48085300	-3.40000000
C	4.00655100	0.85300900	-3.40000000
C	4.76538000	2.15401600	-3.40000000
H	5.84494400	1.97535000	-3.40000000
H	4.50867000	2.75515300	-2.51912900
H	4.50867000	2.75515300	-4.28087100
C	2.54851000	0.88471000	-3.40000000
O	1.87315700	1.93807800	-3.40000000
N	1.90632700	-0.35307900	-3.40000000
H	0.84953300	-0.35557400	-3.40000000
C	2.50989300	-1.59415500	-3.40000000
O	1.87940300	-2.65931900	-3.40000000
H	4.37918300	-2.43460200	-3.40000000
N	-4.94243200	-0.55761400	-3.40000000
C	-5.20886300	0.79788900	-3.40000000
H	-6.22127900	1.17584100	-3.40000000
N	-4.11007100	1.53810600	-3.40000000
C	-3.06845100	0.61038500	-3.40000000
C	-1.66044600	0.75822100	-3.40000000
N	-1.03124200	1.94815100	-3.40000000
H	-0.00517400	1.99208000	-3.40000000
H	-1.57505500	2.80025300	-3.40000000
N	-0.91522700	-0.38280000	-3.40000000
C	-1.52526100	-1.58590000	-3.40000000
H	-0.85467700	-2.44194600	-3.40000000
N	-2.84240100	-1.84172300	-3.40000000
C	-3.56913700	-0.70295400	-3.40000000
H	-5.62455400	-1.30734100	-3.40000000

[A]-T/A-T
Total Energy = -9033.19 kcal mol^{-1}

N	4.05909300	1.04270200	0.00000000
C	3.94582000	2.41546600	0.00000000
H	4.88619300	2.95566000	0.00000000
C	2.73998200	3.04509000	0.00000000
C	2.58917500	4.54365600	0.00000000
H	3.56757700	5.03366400	0.00000000
H	2.02815200	4.87909500	-0.88087100
H	2.02815200	4.87909500	0.88087100
C	1.54176800	2.21372200	0.00000000
O	0.37624200	2.66895200	0.00000000
N	1.74978600	0.83486400	0.00000000
H	0.89628800	0.21167800	0.00000000
C	2.96756700	0.18558000	0.00000000
O	3.08357700	-1.04674900	0.00000000
H	4.97385700	0.60438500	0.00000000
N	-3.67075400	-3.35620800	0.00000000
C	-4.68304600	-2.41618700	0.00000000
H	-5.72426200	-2.70550100	0.00000000
N	-4.22919300	-1.17148500	0.00000000
C	-2.84120400	-1.30977800	0.00000000
C	-1.78900000	-0.36257200	0.00000000
N	-1.97938700	0.96993800	0.00000000
H	-1.17510100	1.60858500	0.00000000
H	-2.92019400	1.33965800	0.00000000
N	-0.51543000	-0.84764900	0.00000000
C	-0.30179300	-2.17954600	0.00000000
H	0.74389200	-2.47794200	0.00000000
N	-1.21701300	-3.16070700	0.00000000
C	-2.47430600	-2.66658800	0.00000000
H	-3.78192400	-4.36369100	0.00000000
N	3.89676000	-1.54231100	-3.40000000
C	4.61201100	-0.36514200	-3.40000000
H	5.69030600	-0.48085300	-3.40000000
C	4.00655100	0.85300900	-3.40000000
C	4.76538000	2.15401600	-3.40000000
H	5.84494400	1.97535000	-3.40000000
H	4.50867000	2.75515300	-2.51912900
H	4.50867000	2.75515300	-4.28087100
C	2.54851000	0.88471000	-3.40000000
O	1.87315700	1.93807800	-3.40000000
N	1.90632700	-0.35307900	-3.40000000
H	0.84953300	-0.35557400	-3.40000000
C	2.50989300	-1.59415500	-3.40000000
O	1.87940300	-2.65931900	-3.40000000
H	4.37918300	-2.43460200	-3.40000000
N	-4.94243200	-0.55761400	-3.40000000
C	-5.20886300	0.79788900	-3.40000000
H	-6.22127900	1.17584100	-3.40000000
N	-4.11007100	1.53810600	-3.40000000
C	-3.06845100	0.61038500	-3.40000000
C	-1.66044600	0.75822100	-3.40000000
N	-1.03124200	1.94815100	-3.40000000

H	-0.00517400	1.99208000	-3.40000000
H	-1.57505500	2.80025300	-3.40000000
N	-0.91522700	-0.38280000	-3.40000000
C	-1.52526100	-1.58590000	-3.40000000
H	-0.85467700	-2.44194600	-3.40000000
N	-2.84240100	-1.84172300	-3.40000000
C	-3.56913700	-0.70295400	-3.40000000
H	-5.62455400	-1.30734100	-3.40000000

[T]-T/A-T

Total Energy = -8890.82 kcal mol^{-1}

N	-1.95270700	0.65325600	0.00000000
C	-3.33692000	0.67520500	0.00000000
N	-3.87125600	1.95550400	0.00000000
C	-3.10813900	3.10151100	0.00000000
C	-1.74860800	3.06779700	0.00000000
C	-1.10287200	1.76212600	0.00000000
O	0.13693900	1.60169900	0.00000000
O	-4.03813900	-0.34167700	0.00000000
C	-0.88854000	4.30396300	0.00000000
H	-1.50547000	-0.28313100	0.00000000
H	-4.88382600	2.01468300	0.00000000
H	-3.66962800	4.02938600	0.00000000
H	-0.23516200	4.32351800	-0.88058300
H	-1.50596500	5.20725700	0.00000000
H	-0.23516200	4.32351800	0.88058300
N	1.45351200	-0.88802200	0.00000000
C	0.60555400	-1.96936500	0.00000000
N	1.24126100	-3.19390300	0.00000000
C	2.61454900	-3.33534200	0.00000000
C	3.45169000	-2.26591600	0.00000000
C	2.86065000	-0.92773200	0.00000000
O	3.50883000	0.12929400	0.00000000
O	-0.63749100	-1.87307200	0.00000000
C	4.95212400	-2.39020200	0.00000000
H	0.99903900	0.04834100	0.00000000
H	0.64133700	-4.01162200	0.00000000
H	2.97027400	-4.35976300	0.00000000
H	5.38261800	-1.89797600	0.88059000
H	5.25705300	-3.44107500	0.00000000
H	5.38261800	-1.89797600	-0.88059000
N	3.89676000	-1.54231100	3.40000000
C	4.61201100	-0.36514200	3.40000000
H	5.69030600	-0.48085300	3.40000000
C	4.00655100	0.85300900	3.40000000
C	4.76538000	2.15401600	3.40000000
H	5.84494400	1.97535000	3.40000000
H	4.50867000	2.75515300	2.51912900
H	4.50867000	2.75515300	4.28087100
C	2.54851000	0.88471000	3.40000000
O	1.87315700	1.93807800	3.40000000

N	1.90632700	-0.35307900	3.40000000
H	0.84953300	-0.35557400	3.40000000
C	2.50989300	-1.59415500	3.40000000
O	1.87940300	-2.65931900	3.40000000
H	4.37918300	-2.43460200	3.40000000
N	-4.94243200	-0.55761400	3.40000000
C	-5.20886300	0.79788900	3.40000000
H	-6.22127900	1.17584100	3.40000000
N	-4.11007100	1.53810600	3.40000000
C	-3.06845100	0.61038500	3.40000000
C	-1.66044600	0.75822100	3.40000000
N	-1.03124200	1.94815100	3.40000000
H	-0.00517400	1.99208000	3.40000000
H	-1.57505500	2.80025300	3.40000000
N	-0.91522700	-0.38280000	3.40000000
C	-1.52526100	-1.58590000	3.40000000
H	-0.85467700	-2.44194600	3.40000000
N	-2.84240100	-1.84172300	3.40000000
C	-3.56913700	-0.70295400	3.40000000
H	-5.62455400	-1.30734100	3.40000000

[G]-T/A-T

Total Energy = -9195.00 kcal mol^{-1}

N	-1.57841000	0.10538400	0.00000000
C	-2.94902300	-0.01195300	0.00000000
N	-3.77465700	1.03293400	0.00000000
C	-3.11799900	2.21821600	0.00000000
C	-1.72995200	2.44607100	0.00000000
C	-0.85814000	1.31713300	0.00000000
N	-3.68268000	3.47330300	0.00000000
C	-2.64366500	4.39236100	0.00000000
N	-1.45673200	3.81441700	0.00000000
O	0.39529100	1.29535800	0.00000000
N	-3.45006600	-1.27283600	0.00000000
H	-1.00890200	-0.76203400	0.00000000
H	-4.67452100	3.68228800	0.00000000
H	-2.83092600	5.45650900	0.00000000
H	-4.45191600	-1.40291400	0.00000000
H	-2.84531700	-2.08228100	0.00000000
N	1.85954500	-1.10995600	0.00000000
C	1.12032000	-2.26529700	0.00000000
N	1.86450500	-3.42437300	0.00000000
C	3.24614500	-3.43940300	0.00000000
C	3.98016400	-2.29747400	0.00000000
C	3.26670400	-1.01966000	0.00000000
O	3.81158400	0.09228500	0.00000000
O	-0.13036600	-2.29057700	0.00000000
C	5.48545100	-2.28154800	0.00000000
H	1.32945300	-0.20993600	0.00000000
H	1.34333600	-4.29428000	0.00000000
H	3.69392300	-4.42693500	0.00000000
H	5.86755500	-1.75089100	0.88053700

H	5.88702200	-3.29938000	0.00000000
H	5.86755500	-1.75089100	-0.88053700
N	3.89676000	-1.54231100	3.40000000
C	4.61201100	-0.36514200	3.40000000
H	5.69030600	-0.48085300	3.40000000
C	4.00655100	0.85300900	3.40000000
C	4.76538000	2.15401600	3.40000000
H	5.84494400	1.97535000	3.40000000
H	4.50867000	2.75515300	2.51912900
H	4.50867000	2.75515300	4.28087100
C	2.54851000	0.88471000	3.40000000
O	1.87315700	1.93807800	3.40000000
N	1.90632700	-0.35307900	3.40000000
H	0.84953300	-0.35557400	3.40000000
C	2.50989300	-1.59415500	3.40000000
O	1.87940300	-2.65931900	3.40000000
H	4.37918300	-2.43460200	3.40000000
N	-4.94243200	-0.55761400	3.40000000
C	-5.20886300	0.79788900	3.40000000
H	-6.22127900	1.17584100	3.40000000
N	-4.11007100	1.53810600	3.40000000
C	-3.06845100	0.61038500	3.40000000
C	-1.66044600	0.75822100	3.40000000
N	-1.03124200	1.94815100	3.40000000
H	-0.00517400	1.99208000	3.40000000
H	-1.57505500	2.80025300	3.40000000
N	-0.91522700	-0.38280000	3.40000000
C	-1.52526100	-1.58590000	3.40000000
H	-0.85467700	-2.44194600	3.40000000
N	-2.84240100	-1.84172300	3.40000000
C	-3.56913700	-0.70295400	3.40000000
H	-5.62455400	-1.30734100	3.40000000

[C]-T/A-T

Total Energy = -8629.65 kcal mol^{-1}

N	-1.38994700	1.05872100	0.00000000
C	-2.69477600	0.63823400	0.00000000
N	-3.69840000	1.63915100	0.00000000
C	-3.41967400	2.97173500	0.00000000
C	-2.12547600	3.39166100	0.00000000
C	-1.10408800	2.37726500	0.00000000
N	0.19249400	2.73792300	0.00000000
O	-3.04462000	-0.55289700	0.00000000
H	-4.65832600	1.30962500	0.00000000
H	-4.26786900	3.64630800	0.00000000
H	-1.87104700	4.44511400	0.00000000
H	0.93269600	2.02199500	0.00000000
H	0.44446800	3.71650800	0.00000000
N	0.79662700	-1.01582200	0.00000000
C	0.49929600	-2.37276000	0.00000000
N	1.62510700	-3.18966700	0.00000000
C	2.91595500	-2.71847900	0.00000000

C	3.19753000	-1.38856800	0.00000000
C	2.07777300	-0.45646000	0.00000000
O	2.22489800	0.78581000	0.00000000
O	-0.64387200	-2.83021900	0.00000000
C	4.60053400	-0.84054100	0.00000000
H	-0.01412600	-0.35745400	0.00000000
H	1.44322600	-4.18750000	0.00000000
H	3.68787300	-3.48036300	0.00000000
H	4.77410500	-0.21061100	0.88094600
H	5.33390700	-1.65266500	0.00000000
H	4.77410500	-0.21061100	-0.88094600
N	3.89676000	-1.54231100	3.40000000
C	4.61201100	-0.36514200	3.40000000
H	5.69030600	-0.48085300	3.40000000
C	4.00655100	0.85300900	3.40000000
C	4.76538000	2.15401600	3.40000000
H	5.84494400	1.97535000	3.40000000
H	4.50867000	2.75515300	2.51912900
H	4.50867000	2.75515300	4.28087100
C	2.54851000	0.88471000	3.40000000
O	1.87315700	1.93807800	3.40000000
N	1.90632700	-0.35307900	3.40000000
H	0.84953300	-0.35557400	3.40000000
C	2.50989300	-1.59415500	3.40000000
O	1.87940300	-2.65931900	3.40000000
H	4.37918300	-2.43460200	3.40000000
N	-4.94243200	-0.55761400	3.40000000
C	-5.20886300	0.79788900	3.40000000
H	-6.22127900	1.17584100	3.40000000
N	-4.11007100	1.53810600	3.40000000
C	-3.06845100	0.61038500	3.40000000
C	-1.66044600	0.75822100	3.40000000
N	-1.03124200	1.94815100	3.40000000
H	-0.00517400	1.99208000	3.40000000
H	-1.57505500	2.80025300	3.40000000
N	-0.91522700	-0.38280000	3.40000000
C	-1.52526100	-1.58590000	3.40000000
H	-0.85467700	-2.44194600	3.40000000
N	-2.84240100	-1.84172300	3.40000000
C	-3.56913700	-0.70295400	3.40000000
H	-5.62455400	-1.30734100	3.40000000

[A]-G/C-G

Total Energy = -9245.41 kcal mol^{-1}

N	1.38446300	0.50784100	0.00000000
C	2.63896900	-0.05916300	0.00000000
N	3.76911700	0.64524600	0.00000000
C	3.55386100	1.98185800	0.00000000
C	2.32562300	2.66328900	0.00000000
C	1.12200900	1.89674900	0.00000000
N	4.51021400	2.97165900	0.00000000
C	3.84265200	4.18787200	0.00000000

N	2.53016800	4.04405500	0.00000000
O	-0.05870900	2.31298300	0.00000000
N	2.70209600	-1.41469400	0.00000000
H	0.55085700	-0.12322200	0.00000000
H	5.51396200	2.83066300	0.00000000
H	4.37769700	5.12664100	0.00000000
H	3.60747400	-1.86279100	0.00000000
H	1.87216600	-1.98661400	0.00000000
N	-0.93761500	-1.28563900	0.00000000
C	-0.82521400	-2.63051900	0.00000000
N	-1.79499300	-3.55494800	0.00000000
C	-3.02040900	-2.98465500	0.00000000
C	-3.29565400	-1.60871300	0.00000000
C	-2.18636900	-0.72598500	0.00000000
N	-4.25799500	-3.59563600	0.00000000
C	-5.20645600	-2.59097000	0.00000000
N	-4.67091300	-1.37914000	0.00000000
N	-2.31500800	0.61023500	0.00000000
H	0.18932500	-3.02406200	0.00000000
H	-4.43496300	-4.59366800	0.00000000
H	-6.26446500	-2.81110900	0.00000000
H	-3.24303900	1.01268700	0.00000000
H	-1.49127000	1.23046900	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[T]-G/C-G

Total Energy = -9105.33 kcal mol^{-1}

N	1.57841000	0.10538400	0.00000000
C	2.94902300	-0.01195300	0.00000000
N	3.77465700	1.03293400	0.00000000
C	3.11799900	2.21821600	0.00000000
C	1.72995200	2.44607100	0.00000000
C	0.85814000	1.31713300	0.00000000
N	3.68268000	3.47330300	0.00000000
C	2.64366500	4.39236100	0.00000000
N	1.45673200	3.81441700	0.00000000
O	-0.39529100	1.29535800	0.00000000
N	3.45006600	-1.27283600	0.00000000
H	1.00890200	-0.76203400	0.00000000
H	4.67452100	3.68228800	0.00000000
H	2.83092600	5.45650900	0.00000000
H	4.45191600	-1.40291400	0.00000000
H	2.84531700	-2.08228100	0.00000000
N	-1.85954500	-1.10995600	0.00000000
C	-1.12032000	-2.26529700	0.00000000
N	-1.86450500	-3.42437300	0.00000000
C	-3.24614500	-3.43940300	0.00000000
C	-3.98016400	-2.29747400	0.00000000
C	-3.26670400	-1.01966000	0.00000000
O	-3.81158400	0.09228500	0.00000000
O	0.13036600	-2.29057700	0.00000000
C	-5.48545100	-2.28154800	0.00000000
H	-1.32945300	-0.20993600	0.00000000
H	-1.34333600	-4.29428000	0.00000000
H	-3.69392300	-4.42693500	0.00000000
H	-5.86755500	-1.75089100	0.88053700
H	-5.88702200	-3.29938000	0.00000000
H	-5.86755500	-1.75089100	-0.88053700
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000

