Supporting Information for

Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, π-stacking and solvent effects

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Table S8. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 0º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in the gas phase and at BP86/TZ2P (see text).

Table S9 Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 0º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1 in water at COSMO-BP86/TZ2P (see text).

Table S10. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in the gas phase and at BP86/TZ2P (see text).

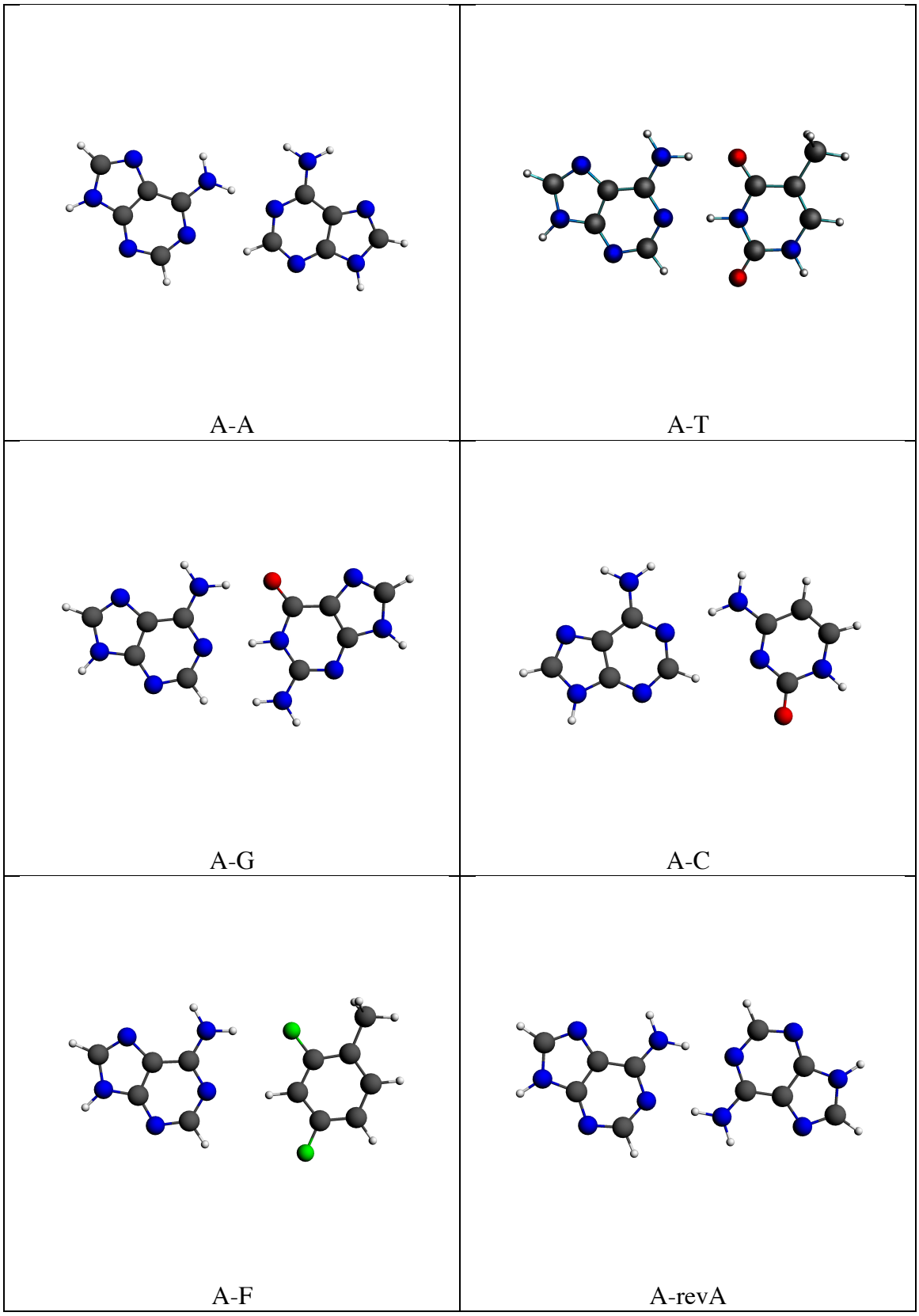
Table S11. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1 in water at COSMO-BP86/TZ2P (see text).

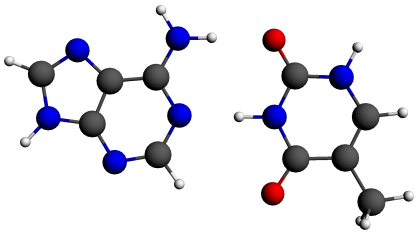
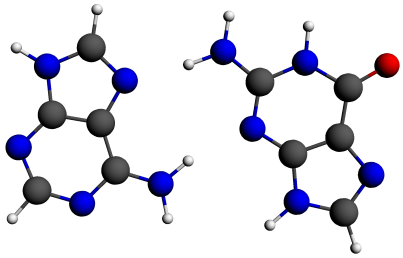
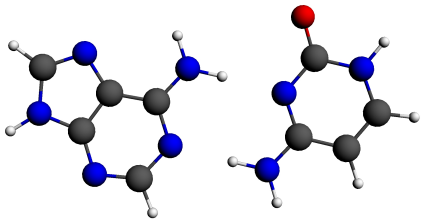
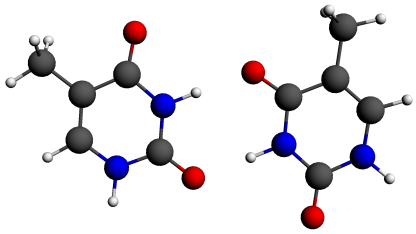
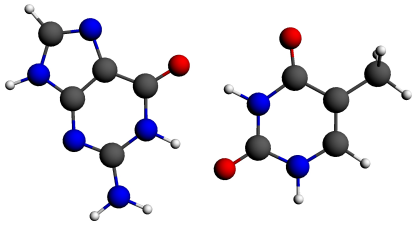
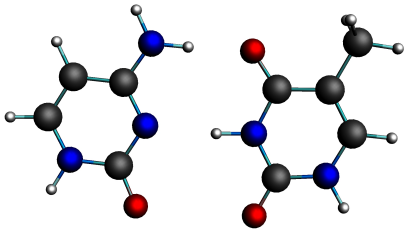
Table S1. Affinities (in kcal/mol) of model template-primer complexes $Y_1/Z\text{-}Y_2$ for model nucleotides X, in a reverse orientation.[a]

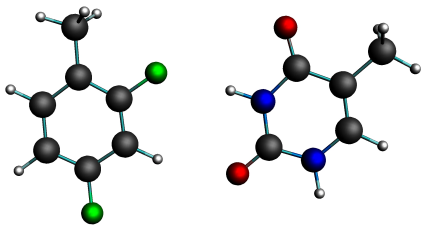
template-primer $Y_1/Z\text{-}Y_2$	incoming nucleotide X	affinity 0º gas	affinity 0º water	affinity 36º gas	affinity 36º water	base pair $X\text{-}Y_1$	affinity gas	affinity water
[X]-A/ T-A	revA	–22.4	–15.0	–23.0	–15.5	A-rA	–16.4	–10.3
	revT	–20.0	–13.6	–20.7	–13.4	A-rT	–17.2	–10.2
	revG	–14.6	–6.5	–14.3	–7.8	A-rG	–13.3	–8.8
	revC	–22.6	–12.7	–25.2	–13.9	A-rC	–19.2	–9.7
[X]-G/ C-G	revA	–13.1	–7.0	–13.5	–8.1	G-rA	–13.3	–8.8
	revT	–21.3	–13.9	–23.3	–14.3	G-rT	–19.4	–10.1
	revG	–36.1	–17.2	–33.0	–16.9	G-rG	–29.7	–11.3
	revC	–13.1	–8.9	–12.9	–8.3	G-rC	–14.5	–9.9

[a] Computed at (COSMO-)BP86-D/TZ2P, in the gas phase and in aqueous solution, with twist angles of 0º and 36º (see Figure 1). X = incoming base, Y_1/Y_2 = template strand, Z = primer. Full structural data are available as Supporting Information.