H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[G]-G/C-G

Total Energy = -9404.07 kcal mol^{-1}

N	-3.61103700	-0.53659600	0.00000000
C	-4.49642600	-1.59645400	0.00000000
N	-4.10217100	-2.86776800	0.00000000
C	-2.75578000	-3.00706100	0.00000000
C	-1.78036400	-1.99830800	0.00000000
C	-2.19572000	-0.63531700	0.00000000
N	-2.04481500	-4.18713700	0.00000000
C	-0.69977600	-3.86156700	0.00000000
N	-0.50372000	-2.55452300	0.00000000
O	-1.50829300	0.40266500	0.00000000
N	-5.81746300	-1.30203700	0.00000000
H	-3.97173300	0.41479700	0.00000000
H	-2.43911100	-5.12112000	0.00000000
H	0.07082100	-4.61830500	0.00000000
H	-6.48392900	-2.06196500	0.00000000
H	-6.15735600	-0.35115400	0.00000000
N	1.27447200	1.08426500	0.00000000
C	2.33676100	0.20498100	0.00000000
N	3.61347700	0.60244800	0.00000000
C	3.75024000	1.94921400	0.00000000
C	2.74344700	2.92687900	0.00000000
C	1.37451200	2.50570500	0.00000000
N	4.93379900	2.65660300	0.00000000
C	4.60686700	4.00468800	0.00000000
N	3.30181900	4.20710700	0.00000000
O	0.34467700	3.20146800	0.00000000
N	2.06161400	-1.11960800	0.00000000
H	0.30784800	0.71916600	0.00000000
H	5.86659200	2.26049800	0.00000000
H	5.36851700	4.77116000	0.00000000
H	2.85379500	-1.74819100	0.00000000
H	1.11461600	-1.52172100	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000

O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[C]-G/C-G
Total Energy = -8852.10 kcal mol^{-1}

N	4.08090700	2.28253600	0.00000000
C	3.56041300	3.56869400	0.00000000
H	4.20300400	4.43747700	0.00000000
N	2.24033700	3.58063600	0.00000000
C	1.87441000	2.23281100	0.00000000
C	0.59078700	1.61135600	0.00000000
O	-0.53606700	2.16546600	0.00000000
N	0.68755800	0.20602400	0.00000000
H	-0.21684900	-0.31756500	0.00000000
C	1.86531500	-0.51541600	0.00000000
N	1.75616700	-1.86071000	0.00000000
H	0.84681100	-2.34438200	0.00000000
H	2.61080600	-2.40054600	0.00000000
N	3.07315200	0.05916500	0.00000000
C	3.01461600	1.40986400	0.00000000
H	5.06184100	2.02770900	0.00000000
N	-3.01695400	-3.28286300	0.00000000
C	-4.22278700	-2.64364400	0.00000000
H	-5.10331500	-3.27460800	0.00000000
C	-4.27248300	-1.28432100	0.00000000
H	-5.21704700	-0.75308300	0.00000000
C	-3.01928900	-0.57800100	0.00000000
N	-2.99186600	0.76322000	0.00000000
H	-2.09339700	1.27527100	0.00000000
H	-3.85803400	1.28459200	0.00000000
N	-1.83545900	-1.23083400	0.00000000

C	-1.79570700	-2.58975000	0.00000000
O	-0.73090400	-3.25301500	0.00000000
H	-2.96727500	-4.29666200	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[A]-C/G-C

Total Energy = -8676.26 kcal mol^{-1}

N	-1.83409000	-1.72905400	0.00000000
C	-2.09253700	-3.06807000	0.00000000
N	-3.45188600	-3.46952500	0.00000000
C	-4.48381600	-2.58003300	0.00000000
C	-4.22774400	-1.24241500	0.00000000
C	-2.84398300	-0.84280000	0.00000000
N	-2.52242200	0.46956200	0.00000000
O	-1.21262500	-3.95129900	0.00000000
H	-3.62947900	-4.46889900	0.00000000
H	-5.48412000	-2.99699500	0.00000000
H	-5.02987400	-0.51308500	0.00000000
H	-1.53304400	0.76597700	0.00000000
H	-3.25499000	1.16584100	0.00000000
N	0.36163500	1.13861800	0.00000000
C	1.03198200	-0.03736900	0.00000000
N	2.36127800	-0.22701000	0.00000000
C	3.03454500	0.94080300	0.00000000

C	2.47153900	2.22887500	0.00000000
C	1.05994700	2.30241800	0.00000000
N	4.39935600	1.15172800	0.00000000
C	4.60056400	2.51807000	0.00000000
N	3.46813300	3.20615700	0.00000000
N	0.38955000	3.47854800	0.00000000
H	0.39795800	-0.92119600	0.00000000
H	5.11584500	0.43469200	0.00000000
H	5.59413900	2.94323300	0.00000000
H	0.89255900	4.35497100	0.00000000
H	-0.62106100	3.49084200	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[T]-C/G-C

Total Energy = -8539.85 kcal mol^{-1}

N	-1.43642100	-0.99475600	0.00000000
C	-1.43972800	-2.36565900	0.00000000
N	-2.70179300	-3.01086200	0.00000000
C	-3.88302500	-2.33398700	0.00000000
C	-3.88247000	-0.97336700	0.00000000
C	-2.60209500	-0.31543500	0.00000000
N	-2.54443600	1.02913700	0.00000000
O	-0.41500300	-3.06646100	0.00000000
H	-2.68502900	-4.02563400	0.00000000

H	-4.78669000	-2.93221300	0.00000000
H	-4.80574000	-0.40585500	0.00000000
H	-1.63481300	1.51187700	0.00000000
H	-3.39726100	1.57117900	0.00000000
N	1.21227600	0.44373100	0.00000000
C	2.41091900	-0.25836400	0.00000000
N	3.53573900	0.55990700	0.00000000
C	3.48650700	1.93318200	0.00000000
C	2.30869800	2.61194100	0.00000000
C	1.07618700	1.83502500	0.00000000
O	-0.05981800	2.35883300	0.00000000
O	2.49273100	-1.48694400	0.00000000
C	2.22104500	4.11562600	0.00000000
H	0.33559400	-0.12389400	0.00000000
H	4.42853100	0.07858100	0.00000000
H	4.44963800	2.43188400	0.00000000
H	1.67558200	4.47536200	0.88094600
H	3.22004500	4.56214500	0.00000000
H	1.67558200	4.47536200	-0.88094600
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[G]-C/G-C
Total Energy = -8852.10 kcal mol^{-1}

N	4.08090700	2.28253600	0.00000000

C	3.56041300	3.56869400	0.00000000
H	4.20300400	4.43747700	0.00000000
N	2.24033700	3.58063600	0.00000000
C	1.87441000	2.23281100	0.00000000
C	0.59078700	1.61135600	0.00000000
O	-0.53606700	2.16546600	0.00000000
N	0.68755800	0.20602400	0.00000000
H	-0.21684900	-0.31756500	0.00000000
C	1.86531500	-0.51541600	0.00000000
N	1.75616700	-1.86071000	0.00000000
H	0.84681100	-2.34438200	0.00000000
H	2.61080600	-2.40054600	0.00000000
N	3.07315200	0.05916500	0.00000000
C	3.01461600	1.40986400	0.00000000
H	5.06184100	2.02770900	0.00000000
N	-3.01695400	-3.28286300	0.00000000
C	-4.22278700	-2.64364400	0.00000000
H	-5.10331500	-3.27460800	0.00000000
C	-4.27248300	-1.28432100	0.00000000
H	-5.21704700	-0.75308300	0.00000000
C	-3.01928900	-0.57800100	0.00000000
N	-2.99186600	0.76322000	0.00000000
H	-2.09339700	1.27527100	0.00000000
H	-3.85803400	1.28459200	0.00000000
N	-1.83545900	-1.23083400	0.00000000
C	-1.79570700	-2.58975000	0.00000000
O	-0.73090400	-3.25301500	0.00000000
H	-2.96727500	-4.29666200	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000
H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000

H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

[C]-C/G-C

Total Energy = -8277.09 kcal mol^{-1}

N	1.84961900	2.70041900	0.00000000
C	3.21352900	2.77901100	0.00000000
N	3.93683500	1.56426300	0.00000000
C	3.33095200	0.34134700	0.00000000
C	1.97295600	0.25452800	0.00000000
C	1.24788900	1.49769000	0.00000000
N	-0.10335300	1.47079400	0.00000000
O	3.85218800	3.85205200	0.00000000
H	4.94887700	1.64054300	0.00000000
H	3.98572900	-0.52253700	0.00000000
H	1.45111000	-0.69689900	0.00000000
H	-0.59333200	2.35726600	0.00000000
H	-0.63274800	0.58935600	0.00000000
N	-1.82764200	-0.98804000	0.00000000
C	-1.22940900	-2.22024300	0.00000000
N	-2.07717000	-3.34989100	0.00000000
C	-3.43522600	-3.25832500	0.00000000
C	-4.03301100	-2.03445600	0.00000000
C	-3.16734200	-0.88886800	0.00000000
N	-3.70631400	0.35143800	0.00000000
O	0.00250400	-2.39631700	0.00000000
H	-1.61952700	-4.25616700	0.00000000
H	-3.98514200	-4.19186200	0.00000000
H	-5.11163000	-1.93055900	0.00000000
H	-3.11045900	1.16805500	0.00000000
H	-4.70728100	0.48738600	0.00000000
N	4.64316400	-0.55208700	-3.40000000
C	4.97806000	0.79437600	-3.40000000
H	6.00858500	1.11953100	-3.40000000
N	3.91711600	1.57995800	-3.40000000
C	2.82884300	0.70463100	-3.40000000
C	1.42508800	0.95635900	-3.40000000
O	0.83914200	2.06699100	-3.40000000
N	0.67734400	-0.23745900	-3.40000000
H	-0.36209500	-0.12945500	-3.40000000
C	1.20611800	-1.51338500	-3.40000000
N	0.32707100	-2.53759500	-3.40000000
H	-0.69290900	-2.39438800	-3.40000000
H	0.70118100	-3.47667600	-3.40000000
N	2.52100900	-1.75848800	-3.40000000
C	3.26757300	-0.63134300	-3.40000000
H	5.28697300	-1.33482500	-3.40000000
N	-4.37038500	-0.88257100	-3.40000000
C	-4.97020200	0.34333900	-3.40000000

H	-6.05343500	0.35044000	-3.40000000
C	-4.21141600	1.47226500	-3.40000000
H	-4.66333100	2.45724600	-3.40000000
C	-2.78239700	1.30708100	-3.40000000
N	-1.97186100	2.37603300	-3.40000000
H	-0.94400800	2.26218400	-3.40000000
H	-2.36615100	3.30695200	-3.40000000
N	-2.20838400	0.08309000	-3.40000000
C	-2.97497400	-1.03966200	-3.40000000
O	-2.50338800	-2.20213000	-3.40000000
H	-4.92609000	-1.73195200	-3.40000000

Cartesian Coordinates of Systems in Ammonia

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in ammonia that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9176.18 kcal mol^{-1}

N	0.98500800	-1.30362900	0.00000000
C	1.82421800	-0.24458200	0.00000000
N	3.16756600	-0.25485900	0.00000000
C	3.65831900	-1.51292500	0.00000000
C	2.90544200	-2.70030900	0.00000000
C	1.49807800	-2.56214500	0.00000000
N	4.97458700	-1.92726500	0.00000000
C	4.96806800	-3.30658700	0.00000000
N	3.74355500	-3.81635400	0.00000000
N	0.65687500	-3.61909700	0.00000000
H	1.33127300	0.72489400	0.00000000
H	5.79369400	-1.32980200	0.00000000
H	5.88614200	-3.87626900	0.00000000
H	1.01697200	-4.56350200	0.00000000
H	-0.34454700	-3.47833000	0.00000000
N	-0.81303200	1.87845200	0.00000000
C	-0.97146300	3.21562400	0.00000000
N	-2.11477200	3.92763800	0.00000000
C	-3.19860500	3.12093400	0.00000000
C	-3.18843300	1.71588100	0.00000000
C	-1.92058000	1.08332600	0.00000000
N	-4.53557400	3.46746600	0.00000000
C	-5.26088100	2.29419600	0.00000000
N	-4.49170300	1.21342200	0.00000000
N	-1.76717100	-0.25641000	0.00000000
H	-0.05085200	3.79536800	0.00000000
H	-4.91408100	4.40788500	0.00000000
H	-6.34142600	2.29681300	0.00000000
H	-2.58896400	-0.84617800	0.00000000
H	-0.82683900	-0.68237900	0.00000000
N	3.90433900	1.53920300	3.40000000
C	4.61727600	0.36189800	3.40000000
H	5.69529300	0.47665900	3.40000000
C	4.00918400	-0.85574900	3.40000000
C	4.76836600	-2.15650800	3.40000000
H	5.84723300	-1.97560500	3.40000000
H	4.51332500	-2.75762500	4.28146800
H	4.51332500	-2.75762500	2.51853200
C	2.55386200	-0.88404000	3.40000000
O	1.87272600	-1.93646400	3.40000000
N	1.91351800	0.35429900	3.40000000
H	0.85868100	0.35913800	3.40000000
C	2.52141200	1.59210400	3.40000000

O	1.88862300	2.65975200	3.40000000
H	4.39185200	2.42904100	3.40000000
N	-4.94968400	0.55303500	3.40000000
C	-5.21362100	-0.80080200	3.40000000
H	-6.22541900	-1.17982100	3.40000000
N	-4.11222100	-1.54001600	3.40000000
C	-3.07230500	-0.60981900	3.40000000
C	-1.66419100	-0.75443300	3.40000000
N	-1.03184600	-1.94230500	3.40000000
H	-0.00576400	-1.98269000	3.40000000
H	-1.57063300	-2.79779400	3.40000000
N	-0.92022700	0.38834200	3.40000000
C	-1.53365900	1.58894100	3.40000000
H	-0.86651800	2.44758700	3.40000000
N	-2.85174700	1.84243100	3.40000000
C	-3.57791000	0.70177100	3.40000000
H	-5.63607200	1.29919600	3.40000000

[T]-A/T-A
Total Energy = -9041.59 kcal mol^{-1}

N	4.06339700	-1.04967100	0.00000000
C	3.94817300	-2.42118500	0.00000000
H	4.88776200	-2.96198400	0.00000000
C	2.74050100	-3.04885500	0.00000000
C	2.59012600	-4.54742700	0.00000000
H	3.56927900	-5.03521500	0.00000000
H	2.03046500	-4.88383100	0.88146800
H	2.03046500	-4.88383100	-0.88146800
C	1.54649200	-2.21632600	0.00000000
O	0.37684200	-2.66739300	0.00000000
N	1.75632000	-0.83810400	0.00000000
H	0.90578400	-0.21417100	0.00000000
C	2.97568000	-0.19401000	0.00000000
O	3.09129100	1.04168000	0.00000000
H	4.98083700	-0.61633000	0.00000000
N	-3.67931300	3.35676600	0.00000000
C	-4.68860800	2.41662700	0.00000000
H	-5.72995100	2.70471400	0.00000000
N	-4.23205500	1.17120400	0.00000000
C	-2.84399000	1.31250200	0.00000000
C	-1.78980300	0.36783800	0.00000000
N	-1.97643900	-0.96485400	0.00000000
H	-1.17005900	-1.60064200	0.00000000
H	-2.91517100	-1.34026800	0.00000000
N	-0.51621800	0.85507100	0.00000000
C	-0.30680000	2.18694200	0.00000000
H	0.73762800	2.48946600	0.00000000
N	-1.22415800	3.16677300	0.00000000
C	-2.48209900	2.67078700	0.00000000
H	-3.79603000	4.36387200	0.00000000
N	3.90433900	1.53920300	3.40000000
C	4.61727600	0.36189800	3.40000000

H	5.69529300	0.47665900	3.40000000
C	4.00918400	-0.85574900	3.40000000
C	4.76836600	-2.15650800	3.40000000
H	5.84723300	-1.97560500	3.40000000
H	4.51332500	-2.75762500	4.28146800
H	4.51332500	-2.75762500	2.51853200
C	2.55386200	-0.88404000	3.40000000
O	1.87272600	-1.93646400	3.40000000
N	1.91351800	0.35429900	3.40000000
H	0.85868100	0.35913800	3.40000000
C	2.52141200	1.59210400	3.40000000
O	1.88862300	2.65975200	3.40000000
H	4.39185200	2.42904100	3.40000000
N	-4.94968400	0.55303500	3.40000000
C	-5.21362100	-0.80080200	3.40000000
H	-6.22541900	-1.17982100	3.40000000
N	-4.11222100	-1.54001600	3.40000000
C	-3.07230500	-0.60981900	3.40000000
C	-1.66419100	-0.75443300	3.40000000
N	-1.03184600	-1.94230500	3.40000000
H	-0.00576400	-1.98269000	3.40000000
H	-1.57063300	-2.79779400	3.40000000
N	-0.92022700	0.38834200	3.40000000
C	-1.53365900	1.58894100	3.40000000
H	-0.86651800	2.44758700	3.40000000
N	-2.85174700	1.84243100	3.40000000
C	-3.57791000	0.70177100	3.40000000
H	-5.63607200	1.29919600	3.40000000

[G]-A/T-A

Total Energy = -9345.50 kcal mol^{-1}

N	1.38544100	-0.50806400	0.00000000
C	2.64076400	0.06010000	0.00000000
N	3.77144000	-0.64730900	0.00000000
C	3.55673400	-1.98326300	0.00000000
C	2.32678700	-2.66158300	0.00000000
C	1.12630500	-1.89392700	0.00000000
N	4.51044000	-2.97497000	0.00000000
C	3.84339100	-4.18863600	0.00000000
N	2.52913200	-4.04387200	0.00000000
O	-0.05615500	-2.31571600	0.00000000
N	2.70516200	1.41272300	0.00000000
H	0.55135100	0.12294300	0.00000000
H	5.51520300	-2.83901800	0.00000000
H	4.37800900	-5.12740000	0.00000000
H	3.60969000	1.86323400	0.00000000
H	1.87614500	1.98609900	0.00000000
N	-0.94205400	1.27935800	0.00000000
C	-0.82381200	2.62343300	0.00000000
N	-1.79126600	3.55112200	0.00000000
C	-3.01995800	2.98616700	0.00000000
C	-3.29896100	1.61067300	0.00000000

C	-2.19283100	0.72517400	0.00000000
N	-4.25448100	3.60105100	0.00000000
C	-5.20620100	2.60261200	0.00000000
N	-4.67581600	1.38667200	0.00000000
N	-2.32411400	-0.61158500	0.00000000
H	0.19178400	3.01277500	0.00000000
H	-4.43029400	4.59953500	0.00000000
H	-6.26284400	2.82812400	0.00000000
H	-3.25134900	-1.01573500	0.00000000
H	-1.50018300	-1.22951300	0.00000000
N	3.90433900	1.53920300	3.40000000
C	4.61727600	0.36189800	3.40000000
H	5.69529300	0.47665900	3.40000000
C	4.00918400	-0.85574900	3.40000000
C	4.76836600	-2.15650800	3.40000000
H	5.84723300	-1.97560500	3.40000000
H	4.51332500	-2.75762500	4.28146800
H	4.51332500	-2.75762500	2.51853200
C	2.55386200	-0.88404000	3.40000000
O	1.87272600	-1.93646400	3.40000000
N	1.91351800	0.35429900	3.40000000
H	0.85868100	0.35913800	3.40000000
C	2.52141200	1.59210400	3.40000000
O	1.88862300	2.65975200	3.40000000
H	4.39185200	2.42904100	3.40000000
N	-4.94968400	0.55303500	3.40000000
C	-5.21362100	-0.80080200	3.40000000
H	-6.22541900	-1.17982100	3.40000000
N	-4.11222100	-1.54001600	3.40000000
C	-3.07230500	-0.60981900	3.40000000
C	-1.66419100	-0.75443300	3.40000000
N	-1.03184600	-1.94230500	3.40000000
H	-0.00576400	-1.98269000	3.40000000
H	-1.57063300	-2.79779400	3.40000000
N	-0.92022700	0.38834200	3.40000000
C	-1.53365900	1.58894100	3.40000000
H	-0.86651800	2.44758700	3.40000000
N	-2.85174700	1.84243100	3.40000000
C	-3.57791000	0.70177100	3.40000000
H	-5.63607200	1.29919600	3.40000000

[C]-A/T-A

Total Energy = -8777.43 kcal mol^{-1}

N	2.22004200	-1.20951700	0.00000000
C	3.57218700	-1.05370500	0.00000000
N	4.36844000	-2.21822600	0.00000000
C	3.83621400	-3.47353300	0.00000000
C	2.48457700	-3.63790700	0.00000000
C	1.68076800	-2.44460000	0.00000000
N	0.33518100	-2.53715200	0.00000000
O	4.14364700	0.06159500	0.00000000
H	5.37509600	-2.08688200	0.00000000

H	4.53989500	-4.29705900	0.00000000
H	2.03415900	-4.62379700	0.00000000
H	-0.24963200	-1.68617500	0.00000000
H	-0.10553200	-3.44720800	0.00000000
N	-1.18504700	0.00243800	0.00000000
C	-0.28275900	1.00909000	0.00000000
N	-0.52055400	2.33129900	0.00000000
C	-1.84305500	2.60266000	0.00000000
C	-2.88635900	1.66024700	0.00000000
C	-2.51195300	0.29649800	0.00000000
N	-2.47366100	3.82994900	0.00000000
C	-3.83194600	3.59114400	0.00000000
N	-4.12815800	2.29812900	0.00000000
N	-3.41182700	-0.71160900	0.00000000
H	0.75594500	0.68655400	0.00000000
H	-2.02247200	4.73787500	0.00000000
H	-4.54791900	4.40035200	0.00000000
H	-4.40353500	-0.51678700	0.00000000
H	-3.10241400	-1.67423200	0.00000000
N	3.90433900	1.53920300	3.40000000
C	4.61727600	0.36189800	3.40000000
H	5.69529300	0.47665900	3.40000000
C	4.00918400	-0.85574900	3.40000000
C	4.76836600	-2.15650800	3.40000000
H	5.84723300	-1.97560500	3.40000000
H	4.51332500	-2.75762500	4.28146800
H	4.51332500	-2.75762500	2.51853200
C	2.55386200	-0.88404000	3.40000000
O	1.87272600	-1.93646400	3.40000000
N	1.91351800	0.35429900	3.40000000
H	0.85868100	0.35913800	3.40000000
C	2.52141200	1.59210400	3.40000000
O	1.88862300	2.65975200	3.40000000
H	4.39185200	2.42904100	3.40000000
N	-4.94968400	0.55303500	3.40000000
C	-5.21362100	-0.80080200	3.40000000
H	-6.22541900	-1.17982100	3.40000000
N	-4.11222100	-1.54001600	3.40000000
C	-3.07230500	-0.60981900	3.40000000
C	-1.66419100	-0.75443300	3.40000000
N	-1.03184600	-1.94230500	3.40000000
H	-0.00576400	-1.98269000	3.40000000
H	-1.57063300	-2.79779400	3.40000000
N	-0.92022700	0.38834200	3.40000000
C	-1.53365900	1.58894100	3.40000000
H	-0.86651800	2.44758700	3.40000000
N	-2.85174700	1.84243100	3.40000000
C	-3.57791000	0.70177100	3.40000000
H	-5.63607200	1.29919600	3.40000000

[A]-T/A-T
Total Energy = -9041.59 kcal mol^{-1}

N	4.06339700	-1.04967100	0.00000000
C	3.94817300	-2.42118500	0.00000000
H	4.88776200	-2.96198400	0.00000000
C	2.74050100	-3.04885500	0.00000000
C	2.59012600	-4.54742700	0.00000000
H	3.56927900	-5.03521500	0.00000000
H	2.03046500	-4.88383100	0.88146800
H	2.03046500	-4.88383100	-0.88146800
C	1.54649200	-2.21632600	0.00000000
O	0.37684200	-2.66739300	0.00000000
N	1.75632000	-0.83810400	0.00000000
H	0.90578400	-0.21417100	0.00000000
C	2.97568000	-0.19401000	0.00000000
O	3.09129100	1.04168000	0.00000000
H	4.98083700	-0.61633000	0.00000000
N	-3.67931300	3.35676600	0.00000000
C	-4.68860800	2.41662700	0.00000000
H	-5.72995100	2.70471400	0.00000000
N	-4.23205500	1.17120400	0.00000000
C	-2.84399000	1.31250200	0.00000000
C	-1.78980300	0.36783800	0.00000000
N	-1.97643900	-0.96485400	0.00000000
H	-1.17005900	-1.60064200	0.00000000
H	-2.91517100	-1.34026800	0.00000000
N	-0.51621800	0.85507100	0.00000000
C	-0.30680000	2.18694200	0.00000000
H	0.73762800	2.48946600	0.00000000
N	-1.22415800	3.16677300	0.00000000
C	-2.48209900	2.67078700	0.00000000
H	-3.79603000	4.36387200	0.00000000
N	3.90433900	1.53920300	3.40000000
C	4.61727600	0.36189800	3.40000000
H	5.69529300	0.47665900	3.40000000
C	4.00918400	-0.85574900	3.40000000
C	4.76836600	-2.15650800	3.40000000
H	5.84723300	-1.97560500	3.40000000
H	4.51332500	-2.75762500	4.28146800
H	4.51332500	-2.75762500	2.51853200
C	2.55386200	-0.88404000	3.40000000
O	1.87272600	-1.93646400	3.40000000
N	1.91351800	0.35429900	3.40000000
H	0.85868100	0.35913800	3.40000000
C	2.52141200	1.59210400	3.40000000
O	1.88862300	2.65975200	3.40000000
H	4.39185200	2.42904100	3.40000000
N	-4.94968400	0.55303500	3.40000000
C	-5.21362100	-0.80080200	3.40000000
H	-6.22541900	-1.17982100	3.40000000
N	-4.11222100	-1.54001600	3.40000000
C	-3.07230500	-0.60981900	3.40000000
C	-1.66419100	-0.75443300	3.40000000
N	-1.03184600	-1.94230500	3.40000000

H	-0.00576400	-1.98269000	3.40000000
H	-1.57063300	-2.79779400	3.40000000
N	-0.92022700	0.38834200	3.40000000
C	-1.53365900	1.58894100	3.40000000
H	-0.86651800	2.44758700	3.40000000
N	-2.85174700	1.84243100	3.40000000
C	-3.57791000	0.70177100	3.40000000
H	-5.63607200	1.29919600	3.40000000

[T]-T/A-T

Total Energy = -8900.52 kcal mol^{-1}

N	-1.93983500	-0.65075900	0.00000000
C	-3.32277300	-0.66574900	0.00000000
N	-3.86598500	-1.93798400	0.00000000
C	-3.11152800	-3.08795300	0.00000000
C	-1.75077100	-3.06351100	0.00000000
C	-1.09916800	-1.76448400	0.00000000
O	0.14439900	-1.60714100	0.00000000
O	-4.01490200	0.36148300	0.00000000
C	-0.90219300	-4.30783300	0.00000000
H	-1.48913900	0.28346600	0.00000000
H	-4.87906100	-1.99463800	0.00000000
H	-3.67972300	-4.01110900	0.00000000
H	-0.24989700	-4.33546500	-0.88135100
H	-1.52942000	-5.20397300	0.00000000
H	-0.24989700	-4.33546500	0.88135100
N	1.43939100	0.89282900	0.00000000
C	0.60370700	1.98381100	0.00000000
N	1.25190800	3.19888600	0.00000000
C	2.62504400	3.32366300	0.00000000
C	3.45106400	2.24395100	0.00000000
C	2.84374600	0.91721700	0.00000000
O	3.47776700	-0.15349100	0.00000000
O	-0.64172100	1.89441500	0.00000000
C	4.95269000	2.35572500	0.00000000
H	0.97672300	-0.03939200	0.00000000
H	0.66542900	4.02679600	0.00000000
H	2.99256500	4.34326200	0.00000000
H	5.38019100	1.86190900	0.88131800
H	5.26406200	3.40445400	0.00000000
H	5.38019100	1.86190900	-0.88131800
N	3.90433900	1.53920300	-3.40000000
C	4.61727600	0.36189800	-3.40000000
H	5.69529300	0.47665900	-3.40000000
C	4.00918400	-0.85574900	-3.40000000
C	4.76836600	-2.15650800	-3.40000000
H	5.84723300	-1.97560500	-3.40000000
H	4.51332500	-2.75762500	-4.28146800
H	4.51332500	-2.75762500	-2.51853200
C	2.55386200	-0.88404000	-3.40000000
O	1.87272600	-1.93646400	-3.40000000

N	1.91351800	0.35429900	-3.40000000
H	0.85868100	0.35913800	-3.40000000
C	2.52141200	1.59210400	-3.40000000
O	1.88862300	2.65975200	-3.40000000
H	4.39185200	2.42904100	-3.40000000
N	-4.94968400	0.55303500	-3.40000000
C	-5.21362100	-0.80080200	-3.40000000
H	-6.22541900	-1.17982100	-3.40000000
N	-4.11222100	-1.54001600	-3.40000000
C	-3.07230500	-0.60981900	-3.40000000
C	-1.66419100	-0.75443300	-3.40000000
N	-1.03184600	-1.94230500	-3.40000000
H	-0.00576400	-1.98269000	-3.40000000
H	-1.57063300	-2.79779400	-3.40000000
N	-0.92022700	0.38834200	-3.40000000
C	-1.53365900	1.58894100	-3.40000000
H	-0.86651800	2.44758700	-3.40000000
N	-2.85174700	1.84243100	-3.40000000
C	-3.57791000	0.70177100	-3.40000000
H	-5.63607200	1.29919600	-3.40000000

[G]-T/A-T
Total Energy = -9205.09 kcal mol^{-1}

N	-1.57618700	-0.10371900	0.00000000
C	-2.94804900	0.01504100	0.00000000
N	-3.77364700	-1.03254500	0.00000000
C	-3.11840200	-2.21744200	0.00000000
C	-1.73001500	-2.44267600	0.00000000
C	-0.86118300	-1.31421700	0.00000000
N	-3.68082600	-3.47305700	0.00000000
C	-2.64356800	-4.39078700	0.00000000
N	-1.45503300	-3.81190500	0.00000000
O	0.39614300	-1.29849000	0.00000000
N	-3.44883800	1.27273700	0.00000000
H	-1.00758300	0.76457700	0.00000000
H	-4.67241400	-3.68466900	0.00000000
H	-2.82996000	-5.45486400	0.00000000
H	-4.45078400	1.40481800	0.00000000
H	-2.84560800	2.08352000	0.00000000
N	1.85720600	1.11523700	0.00000000
C	1.12270700	2.27503700	0.00000000
N	1.87191400	3.42831500	0.00000000
C	3.25111100	3.43465400	0.00000000
C	3.98016400	2.28758600	0.00000000
C	3.25938200	1.01872800	0.00000000
O	3.79702100	-0.10274200	0.00000000
O	-0.12827400	2.29877000	0.00000000
C	5.48581100	2.26831800	0.00000000
H	1.32247900	0.21970200	0.00000000
H	1.35919400	4.30377200	0.00000000
H	3.70456300	4.41902100	0.00000000
H	5.86857700	1.73904100	0.88128300

H	5.88723700	3.28587700	0.00000000
H	5.86857700	1.73904100	-0.88128300
N	3.90433900	1.53920300	-3.40000000
C	4.61727600	0.36189800	-3.40000000
H	5.69529300	0.47665900	-3.40000000
C	4.00918400	-0.85574900	-3.40000000
C	4.76836600	-2.15650800	-3.40000000
H	5.84723300	-1.97560500	-3.40000000
H	4.51332500	-2.75762500	-4.28146800
H	4.51332500	-2.75762500	-2.51853200
C	2.55386200	-0.88404000	-3.40000000
O	1.87272600	-1.93646400	-3.40000000
N	1.91351800	0.35429900	-3.40000000
H	0.85868100	0.35913800	-3.40000000
C	2.52141200	1.59210400	-3.40000000
O	1.88862300	2.65975200	-3.40000000
H	4.39185200	2.42904100	-3.40000000
N	-4.94968400	0.55303500	-3.40000000
C	-5.21362100	-0.80080200	-3.40000000
H	-6.22541900	-1.17982100	-3.40000000
N	-4.11222100	-1.54001600	-3.40000000
C	-3.07230500	-0.60981900	-3.40000000
C	-1.66419100	-0.75443300	-3.40000000
N	-1.03184600	-1.94230500	-3.40000000
H	-0.00576400	-1.98269000	-3.40000000
H	-1.57063300	-2.79779400	-3.40000000
N	-0.92022700	0.38834200	-3.40000000
C	-1.53365900	1.58894100	-3.40000000
H	-0.86651800	2.44758700	-3.40000000
N	-2.85174700	1.84243100	-3.40000000
C	-3.57791000	0.70177100	-3.40000000
H	-5.63607200	1.29919600	-3.40000000

[C]-T/A-T

Total Energy = -8639.91 kcal mol^{-1}

N	-1.39583400	-1.05886900	0.00000000
C	-2.70131000	-0.64858100	0.00000000
N	-3.69940800	-1.64659400	0.00000000
C	-3.41670100	-2.97927500	0.00000000
C	-2.12137700	-3.39499300	0.00000000
C	-1.10374400	-2.37919100	0.00000000
N	0.19310600	-2.73409700	0.00000000
O	-3.05362500	0.54789600	0.00000000
H	-4.66204900	-1.32455700	0.00000000
H	-4.26378400	-3.65446000	0.00000000
H	-1.86289000	-4.44723700	0.00000000
H	0.93157600	-2.01754100	0.00000000
H	0.44816300	-3.71235000	0.00000000
N	0.80366500	1.01359200	0.00000000
C	0.50013100	2.36666200	0.00000000
N	1.61467000	3.19055700	0.00000000
C	2.90854800	2.72877200	0.00000000

C	3.19995000	1.40034300	0.00000000
C	2.08846200	0.46219800	0.00000000
O	2.23859000	-0.78133900	0.00000000
O	-0.65240100	2.81265400	0.00000000
C	4.60782000	0.86524100	0.00000000
H	-0.00307900	0.35174300	0.00000000
H	1.42990300	4.18814900	0.00000000
H	3.67368400	3.49678600	0.00000000
H	4.78762100	0.23766200	0.88140200
H	5.33248100	1.68476700	0.00000000
H	4.78762100	0.23766200	-0.88140200
N	3.90433900	1.53920300	-3.40000000
C	4.61727600	0.36189800	-3.40000000
H	5.69529300	0.47665900	-3.40000000
C	4.00918400	-0.85574900	-3.40000000
C	4.76836600	-2.15650800	-3.40000000
H	5.84723300	-1.97560500	-3.40000000
H	4.51332500	-2.75762500	-4.28146800
H	4.51332500	-2.75762500	-2.51853200
C	2.55386200	-0.88404000	-3.40000000
O	1.87272600	-1.93646400	-3.40000000
N	1.91351800	0.35429900	-3.40000000
H	0.85868100	0.35913800	-3.40000000
C	2.52141200	1.59210400	-3.40000000
O	1.88862300	2.65975200	-3.40000000
H	4.39185200	2.42904100	-3.40000000
N	-4.94968400	0.55303500	-3.40000000
C	-5.21362100	-0.80080200	-3.40000000
H	-6.22541900	-1.17982100	-3.40000000
N	-4.11222100	-1.54001600	-3.40000000
C	-3.07230500	-0.60981900	-3.40000000
C	-1.66419100	-0.75443300	-3.40000000
N	-1.03184600	-1.94230500	-3.40000000
H	-0.00576400	-1.98269000	-3.40000000
H	-1.57063300	-2.79779400	-3.40000000
N	-0.92022700	0.38834200	-3.40000000
C	-1.53365900	1.58894100	-3.40000000
H	-0.86651800	2.44758700	-3.40000000
N	-2.85174700	1.84243100	-3.40000000
C	-3.57791000	0.70177100	-3.40000000
H	-5.63607200	1.29919600	-3.40000000

[A]-G/C-G

Total Energy = -9256.69 kcal mol^{-1}

N	1.38544100	0.50806400	0.00000000
C	2.64076400	-0.06010000	0.00000000
N	3.77144000	0.64730900	0.00000000
C	3.55673400	1.98326300	0.00000000
C	2.32678700	2.66158300	0.00000000
C	1.12630500	1.89392700	0.00000000
N	4.51044000	2.97497000	0.00000000
C	3.84339100	4.18863600	0.00000000