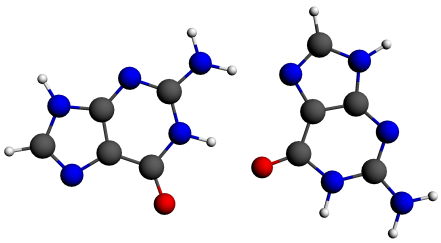
Figure S1. Structures of Watson-Crick pairs and mismatched DNA base pairs in the gas phase, optimized in C_s symmetry at BP86/TZ2P (atom color code: C black, H white, N blue, O red, F green).



 A-revT	 A-revG
 A-revC	 T-T
 G-T	 C-T



F-T



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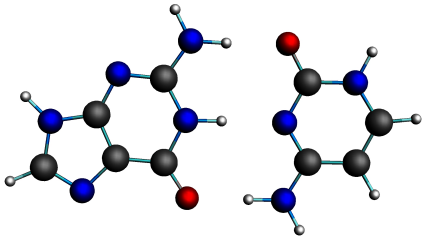

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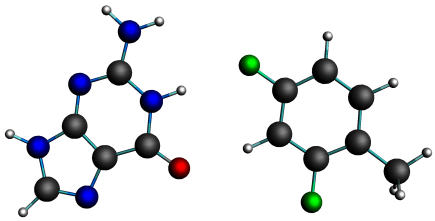

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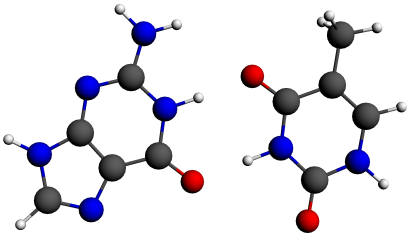

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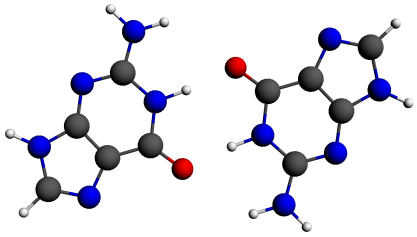

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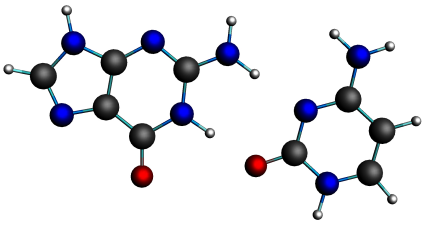

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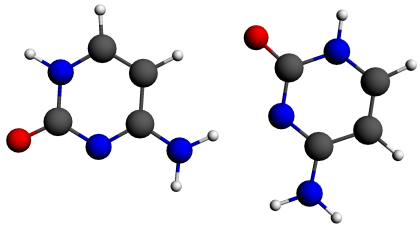
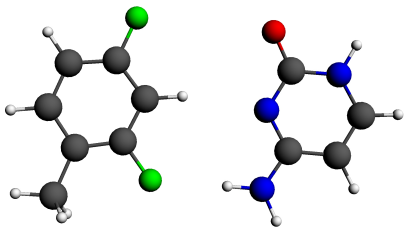


C-C



F-C

Table S2. Cartesian coordinates (in Å) of Watson-Crick pairs and mismatched DNA base pairs in the gas phase, optimized in C_s symmetry at BP86/TZ2P.

A-A			
N	0.0000	0.0000	0.0000
C	1.3527	0.0000	0.0000
N	2.1761	1.0527	0.0000
C	1.4952	2.2063	0.0000
C	0.1029	2.3664	0.0000
C	-0.6558	1.1777	0.0000
N	1.9866	3.4948	0.0000
C	0.8954	4.3403	0.0000
N	-0.2563	3.7043	0.0000
N	-2.0101	1.1928	0.0000
H	1.8055	-0.9941	0.0000
H	2.9663	3.7528	0.0000
H	1.0145	5.4184	0.0000
H	-2.5007	2.0759	0.0000
H	-2.5273	0.3256	0.0000
N	1.5699	-3.3792	0.0000
C	2.5486	-4.3006	0.0000
N	2.4506	-5.6368	0.0000
C	1.1652	-6.0203	0.0000
C	0.0369	-5.1907	0.0000
C	0.2835	-3.7973	0.0000
N	0.6503	-7.3008	0.0000
C	-0.7250	-7.1795	0.0000
N	-1.1359	-5.9295	0.0000
N	-0.7138	-2.8907	0.0000
H	3.5637	-3.8997	0.0000
H	1.1929	-8.1558	0.0000
H	-1.3706	-8.0511	0.0000
H	-1.6645	-3.2348	0.0000
H	-0.5205	-1.8771	0.0000
A-T			
N	-0.5475	-0.7023	0.0000
C	-1.0248	-1.9633	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4092	0.3462	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9232	1.5977	0.0000
H	-0.2608	-2.7414	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5757	2.3696	0.0000
H	0.0957	1.7650	0.0000
N	2.2332	-0.3395	0.0000
C	2.9879	-1.4952	0.0000
N	4.3636	-1.2570	0.0000
C	4.9204	0.0000	0.0000
C	4.1638	1.1274	0.0000
C	2.7087	0.9683	0.0000
O	1.9192	1.9281	0.0000
O	2.5217	-2.6286	0.0000
C	4.7347	2.5143	0.0000
H	1.1749	-0.4774	0.0000
H	4.9433	-2.0886	0.0000
H	6.0089	0.0278	0.0000
H	4.3937	3.0763	0.8802
H	5.8313	2.4920	0.0000
H	4.3937	3.0763	-0.8802
A-G			
N	0.0000	0.0000	0.0000

C	1.3696	0.0000	0.0000
N	2.1155	1.0903	0.0000
C	1.3698	2.2163	0.0000
C	-0.0253	2.3509	0.0000
C	-0.8176	1.1585	0.0000
N	1.8453	3.5034	0.0000
C	0.7392	4.3399	0.0000
N	-0.3956	3.6845	0.0000
O	-2.0521	1.0437	0.0000
N	1.9828	-1.2160	0.0000
H	-0.5038	-0.9195	0.0000
H	2.8231	3.7679	0.0000
H	0.8460	5.4190	0.0000
H	2.9917	-1.2391	0.0000
H	1.4554	-2.0749	0.0000
N	-1.3956	-2.5980	0.0000
C	-0.7922	-3.8029	0.0000
N	-1.3307	-5.0214	0.0000
C	-2.6734	-4.9487	0.0000
C	-3.4512	-3.7871	0.0000
C	-2.7587	-2.5499	0.0000
N	-3.5885	-5.9785	0.0000
C	-4.8417	-5.3980	0.0000
N	-4.8026	-4.0831	0.0000
N	-3.3905	-1.3724	0.0000
H	0.3012	-3.7852	0.0000
H	-3.3680	-6.9672	0.0000
H	-5.7448	-5.9984	0.0000
H	-4.4025	-1.3815	0.0000
H	-2.8770	-0.4664	0.0000

A-C

N	0.0000	0.0000	0.0000
C	1.3676	0.0000	0.0000
N	2.0004	1.2859	0.0000
C	1.3125	2.4537	0.0000
C	-0.0480	2.4390	0.0000
C	-0.6801	1.1426	0.0000
N	-2.0310	1.0637	0.0000
O	2.0840	-0.9954	0.0000
H	3.0151	1.2666	0.0000
H	1.8965	3.3722	0.0000
H	-0.6210	3.3627	0.0000
H	-2.5038	0.1422	0.0000
H	-2.5799	1.9108	0.0000
N	-3.2696	-1.6394	0.0000
C	-2.2299	-2.5088	0.0000
N	-2.2791	-3.8439	0.0000
C	-3.5408	-4.2906	0.0000
C	-4.7110	-3.5199	0.0000
C	-4.5278	-2.1223	0.0000
N	-3.9912	-5.5942	0.0000
C	-5.3703	-5.5422	0.0000
N	-5.8457	-4.3151	0.0000
N	-5.5793	-1.2661	0.0000
H	-1.2434	-2.0401	0.0000
H	-3.4046	-6.4203	0.0000
H	-5.9710	-6.4453	0.0000
H	-6.5210	-1.6320	0.0000
H	-5.4231	-0.2690	0.0000

A-F

N	0.0000	0.0000	0.0000
C	1.3460	0.0000	0.0000
N	2.1849	1.0427	0.0000
C	1.5116	2.2018	0.0000
C	0.1202	2.3701	0.0000
C	-0.6475	1.1844	0.0000
N	2.0122	3.4871	0.0000
C	0.9265	4.3399	0.0000
N	-0.2290	3.7110	0.0000
N	-1.9985	1.1999	0.0000
H	1.8115	-0.9866	0.0000

H	2.9932	3.7394	0.0000
H	1.0527	5.4172	0.0000
H	-2.4865	2.0844	0.0000
H	-2.5175	0.3300	0.0000
C	-1.7547	-2.9334	0.0000
C	-1.2636	-4.2338	0.0000
C	-2.0924	-5.3480	0.0000
C	-3.4751	-5.1459	0.0000
C	-4.0404	-3.8631	0.0000
C	-3.1348	-2.8002	0.0000
F	-3.6500	-1.5237	0.0000
F	0.0857	-4.4153	0.0000
C	-5.5282	-3.6237	0.0000
H	-1.0985	-2.0589	0.0000
H	-1.6597	-6.3461	0.0000
H	-4.1397	-6.0105	0.0000
H	-5.8416	-3.0490	0.8828
H	-6.0716	-4.5756	0.0000
H	-5.8416	-3.0490	-0.8828

A-revA

N	1.7606	0.6390	0.0000
C	3.1076	0.6390	0.0000
N	3.9459	1.6781	0.0000
C	3.2695	2.8387	0.0000
C	1.8799	3.0062	0.0000
C	1.0988	1.8253	0.0000
N	3.7709	4.1230	0.0000
C	2.6854	4.9764	0.0000
N	1.5306	4.3460	0.0000
N	-0.2426	1.8413	0.0000
H	3.5726	-0.3485	0.0000
H	4.7521	4.3745	0.0000
H	2.8113	6.0536	0.0000
H	-0.7023	2.7424	0.0000
H	-0.7993	0.9617	0.0000
N	-1.7606	-0.6390	0.0000
C	-3.1076	-0.6390	0.0000
N	-3.9459	-1.6781	0.0000
C	-3.2695	-2.8387	0.0000
C	-1.8799	-3.0062	0.0000
C	-1.0988	-1.8253	0.0000
N	-3.7709	-4.1230	0.0000
C	-2.6854	-4.9764	0.0000
N	-1.5306	-4.3460	0.0000
N	0.2426	-1.8413	0.0000
H	-3.5726	0.3485	0.0000
H	-4.7521	-4.3745	0.0000
H	-2.8113	-6.0536	0.0000
H	0.7023	-2.7424	0.0000
H	0.7993	-0.9617	0.0000

A-revT

N	0.0000	0.0000	0.0000
C	1.3486	0.0000	0.0000
N	2.1720	1.0503	0.0000
C	1.4845	2.2035	0.0000
C	0.0927	2.3631	0.0000
C	-0.6754	1.1757	0.0000
N	1.9769	3.4911	0.0000
C	0.8864	4.3378	0.0000
N	-0.2648	3.7010	0.0000
N	-2.0188	1.1660	0.0000
H	1.8048	-0.9909	0.0000
H	2.9568	3.7477	0.0000
H	1.0059	5.4157	0.0000
H	-2.5092	2.0499	0.0000
H	-2.5360	0.2759	0.0000
N	-1.2849	-2.4947	0.0000
C	-2.6521	-2.4481	0.0000
N	-3.2639	-3.6929	0.0000
C	-2.5652	-4.8825	0.0000
C	-1.2109	-4.9231	0.0000

C	-0.4809	-3.6478	0.0000
O	0.7450	-3.5503	0.0000
O	-3.3201	-1.4057	0.0000
C	-0.4144	-6.1930	0.0000
H	-0.7830	-1.5537	0.0000
H	-4.2774	-3.6787	0.0000
H	-3.1798	-5.7813	0.0000
H	0.2426	-6.2376	-0.8795
H	-1.0676	-7.0743	0.0000
H	0.2426	-6.2376	0.8795

A-revG

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

A-revC

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000

H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

T-T

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-T

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

C-T

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000

N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

F-T

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-G

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000

N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-C

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-F

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000

C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-revA

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-revT

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000

N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-revG

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

G-revC

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000

H	-2.6254	6.1731	0.0000

C-C

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

F-C

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000

Table S3. Cartesian coordinates (in Å) of Watson-Crick pairs and mismatched DNA base pairs X-Y_1 in water, optimized in C_s symmetry at COSMO-BP86/TZ2P.

A-A			
N	-5.8246	-4.5339	0.0000
C	-6.0948	-5.8497	0.0000
N	-7.2878	-6.4641	0.0000
C	-8.2968	-5.5702	0.0000
C	-8.1736	-4.1745	0.0000
C	-6.8583	-3.6513	0.0000
N	-9.6515	-5.8039	0.0000
C	-10.2723	-4.5816	0.0000
N	-9.4223	-3.5677	0.0000
N	-6.5948	-2.3338	0.0000
H	-5.2227	-6.5055	0.0000
H	-10.1095	-6.7091	0.0000
H	-11.3523	-4.4951	0.0000
H	-7.3657	-1.6778	0.0000
H	-5.6213	-1.9809	0.0000
N	-3.7890	-1.4231	0.0000
C	-2.9933	-2.5102	0.0000
N	-1.6562	-2.5590	0.0000
C	-1.1181	-1.3235	0.0000
C	-1.8162	-0.1077	0.0000
C	-3.2273	-0.1881	0.0000
N	0.2079	-0.9666	0.0000
C	0.2580	0.4031	0.0000
N	-0.9386	0.9669	0.0000
N	-4.0216	0.8970	0.0000
H	-3.5254	-3.4633	0.0000
H	1.0033	-1.5965	0.0000
H	1.2020	0.9346	0.0000
H	-3.6239	1.8269	0.0000
H	-5.0284	0.7979	0.0000
A-T			
N	2.7515	-2.3309	0.0000
C	3.3756	-3.5227	0.0000
N	4.6899	-3.7694	0.0000
C	5.4050	-2.6255	0.0000
C	4.8953	-1.3201	0.0000
C	3.4870	-1.1855	0.0000
N	6.7694	-2.4697	0.0000
C	7.0225	-1.1226	0.0000
N	5.9225	-0.3878	0.0000
N	2.8494	-0.0068	0.0000
H	2.7152	-4.3903	0.0000
H	7.4630	-3.2102	0.0000
H	8.0348	-0.7369	0.0000
H	3.3828	0.8529	0.0000
H	1.8191	0.0267	0.0000
N	-0.1101	-2.2689	0.0000
C	-0.7434	-3.4911	0.0000
N	-2.1199	-3.4086	0.0000
C	-2.8071	-2.2232	0.0000
C	-2.1756	-1.0175	0.0000
C	-0.7239	-1.0220	0.0000
O	-0.0230	0.0150	0.0000
O	-0.1349	-4.5690	0.0000
C	-2.9058	0.2936	0.0000
H	0.9473	-2.2946	0.0000
H	-2.6260	-4.2892	0.0000
H	-3.8899	-2.3172	0.0000
H	-2.6401	0.8924	0.8825
H	-3.9902	0.1352	0.0000
H	-2.6401	0.8924	-0.8825
A-G			
N	2.7871	-2.2949	0.0000