N	2.52913200	4.04387200	0.00000000
O	-0.05615500	2.31571600	0.00000000
N	2.70516200	-1.41272300	0.00000000
H	0.55135100	-0.12294300	0.00000000
H	5.51520300	2.83901800	0.00000000
H	4.37800900	5.12740000	0.00000000
H	3.60969000	-1.86323400	0.00000000
H	1.87614500	-1.98609900	0.00000000
N	-0.94205400	-1.27935800	0.00000000
C	-0.82381200	-2.62343300	0.00000000
N	-1.79126600	-3.55112200	0.00000000
C	-3.01995800	-2.98616700	0.00000000
C	-3.29896100	-1.61067300	0.00000000
C	-2.19283100	-0.72517400	0.00000000
N	-4.25448100	-3.60105100	0.00000000
C	-5.20620100	-2.60261200	0.00000000
N	-4.67581600	-1.38667200	0.00000000
N	-2.32411400	0.61158500	0.00000000
H	0.19178400	-3.01277500	0.00000000
H	-4.43029400	-4.59953500	0.00000000
H	-6.26284400	-2.82812400	0.00000000
H	-3.25134900	1.01573500	0.00000000
H	-1.50018300	1.22951300	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[T]-G/C-G

Total Energy = -9117.28 kcal mol^{-1}

N	1.57618700	0.10371900	0.00000000
C	2.94804900	-0.01504100	0.00000000
N	3.77364700	1.03254500	0.00000000
C	3.11840200	2.21744200	0.00000000
C	1.73001500	2.44267600	0.00000000
C	0.86118300	1.31421700	0.00000000
N	3.68082600	3.47305700	0.00000000
C	2.64356800	4.39078700	0.00000000
N	1.45503300	3.81190500	0.00000000
O	-0.39614300	1.29849000	0.00000000
N	3.44883800	-1.27273700	0.00000000
H	1.00758300	-0.76457700	0.00000000
H	4.67241400	3.68466900	0.00000000
H	2.82996000	5.45486400	0.00000000
H	4.45078400	-1.40481800	0.00000000
H	2.84560800	-2.08352000	0.00000000
N	-1.85720600	-1.11523700	0.00000000
C	-1.12270700	-2.27503700	0.00000000
N	-1.87191400	-3.42831500	0.00000000
C	-3.25111100	-3.43465400	0.00000000
C	-3.98016400	-2.28758600	0.00000000
C	-3.25938200	-1.01872800	0.00000000
O	-3.79702100	0.10274200	0.00000000
O	0.12827400	-2.29877000	0.00000000
C	-5.48581100	-2.26831800	0.00000000
H	-1.32247900	-0.21970200	0.00000000
H	-1.35919400	-4.30377200	0.00000000
H	-3.70456300	-4.41902100	0.00000000
H	-5.86857700	-1.73904100	0.88128300
H	-5.88723700	-3.28587700	0.00000000
H	-5.86857700	-1.73904100	-0.88128300
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000

H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[G]-G/C-G

Total Energy = -9418.68 kcal mol^{-1}

N	-3.60996100	-0.53557000	0.00000000
C	-4.48887500	-1.60179700	0.00000000
N	-4.08334200	-2.87161700	0.00000000
C	-2.73661700	-3.00058800	0.00000000
C	-1.77053300	-1.98167700	0.00000000
C	-2.19958500	-0.62552700	0.00000000
N	-2.01469500	-4.17318400	0.00000000
C	-0.67416100	-3.83691300	0.00000000
N	-0.48848700	-2.52735300	0.00000000
O	-1.51357700	0.41996700	0.00000000
N	-5.80871700	-1.31480700	0.00000000
H	-3.98353400	0.41063400	0.00000000
H	-2.39783000	-5.11205100	0.00000000
H	0.10234500	-4.58735700	0.00000000
H	-6.47400200	-2.07598600	0.00000000
H	-6.15181800	-0.36455400	0.00000000
N	1.26877300	1.06580800	0.00000000
C	2.33828700	0.19225900	0.00000000
N	3.61312400	0.60155600	0.00000000
C	3.74096000	1.94816500	0.00000000
C	2.72430200	2.91596400	0.00000000
C	1.36288000	2.48164400	0.00000000
N	4.91680100	2.66676100	0.00000000
C	4.57950400	4.01012300	0.00000000
N	3.27118500	4.20231300	0.00000000
O	0.32678800	3.17765300	0.00000000
N	2.07111500	-1.13075200	0.00000000
H	0.30294700	0.69398800	0.00000000
H	5.85426400	2.28084700	0.00000000
H	5.33401300	4.78329900	0.00000000
H	2.86514100	-1.75773500	0.00000000
H	1.12250700	-1.53609200	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000

O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[C]-G/C-G

Total Energy = -8863.55 kcal mol^{-1}

N	4.08603100	2.27851900	0.00000000
C	3.57180900	3.56492400	0.00000000
H	4.21679700	4.43167900	0.00000000
N	2.24991300	3.58156100	0.00000000
C	1.87965800	2.23388800	0.00000000
C	0.59523900	1.61676900	0.00000000
O	-0.52961500	2.17990200	0.00000000
N	0.68388700	0.21323900	0.00000000
H	-0.22241700	-0.30910000	0.00000000
C	1.85945900	-0.51290800	0.00000000
N	1.74613200	-1.85640700	0.00000000
H	0.83415300	-2.33682400	0.00000000
H	2.59799400	-2.40128100	0.00000000
N	3.07034200	0.05825200	0.00000000
C	3.01797000	1.40909300	0.00000000
H	5.06670000	2.02141400	0.00000000
N	-3.01436100	-3.28624400	0.00000000
C	-4.22212000	-2.65109000	0.00000000
H	-5.09958300	-3.28553400	0.00000000
C	-4.27534600	-1.29174700	0.00000000
H	-5.22055300	-0.76216100	0.00000000
C	-3.02574300	-0.58309200	0.00000000
N	-3.00309500	0.75871900	0.00000000
H	-2.10872200	1.27192300	0.00000000
H	-3.87139600	1.27702600	0.00000000
N	-1.83817600	-1.23230300	0.00000000

C	-1.79909000	-2.59092000	0.00000000
O	-0.72828900	-3.25134800	0.00000000
H	-2.96549500	-4.30023400	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[A]-C/G-C

Total Energy = -8688.34 kcal mol^{-1}

N	-1.83635000	-1.73762400	0.00000000
C	-2.10599900	-3.07173900	0.00000000
N	-3.45958100	-3.46916400	0.00000000
C	-4.48898200	-2.57507600	0.00000000
C	-4.22763200	-1.23879800	0.00000000
C	-2.84433900	-0.84308300	0.00000000
N	-2.51655200	0.46524700	0.00000000
O	-1.22187700	-3.95987600	0.00000000
H	-3.64573900	-4.46713800	0.00000000
H	-5.48965000	-2.98983300	0.00000000
H	-5.02608200	-0.50576900	0.00000000
H	-1.52650700	0.75847100	0.00000000
H	-3.24587900	1.16561300	0.00000000
N	0.36851800	1.12629300	0.00000000
C	1.04707900	-0.04290600	0.00000000
N	2.37805700	-0.22533500	0.00000000
C	3.04481200	0.94858300	0.00000000

C	2.47092300	2.23204600	0.00000000
C	1.05822300	2.29738600	0.00000000
N	4.40690100	1.16907200	0.00000000
C	4.59951700	2.53467300	0.00000000
N	3.46132100	3.21595000	0.00000000
N	0.37753300	3.46473900	0.00000000
H	0.41935200	-0.93110300	0.00000000
H	5.13096500	0.45940100	0.00000000
H	5.59036800	2.96554400	0.00000000
H	0.86927400	4.34770600	0.00000000
H	-0.63359000	3.46793700	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[T]-C/G-C

Total Energy = -8688.34 kcal mol^{-1}

N	-1.43838100	-1.00030800	0.00000000
C	-1.45158800	-2.36867600	0.00000000
N	-2.70918300	-3.00952000	0.00000000
C	-3.88927800	-2.32882900	0.00000000
C	-3.88437200	-0.96843900	0.00000000
C	-2.60382000	-0.31451300	0.00000000
N	-2.54060800	1.02853700	0.00000000
O	-0.42254200	-3.07347900	0.00000000
H	-2.70038100	-4.02456200	0.00000000

H	-4.79318000	-2.92581000	0.00000000
H	-4.80523800	-0.39744200	0.00000000
H	-1.63092300	1.50943600	0.00000000
H	-3.39216500	1.57340800	0.00000000
N	1.21233000	0.45111300	0.00000000
C	2.40537800	-0.25568600	0.00000000
N	3.53336100	0.54970600	0.00000000
C	3.49400700	1.92295700	0.00000000
C	2.32064400	2.61060300	0.00000000
C	1.08494700	1.84341900	0.00000000
O	-0.05133500	2.37047300	0.00000000
O	2.47339000	-1.48962800	0.00000000
C	2.24678800	4.11492300	0.00000000
H	0.33357600	-0.11162300	0.00000000
H	4.42503100	0.06570900	0.00000000
H	4.46087200	2.41331500	0.00000000
H	1.70548600	4.47985700	0.88140200
H	3.25013600	4.55086900	0.00000000
H	1.70548600	4.47985700	-0.88140200
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[G]-C/G-C
Total Energy = -8863.55 kcal mol^{-1}

N	4.08603100	2.27851900	0.00000000

C	3.57180900	3.56492400	0.00000000
H	4.21679700	4.43167900	0.00000000
N	2.24991300	3.58156100	0.00000000
C	1.87965800	2.23388800	0.00000000
C	0.59523900	1.61676900	0.00000000
O	-0.52961500	2.17990200	0.00000000
N	0.68388700	0.21323900	0.00000000
H	-0.22241700	-0.30910000	0.00000000
C	1.85945900	-0.51290800	0.00000000
N	1.74613200	-1.85640700	0.00000000
H	0.83415300	-2.33682400	0.00000000
H	2.59799400	-2.40128100	0.00000000
N	3.07034200	0.05825200	0.00000000
C	3.01797000	1.40909300	0.00000000
H	5.06670000	2.02141400	0.00000000
N	-3.01436100	-3.28624400	0.00000000
C	-4.22212000	-2.65109000	0.00000000
H	-5.09958300	-3.28553400	0.00000000
C	-4.27534600	-1.29174700	0.00000000
H	-5.22055300	-0.76216100	0.00000000
C	-3.02574300	-0.58309200	0.00000000
N	-3.00309500	0.75871900	0.00000000
H	-2.10872200	1.27192300	0.00000000
H	-3.87139600	1.27702600	0.00000000
N	-1.83817600	-1.23230300	0.00000000
C	-1.79909000	-2.59092000	0.00000000
O	-0.72828900	-3.25134800	0.00000000
H	-2.96549500	-4.30023400	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000
H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000

H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

[C]-C/G-C

Total Energy = -8290.12 kcal mol^{-1}

N	1.84652000	2.69553800	0.00000000
C	3.20865500	2.76715800	0.00000000
N	3.93091500	1.55882900	0.00000000
C	3.32379500	0.33587400	0.00000000
C	1.96583700	0.25054000	0.00000000
C	1.23859300	1.49144500	0.00000000
N	-0.10951500	1.46523100	0.00000000
O	3.84588500	3.84749700	0.00000000
H	4.94356100	1.62968900	0.00000000
H	3.97918700	-0.52699700	0.00000000
H	1.44380400	-0.70088500	0.00000000
H	-0.60727500	2.34770800	0.00000000
H	-0.63763000	0.58073100	0.00000000
N	-1.81070300	-0.99017600	0.00000000
C	-1.23098000	-2.22873500	0.00000000
N	-2.08634700	-3.34654400	0.00000000
C	-3.44421500	-3.24016200	0.00000000
C	-4.02843800	-2.01016000	0.00000000
C	-3.15251500	-0.87362100	0.00000000
N	-3.67656500	0.37044400	0.00000000
O	0.00440300	-2.41574500	0.00000000
H	-1.64260300	-4.25979100	0.00000000
H	-4.00252800	-4.16818900	0.00000000
H	-5.10561100	-1.89364500	0.00000000
H	-3.07532500	1.18330200	0.00000000
H	-4.67672800	0.51496900	0.00000000
N	4.64494800	-0.55834800	-3.40000000
C	4.98506400	0.78462800	-3.40000000
H	6.01633600	1.10673300	-3.40000000
N	3.92540700	1.57507800	-3.40000000
C	2.83372200	0.70241800	-3.40000000
C	1.43187100	0.95812100	-3.40000000
O	0.85284700	2.07487800	-3.40000000
N	0.67861500	-0.22946500	-3.40000000
H	-0.36162400	-0.11933400	-3.40000000
C	1.20285400	-1.50791400	-3.40000000
N	0.32148200	-2.52821500	-3.40000000
H	-0.69870700	-2.38083300	-3.40000000
H	0.69038400	-3.46974000	-3.40000000
N	2.51819900	-1.75757500	-3.40000000
C	3.26983300	-0.63393800	-3.40000000
H	5.28720400	-1.34277300	-3.40000000
N	-4.37027500	-0.88683000	-3.40000000
C	-4.97403900	0.33692300	-3.40000000

H	-6.05683800	0.33940700	-3.40000000
C	-4.21809800	1.46794000	-3.40000000
H	-4.67150300	2.45196300	-3.40000000
C	-2.79061000	1.30675600	-3.40000000
N	-1.98359100	2.37899100	-3.40000000
H	-0.95837400	2.26848300	-3.40000000
H	-2.38140800	3.30868500	-3.40000000
N	-2.21144500	0.08349900	-3.40000000
C	-2.97839900	-1.03862000	-3.40000000
O	-2.50029300	-2.20231800	-3.40000000
H	-4.92675000	-1.73588800	-3.40000000

Cartesian Coordinates of Systems in Methanol

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in methanol that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9177.53 kcal mol^{-1}

N	-1.53762100	0.53951300	0.00000000
C	-0.79452900	1.66753900	0.00000000
N	-1.22458000	2.94035900	0.00000000
C	-2.57332200	3.01272900	0.00000000
C	-3.46554900	1.92605400	0.00000000
C	-2.89405100	0.63217200	0.00000000
N	-3.37817800	4.13343800	0.00000000
C	-4.68618700	3.69659900	0.00000000
N	-4.78764500	2.37391900	0.00000000
N	-3.63209600	-0.49865400	0.00000000
H	0.28055500	1.50262800	0.00000000
H	-3.06732300	5.09848800	0.00000000
H	-5.51444600	4.39035300	0.00000000
H	-4.64192000	-0.45534800	0.00000000
H	-3.18180400	-1.40435300	0.00000000
N	2.03853300	-0.19164700	0.00000000
C	3.35932900	0.07006200	0.00000000
N	4.38908200	-0.79840200	0.00000000
C	3.95591400	-2.07843500	0.00000000
C	2.61608600	-2.50179600	0.00000000
C	1.62331200	-1.49081000	0.00000000
N	4.69786000	-3.24300200	0.00000000
C	3.80590700	-4.29465600	0.00000000
N	2.54032600	-3.89648600	0.00000000
N	0.30163800	-1.75689400	0.00000000
H	3.62709200	1.12452600	0.00000000
H	5.70918800	-3.31384700	0.00000000
H	4.14213000	-5.32156400	0.00000000
H	-0.00867000	-2.71965300	0.00000000
H	-0.39252400	-0.99257800	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000

O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000
N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000
H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000

[T]-A/T-A
Total Energy = -9042.61 kcal mol^{-1}

N	4.06322600	-1.04838400	0.00000000
C	3.94914000	-2.41975300	0.00000000
H	4.88924300	-2.95940500	0.00000000
C	2.74184300	-3.04865700	0.00000000
C	2.59346200	-4.54762700	0.00000000
H	3.57325600	-5.03406600	0.00000000
H	2.03441300	-4.88505900	0.88148600
H	2.03441300	-4.88505900	-0.88148600
C	1.54744200	-2.21725800	0.00000000
O	0.37760100	-2.66860900	0.00000000
N	1.75630300	-0.83887100	0.00000000
H	0.90541800	-0.21567500	0.00000000
C	2.97506200	-0.19400400	0.00000000
O	3.08896100	1.04224600	0.00000000
H	4.98069100	-0.61488700	0.00000000
N	-3.67882300	3.35748600	0.00000000
C	-4.68874900	2.41851800	0.00000000
H	-5.72977000	2.70756000	0.00000000
N	-4.23308900	1.17256800	0.00000000
C	-2.84475200	1.31250500	0.00000000
C	-1.79102200	0.36711300	0.00000000
N	-1.97731400	-0.96548500	0.00000000
H	-1.17050100	-1.60057400	0.00000000
H	-2.91574100	-1.34184600	0.00000000
N	-0.51701100	0.85409800	0.00000000
C	-0.30691600	2.18578900	0.00000000
H	0.73762700	2.48790400	0.00000000
N	-1.22388800	3.16602500	0.00000000
C	-2.48228900	2.67068900	0.00000000
H	-3.79571300	4.36466300	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000

H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000
N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000
H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000

[G]-A/T-A

Total Energy = -9346.93 kcal mol^{-1}

N	1.38327600	-0.51140300	0.00000000
C	2.63784700	0.05983800	0.00000000
N	3.77007400	-0.64551500	0.00000000
C	3.55855000	-1.98200800	0.00000000
C	2.32954500	-2.66216700	0.00000000
C	1.12782300	-1.89733100	0.00000000
N	4.51391800	-2.97218900	0.00000000
C	3.84914200	-4.18672400	0.00000000
N	2.53438600	-4.04417000	0.00000000
O	-0.05407400	-2.32269000	0.00000000
N	2.69737400	1.41209200	0.00000000
H	0.54888800	0.11885800	0.00000000
H	5.51856800	-2.83541400	0.00000000
H	4.38486300	-5.12483900	0.00000000
H	3.59977100	1.86698500	0.00000000
H	1.86543400	1.98103800	0.00000000
N	-0.94140700	1.28306800	0.00000000
C	-0.82506200	2.62763800	0.00000000
N	-1.79442400	3.55359500	0.00000000
C	-3.02244400	2.98715500	0.00000000
C	-3.29860800	1.61111900	0.00000000