C	3.6112	-1.1940	0.0000
N	4.9401	-1.2676	0.0000
C	5.3926	-2.5380	0.0000
C	4.6459	-3.7233	0.0000
C	3.2266	-3.6272	0.0000
N	6.7002	-2.9464	0.0000
C	6.6988	-4.3224	0.0000
N	5.4823	-4.8322	0.0000
O	2.3966	-4.5666	0.0000
N	3.0210	0.0181	0.0000
H	1.7482	-2.1483	0.0000
H	7.5172	-2.3447	0.0000
H	7.6221	-4.8888	0.0000
H	3.6012	0.8462	0.0000
H	2.0179	0.1276	0.0000
N	-0.1488	-1.8950	0.0000
C	-0.7184	-0.6748	0.0000
N	-2.0153	-0.3539	0.0000
C	-2.7934	-1.4557	0.0000
C	-2.3522	-2.7838	0.0000
C	-0.9530	-2.9968	0.0000
N	-4.1638	-1.5391	0.0000
C	-4.4863	-2.8715	0.0000
N	-3.4254	-3.6620	0.0000
N	-0.3996	-4.2157	0.0000
H	-0.0305	0.1714	0.0000
H	-4.8178	-0.7634	0.0000
H	-5.5172	-3.2045	0.0000
H	-0.9994	-5.0310	0.0000
H	0.6267	-4.3363	0.0000

A-C

N	2.5674	-0.3433	0.0000
C	3.6021	-1.2220	0.0000
N	4.9062	-0.7046	0.0000
C	5.1676	0.6289	0.0000
C	4.1406	1.5208	0.0000
C	2.8106	0.9808	0.0000
N	1.7504	1.8065	0.0000
O	3.4541	-2.4648	0.0000
H	5.6679	-1.3769	0.0000
H	6.2144	0.9182	0.0000
H	4.3206	2.5922	0.0000
H	0.7848	1.4339	0.0000
H	1.8961	2.8079	0.0000
N	-0.9884	0.6532	0.0000
C	-0.8735	-0.6895	0.0000
N	-1.8490	-1.6056	0.0000
C	-3.0669	-1.0293	0.0000
C	-3.3401	0.3455	0.0000
C	-2.2242	1.2129	0.0000
N	-4.3007	-1.6322	0.0000
C	-5.2390	-0.6330	0.0000
N	-4.7079	0.5787	0.0000
N	-2.3422	2.5526	0.0000
H	0.1543	-1.0572	0.0000
H	-4.4859	-2.6297	0.0000
H	-6.2997	-0.8532	0.0000
H	-3.2545	2.9891	0.0000
H	-1.5202	3.1425	0.0000

A-F

N	1.2602	0.5067	0.0000
C	1.9318	1.6710	0.0000
N	3.2570	1.8740	0.0000
C	3.9319	0.7080	0.0000
C	3.3745	-0.5784	0.0000
C	1.9627	-0.6537	0.0000
N	5.2903	0.5022	0.0000
C	5.4937	-0.8534	0.0000
N	4.3678	-1.5481	0.0000
N	1.2924	-1.8206	0.0000
H	1.3124	2.5687	0.0000

H	6.0106	1.2166	0.0000
H	6.4916	-1.2754	0.0000
H	1.7891	-2.7015	0.0000
H	0.2791	-1.8272	0.0000
C	-2.2312	0.4858	0.0000
C	-3.1065	1.5648	0.0000
C	-4.4864	1.4166	0.0000
C	-5.0097	0.1189	0.0000
C	-4.1877	-1.0186	0.0000
C	-2.8120	-0.7747	0.0000
F	-1.9675	-1.8587	0.0000
F	-2.5746	2.8254	0.0000
C	-4.7351	-2.4225	0.0000
H	-1.1467	0.6107	0.0000
H	-5.1323	2.2918	0.0000
H	-6.0913	-0.0171	0.0000
H	-4.3971	-2.9830	0.8827
H	-5.8304	-2.4075	0.0000
H	-4.3971	-2.9830	-0.8827

A-revA

N	-1.7024	0.7545	0.0000
C	-2.6473	1.7118	0.0000
N	-3.9780	1.5690	0.0000
C	-4.3312	0.2672	0.0000
C	-3.4645	-0.8336	0.0000
C	-2.0769	-0.5546	0.0000
N	-5.5920	-0.2780	0.0000
C	-5.4430	-1.6407	0.0000
N	-4.1768	-2.0241	0.0000
N	-1.1303	-1.5041	0.0000
H	-2.2741	2.7367	0.0000
H	-6.4706	0.2294	0.0000
H	-6.2996	-2.3040	0.0000
H	-1.4079	-2.4774	0.0000
H	-0.1227	-1.2532	0.0000
N	1.7024	-0.7545	0.0000
C	2.6473	-1.7118	0.0000
N	3.9780	-1.5690	0.0000
C	4.3312	-0.2672	0.0000
C	3.4645	0.8336	0.0000
C	2.0769	0.5546	0.0000
N	5.5920	0.2780	0.0000
C	5.4430	1.6407	0.0000
N	4.1768	2.0241	0.0000
N	1.1303	1.5041	0.0000
H	2.2741	-2.7367	0.0000
H	6.4706	-0.2294	0.0000
H	6.2996	2.3040	0.0000
H	1.4079	2.4774	0.0000
H	0.1227	1.2532	0.0000

A-revT

N	2.8020	-0.0035	0.0000
C	3.4136	-1.2017	0.0000
N	4.7253	-1.4614	0.0000
C	5.4512	-0.3246	0.0000
C	4.9549	0.9863	0.0000
C	3.5480	1.1344	0.0000
N	6.8170	-0.1830	0.0000
C	7.0841	1.1613	0.0000
N	5.9919	1.9077	0.0000
N	2.9216	2.3198	0.0000
H	2.7426	-2.0614	0.0000
H	7.5025	-0.9310	0.0000
H	8.1006	1.5361	0.0000
H	3.4612	3.1756	0.0000
H	1.8945	2.3622	0.0000
N	-0.0541	0.0188	0.0000
C	-0.6352	1.2594	0.0000
N	-2.0093	1.2455	0.0000
C	-2.7507	0.0904	0.0000
C	-2.1746	-1.1413	0.0000

C	-0.7203	-1.2091	0.0000
O	-0.0600	-2.2634	0.0000
O	0.0170	2.3206	0.0000
C	-2.9643	-2.4170	0.0000
H	1.0036	-0.0025	0.0000
H	-2.4736	2.1486	0.0000
H	-3.8279	0.2352	0.0000
H	-2.7254	-3.0272	-0.8824
H	-4.0405	-2.2098	0.0000
H	-2.7254	-3.0272	0.8824

A-revG

N	3.4760	-2.1639	0.0000
C	4.7637	-1.7805	0.0000
N	5.2679	-0.5380	0.0000
C	4.2888	0.3859	0.0000
C	2.9085	0.1414	0.0000
C	2.5038	-1.2146	0.0000
N	4.4075	1.7555	0.0000
C	3.1430	2.2736	0.0000
N	2.2058	1.3387	0.0000
N	1.2188	-1.6094	0.0000
H	5.4937	-2.5909	0.0000
H	5.2718	2.2871	0.0000
H	2.9639	3.3419	0.0000
H	0.4275	-0.9543	0.0000
H	1.0300	-2.6050	0.0000
N	-2.8897	1.8070	0.0000
C	-1.6196	1.2703	0.0000
N	-1.4036	-0.0478	0.0000
C	-2.5461	-0.7722	0.0000
C	-3.8704	-0.3129	0.0000
C	-4.1060	1.0932	0.0000
N	-2.6525	-2.1386	0.0000
C	-3.9939	-2.4477	0.0000
N	-4.7620	-1.3767	0.0000
O	-5.1872	1.7094	0.0000
N	-0.5870	2.1255	0.0000
H	-2.9866	2.8207	0.0000
H	-1.8903	-2.8072	0.0000
H	-4.3372	-3.4749	0.0000
H	0.3910	1.7774	0.0000
H	-0.7521	3.1233	0.0000