C	-2.19137900	0.72727700	0.00000000
N	-4.25823100	3.59967400	0.00000000
C	-5.20782100	2.59956600	0.00000000
N	-4.67503600	1.38442000	0.00000000
N	-2.32166000	-0.60978400	0.00000000
H	0.18954800	3.01946500	0.00000000
H	-4.43737500	4.59765800	0.00000000
H	-6.26487700	2.82287700	0.00000000
H	-3.24837300	-1.01515500	0.00000000
H	-1.49803600	-1.22757700	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000
N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000
H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000

[C]-A/T-A

Total Energy = -8778.75 kcal mol^{-1}

N	2.22125900	-1.20888500	0.00000000
C	3.57340700	-1.05542800	0.00000000
N	4.36863100	-2.21938100	0.00000000
C	3.83567200	-3.47467600	0.00000000
C	2.48403300	-3.63774200	0.00000000
C	1.68062700	-2.44448700	0.00000000
N	0.33560000	-2.53693900	0.00000000
O	4.14624600	0.06030100	0.00000000
H	5.37541400	-2.08896800	0.00000000

H	4.53903200	-4.29844700	0.00000000
H	2.03274100	-4.62309200	0.00000000
H	-0.24918200	-1.68608500	0.00000000
H	-0.10598500	-3.44678900	0.00000000
N	-1.18142000	0.00527200	0.00000000
C	-0.28221500	1.01398700	0.00000000
N	-0.52261800	2.33583400	0.00000000
C	-1.84610700	2.60428500	0.00000000
C	-2.88718000	1.65937300	0.00000000
C	-2.50971300	0.29600200	0.00000000
N	-2.47903100	3.83023400	0.00000000
C	-3.83659600	3.58901800	0.00000000
N	-4.13017800	2.29529700	0.00000000
N	-3.40578100	-0.71461200	0.00000000
H	0.75733100	0.69375500	0.00000000
H	-2.03039500	4.73950100	0.00000000
H	-4.55448700	4.39644700	0.00000000
H	-4.39807700	-0.52262700	0.00000000
H	-3.09400300	-1.67673800	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000
N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000
H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000

[A]-T/A-T
Total Energy = -9042.61 kcal mol^{-1}

N	4.06322600	-1.04838400	0.00000000
C	3.94914000	-2.41975300	0.00000000
H	4.88924300	-2.95940500	0.00000000
C	2.74184300	-3.04865700	0.00000000
C	2.59346200	-4.54762700	0.00000000
H	3.57325600	-5.03406600	0.00000000
H	2.03441300	-4.88505900	0.88148600
H	2.03441300	-4.88505900	-0.88148600
C	1.54744200	-2.21725800	0.00000000
O	0.37760100	-2.66860900	0.00000000
N	1.75630300	-0.83887100	0.00000000
H	0.90541800	-0.21567500	0.00000000
C	2.97506200	-0.19400400	0.00000000
O	3.08896100	1.04224600	0.00000000
H	4.98069100	-0.61488700	0.00000000
N	-3.67882300	3.35748600	0.00000000
C	-4.68874900	2.41851800	0.00000000
H	-5.72977000	2.70756000	0.00000000
N	-4.23308900	1.17256800	0.00000000
C	-2.84475200	1.31250500	0.00000000
C	-1.79102200	0.36711300	0.00000000
N	-1.97731400	-0.96548500	0.00000000
H	-1.17050100	-1.60057400	0.00000000
H	-2.91574100	-1.34184600	0.00000000
N	-0.51701100	0.85409800	0.00000000
C	-0.30691600	2.18578900	0.00000000
H	0.73762700	2.48790400	0.00000000
N	-1.22388800	3.16602500	0.00000000
C	-2.48228900	2.67068900	0.00000000
H	-3.79571300	4.36466300	0.00000000
N	3.90344300	1.54014400	3.40000000
C	4.61721700	0.36362500	3.40000000
H	5.69497500	0.47961600	3.40000000
C	4.01015300	-0.85480000	3.40000000
C	4.77118300	-2.15470900	3.40000000
H	5.84977500	-1.97233800	3.40000000
H	4.51724000	-2.75629800	4.28148600
H	4.51724000	-2.75629800	2.51851400
C	2.55517800	-0.88423600	3.40000000
O	1.87405500	-1.93700200	3.40000000
N	1.91395500	0.35366800	3.40000000
H	0.85926900	0.35770600	3.40000000
C	2.52090800	1.59174500	3.40000000
O	1.88640500	2.65884000	3.40000000
H	4.39088500	2.43012300	3.40000000
N	-4.94971100	0.55390500	3.40000000
C	-5.21484700	-0.79935500	3.40000000
H	-6.22694500	-1.17741200	3.40000000
N	-4.11385900	-1.53952000	3.40000000
C	-3.07292400	-0.61026400	3.40000000
C	-1.66475100	-0.75573600	3.40000000
N	-1.03218300	-1.94333000	3.40000000

H	-0.00616100	-1.98289500	3.40000000
H	-1.57016700	-2.79940600	3.40000000
N	-0.92029700	0.38708800	3.40000000
C	-1.53307500	1.58794000	3.40000000
H	-0.86560000	2.44632300	3.40000000
N	-2.85108900	1.84198500	3.40000000
C	-3.57800600	0.70158000	3.40000000
H	-5.63628100	1.30002200	3.40000000

[T]-T/A-T

Total Energy = -8899.76 kcal mol^{-1}

N	1.21561600	1.64032800	0.00000000
C	1.65506000	2.95124500	0.00000000
N	3.03199800	3.07721900	0.00000000
C	3.89454400	2.00582200	0.00000000
C	3.45300000	0.71831800	0.00000000
C	2.01681200	0.49749200	0.00000000
O	1.48419600	-0.63729500	0.00000000
O	0.88888600	3.92530500	0.00000000
C	4.37656400	-0.47136600	0.00000000
H	0.18783800	1.50001100	0.00000000
H	3.39797900	4.02363700	0.00000000
H	4.94751000	2.26299600	0.00000000
H	4.20251300	-1.10046700	0.88143500
H	5.42203200	-0.14967600	0.00000000
H	4.20251300	-1.10046700	-0.88143500
N	-1.29260400	-1.08851300	0.00000000
C	-2.07507100	0.04115600	0.00000000
N	-3.42992300	-0.20309700	0.00000000
C	-3.96929300	-1.47170900	0.00000000
C	-3.19451100	-2.58909900	0.00000000
C	-1.74610000	-2.41726800	0.00000000
O	-0.91989200	-3.34860500	0.00000000
O	-1.60748500	1.19937600	0.00000000
C	-3.76126300	-3.98422800	0.00000000
H	-0.26297000	-0.93507800	0.00000000
H	-4.03896300	0.60848000	0.00000000
H	-5.05242200	-1.50890600	0.00000000
H	-3.42248000	-4.54256100	-0.88138700
H	-4.85487800	-3.95911300	0.00000000
H	-3.42248000	-4.54256100	0.88138700
N	3.90344300	1.54014400	-3.40000000
C	4.61721700	0.36362500	-3.40000000
H	5.69497500	0.47961600	-3.40000000
C	4.01015300	-0.85480000	-3.40000000
C	4.77118300	-2.15470900	-3.40000000
H	5.84977500	-1.97233800	-3.40000000
H	4.51724000	-2.75629800	-4.28148600
H	4.51724000	-2.75629800	-2.51851400
C	2.55517800	-0.88423600	-3.40000000
O	1.87405500	-1.93700200	-3.40000000

N	1.91395500	0.35366800	-3.40000000
H	0.85926900	0.35770600	-3.40000000
C	2.52090800	1.59174500	-3.40000000
O	1.88640500	2.65884000	-3.40000000
H	4.39088500	2.43012300	-3.40000000
N	-4.94971100	0.55390500	-3.40000000
C	-5.21484700	-0.79935500	-3.40000000
H	-6.22694500	-1.17741200	-3.40000000
N	-4.11385900	-1.53952000	-3.40000000
C	-3.07292400	-0.61026400	-3.40000000
C	-1.66475100	-0.75573600	-3.40000000
N	-1.03218300	-1.94333000	-3.40000000
H	-0.00616100	-1.98289500	-3.40000000
H	-1.57016700	-2.79940600	-3.40000000
N	-0.92029700	0.38708800	-3.40000000
C	-1.53307500	1.58794000	-3.40000000
H	-0.86560000	2.44632300	-3.40000000
N	-2.85108900	1.84198500	-3.40000000
C	-3.57800600	0.70158000	-3.40000000
H	-5.63628100	1.30002200	-3.40000000

[G]-T/A-T
Total Energy = -9206.24 kcal mol^{-1}

N	-1.57942500	-0.10255100	0.00000000
C	-2.95231400	0.01357700	0.00000000
N	-3.77566400	-1.03636200	0.00000000
C	-3.11865000	-2.22010100	0.00000000
C	-1.72978500	-2.44187200	0.00000000
C	-0.86328800	-1.31216500	0.00000000
N	-3.67834200	-3.47700900	0.00000000
C	-2.63947300	-4.39235800	0.00000000
N	-1.45199300	-3.81070800	0.00000000
O	0.39467700	-1.29647200	0.00000000
N	-3.45555000	1.26967900	0.00000000
H	-1.01225700	0.76661100	0.00000000
H	-4.66935600	-3.69136600	0.00000000
H	-2.82350500	-5.45686800	0.00000000
H	-4.45793200	1.39923900	0.00000000
H	-2.85516300	2.08264700	0.00000000
N	1.85746000	1.11757800	0.00000000
C	1.12424300	2.27885400	0.00000000
N	1.87539300	3.43074500	0.00000000
C	3.25411000	3.43477300	0.00000000
C	3.98151300	2.28635700	0.00000000
C	3.25939600	1.01907100	0.00000000
O	3.79538500	-0.10390900	0.00000000
O	-0.12657000	2.30420900	0.00000000
C	5.48713600	2.26538600	0.00000000
H	1.32158200	0.22315100	0.00000000
H	1.36451100	4.30743300	0.00000000
H	3.70916500	4.41831500	0.00000000
H	5.86939700	1.73598000	-0.88140800

H	5.88948800	3.28259200	0.00000000
H	5.86939700	1.73598000	0.88140800
N	3.90344300	1.54014400	-3.40000000
C	4.61721700	0.36362500	-3.40000000
H	5.69497500	0.47961600	-3.40000000
C	4.01015300	-0.85480000	-3.40000000
C	4.77118300	-2.15470900	-3.40000000
H	5.84977500	-1.97233800	-3.40000000
H	4.51724000	-2.75629800	-4.28148600
H	4.51724000	-2.75629800	-2.51851400
C	2.55517800	-0.88423600	-3.40000000
O	1.87405500	-1.93700200	-3.40000000
N	1.91395500	0.35366800	-3.40000000
H	0.85926900	0.35770600	-3.40000000
C	2.52090800	1.59174500	-3.40000000
O	1.88640500	2.65884000	-3.40000000
H	4.39088500	2.43012300	-3.40000000
N	-4.94971100	0.55390500	-3.40000000
C	-5.21484700	-0.79935500	-3.40000000
H	-6.22694500	-1.17741200	-3.40000000
N	-4.11385900	-1.53952000	-3.40000000
C	-3.07292400	-0.61026400	-3.40000000
C	-1.66475100	-0.75573600	-3.40000000
N	-1.03218300	-1.94333000	-3.40000000
H	-0.00616100	-1.98289500	-3.40000000
H	-1.57016700	-2.79940600	-3.40000000
N	-0.92029700	0.38708800	-3.40000000
C	-1.53307500	1.58794000	-3.40000000
H	-0.86560000	2.44632300	-3.40000000
N	-2.85108900	1.84198500	-3.40000000
C	-3.57800600	0.70158000	-3.40000000
H	-5.63628100	1.30002200	-3.40000000

[C]-T/A-T

Total Energy = -8641.15 kcal mol^{-1}

N	-1.39415600	-1.05819300	0.00000000
C	-2.69977300	-0.64919900	0.00000000
N	-3.69709400	-1.64633600	0.00000000
C	-3.41455800	-2.97926800	0.00000000
C	-2.11919100	-3.39462700	0.00000000
C	-1.10181800	-2.37913100	0.00000000
N	0.19472500	-2.73406600	0.00000000
O	-3.05266500	0.54811700	0.00000000
H	-4.65990300	-1.32471400	0.00000000
H	-4.26148600	-3.65448500	0.00000000
H	-1.86003500	-4.44672300	0.00000000
H	0.93314100	-2.01778600	0.00000000
H	0.44992500	-3.71233800	0.00000000
N	0.80426300	1.01042400	0.00000000
C	0.49669600	2.36217300	0.00000000
N	1.60779900	3.18960500	0.00000000
C	2.90301700	2.73183400	0.00000000

C	3.19899600	1.40412600	0.00000000
C	2.09071500	0.46268600	0.00000000
O	2.24268400	-0.78074500	0.00000000
O	-0.65846200	2.80284700	0.00000000
C	4.60948000	0.87529800	0.00000000
H	-0.00105900	0.34649900	0.00000000
H	1.42138500	4.18700000	0.00000000
H	3.66560000	3.50212900	0.00000000
H	4.79279300	0.24883300	0.88153000
H	5.33002900	1.69842300	0.00000000
H	4.79279300	0.24883300	-0.88153000
N	3.90344300	1.54014400	-3.40000000
C	4.61721700	0.36362500	-3.40000000
H	5.69497500	0.47961600	-3.40000000
C	4.01015300	-0.85480000	-3.40000000
C	4.77118300	-2.15470900	-3.40000000
H	5.84977500	-1.97233800	-3.40000000
H	4.51724000	-2.75629800	-4.28148600
H	4.51724000	-2.75629800	-2.51851400
C	2.55517800	-0.88423600	-3.40000000
O	1.87405500	-1.93700200	-3.40000000
N	1.91395500	0.35366800	-3.40000000
H	0.85926900	0.35770600	-3.40000000
C	2.52090800	1.59174500	-3.40000000
O	1.88640500	2.65884000	-3.40000000
H	4.39088500	2.43012300	-3.40000000
N	-4.94971100	0.55390500	-3.40000000
C	-5.21484700	-0.79935500	-3.40000000
H	-6.22694500	-1.17741200	-3.40000000
N	-4.11385900	-1.53952000	-3.40000000
C	-3.07292400	-0.61026400	-3.40000000
C	-1.66475100	-0.75573600	-3.40000000
N	-1.03218300	-1.94333000	-3.40000000
H	-0.00616100	-1.98289500	-3.40000000
H	-1.57016700	-2.79940600	-3.40000000
N	-0.92029700	0.38708800	-3.40000000
C	-1.53307500	1.58794000	-3.40000000
H	-0.86560000	2.44632300	-3.40000000
N	-2.85108900	1.84198500	-3.40000000
C	-3.57800600	0.70158000	-3.40000000
H	-5.63628100	1.30002200	-3.40000000

[A]-G/C-G

Total Energy = -9257.87 kcal mol^{-1}

N	1.38327600	-0.51140300	0.00000000
C	2.63784700	0.05983800	0.00000000
N	3.77007400	-0.64551500	0.00000000
C	3.55855000	-1.98200800	0.00000000
C	2.32954500	-2.66216700	0.00000000
C	1.12782300	-1.89733100	0.00000000
N	4.51391800	-2.97218900	0.00000000
C	3.84914200	-4.18672400	0.00000000

N	2.53438600	-4.04417000	0.00000000
O	-0.05407400	-2.32269000	0.00000000
N	2.69737400	1.41209200	0.00000000
H	0.54888800	0.11885800	0.00000000
H	5.51856800	-2.83541400	0.00000000
H	4.38486300	-5.12483900	0.00000000
H	3.59977100	1.86698500	0.00000000
H	1.86543400	1.98103800	0.00000000
N	-0.94140700	1.28306800	0.00000000
C	-0.82506200	2.62763800	0.00000000
N	-1.79442400	3.55359500	0.00000000
C	-3.02244400	2.98715500	0.00000000
C	-3.29860800	1.61111900	0.00000000
C	-2.19137900	0.72727700	0.00000000
N	-4.25823100	3.59967400	0.00000000
C	-5.20782100	2.59956600	0.00000000
N	-4.67503600	1.38442000	0.00000000
N	-2.32166000	-0.60978400	0.00000000
H	0.18954800	3.01946500	0.00000000
H	-4.43737500	4.59765800	0.00000000
H	-6.26487700	2.82287700	0.00000000
H	-3.24837300	-1.01515500	0.00000000
H	-1.49803600	-1.22757700	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[T]-G/C-G

Total Energy = -9118.78 kcal mol^{-1}

N	1.57942500	-0.10255100	0.00000000
C	2.95231400	0.01357700	0.00000000
N	3.77566400	-1.03636200	0.00000000
C	3.11865000	-2.22010100	0.00000000
C	1.72978500	-2.44187200	0.00000000
C	0.86328800	-1.31216500	0.00000000
N	3.67834200	-3.47700900	0.00000000
C	2.63947300	-4.39235800	0.00000000
N	1.45199300	-3.81070800	0.00000000
O	-0.39467700	-1.29647200	0.00000000
N	3.45555000	1.26967900	0.00000000
H	1.01225700	0.76661100	0.00000000
H	4.66935600	-3.69136600	0.00000000
H	2.82350500	-5.45686800	0.00000000
H	4.45793200	1.39923900	0.00000000
H	2.85516300	2.08264700	0.00000000
N	-1.85746000	1.11757800	0.00000000
C	-1.12424300	2.27885400	0.00000000
N	-1.87539300	3.43074500	0.00000000
C	-3.25411000	3.43477300	0.00000000
C	-3.98151300	2.28635700	0.00000000
C	-3.25939600	1.01907100	0.00000000
O	-3.79538500	-0.10390900	0.00000000
O	0.12657000	2.30420900	0.00000000
C	-5.48713600	2.26538600	0.00000000
H	-1.32158200	0.22315100	0.00000000
H	-1.36451100	4.30743300	0.00000000
H	-3.70916500	4.41831500	0.00000000
H	-5.86939700	1.73598000	-0.88140800
H	-5.88948800	3.28259200	0.00000000
H	-5.86939700	1.73598000	0.88140800
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000

H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[G]-G/C-G

Total Energy = -9420.63 kcal mol^{-1}

N	-3.60757900	0.53363400	0.00000000
C	-4.48671900	1.59994100	0.00000000
N	-4.08056100	2.87000600	0.00000000
C	-2.73404300	2.99887300	0.00000000
C	-1.76838800	1.97935000	0.00000000
C	-2.19814400	0.62400200	0.00000000
N	-2.01150000	4.17090100	0.00000000
C	-0.67137200	3.83432500	0.00000000
N	-0.48592200	2.52455500	0.00000000
O	-1.51096600	-0.42191100	0.00000000
N	-5.80583200	1.31295900	0.00000000
H	-3.98213800	-0.41225000	0.00000000
H	-2.39379300	5.11019300	0.00000000
H	0.10528800	4.58460700	0.00000000
H	-6.47193400	2.07349000	0.00000000
H	-6.14874700	0.36258500	0.00000000
N	1.26706600	-1.06202400	0.00000000
C	2.33792900	-0.18933200	0.00000000
N	3.61239200	-0.60071700	0.00000000
C	3.73882400	-1.94727500	0.00000000
C	2.72049800	-2.91339300	0.00000000
C	1.36035900	-2.47711300	0.00000000
N	4.91326600	-2.66792800	0.00000000
C	4.57424000	-4.01037800	0.00000000
N	3.26536400	-4.20089000	0.00000000
O	0.32343100	-3.17333500	0.00000000
N	2.07214900	1.13341500	0.00000000
H	0.30097300	-0.68937300	0.00000000
H	5.85174000	-2.28415900	0.00000000
H	5.32773800	-4.78452900	0.00000000
H	2.86655800	1.76008900	0.00000000
H	1.12334800	1.53965400	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000

O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[C]-G/C-G
Total Energy = -9420.63 kcal mol^{-1}

N	4.08648800	-2.27914700	0.00000000
C	3.57244800	-3.56517900	0.00000000
H	4.21725800	-4.43199900	0.00000000
N	2.25021100	-3.58170800	0.00000000
C	1.88022300	-2.23377900	0.00000000
C	0.59604100	-1.61697200	0.00000000
O	-0.52862600	-2.18135300	0.00000000
N	0.68375800	-0.21375000	0.00000000
H	-0.22281100	0.30856100	0.00000000
C	1.85947100	0.51260900	0.00000000
N	1.74602000	1.85582300	0.00000000
H	0.83383000	2.33602900	0.00000000
H	2.59754400	2.40136900	0.00000000
N	3.07054400	-0.05861000	0.00000000
C	3.01871300	-1.40945200	0.00000000
H	5.06747100	-2.02287400	0.00000000
N	-3.01359000	3.28697900	0.00000000
C	-4.22195900	2.65276400	0.00000000
H	-5.09886900	3.28775800	0.00000000
C	-4.27614000	1.29344900	0.00000000
H	-5.22174300	0.76455200	0.00000000
C	-3.02741800	0.58391500	0.00000000
N	-3.00573900	-0.75786000	0.00000000
H	-2.11215300	-1.27139100	0.00000000
H	-3.87436500	-1.27572800	0.00000000
N	-1.83890300	1.23239200	0.00000000

C	-1.79937400	2.59102200	0.00000000
O	-0.72737200	3.25053900	0.00000000
H	-2.96482200	4.30105400	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[A]-C/G-C

Total Energy = -8689.95 kcal mol^{-1}

N	-1.83612500	1.73897700	0.00000000
C	-2.10801500	3.07236700	0.00000000
N	-3.46073800	3.46898900	0.00000000
C	-4.48990100	2.57420700	0.00000000
C	-4.22730700	1.23833200	0.00000000
C	-2.84418800	0.84298300	0.00000000
N	-2.51647900	-0.46478200	0.00000000
O	-1.22391000	3.96194800	0.00000000
H	-3.64782100	4.46679600	0.00000000
H	-5.49070400	2.98858300	0.00000000
H	-5.02497300	0.50463700	0.00000000
H	-1.52656000	-0.75801500	0.00000000
H	-3.24534000	-1.16591400	0.00000000
N	0.37009300	-1.12196800	0.00000000
C	1.05156900	0.04493600	0.00000000
N	2.38300800	0.22477300	0.00000000
C	3.04730000	-0.95098400	0.00000000

C	2.47034500	-2.23309700	0.00000000
C	1.05705900	-2.29540900	0.00000000
N	4.40883200	-1.17409100	0.00000000
C	4.59893200	-2.53975200	0.00000000
N	3.45925200	-3.21874700	0.00000000
N	0.37280800	-3.45991700	0.00000000
H	0.42577200	0.93464700	0.00000000
H	5.13496000	-0.46643500	0.00000000
H	5.58868300	-2.97299800	0.00000000
H	0.86203300	-4.34432100	0.00000000
H	-0.63857300	-3.46071200	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[T]-C/G-C

Total Energy = -8552.01 kcal mol^{-1}

N	-1.43721900	0.99892100	0.00000000
C	-1.45170100	2.36702300	0.00000000
N	-2.70822300	3.00740000	0.00000000
C	-3.88860900	2.32679300	0.00000000
C	-3.88334800	0.96647300	0.00000000
C	-2.60316800	0.31269900	0.00000000
N	-2.54007800	-1.03006700	0.00000000
O	-0.42203600	3.07263400	0.00000000
H	-2.69986700	4.02247200	0.00000000

H	-4.79249300	2.92361600	0.00000000
H	-4.80386700	0.39488600	0.00000000
H	-1.63067200	-1.51100000	0.00000000
H	-3.39160900	-1.57508000	0.00000000
N	1.20950100	-0.45266200	0.00000000
C	2.40004700	0.25756500	0.00000000
N	3.53033200	-0.54346600	0.00000000
C	3.49521100	-1.91675000	0.00000000
C	2.32394700	-2.60852700	0.00000000
C	1.08610700	-1.84541100	0.00000000
O	-0.04950500	-2.37418200	0.00000000
O	2.46219000	1.49236200	0.00000000
C	2.25686500	-4.11339500	0.00000000
H	0.32921300	0.10808100	0.00000000
H	4.42130600	-0.05796400	0.00000000
H	4.46345500	-2.40397500	0.00000000
H	1.71770800	-4.48132300	0.88153000
H	3.26236600	-4.54431700	0.00000000
H	1.71770800	-4.48132300	-0.88153000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[G]-C/G-C
Total Energy = -8865.35 kcal mol^{-1}

N	4.08648800	-2.27914700	0.00000000

C	3.57244800	-3.56517900	0.00000000
H	4.21725800	-4.43199900	0.00000000
N	2.25021100	-3.58170800	0.00000000
C	1.88022300	-2.23377900	0.00000000
C	0.59604100	-1.61697200	0.00000000
O	-0.52862600	-2.18135300	0.00000000
N	0.68375800	-0.21375000	0.00000000
H	-0.22281100	0.30856100	0.00000000
C	1.85947100	0.51260900	0.00000000
N	1.74602000	1.85582300	0.00000000
H	0.83383000	2.33602900	0.00000000
H	2.59754400	2.40136900	0.00000000
N	3.07054400	-0.05861000	0.00000000
C	3.01871300	-1.40945200	0.00000000
H	5.06747100	-2.02287400	0.00000000
N	-3.01359000	3.28697900	0.00000000
C	-4.22195900	2.65276400	0.00000000
H	-5.09886900	3.28775800	0.00000000
C	-4.27614000	1.29344900	0.00000000
H	-5.22174300	0.76455200	0.00000000
C	-3.02741800	0.58391500	0.00000000
N	-3.00573900	-0.75786000	0.00000000
H	-2.11215300	-1.27139100	0.00000000
H	-3.87436500	-1.27572800	0.00000000
N	-1.83890300	1.23239200	0.00000000
C	-1.79937400	2.59102200	0.00000000
O	-0.72737200	3.25053900	0.00000000
H	-2.96482200	4.30105400	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000
H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000

H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

[C]-C/G-C

Total Energy = -8292.16 kcal mol^{-1}

N	1.84585400	-2.69481600	0.00000000
C	3.20760800	-2.76571900	0.00000000
N	3.93011200	-1.55885100	0.00000000
C	3.32325900	-0.33566300	0.00000000
C	1.96526500	-0.25003700	0.00000000
C	1.23735800	-1.49029300	0.00000000
N	-0.11035900	-1.46432500	0.00000000
O	3.84411100	-3.84766000	0.00000000
H	4.94286100	-1.62929000	0.00000000
H	3.97912900	0.52674700	0.00000000
H	1.44330000	0.70151700	0.00000000
H	-0.60768300	-2.34716200	0.00000000
H	-0.63889200	-0.57952000	0.00000000
N	-1.80943700	0.98966000	0.00000000
C	-1.23049000	2.22823400	0.00000000
N	-2.08504400	3.34557700	0.00000000
C	-3.44316700	3.23950200	0.00000000
C	-4.02746700	2.00963300	0.00000000
C	-3.15185000	0.87312300	0.00000000
N	-3.67624300	-0.37021200	0.00000000
O	0.00586300	2.41472200	0.00000000
H	-1.64174400	4.25905400	0.00000000
H	-4.00097600	4.16776100	0.00000000
H	-5.10465800	1.89248200	0.00000000
H	-3.07645000	-1.18392200	0.00000000
H	-4.67649400	-0.51402700	0.00000000
N	4.64568700	0.55810900	3.40000000
C	4.98573100	-0.78445800	3.40000000
H	6.01689700	-1.10672000	3.40000000
N	3.92573400	-1.57502200	3.40000000
C	2.83411500	-0.70199800	3.40000000
C	1.43264000	-0.95781400	3.40000000
O	0.85450000	-2.07547000	3.40000000
N	0.67881100	0.22897600	3.40000000
H	-0.36162500	0.11866600	3.40000000
C	1.20304000	1.50767900	3.40000000
N	0.32173500	2.52767700	3.40000000
H	-0.69850100	2.38000000	3.40000000
H	0.68996800	3.46954600	3.40000000
N	2.51857200	1.75740400	3.40000000
C	3.27064500	0.63408400	3.40000000
H	5.28868600	1.34204500	3.40000000
N	-4.37008300	0.88787800	3.40000000
C	-4.97489200	-0.33547400	3.40000000

H	-6.05756700	-0.33718800	3.40000000
C	-4.21974000	-1.46703000	3.40000000
H	-4.67387100	-2.45072800	3.40000000
C	-2.79244900	-1.30707400	3.40000000
N	-1.98623500	-2.37985100	3.40000000
H	-0.96146300	-2.27006900	3.40000000
H	-2.38457300	-3.30938000	3.40000000
N	-2.21208600	-0.08385400	3.40000000
C	-2.97868900	1.03853500	3.40000000
O	-2.49907500	2.20220300	3.40000000
H	-4.92668800	1.73694700	3.40000000

Cartesian Coordinates of Systems in Water

Cartesian coordinates (in Å) and ADF total energies (in kcal mol^{-1}) of template-primer complexes Y_1/Z-Y_2 binding an incoming nucleotide [X] with 3.4 Å stacking distance and a twist angle of 36°, based on DNA base pairs in water that were optimized in C_s symmetry at BLYP-D3(BJ)/TZ2P (see above section for description).

[A]-A/T-A
Total Energy = -9179.50 kcal mol^{-1}

N	0.99116200	-1.29373700	0.00000000
C	1.83617200	-0.23999400	0.00000000
N	3.17961700	-0.25769600	0.00000000
C	3.66350300	-1.51916600	0.00000000
C	2.90342000	-2.70214900	0.00000000
C	1.49640000	-2.55627200	0.00000000
N	4.97704700	-1.94047500	0.00000000
C	4.96363000	-3.31895700	0.00000000
N	3.73609800	-3.82255900	0.00000000
N	0.64768800	-3.60619000	0.00000000
H	1.34921400	0.73248400	0.00000000
H	5.79986200	-1.34805500	0.00000000
H	5.87881900	-3.89311300	0.00000000
H	0.99933500	-4.55382100	0.00000000
H	-0.35272500	-3.45753600	0.00000000
N	-0.81341200	1.88396900	0.00000000
C	-0.97494800	3.22074100	0.00000000
N	-2.12009100	3.92989000	0.00000000
C	-3.20261100	3.12057500	0.00000000
C	-3.18887800	1.71544900	0.00000000
C	-1.91948500	1.08559200	0.00000000
N	-4.53988100	3.46428400	0.00000000
C	-5.26284100	2.29043400	0.00000000
N	-4.49154800	1.21064200	0.00000000
N	-1.76110800	-0.25312300	0.00000000
H	-0.05572100	3.80269300	0.00000000
H	-4.92141100	4.40358700	0.00000000
H	-6.34336100	2.29152900	0.00000000
H	-2.57962700	-0.84750800	0.00000000
H	-0.81867700	-0.67484300	0.00000000
N	3.90683800	1.53839200	3.40000000
C	4.61926800	0.36132900	3.40000000
H	5.69705300	0.47596000	3.40000000
C	4.01069600	-0.85634200	3.40000000
C	4.77077400	-2.15664300	3.40000000
H	5.84931200	-1.97433000	3.40000000
H	4.51677200	-2.75800900	2.51835800
H	4.51677200	-2.75800900	4.28164200
C	2.55637400	-0.88387000	3.40000000
O	1.87362600	-1.93629500	3.40000000
N	1.91623400	0.35435700	3.40000000
H	0.86217800	0.35997400	3.40000000
C	2.52524200	1.59117000	3.40000000

O	1.89140800	2.65957600	3.40000000
H	4.39596300	2.42745300	3.40000000
N	-4.95282400	0.55076600	3.40000000
C	-5.21572700	-0.80244200	3.40000000
H	-6.22725600	-1.18194500	3.40000000
N	-4.11346800	-1.54117000	3.40000000
C	-3.07392000	-0.61014700	3.40000000
C	-1.66543600	-0.75306300	3.40000000
N	-1.03053200	-1.93932100	3.40000000
H	-0.00437000	-1.97692100	3.40000000
H	-1.56675200	-2.79644100	3.40000000
N	-0.92255600	0.39102300	3.40000000
C	-1.53765400	1.59049300	3.40000000
H	-0.87231200	2.45049100	3.40000000
N	-2.85621700	1.84251100	3.40000000
C	-3.58162900	0.70078100	3.40000000
H	-5.64076900	1.29555400	3.40000000

[T]-A/T-A
Total Energy = -9044.89 kcal mol^{-1}

N	0.00000000	1.53316000	3.90890000
C	0.00000000	0.35514000	4.61975000
H	0.00000000	0.46833000	5.69769000
C	0.00000000	-0.86171000	4.00955000
C	0.00000000	-2.16303000	4.76789000
H	0.00000000	-1.98216000	5.84667000
H	-0.88164000	-2.76405000	4.51308000
H	0.88164000	-2.76405000	4.51308000
C	0.00000000	-0.88729000	2.55519000
O	0.00000000	-1.93880000	1.87104000
N	0.00000000	0.35179000	1.91671000
H	0.00000000	0.35882000	0.86266000
C	0.00000000	1.58779000	2.52737000
O	0.00000000	2.65704000	1.89497000
H	0.00000000	2.42157000	4.39921000
N	0.00000000	0.55739000	-4.95208000
C	0.00000000	-0.79546000	-5.21679000
H	-0.00000000	-1.17361000	-6.22883000
N	0.00000000	-1.53566000	-4.11552000
C	0.00000000	-0.60603000	-3.07473000
C	0.00000000	-0.75083000	-1.66644000
N	0.00000000	-1.93794000	-1.03312000
H	0.00000000	-1.97691000	-0.00701000
H	0.00000000	-2.79434000	-1.57049000
N	0.00000000	0.39226000	-0.92203000
C	0.00000000	1.59255000	-1.53552000
H	0.00000000	2.45166000	-0.86903000
N	0.00000000	1.84633000	-2.85375000
C	0.00000000	0.70557000	-3.58069000
H	-0.00000000	1.30310000	-5.63903000
N	3.40000000	-1.05716000	4.06355000
C	3.40000000	-2.42803000	3.94625000

H	3.40000000	-2.97004000	4.88486000
C	3.40000000	-3.05384000	2.73735000
C	3.40000000	-4.55237000	2.58599000
H	3.40000000	-5.04012000	3.56506000
H	2.51836000	-4.88885000	2.02658000
H	4.28164000	-4.88885000	2.02658000
C	3.40000000	-2.21971000	1.54570000
O	3.40000000	-2.66828000	0.37415000
N	3.40000000	-0.84198000	1.75744000
H	3.40000000	-0.21675000	0.90882000
C	3.40000000	-0.20095000	2.97797000
O	3.40000000	1.03581000	3.09481000
H	3.40000000	-0.62661000	4.98241000
N	3.40000000	3.36163000	-3.67875000
C	3.40000000	2.42273000	-4.68808000
H	3.40000000	2.71164000	-5.72911000
N	3.40000000	1.17659000	-4.23219000
C	3.40000000	1.31694000	-2.84375000
C	3.40000000	0.37204000	-1.78951000
N	3.40000000	-0.96061000	-1.97489000
H	3.40000000	-1.59526000	-1.16765000
H	3.40000000	-1.33761000	-2.91300000
N	3.40000000	0.85929000	-0.51539000
C	3.40000000	2.19095000	-0.30623000
H	3.40000000	2.49425000	0.73794000
N	3.40000000	3.17108000	-1.22354000
C	3.40000000	2.67545000	-2.48216000
H	3.40000000	4.36870000	-3.79621000