A-revC

N	-3.0633	1.0411	0.0000
C	-3.8391	2.1579	0.0000
N	-5.2290	1.9834	0.0000
C	-5.8170	0.7581	0.0000
C	-5.0499	-0.3653	0.0000
C	-3.6275	-0.1842	0.0000
N	-2.8058	-1.2437	0.0000
O	-3.3744	3.3173	0.0000
H	-5.7973	2.8257	0.0000
H	-6.9028	0.7426	0.0000
H	-5.4949	-1.3560	0.0000
H	-1.7756	-1.1154	0.0000
H	-3.1941	-2.1782	0.0000
N	0.1141	-0.8421	0.0000
C	0.9324	-1.9095	0.0000
N	2.2707	-1.9346	0.0000
C	2.7842	-0.6872	0.0000
C	2.0621	0.5132	0.0000
C	0.6501	0.4103	0.0000
N	4.1034	-0.3042	0.0000
C	4.1263	1.0663	0.0000
N	2.9180	1.6052	0.0000
N	-0.1695	1.4707	0.0000
H	0.4345	-2.8800	0.0000
H	4.9114	-0.9177	0.0000
H	5.0593	1.6170	0.0000
H	0.2283	2.4015	0.0000
H	-1.2016	1.3486	0.0000

T-T

N	3.4506	1.5900	0.0000
C	3.2221	2.9408	0.0000
N	1.8966	3.2945	0.0000
C	0.8731	2.3793	0.0000
C	1.0984	1.0385	0.0000
C	2.4804	0.5825	0.0000
O	2.8336	-0.6090	0.0000
O	4.1362	3.7884	0.0000
C	-0.0030	0.0199	0.0000
H	4.4537	1.2981	0.0000
H	1.6900	4.2887	0.0000
H	-0.1259	2.8072	0.0000
H	0.0650	-0.6319	-0.8824
H	-0.9849	0.5065	0.0000
H	0.0650	-0.6319	0.8824
N	6.8753	3.0345	0.0000
C	7.8163	4.0420	0.0000
N	9.1167	3.5862	0.0000
C	9.4560	2.2590	0.0000
C	8.5211	1.2696	0.0000
C	7.1271	1.6679	0.0000
O	6.1699	0.8605	0.0000
O	7.5241	5.2434	0.0000
C	8.8668	-0.1905	0.0000
H	5.8766	3.3311	0.0000
H	9.8432	4.2960	0.0000
H	10.5237	2.0556	0.0000
H	8.4482	-0.6937	0.8827
H	9.9533	-0.3326	0.0000
H	8.4482	-0.6937	-0.8827

G-T

N	5.9037	0.0016	0.0000
C	6.4252	-1.2642	0.0000
N	7.7948	-1.3187	0.0000
C	8.5932	-0.2014	0.0000
C	8.0786	1.0568	0.0000
C	6.6301	1.1976	0.0000
O	6.0241	2.2823	0.0000
O	5.7217	-2.2954	0.0000
C	8.9284	2.2929	0.0000
H	4.8589	0.0712	0.0000
H	8.2142	-2.2436	0.0000
H	9.6617	-0.4000	0.0000
H	8.7181	2.9135	-0.8823
H	9.9934	2.0347	0.0000
H	8.7181	2.9135	0.8823
N	2.9202	-2.1463	0.0000
C	2.2160	-3.3264	0.0000
N	0.8863	-3.3853	0.0000
C	0.3114	-2.1648	0.0000
C	0.9354	-0.9087	0.0000
C	2.3568	-0.8655	0.0000
N	-1.0303	-1.8888	0.0000
C	-1.1672	-0.5197	0.0000
N	-0.0084	0.1100	0.0000
O	3.0999	0.1467	0.0000
N	2.9355	-4.4664	0.0000
H	3.9627	-2.1826	0.0000
H	-1.7833	-2.5690	0.0000
H	-2.1428	-0.0491	0.0000
H	2.4495	-5.3532	0.0000
H	3.9463	-4.4620	0.0000

C-T

N	5.1126	-1.0994	0.0000
C	5.8080	0.0740	0.0000
N	7.2096	0.0036	0.0000
C	7.8929	-1.1698	0.0000

C	7.2125	-2.3465	0.0000
C	5.7801	-2.2739	0.0000
N	5.0560	-3.4014	0.0000
O	5.2687	1.1979	0.0000
H	7.7085	0.8887	0.0000
H	8.9767	-1.1016	0.0000
H	7.7286	-3.3020	0.0000
H	4.0246	-3.3637	0.0000
H	5.5219	-4.2994	0.0000
N	2.0612	-1.0698	0.0000
C	1.3673	0.1252	0.0000
N	-0.0035	-0.0251	0.0000
C	-0.6386	-1.2376	0.0000
C	0.0476	-2.4120	0.0000
C	1.4968	-2.3435	0.0000
O	2.2338	-3.3536	0.0000
O	1.9128	1.2325	0.0000
C	-0.6212	-3.7553	0.0000
H	3.1049	-1.0071	0.0000
H	-0.5465	0.8331	0.0000
H	-1.7245	-1.1918	0.0000
H	-0.3289	-4.3411	-0.8826
H	-1.7116	-3.6457	0.0000
H	-0.3289	-4.3411	0.8826

F-T

N	3.1396	1.6595	0.0000
C	2.8313	3.0044	0.0000
N	1.4776	3.2524	0.0000
C	0.5234	2.2661	0.0000
C	0.8382	0.9426	0.0000
C	2.2464	0.5807	0.0000
O	2.6886	-0.5796	0.0000
O	3.6877	3.8960	0.0000
C	-0.1928	-0.1475	0.0000
H	4.1337	1.4315	0.0000
H	1.1974	4.2284	0.0000
H	-0.5036	2.6220	0.0000
H	-0.0827	-0.7930	-0.8826
H	-1.2044	0.2737	0.0000
H	-0.0827	-0.7930	0.8826
C	7.1740	3.3572	0.0000
C	8.2571	4.2279	0.0000
C	9.5742	3.7907	0.0000
C	9.8108	2.4116	0.0000
C	8.7668	1.4736	0.0000
C	7.4733	2.0019	0.0000
F	6.4189	1.1219	0.0000
F	8.0038	5.5720	0.0000
C	9.0060	-0.0140	0.0000
H	6.1433	3.7081	0.0000
H	10.3907	4.5093	0.0000
H	10.8391	2.0499	0.0000
H	8.5572	-0.4903	0.8826
H	10.0799	-0.2300	0.0000
H	8.5572	-0.4903	-0.8826

G-G

N	3.2214	-1.6792	0.0000
C	4.5577	-1.3429	0.0000
N	4.9844	-0.0830	0.0000
C	3.9765	0.8131	0.0000
C	2.5979	0.5673	0.0000
C	2.1441	-0.7780	0.0000
N	4.0875	2.1792	0.0000
C	2.8159	2.6975	0.0000
N	1.8891	1.7580	0.0000
O	0.9730	-1.2138	0.0000
N	5.4462	-2.3529	0.0000
H	2.9635	-2.6643	0.0000
H	4.9514	2.7116	0.0000
H	2.6356	3.7651	0.0000
H	6.4337	-2.1344	0.0000

H	5.1598	-3.3222	0.0000
N	-1.6570	-0.1288	0.0000
C	-1.9981	1.2058	0.0000
N	-3.2636	1.6332	0.0000
C	-4.1607	0.6262	0.0000
C	-3.9191	-0.7529	0.0000
C	-2.5669	-1.2070	0.0000
N	-5.5275	0.7434	0.0000
C	-6.0477	-0.5306	0.0000
N	-5.1139	-1.4625	0.0000
O	-2.1472	-2.3807	0.0000
N	-1.0024	2.1103	0.0000
H	-0.6540	-0.4021	0.0000
H	-6.0564	1.6092	0.0000
H	-7.1165	-0.7060	0.0000
H	-1.2748	3.0855	0.0000
H	0.0072	1.8821	0.0000

G-C

N	-2.6972	-0.0668	0.0000
O	1.2491	2.3281	0.0000
N	-0.7665	1.2158	0.0000
C	-2.1430	1.1574	0.0000
N	-2.9196	2.2436	0.0000
C	-2.2125	3.3914	0.0000
C	-0.8201	3.5561	0.0000
C	-0.0052	2.3893	0.0000
N	-2.7155	4.6668	0.0000
C	-1.6440	5.5305	0.0000
N	-0.4832	4.9043	0.0000
H	-2.1312	-0.9330	0.0000
H	-3.7073	-0.1274	0.0000
H	-0.2269	0.3130	0.0000
H	-3.6966	4.9251	0.0000
H	-1.7832	6.6047	0.0000
O	-1.2201	-2.4749	0.0000
N	2.7211	-0.1106	0.0000
N	0.7351	-1.2687	0.0000
C	2.8237	-2.5172	0.0000
C	0.0352	-2.4294	0.0000
N	0.7464	-3.6276	0.0000
C	2.1057	-3.6717	0.0000
C	2.0867	-1.2882	0.0000
H	3.9097	-2.5247	0.0000
H	0.2041	-4.4868	0.0000
H	2.5566	-4.6592	0.0000
H	2.1870	0.7746	0.0000
H	3.7324	-0.0820	0.0000

G-F

N	2.3504	-3.0361	0.0000
O	0.7338	1.2949	0.0000
N	1.6337	-0.8222	0.0000
C	2.6708	-1.7278	0.0000
N	3.9482	-1.3609	0.0000
C	4.1101	-0.0200	0.0000
C	3.1263	0.9784	0.0000
C	1.7563	0.5852	0.0000
N	5.2993	0.6600	0.0000
C	5.0033	2.0035	0.0000
N	3.7057	2.2401	0.0000
H	1.3932	-3.3593	0.0000
H	3.0945	-3.7212	0.0000
H	0.6754	-1.1706	0.0000
H	6.2265	0.2478	0.0000
H	5.7834	2.7550	0.0000
C	-2.4362	0.1943	0.0000
C	-2.6075	-1.1833	0.0000
C	-3.8527	-1.7935	0.0000
C	-4.9845	-0.9696	0.0000
C	-4.8904	0.4304	0.0000
C	-3.5955	0.9580	0.0000
F	-3.4544	2.3200	0.0000

F	-1.4812	-1.9705	0.0000
C	-6.0988	1.3301	0.0000
H	-1.4448	0.6480	0.0000
H	-3.9358	-2.8780	0.0000
H	-5.9739	-1.4271	0.0000
H	-6.1080	1.9849	-0.8824
H	-7.0195	0.7368	0.0000
H	-6.1080	1.9849	0.8824

G-revT

N	5.6748	-1.8806	0.0000
C	6.6808	-2.8229	0.0000
N	7.9491	-2.2834	0.0000
C	8.2004	-0.9375	0.0000
C	7.2021	-0.0117	0.0000
C	5.8385	-0.5018	0.0000
O	4.8310	0.2454	0.0000
O	6.4692	-4.0411	0.0000
C	7.4520	1.4679	0.0000
H	4.6943	-2.2512	0.0000
H	8.7200	-2.9445	0.0000
H	9.2523	-0.6641	0.0000
H	7.0016	1.9428	-0.8826
H	8.5271	1.6797	0.0000
H	7.0016	1.9428	0.8826
N	2.2374	-0.7221	0.0000
C	1.2333	0.2118	0.0000
N	-0.0611	-0.0988	0.0000
C	-0.2734	-1.4311	0.0000
C	0.6759	-2.4639	0.0000
C	2.0530	-2.1080	0.0000
N	-1.4854	-2.0693	0.0000
C	-1.2360	-3.4224	0.0000
N	0.0523	-3.7050	0.0000
O	3.0504	-2.8723	0.0000
N	1.6120	1.5064	0.0000
H	3.2322	-0.3914	0.0000
H	-2.3977	-1.6250	0.0000
H	-2.0422	-4.1458	0.0000
H	0.9040	2.2282	0.0000
H	2.5868	1.7748	0.0000

G-revG

N	-1.5712	0.8486	0.0000
C	-2.4021	1.9425	0.0000
N	-3.7306	1.8552	0.0000
C	-4.1660	0.5786	0.0000
C	-3.4056	-0.6008	0.0000
C	-1.9897	-0.4836	0.0000
N	-5.4684	0.1546	0.0000
C	-5.4518	-1.2213	0.0000
N	-4.2302	-1.7183	0.0000
O	-1.1379	-1.4104	0.0000
N	-1.8088	3.1530	0.0000
H	-0.5346	1.0152	0.0000
H	-6.2924	0.7466	0.0000
H	-6.3690	-1.7974	0.0000
H	-2.3850	3.9839	0.0000
H	-0.8025	3.2526	0.0000
N	1.5712	-0.8486	0.0000
C	2.4021	-1.9425	0.0000
N	3.7306	-1.8552	0.0000
C	4.1660	-0.5786	0.0000
C	3.4056	0.6008	0.0000
C	1.9897	0.4836	0.0000
N	5.4684	-0.1546	0.0000
C	5.4518	1.2213	0.0000
N	4.2302	1.7183	0.0000
O	1.1379	1.4104	0.0000
N	1.8088	-3.1530	0.0000
H	0.5346	-1.0152	0.0000
H	6.2924	-0.7466	0.0000
H	6.3690	1.7974	0.0000

H	2.3850	-3.9839	0.0000
H	0.8025	-3.2526	0.0000

G-revC

N	2.1261	1.0574	0.0000
C	1.4103	-0.0948	0.0000
N	0.0201	-0.0104	0.0000
C	-0.6417	1.1760	0.0000
C	0.0579	2.3423	0.0000
C	1.4858	2.2431	0.0000
N	2.2329	3.3579	0.0000
O	1.9381	-1.2345	0.0000
H	-0.4946	-0.8867	0.0000
H	-1.7260	1.1253	0.0000
H	-0.4442	3.3051	0.0000
H	3.2434	3.3013	0.0000
H	1.8018	4.2728	0.0000
N	4.6757	-1.7861	0.0000
C	5.5667	-0.7380	0.0000
N	6.8911	-0.9017	0.0000
C	7.2552	-2.2017	0.0000
C	6.4329	-3.3357	0.0000
C	5.0175	-3.1502	0.0000
N	8.5348	-2.6959	0.0000
C	8.4440	-4.0688	0.0000
N	7.1960	-4.4968	0.0000
O	4.1235	-4.0207	0.0000
N	5.0473	0.5048	0.0000
H	3.6530	-1.5641	0.0000
H	9.3897	-2.1496	0.0000
H	9.3280	-4.6948	0.0000
H	5.6966	1.2810	0.0000
H	4.0304	0.6881	0.0000