[G]-A/T-A

Total Energy = -9044.89 kcal mol^{-1}

N	1.92447953	0.56733630	2.69738131
C	1.98594235	0.19428260	4.01743663
N	2.92097565	-0.59397938	4.52619619
C	3.81924714	-0.99681799	3.59539558
C	3.86428118	-0.68657694	2.22527692
C	2.84665322	0.16748715	1.68690761
N	4.90501366	-1.81808131	3.80939905
C	5.54914355	-1.96663767	2.57997909
N	4.95266627	-1.30383079	1.61477259
O	2.69627282	0.56520741	0.51990593
N	1.00809040	0.68048964	4.83973427
H	1.14682931	1.19360211	2.39167600
H	5.16572756	-2.22464076	4.69929817
H	6.44000609	-2.57117691	2.47800706
H	1.03214749	0.42020176	5.81409091
H	0.27854855	1.28260894	4.49447910
N	-0.27238036	2.32361461	1.88551540
C	-1.22713235	2.79076711	2.71870194
N	-2.26482181	3.59090982	2.45311806
C	-2.29038841	3.93445164	1.14959133
C	-1.37774105	3.53551842	0.16243122

C	-0.31657900	2.68412929	0.56678236
N	-3.19689999	4.74142591	0.48510200
C	-2.79438143	4.78865933	-0.84415584
N	-1.70742102	4.07789977	-1.07611938
N	0.61652211	2.23733168	-0.28660561
H	-1.14581482	2.47360477	3.75866748
H	-3.99585760	5.20200136	0.90336385
H	-3.34175644	5.35988211	-1.58162878
H	0.54942182	2.52622499	-1.25361756
H	1.38910856	1.61563450	0.01514401
N	-0.54292428	-2.56164408	5.19642901
C	0.58889680	-3.33801583	5.10019105
H	0.91161308	-3.79768414	6.02718621
C	1.25194230	-3.51331346	3.92429822
C	2.49209623	-4.35839914	3.79643229
H	2.76547645	-4.79289156	4.76233179
H	3.33591243	-3.76136679	3.42903975
H	2.33832760	-5.17202049	3.07683087
C	0.72326224	-2.84509786	2.74540232
O	1.23716556	-2.92345947	1.60369042
N	-0.42611821	-2.07938831	2.93407871
H	-0.82803754	-1.58543888	2.09411418
C	-1.10303290	-1.89707444	4.12115297
O	-2.12553123	-1.19835775	4.21876993
H	-1.01013266	-2.45455153	6.09081161
N	-3.16249922	1.19984716	-2.44935589
C	-2.26963073	0.81213790	-3.42544874
H	-2.37315423	1.14099034	-4.44933956
N	-1.31204802	0.01919320	-2.96180230
C	-1.60229041	-0.11471942	-1.60338754
C	-0.96595066	-0.82583206	-0.55761382
N	0.14335328	-1.56949759	-0.72106866
H	0.55819334	-2.06249431	0.07848382
H	0.56937082	-1.64256824	-1.63504695
N	-1.52436029	-0.74095725	0.68406989
C	-2.63587565	-0.00155026	0.87084444
H	-3.01527245	0.01235652	1.88973659
N	-3.31826599	0.70875392	-0.04125909
C	-2.75499120	0.61661701	-1.26763678
H	-3.96816242	1.80175528	-2.57816162

[C]-A/T-A

Total Energy = -8780.94 kcal mol^{-1}

N	2.22378900	-1.20952500	0.00000000
C	3.57555900	-1.05864900	0.00000000
N	4.36956200	-2.22162600	0.00000000
C	3.83503800	-3.47625900	0.00000000
C	2.48333000	-3.63833400	0.00000000
C	1.68135000	-2.44466700	0.00000000
N	0.33623100	-2.53451100	0.00000000
O	4.14829900	0.05876500	0.00000000
H	5.37672100	-2.09371600	0.00000000

H	4.53760000	-4.30050200	0.00000000
H	2.03097200	-4.62323500	0.00000000
H	-0.24753500	-1.68298500	0.00000000
H	-0.10617000	-3.44393400	0.00000000
N	-1.18195600	0.00621800	0.00000000
C	-0.28287600	1.01490700	0.00000000
N	-0.52317300	2.33692300	0.00000000
C	-1.84705600	2.60558300	0.00000000
C	-2.88757800	1.66000500	0.00000000
C	-2.51041700	0.29663300	0.00000000
N	-2.48055200	3.83090700	0.00000000
C	-3.83764100	3.58924500	0.00000000
N	-4.13087800	2.29509600	0.00000000
N	-3.40653700	-0.71351800	0.00000000
H	0.75662800	0.69500800	0.00000000
H	-2.03262200	4.74049900	0.00000000
H	-4.55531100	4.39683300	0.00000000
H	-4.39901600	-0.52220600	0.00000000
H	-3.09539500	-1.67583900	0.00000000
N	3.90683800	1.53839200	3.40000000
C	4.61926800	0.36132900	3.40000000
H	5.69705300	0.47596000	3.40000000
C	4.01069600	-0.85634200	3.40000000
C	4.77077400	-2.15664300	3.40000000
H	5.84931200	-1.97433000	3.40000000
H	4.51677200	-2.75800900	2.51835800
H	4.51677200	-2.75800900	4.28164200
C	2.55637400	-0.88387000	3.40000000
O	1.87362600	-1.93629500	3.40000000
N	1.91623400	0.35435700	3.40000000
H	0.86217800	0.35997400	3.40000000
C	2.52524200	1.59117000	3.40000000
O	1.89140800	2.65957600	3.40000000
H	4.39596300	2.42745300	3.40000000
N	-4.95282400	0.55076600	3.40000000
C	-5.21572700	-0.80244200	3.40000000
H	-6.22725600	-1.18194500	3.40000000
N	-4.11346800	-1.54117000	3.40000000
C	-3.07392000	-0.61014700	3.40000000
C	-1.66543600	-0.75306300	3.40000000
N	-1.03053200	-1.93932100	3.40000000
H	-0.00437000	-1.97692100	3.40000000
H	-1.56675200	-2.79644100	3.40000000
N	-0.92255600	0.39102300	3.40000000
C	-1.53765400	1.59049300	3.40000000
H	-0.87231200	2.45049100	3.40000000
N	-2.85621700	1.84251100	3.40000000
C	-3.58162900	0.70078100	3.40000000
H	-5.64076900	1.29555400	3.40000000

[A]-T/A-T
Total Energy = -9044.89 kcal mol^{-1}

N	0.00000000	1.53316000	3.90890000
C	0.00000000	0.35514000	4.61975000
H	0.00000000	0.46833000	5.69769000
C	0.00000000	-0.86171000	4.00955000
C	0.00000000	-2.16303000	4.76789000
H	0.00000000	-1.98216000	5.84667000
H	-0.88164000	-2.76405000	4.51308000
H	0.88164000	-2.76405000	4.51308000
C	0.00000000	-0.88729000	2.55519000
O	0.00000000	-1.93880000	1.87104000
N	0.00000000	0.35179000	1.91671000
H	0.00000000	0.35882000	0.86266000
C	0.00000000	1.58779000	2.52737000
O	0.00000000	2.65704000	1.89497000
H	0.00000000	2.42157000	4.39921000
N	0.00000000	0.55739000	-4.95208000
C	0.00000000	-0.79546000	-5.21679000
H	-0.00000000	-1.17361000	-6.22883000
N	0.00000000	-1.53566000	-4.11552000
C	0.00000000	-0.60603000	-3.07473000
C	0.00000000	-0.75083000	-1.66644000
N	0.00000000	-1.93794000	-1.03312000
H	0.00000000	-1.97691000	-0.00701000
H	0.00000000	-2.79434000	-1.57049000
N	0.00000000	0.39226000	-0.92203000
C	0.00000000	1.59255000	-1.53552000
H	0.00000000	2.45166000	-0.86903000
N	0.00000000	1.84633000	-2.85375000
C	0.00000000	0.70557000	-3.58069000
H	-0.00000000	1.30310000	-5.63903000
N	3.40000000	-1.05716000	4.06355000
C	3.40000000	-2.42803000	3.94625000
H	3.40000000	-2.97004000	4.88486000
C	3.40000000	-3.05384000	2.73735000
C	3.40000000	-4.55237000	2.58599000
H	3.40000000	-5.04012000	3.56506000
H	2.51836000	-4.88885000	2.02658000
H	4.28164000	-4.88885000	2.02658000
C	3.40000000	-2.21971000	1.54570000
O	3.40000000	-2.66828000	0.37415000
N	3.40000000	-0.84198000	1.75744000
H	3.40000000	-0.21675000	0.90882000
C	3.40000000	-0.20095000	2.97797000
O	3.40000000	1.03581000	3.09481000
H	3.40000000	-0.62661000	4.98241000
N	3.40000000	3.36163000	-3.67875000
C	3.40000000	2.42273000	-4.68808000
H	3.40000000	2.71164000	-5.72911000
N	3.40000000	1.17659000	-4.23219000
C	3.40000000	1.31694000	-2.84375000
C	3.40000000	0.37204000	-1.78951000
N	3.40000000	-0.96061000	-1.97489000

H	3.40000000	-1.59526000	-1.16765000
H	3.40000000	-1.33761000	-2.91300000
N	3.40000000	0.85929000	-0.51539000
C	3.40000000	2.19095000	-0.30623000
H	3.40000000	2.49425000	0.73794000
N	3.40000000	3.17108000	-1.22354000
C	3.40000000	2.67545000	-2.48216000
H	3.40000000	4.36870000	-3.79621000

[T]-T/A-T

Total Energy = -8902.98 kcal mol^{-1}

N	-1.98458000	-0.65748700	0.00000000
C	-3.37442600	-0.69857500	0.00000000
N	-3.88059800	-2.00617500	0.00000000
C	-3.09224300	-3.13844600	0.00000000
C	-1.73640700	-3.07640700	0.00000000
C	-1.11219900	-1.75144100	0.00000000
O	0.11911800	-1.58203600	0.00000000
O	-4.10069600	0.28597700	0.00000000
C	-0.84137400	-4.28697900	0.00000000
H	-1.54890700	0.28546400	0.00000000
H	-4.89156100	-2.07260100	0.00000000
H	-3.63199000	-4.08099200	0.00000000
H	-0.18555600	-4.28355400	-0.87875000
H	-1.42910100	-5.21093600	0.00000000
H	-0.18555600	-4.28355400	0.87875000
N	1.48142500	0.87997000	0.00000000
C	0.60563500	1.93884000	0.00000000
N	1.21898100	3.18596500	0.00000000
C	2.59337200	3.36131000	0.00000000
C	3.45283400	2.31443300	0.00000000
C	2.89747700	0.94946700	0.00000000
O	3.57338800	-0.07564000	0.00000000
O	-0.62975800	1.83365400	0.00000000
C	4.95024500	2.46254700	0.00000000
H	1.04594500	-0.06496600	0.00000000
H	0.58836700	3.97864900	0.00000000
H	2.92650700	4.39486400	0.00000000
H	5.38534400	1.97137700	0.87866000
H	5.24428000	3.51745700	0.00000000
H	5.38534400	1.97137700	-0.87866000
N	3.90683800	1.53839200	-3.40000000
C	4.61926800	0.36132900	-3.40000000
H	5.69705300	0.47596000	-3.40000000
C	4.01069600	-0.85634200	-3.40000000
C	4.77077400	-2.15664300	-3.40000000
H	5.84931200	-1.97433000	-3.40000000
H	4.51677200	-2.75800900	-2.51835800
H	4.51677200	-2.75800900	-4.28164200
C	2.55637400	-0.88387000	-3.40000000
O	1.87362600	-1.93629500	-3.40000000

N	1.91623400	0.35435700	-3.40000000
H	0.86217800	0.35997400	-3.40000000
C	2.52524200	1.59117000	-3.40000000
O	1.89140800	2.65957600	-3.40000000
H	4.39596300	2.42745300	-3.40000000
N	-4.95282400	0.55076600	-3.40000000
C	-5.21572700	-0.80244200	-3.40000000
H	-6.22725600	-1.18194500	-3.40000000
N	-4.11346800	-1.54117000	-3.40000000
C	-3.07392000	-0.61014700	-3.40000000
C	-1.66543600	-0.75306300	-3.40000000
N	-1.03053200	-1.93932100	-3.40000000
H	-0.00437000	-1.97692100	-3.40000000
H	-1.56675200	-2.79644100	-3.40000000
N	-0.92255600	0.39102300	-3.40000000
C	-1.53765400	1.59049300	-3.40000000
H	-0.87231200	2.45049100	-3.40000000
N	-2.85621700	1.84251100	-3.40000000
C	-3.58162900	0.70078100	-3.40000000
H	-5.64076900	1.29555400	-3.40000000

[G]-T/A-T
Total Energy = -9207.90 kcal mol^{-1}

N	-1.57691700	-0.10984500	0.00000000
C	-2.94393700	0.00634000	0.00000000
N	-3.77231200	-1.02735400	0.00000000
C	-3.11421500	-2.21324900	0.00000000
C	-1.72766900	-2.45602500	0.00000000
C	-0.84305600	-1.32753000	0.00000000
N	-3.69182100	-3.46451900	0.00000000
C	-2.64964700	-4.39327000	0.00000000
N	-1.46610200	-3.82297300	0.00000000
O	0.39929700	-1.29104500	0.00000000
N	-3.44166700	1.27880000	0.00000000
H	-1.00679800	0.75532500	0.00000000
H	-4.68721300	-3.64977600	0.00000000
H	-2.84091500	-5.45769100	0.00000000
H	-4.44304000	1.40106900	0.00000000
H	-2.82882200	2.08123200	0.00000000
N	1.85713100	1.09398900	0.00000000
C	1.10946900	2.24080600	0.00000000
N	1.84677400	3.41441100	0.00000000
C	3.23388000	3.44773600	0.00000000
C	3.97593700	2.31642500	0.00000000
C	3.27856900	1.01690700	0.00000000
O	3.84309700	-0.07012700	0.00000000
O	-0.13805600	2.27920300	0.00000000
C	5.48014900	2.30230000	0.00000000
H	1.33700300	0.18129600	0.00000000
H	1.30383700	4.26910200	0.00000000
H	3.67120600	4.44152700	0.00000000
H	5.85842000	1.76598500	0.87844000

H	5.88678700	3.31903500	0.00000000
H	5.85842000	1.76598500	-0.87844000
N	3.90683800	1.53839200	-3.40000000
C	4.61926800	0.36132900	-3.40000000
H	5.69705300	0.47596000	-3.40000000
C	4.01069600	-0.85634200	-3.40000000
C	4.77077400	-2.15664300	-3.40000000
H	5.84931200	-1.97433000	-3.40000000
H	4.51677200	-2.75800900	-2.51835800
H	4.51677200	-2.75800900	-4.28164200
C	2.55637400	-0.88387000	-3.40000000
O	1.87362600	-1.93629500	-3.40000000
N	1.91623400	0.35435700	-3.40000000
H	0.86217800	0.35997400	-3.40000000
C	2.52524200	1.59117000	-3.40000000
O	1.89140800	2.65957600	-3.40000000
H	4.39596300	2.42745300	-3.40000000
N	-4.95282400	0.55076600	-3.40000000
C	-5.21572700	-0.80244200	-3.40000000
H	-6.22725600	-1.18194500	-3.40000000
N	-4.11346800	-1.54117000	-3.40000000
C	-3.07392000	-0.61014700	-3.40000000
C	-1.66543600	-0.75306300	-3.40000000
N	-1.03053200	-1.93932100	-3.40000000
H	-0.00437000	-1.97692100	-3.40000000
H	-1.56675200	-2.79644100	-3.40000000
N	-0.92255600	0.39102300	-3.40000000
C	-1.53765400	1.59049300	-3.40000000
H	-0.87231200	2.45049100	-3.40000000
N	-2.85621700	1.84251100	-3.40000000
C	-3.58162900	0.70078100	-3.40000000
H	-5.64076900	1.29555400	-3.40000000

[C]-T/A-T

Total Energy = -8642.09 kcal mol^{-1}

N	-1.37124800	-1.05420500	0.00000000
C	-2.67495500	-0.60825700	0.00000000
N	-3.69199600	-1.62495000	0.00000000
C	-3.41792000	-2.95649400	0.00000000
C	-2.12542100	-3.38109400	0.00000000
C	-1.09743900	-2.36583400	0.00000000
N	0.19951500	-2.73875500	0.00000000
O	-3.02556000	0.56551300	0.00000000
H	-4.64446900	-1.27661300	0.00000000
H	-4.26540000	-3.63479400	0.00000000
H	-1.87794100	-4.43672700	0.00000000
H	0.94529100	-2.02316300	0.00000000
H	0.44182400	-3.71823300	0.00000000
N	0.77552800	1.01692800	0.00000000
C	0.48795000	2.38269200	0.00000000
N	1.64411200	3.18510300	0.00000000
C	2.92870700	2.69302000	0.00000000

C	3.18751100	1.36078700	0.00000000
C	2.04829900	0.44060700	0.00000000
O	2.19362500	-0.79687000	0.00000000
O	-0.63012100	2.86781600	0.00000000
C	4.57694400	0.78041400	0.00000000
H	-0.04287900	0.36438600	0.00000000
H	1.46327500	4.18196400	0.00000000
H	3.71705100	3.44042900	0.00000000
H	4.73275200	0.14403900	-0.87947000
H	5.33299600	1.57286500	0.00000000
H	4.73275200	0.14403900	0.87947000
N	3.90683800	1.53839200	-3.40000000
C	4.61926800	0.36132900	-3.40000000
H	5.69705300	0.47596000	-3.40000000
C	4.01069600	-0.85634200	-3.40000000
C	4.77077400	-2.15664300	-3.40000000
H	5.84931200	-1.97433000	-3.40000000
H	4.51677200	-2.75800900	-2.51835800
H	4.51677200	-2.75800900	-4.28164200
C	2.55637400	-0.88387000	-3.40000000
O	1.87362600	-1.93629500	-3.40000000
N	1.91623400	0.35435700	-3.40000000
H	0.86217800	0.35997400	-3.40000000
C	2.52524200	1.59117000	-3.40000000
O	1.89140800	2.65957600	-3.40000000
H	4.39596300	2.42745300	-3.40000000
N	-4.95282400	0.55076600	-3.40000000
C	-5.21572700	-0.80244200	-3.40000000
H	-6.22725600	-1.18194500	-3.40000000
N	-4.11346800	-1.54117000	-3.40000000
C	-3.07392000	-0.61014700	-3.40000000
C	-1.66543600	-0.75306300	-3.40000000
N	-1.03053200	-1.93932100	-3.40000000
H	-0.00437000	-1.97692100	-3.40000000
H	-1.56675200	-2.79644100	-3.40000000
N	-0.92255600	0.39102300	-3.40000000
C	-1.53765400	1.59049300	-3.40000000
H	-0.87231200	2.45049100	-3.40000000
N	-2.85621700	1.84251100	-3.40000000
C	-3.58162900	0.70078100	-3.40000000
H	-5.64076900	1.29555400	-3.40000000