C-C

N	3.0745	-1.1295	0.0000
C	4.2359	-0.4237	0.0000
N	4.1558	0.9748	0.0000
C	2.9716	1.6440	0.0000
C	1.8003	0.9532	0.0000
C	1.8957	-0.4781	0.0000
N	0.7742	-1.2185	0.0000
O	5.3676	-0.9600	0.0000
H	5.0339	1.4858	0.0000
H	3.0302	2.7288	0.0000
H	0.8311	1.4484	0.0000
H	0.8676	-2.2282	0.0000
H	-0.1687	-0.7992	0.0000
N	-2.0840	-0.2389	0.0000
C	-2.2938	1.1079	0.0000
N	-3.6186	1.5616	0.0000
C	-4.6867	0.7237	0.0000
C	-4.4917	-0.6225	0.0000
C	-3.1348	-1.0802	0.0000
N	-2.8809	-2.4002	0.0000
O	-1.3712	1.9488	0.0000
H	-3.7563	2.5684	0.0000
H	-5.6683	1.1880	0.0000
H	-5.3260	-1.3179	0.0000
H	-1.9284	-2.7413	0.0000
H	-3.6334	-3.0754	0.0000

F-C

O	-2.3239	-2.2759	0.0000
N	-1.8438	2.2946	0.0000
N	-2.0456	0.0068	0.0000
C	-4.0656	1.3748	0.0000
C	-2.8033	-1.1227	0.0000
N	-4.1996	-0.9744	0.0000
C	-4.8124	0.2373	0.0000
C	-2.6418	1.2106	0.0000
H	-4.5276	2.3578	0.0000
H	-4.7517	-1.8275	0.0000

H	-5.8983	0.2324	0.0000
H	-0.8366	2.1795	0.0000
H	-2.2298	3.2291	0.0000
C	1.4870	-0.4131	0.0000
C	2.2837	-1.5519	0.0000
C	3.6707	-1.5022	0.0000
C	4.2856	-0.2454	0.0000
C	3.5465	0.9476	0.0000
C	2.1568	0.8027	0.0000
F	1.3934	1.9450	0.0000
F	1.6654	-2.7720	0.0000
C	4.1930	2.3084	0.0000
H	0.3965	-0.4601	0.0000
H	4.2520	-2.4217	0.0000
H	5.3740	-0.1863	0.0000
H	3.8954	2.8913	0.8827
H	5.2843	2.2143	0.0000
H	3.8954	2.8913	-0.8827

Table S4. Cartesian coordinates (in Å) of models 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 0º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P (see text).

[A]-A/T-A			
N	0.0000	0.0000	0.0000
C	1.3527	0.0000	0.0000
N	2.1761	1.0527	0.0000
C	1.4952	2.2063	0.0000
C	0.1029	2.3664	0.0000
C	-0.6558	1.1777	0.0000
N	1.9866	3.4948	0.0000
C	0.8954	4.3403	0.0000
N	-0.2563	3.7043	0.0000
N	-2.0101	1.1928	0.0000
H	1.8055	-0.9941	0.0000
H	2.9663	3.7528	0.0000
H	1.0145	5.4184	0.0000
H	-2.5007	2.0759	0.0000
H	-2.5273	0.3256	0.0000
N	1.5699	-3.3792	0.0000
C	2.5486	-4.3006	0.0000
N	2.4506	-5.6368	0.0000
C	1.1652	-6.0203	0.0000
C	0.0369	-5.1907	0.0000
C	0.2835	-3.7973	0.0000
N	0.6503	-7.3008	0.0000
C	-0.7250	-7.1795	0.0000
N	-1.1359	-5.9295	0.0000
N	-0.7138	-2.8907	0.0000
H	3.5637	-3.8997	0.0000
H	1.1929	-8.1558	0.0000
H	-1.3706	-8.0511	0.0000
H	-1.6645	-3.2348	0.0000
H	-0.5205	-1.8771	0.0000
N	1.5677	-3.3662	3.4000
C	2.5731	-4.2646	3.4000
N	2.4893	-5.5965	3.4000
C	1.2083	-6.0000	3.4000
C	0.0632	-5.1924	3.4000
C	0.2797	-3.7938	3.4000
N	0.7193	-7.2890	3.4000
C	-0.6584	-7.1951	3.4000
N	-1.0940	-5.9533	3.4000
N	-0.7138	-2.8907	3.4000
H	3.5737	-3.8310	3.4000
H	1.2796	-8.1329	3.4000
H	-1.2865	-8.0789	3.4000
H	-1.6685	-3.2224	3.4000
H	-0.5040	-1.8798	3.4000
N	2.2278	-0.6407	3.4000
C	3.5775	-0.3515	3.4000
N	3.8493	1.0179	3.4000
C	2.8762	1.9891	3.4000
C	1.5523	1.6879	3.4000
C	1.1781	0.2727	3.4000
O	-0.0012	-0.1194	3.4000
O	4.4678	-1.1937	3.4000
C	0.4630	2.7188	3.4000
H	1.9764	-1.6779	3.4000
H	4.8336	1.2603	3.4000
H	3.2412	3.0149	3.4000
H	-0.1840	2.6024	4.2802
H	0.8777	3.7342	3.4000
H	-0.1840	2.6024	2.5198
[T]-A/T-A			
N	-0.5475	-0.7023	-1.7000
C	-1.0248	-1.9633	-1.7000

N	-2.2980	-2.3635	-1.7000
C	-3.1346	-1.3129	-1.7000
C	-2.7921	0.0458	-1.7000
C	-1.4092	0.3462	-1.7000
N	-4.5132	-1.3195	-1.7000
C	-4.9204	0.0000	-1.7000
N	-3.9180	0.8525	-1.7000
N	-0.9232	1.5977	-1.7000
H	-0.2608	-2.7414	-1.7000
H	-5.0996	-2.1456	-1.7000
H	-5.9709	0.2687	-1.7000
H	-1.5757	2.3696	-1.7000
H	0.0957	1.7650	-1.7000
N	2.2332	-0.3395	-1.7000
C	2.9879	-1.4952	-1.7000
N	4.3636	-1.2570	-1.7000
C	4.9204	0.0000	-1.7000
C	4.1638	1.1274	-1.7000
C	2.7087	0.9683	-1.7000
O	1.9192	1.9281	-1.7000
O	2.5217	-2.6286	-1.7000
C	4.7347	2.5143	-1.7000
H	1.1749	-0.4774	-1.7000
H	4.9433	-2.0886	-1.7000
H	6.0089	0.0278	-1.7000
H	4.3937	3.0763	-0.8198
H	5.8313	2.4920	-1.7000
H	4.3937	3.0763	-2.5802
N	-0.5475	-0.7023	1.7000
C	-1.0248	-1.9633	1.7000
N	-2.2980	-2.3635	1.7000
C	-3.1346	-1.3129	1.7000
C	-2.7921	0.0458	1.7000
C	-1.4092	0.3462	1.7000
N	-4.5132	-1.3195	1.7000
C	-4.9204	0.0000	1.7000
N	-3.9180	0.8525	1.7000
N	-0.9232	1.5977	1.7000
H	-0.2608	-2.7414	1.7000
H	-5.0996	-2.1456	1.7000
H	-5.9709	0.2687	1.7000
H	-1.5757	2.3696	1.7000
H	0.0957	1.7650	1.7000
N	2.2332	-0.3395	1.7000
C	2.9879	-1.4952	1.7000
N	4.3636	-1.2570	1.7000
C	4.9204	0.0000	1.7000
C	4.1638	1.1274	1.7000
C	2.7087	0.9683	1.7000
O	1.9192	1.9281	1.7000
O	2.5217	-2.6286	1.7000
C	4.7347	2.5143	1.7000
H	1.1749	-0.4774	1.7000
H	4.9433	-2.0886	1.7000
H	6.0089	0.0278	1.7000
H	4.3937	3.0763	2.5802
H	5.8313	2.4920	1.7000
H	4.3937	3.0763	0.8198