[A]-G/C-G

Total Energy = -9259.17 kcal mol^{-1}

N	-1.37903300	-0.50465500	0.00000000
C	-2.63221600	0.05661600	0.00000000
N	-3.75986600	-0.63828400	0.00000000
C	-3.54229100	-1.97552800	0.00000000
C	-2.31856300	-2.66689800	0.00000000
C	-1.10535300	-1.90338300	0.00000000
N	-4.50645000	-2.96018900	0.00000000
C	-3.83544500	-4.18419800	0.00000000

N	-2.52899100	-4.04313200	0.00000000
O	0.07046900	-2.30354700	0.00000000
N	-2.69406500	1.42224400	0.00000000
H	-0.54879200	0.12867300	0.00000000
H	-5.50638100	-2.80106400	0.00000000
H	-4.37217200	-5.12304100	0.00000000
H	-3.60398800	1.85783500	0.00000000
H	-1.86161100	1.98881300	0.00000000
N	0.91897100	1.30890800	0.00000000
C	0.83080300	2.65657600	0.00000000
N	1.80822200	3.56883400	0.00000000
C	3.02086600	2.97946900	0.00000000
C	3.27992000	1.60126400	0.00000000
C	2.15873000	0.73099900	0.00000000
N	4.27105200	3.57238700	0.00000000
C	5.20445900	2.54285800	0.00000000
N	4.64814200	1.34662200	0.00000000
N	2.28072600	-0.60455100	0.00000000
H	-0.17974900	3.06586500	0.00000000
H	4.45291800	4.56854500	0.00000000
H	6.26748300	2.74226000	0.00000000
H	3.21436600	-0.99364000	0.00000000
H	1.45769200	-1.23468200	0.00000000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000
O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000
H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000

[T]-G/C-G

Total Energy = -9118.94 kcal mol^{-1}

N	-1.57691700	-0.10984500	0.00000000
C	-2.94393700	0.00634000	0.00000000
N	-3.77231200	-1.02735400	0.00000000
C	-3.11421500	-2.21324900	0.00000000
C	-1.72766900	-2.45602500	0.00000000
C	-0.84305600	-1.32753000	0.00000000
N	-3.69182100	-3.46451900	0.00000000
C	-2.64964700	-4.39327000	0.00000000
N	-1.46610200	-3.82297300	0.00000000
O	0.39929700	-1.29104500	0.00000000
N	-3.44166700	1.27880000	0.00000000
H	-1.00679800	0.75532500	0.00000000
H	-4.68721300	-3.64977600	0.00000000
H	-2.84091500	-5.45769100	0.00000000
H	-4.44304000	1.40106900	0.00000000
H	-2.82882200	2.08123200	0.00000000
N	1.85713100	1.09398900	0.00000000
C	1.10946900	2.24080600	0.00000000
N	1.84677400	3.41441100	0.00000000
C	3.23388000	3.44773600	0.00000000
C	3.97593700	2.31642500	0.00000000
C	3.27856900	1.01690700	0.00000000
O	3.84309700	-0.07012700	0.00000000
O	-0.13805600	2.27920300	0.00000000
C	5.48014900	2.30230000	0.00000000
H	1.33700300	0.18129600	0.00000000
H	1.30383700	4.26910200	0.00000000
H	3.67120600	4.44152700	0.00000000
H	5.85842000	1.76598500	0.87844000
H	5.88678700	3.31903500	0.00000000
H	5.85842000	1.76598500	-0.87844000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000
O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000

H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000

[G]-G/C-G

Total Energy = -9421.43 kcal mol^{-1}

N	3.62911900	0.55312900	0.00000000
C	4.53534900	1.59254800	0.00000000
N	4.17832100	2.86660500	0.00000000
C	2.83450600	3.03984800	0.00000000
C	1.82744000	2.06507600	0.00000000
C	2.19666200	0.68159800	0.00000000
N	2.15971500	4.24343000	0.00000000
C	0.79992500	3.95247900	0.00000000
N	0.56943400	2.65542500	0.00000000
O	1.50221900	-0.33303100	0.00000000
N	5.86133900	1.27336700	0.00000000
H	3.94776300	-0.41312400	0.00000000
H	2.59154400	5.15965500	0.00000000
H	0.04962000	4.73031500	0.00000000
H	6.52885700	2.03130700	0.00000000
H	6.19286200	0.32125400	0.00000000
N	-1.30203500	-1.16969700	0.00000000
C	-2.33399800	-0.26245100	0.00000000
N	-3.61710400	-0.61197400	0.00000000
C	-3.79291200	-1.95571200	0.00000000
C	-2.82869300	-2.97584700	0.00000000
C	-1.43390400	-2.61042200	0.00000000
N	-5.00698500	-2.61388500	0.00000000
C	-4.72756500	-3.98111400	0.00000000
N	-3.43644500	-4.22941400	0.00000000
O	-0.42664500	-3.31234500	0.00000000
N	-2.02116000	1.06412200	0.00000000
H	-0.33242000	-0.83489100	0.00000000
H	-5.91441900	-2.16565900	0.00000000
H	-5.51709800	-4.72030100	0.00000000
H	-2.80344200	1.70226300	0.00000000
H	-1.07594500	1.44615700	0.00000000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000

O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000
H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000

[C]-G/C-G

Total Energy = -8865.22 kcal mol^{-1}

N	0.00000000	0.54203000	4.63285000
C	0.00000000	-0.81577000	4.95922000
H	0.00000000	-1.14936000	5.98799000
N	0.00000000	-1.59019000	3.89791000
C	0.00000000	-0.71224000	2.81568000
C	0.00000000	-0.95497000	1.40594000
O	0.00000000	-2.04801000	0.80067000
N	0.00000000	0.25658000	0.67314000
H	0.00000000	0.15547000	-0.36303000
C	0.00000000	1.52584000	1.21247000
N	0.00000000	2.56104000	0.33848000
H	0.00000000	2.43092000	-0.68079000
H	0.00000000	3.49044000	0.73250000
N	0.00000000	1.76062000	2.52393000
C	0.00000000	0.62532000	3.25564000
H	0.00000000	1.33226000	5.26557000
N	0.00000000	0.86619000	-4.37352000
C	0.00000000	-0.36781000	-4.95721000
H	-0.00000000	-0.39342000	-6.04166000
C	0.00000000	-1.48766000	-4.18632000
H	0.00000000	-2.47613000	-4.63190000
C	0.00000000	-1.30615000	-2.75280000
N	0.00000000	-2.36297000	-1.92727000
H	0.00000000	-2.23389000	-0.88718000
H	0.00000000	-3.29730000	-2.31142000
N	0.00000000	-0.07985000	-2.19844000

C	0.00000000	1.04399000	-2.96504000
O	0.00000000	2.20346000	-2.51832000
H	0.00000000	1.71611000	-4.92704000
N	3.40000000	-2.28454000	4.06669000
C	3.40000000	-3.57486000	3.53266000
H	3.40000000	-4.44943000	4.16889000
N	3.40000000	-3.57758000	2.21885000
C	3.40000000	-2.23120000	1.85933000
C	3.40000000	-1.59897000	0.57614000
O	3.40000000	-2.12751000	-0.55600000
N	3.40000000	-0.18807000	0.69540000
H	3.40000000	0.33916000	-0.20232000
C	3.40000000	0.52179000	1.87776000
N	3.40000000	1.87300000	1.77914000
H	3.40000000	2.36683000	0.87804000
H	3.40000000	2.39332000	2.64419000
N	3.40000000	-0.05910000	3.07677000
C	3.40000000	-1.40767000	3.00145000
H	3.40000000	-2.01711000	5.04305000
N	3.40000000	3.27140000	-3.02918000
C	3.40000000	2.61613000	-4.22671000
H	3.40000000	3.23282000	-5.11911000
C	3.40000000	1.25703000	-4.26125000
H	3.40000000	0.71923000	-5.20273000
C	3.40000000	0.56130000	-2.99481000
N	3.40000000	-0.77892000	-2.94810000
H	3.40000000	-1.28582000	-2.03077000
H	3.40000000	-1.30903000	-3.80806000
N	3.40000000	1.22758000	-1.82554000
C	3.40000000	2.58738000	-1.78518000
O	3.40000000	3.26285000	-0.74227000
H	3.40000000	4.28435000	-2.97744000

[A]-C/G-C

Total Energy = -8691.89 kcal mol^{-1}

N	1.83751500	1.74118500	0.00000000
C	2.11174300	3.07341800	0.00000000
N	3.46316100	3.46918000	0.00000000
C	4.49121100	2.57311500	0.00000000
C	4.22765200	1.23748000	0.00000000
C	2.84458200	0.84361600	0.00000000
N	2.51436500	-0.46343200	0.00000000
O	1.22600600	3.96342600	0.00000000
H	3.65274100	4.46657100	0.00000000
H	5.49221600	2.98658600	0.00000000
H	5.02456200	0.50291100	0.00000000
H	1.52412200	-0.75549100	0.00000000
H	3.24256700	-1.16520800	0.00000000
N	-0.37115800	-1.12218500	0.00000000
C	-1.05264800	0.04459300	0.00000000
N	-2.38421500	0.22458200	0.00000000
C	-3.04882900	-0.95148500	0.00000000

C	-2.47106900	-2.23328000	0.00000000
C	-1.05787600	-2.29588400	0.00000000
N	-4.40994200	-1.17533000	0.00000000
C	-4.59947100	-2.54067600	0.00000000
N	-3.45927700	-3.21947500	0.00000000
N	-0.37408200	-3.46029800	0.00000000
H	-0.42718100	0.93436500	0.00000000
H	-5.13659700	-0.46824400	0.00000000
H	-5.58930500	-2.97366200	0.00000000
H	-0.86272400	-4.34508300	0.00000000
H	0.63728800	-3.46175900	0.00000000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000
O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000
H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000

[T]-C/G-C

Total Energy = -8552.03 kcal mol^{-1}

N	1.42634800	0.97836700	0.00000000
C	1.40509400	2.35607200	0.00000000
N	2.68630800	3.00916000	0.00000000
C	3.86798800	2.33702800	0.00000000
C	3.87240300	0.97658000	0.00000000
C	2.58916900	0.31264400	0.00000000
N	2.54305700	-1.03607100	0.00000000
O	0.39711500	3.05223100	0.00000000
H	2.64935100	4.02265800	0.00000000

H	4.77497500	2.93342300	0.00000000
H	4.79989400	0.41500400	0.00000000
H	1.63203100	-1.52421700	0.00000000
H	3.39971800	-1.56919700	0.00000000
N	-1.20680800	-0.42332300	0.00000000
C	-2.41685900	0.27222400	0.00000000
N	-3.53727200	-0.57939200	0.00000000
C	-3.46623400	-1.95317700	0.00000000
C	-2.27918000	-2.61099700	0.00000000
C	-1.05200100	-1.81189400	0.00000000
O	0.08000200	-2.33250800	0.00000000
O	-2.53273700	1.48548500	0.00000000
C	-2.15657100	-4.11177100	0.00000000
H	-0.33330100	0.15338200	0.00000000
H	-4.42946100	-0.09936000	0.00000000
H	-4.42067500	-2.47197400	0.00000000
H	-1.59949000	-4.45660400	-0.87947000
H	-3.14387000	-4.58593900	0.00000000
H	-1.59949000	-4.45660400	0.87947000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000
O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000
H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000

[G]-C/G-C
Total Energy = -8865.22 kcal mol^{-1}

N	0.00000000	0.54203000	4.63285000

C	0.00000000	-0.81577000	4.95922000
H	0.00000000	-1.14936000	5.98799000
N	0.00000000	-1.59019000	3.89791000
C	0.00000000	-0.71224000	2.81568000
C	0.00000000	-0.95497000	1.40594000
O	0.00000000	-2.04801000	0.80067000
N	0.00000000	0.25658000	0.67314000
H	0.00000000	0.15547000	-0.36303000
C	0.00000000	1.52584000	1.21247000
N	0.00000000	2.56104000	0.33848000
H	0.00000000	2.43092000	-0.68079000
H	0.00000000	3.49044000	0.73250000
N	0.00000000	1.76062000	2.52393000
C	0.00000000	0.62532000	3.25564000
H	0.00000000	1.33226000	5.26557000
N	0.00000000	0.86619000	-4.37352000
C	0.00000000	-0.36781000	-4.95721000
H	-0.00000000	-0.39342000	-6.04166000
C	0.00000000	-1.48766000	-4.18632000
H	0.00000000	-2.47613000	-4.63190000
C	0.00000000	-1.30615000	-2.75280000
N	0.00000000	-2.36297000	-1.92727000
H	0.00000000	-2.23389000	-0.88718000
H	0.00000000	-3.29730000	-2.31142000
N	0.00000000	-0.07985000	-2.19844000
C	0.00000000	1.04399000	-2.96504000
O	0.00000000	2.20346000	-2.51832000
H	0.00000000	1.71611000	-4.92704000
N	3.40000000	-2.28454000	4.06669000
C	3.40000000	-3.57486000	3.53266000
H	3.40000000	-4.44943000	4.16889000
N	3.40000000	-3.57758000	2.21885000
C	3.40000000	-2.23120000	1.85933000
C	3.40000000	-1.59897000	0.57614000
O	3.40000000	-2.12751000	-0.55600000
N	3.40000000	-0.18807000	0.69540000
H	3.40000000	0.33916000	-0.20232000
C	3.40000000	0.52179000	1.87776000
N	3.40000000	1.87300000	1.77914000
H	3.40000000	2.36683000	0.87804000
H	3.40000000	2.39332000	2.64419000
N	3.40000000	-0.05910000	3.07677000
C	3.40000000	-1.40767000	3.00145000
H	3.40000000	-2.01711000	5.04305000
N	3.40000000	3.27140000	-3.02918000
C	3.40000000	2.61613000	-4.22671000
H	3.40000000	3.23282000	-5.11911000
C	3.40000000	1.25703000	-4.26125000
H	3.40000000	0.71923000	-5.20273000
C	3.40000000	0.56130000	-2.99481000
N	3.40000000	-0.77892000	-2.94810000
H	3.40000000	-1.28582000	-2.03077000

H	3.40000000	-1.30903000	-3.80806000
N	3.40000000	1.22758000	-1.82554000
C	3.40000000	2.58738000	-1.78518000
O	3.40000000	3.26285000	-0.74227000
H	3.40000000	4.28435000	-2.97744000

[C]-C/G-C

Total Energy = -8292.06 kcal mol^{-1}

N	-1.86600000	-2.71613100	0.00000000
C	-3.23451100	-2.82755000	0.00000000
N	-3.96964000	-1.59165200	0.00000000
C	-3.37383100	-0.36540300	0.00000000
C	-2.01666700	-0.26749300	0.00000000
C	-1.29104500	-1.51468500	0.00000000
N	0.06979400	-1.47675000	0.00000000
O	-3.87241000	-3.88028000	0.00000000
H	-4.97890600	-1.69057600	0.00000000
H	-4.03026700	0.49951900	0.00000000
H	-1.50223800	0.68708900	0.00000000
H	0.54455500	-2.37012100	0.00000000
H	0.59669400	-0.60226500	0.00000000
N	1.88027400	0.99558500	0.00000000
C	1.24175400	2.21464200	0.00000000
N	2.08626900	3.37025700	0.00000000
C	3.44364300	3.30188300	0.00000000
C	4.06291900	2.08816500	0.00000000
C	3.20982400	0.92864000	0.00000000
N	3.77411200	-0.30983900	0.00000000
O	0.02396900	2.37752400	0.00000000
H	1.60029800	4.26124400	0.00000000
H	3.98387200	4.24284900	0.00000000
H	5.14389400	2.00660900	0.00000000
H	3.17823800	-1.12625600	0.00000000
H	4.77495900	-0.43466700	0.00000000
N	-4.63284900	0.54203200	-3.40000000
C	-4.95921900	-0.81576800	-3.40000000
H	-5.98799000	-1.14935700	-3.40000000
N	-3.89791000	-1.59018800	-3.40000000
C	-2.81567900	-0.71223800	-3.40000000
C	-1.40593900	-0.95496900	-3.40000000
O	-0.80067000	-2.04800900	-3.40000000
N	-0.67313900	0.25658100	-3.40000000
H	0.36303100	0.15547000	-3.40000000
C	-1.21246800	1.52584100	-3.40000000
N	-0.33847800	2.56104100	-3.40000000
H	0.68079200	2.43092000	-3.40000000
H	-0.73249800	3.49044100	-3.40000000
N	-2.52392800	1.76062100	-3.40000000
C	-3.25563900	0.62532200	-3.40000000
H	-5.26556900	1.33226300	-3.40000000
N	4.37352100	0.86618900	-3.40000000
C	4.95721100	-0.36781200	-3.40000000

H	6.04166100	-0.39342200	-3.40000000
C	4.18632000	-1.48766100	-3.40000000
H	4.63190000	-2.47613100	-3.40000000
C	2.75280000	-1.30615100	-3.40000000
N	1.92727000	-2.36297000	-3.40000000
H	0.88718000	-2.23389000	-3.40000000
H	2.31142000	-3.29730100	-3.40000000
N	2.19844100	-0.07985000	-3.40000000
C	2.96504100	1.04398900	-3.40000000
O	2.51832200	2.20345900	-3.40000000
H	4.92704200	1.71610800	-3.40000000