[G]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3696	0.0000	0.0000
N	2.1155	1.0903	0.0000
C	1.3698	2.2163	0.0000
C	-0.0253	2.3509	0.0000
C	-0.8176	1.1585	0.0000
N	1.8453	3.5034	0.0000
C	0.7392	4.3399	0.0000
N	-0.3956	3.6845	0.0000
O	-2.0521	1.0437	0.0000
N	1.9828	-1.2160	0.0000
H	-0.5038	-0.9195	0.0000
H	2.8231	3.7679	0.0000

H	0.8460	5.4190	0.0000
H	2.9917	-1.2391	0.0000
H	1.4554	-2.0749	0.0000
N	-1.3956	-2.5980	0.0000
C	-0.7922	-3.8029	0.0000
N	-1.3307	-5.0214	0.0000
C	-2.6734	-4.9487	0.0000
C	-3.4512	-3.7871	0.0000
C	-2.7587	-2.5499	0.0000
N	-3.5885	-5.9785	0.0000
C	-4.8417	-5.3980	0.0000
N	-4.8026	-4.0831	0.0000
N	-3.3905	-1.3724	0.0000
H	0.3012	-3.7852	0.0000
H	-3.3680	-6.9672	0.0000
H	-5.7448	-5.9984	0.0000
H	-4.4025	-1.3815	0.0000
H	-2.8770	-0.4664	0.0000
N	-1.3956	-2.5980	3.4000
C	-0.7918	-3.8036	3.4000
N	-1.3606	-5.0109	3.4000
C	-2.7001	-4.9140	3.4000
C	-3.4670	-3.7413	3.4000
C	-2.7505	-2.5209	3.4000
N	-3.6297	-5.9321	3.4000
C	-4.8758	-5.3372	3.4000
N	-4.8232	-4.0223	3.4000
N	-3.3413	-1.3153	3.4000
H	0.2981	-3.7692	3.4000
H	-3.4197	-6.9232	3.4000
H	-5.7854	-5.9274	3.4000
H	-4.3511	-1.2719	3.4000
H	-2.7737	-0.4528	3.4000
N	0.2224	-0.3075	3.4000
C	1.5837	-0.5359	3.4000
N	2.3409	0.6370	3.4000
C	1.7941	1.8984	3.4000
C	0.4524	2.1062	3.4000
C	-0.4169	0.9285	3.4000
O	-1.6577	0.9985	3.4000
O	2.1010	-1.6470	3.4000
C	-0.1804	3.4660	3.4000
H	-0.3935	-1.1791	3.4000
H	3.3453	0.4996	3.4000
H	2.5115	2.7176	3.4000
H	-0.8247	3.5962	4.2802
H	0.5792	4.2571	3.4000
H	-0.8247	3.5962	2.5198

[C]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3676	0.0000	0.0000
N	2.0004	1.2859	0.0000
C	1.3125	2.4537	0.0000
C	-0.0480	2.4390	0.0000
C	-0.6801	1.1426	0.0000
N	-2.0310	1.0637	0.0000
O	2.0840	-0.9954	0.0000
H	3.0151	1.2666	0.0000
H	1.8965	3.3722	0.0000
H	-0.6210	3.3627	0.0000
H	-2.5038	0.1422	0.0000
H	-2.5799	1.9108	0.0000
N	-3.2696	-1.6394	0.0000
C	-2.2299	-2.5088	0.0000
N	-2.2791	-3.8439	0.0000
C	-3.5408	-4.2906	0.0000
C	-4.7110	-3.5199	0.0000
C	-4.5278	-2.1223	0.0000
N	-3.9912	-5.5942	0.0000
C	-5.3703	-5.5422	0.0000
N	-5.8457	-4.3151	0.0000
N	-5.5793	-1.2661	0.0000

H	-1.2434	-2.0401	0.0000
H	-3.4046	-6.4203	0.0000
H	-5.9710	-6.4453	0.0000
H	-6.5210	-1.6320	0.0000
H	-5.4231	-0.2690	0.0000
N	-3.2643	-1.6439	3.4000
C	-2.2299	-2.5088	3.4000
N	-2.2701	-3.8428	3.4000
C	-3.5371	-4.2881	3.4000
C	-4.7080	-3.5184	3.4000
C	-4.5376	-2.1135	3.4000
N	-3.9836	-5.5924	3.4000
C	-5.3637	-5.5437	3.4000
N	-5.8397	-4.3169	3.4000
N	-5.5601	-1.2435	3.4000
H	-1.2441	-2.0427	3.4000
H	-3.3959	-6.4175	3.4000
H	-5.9624	-6.4476	3.4000
H	-6.5034	-1.6063	3.4000
H	-5.3835	-0.2262	3.4000
N	-2.6938	1.1017	3.4000
C	-1.3543	1.4350	3.4000
N	-1.1276	2.8126	3.4000
C	-2.1320	3.7514	3.4000
C	-3.4453	3.4070	3.4000
C	-3.7729	1.9803	3.4000
O	-4.9387	1.5497	3.4000
O	-0.4369	0.6225	3.4000
C	-4.5679	4.4016	3.4000
H	-2.9111	0.0568	3.4000
H	-0.1517	3.0872	3.4000
H	-1.8008	4.7887	3.4000
H	-5.2106	4.2641	4.2802
H	-4.1867	5.4301	3.4000
H	-5.2106	4.2641	2.5198

[F]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3460	0.0000	0.0000
N	2.1849	1.0427	0.0000
C	1.5116	2.2018	0.0000
C	0.1202	2.3701	0.0000
C	-0.6475	1.1844	0.0000
N	2.0122	3.4871	0.0000
C	0.9265	4.3399	0.0000
N	-0.2290	3.7110	0.0000
N	-1.9985	1.1999	0.0000
H	1.8115	-0.9866	0.0000
H	2.9932	3.7394	0.0000
H	1.0527	5.4172	0.0000
H	-2.4865	2.0844	0.0000
H	-2.5175	0.3300	0.0000
C	-1.7547	-2.9334	0.0000
C	-1.2636	-4.2338	0.0000
C	-2.0924	-5.3480	0.0000
C	-3.4751	-5.1459	0.0000
C	-4.0404	-3.8631	0.0000
C	-3.1348	-2.8002	0.0000
F	-3.6500	-1.5237	0.0000
F	0.0857	-4.4153	0.0000
C	-5.5282	-3.6237	0.0000
H	-1.0985	-2.0589	0.0000
H	-1.6597	-6.3461	0.0000
H	-4.1397	-6.0105	0.0000
H	-5.8416	-3.0490	0.8828
H	-6.0716	-4.5756	0.0000
N	0.0000	0.0000	-3.4000
C	1.3483	0.0000	-3.4000
N	2.1732	1.0492	-3.4000
C	1.4868	2.2035	-3.4000
C	0.0948	2.3641	-3.4000
C	-0.6756	1.1770	-3.4000
N	1.9810	3.4905	-3.4000

C	0.8910	4.3384	-3.4000
N	-0.2612	3.7026	-3.4000
N	-2.0181	1.1655	-3.4000
H	1.8056	-0.9899	-3.4000
H	2.9611	3.7465	-3.4000
H	1.0115	5.4160	-3.4000
H	-2.5091	2.0489	-3.4000
H	-2.5352	0.2718	-3.4000
N	-1.3236	-2.4723	-3.4000
C	-0.5098	-3.5872	-3.4000
N	-1.2196	-4.7894	-3.4000
C	-2.5923	-4.8654	-3.4000
C	-3.3788	-3.7587	-3.4000
C	-2.7150	-2.4540	-3.4000
O	-3.3332	-1.3759	-3.4000
O	0.7152	-3.5523	-3.4000
C	-4.8780	-3.8017	-3.4000
H	-0.8200	-1.5313	-3.4000
H	-0.6470	-5.6260	-3.4000
H	-3.0035	-5.8736	-3.4000
H	-5.2829	-3.2839	-4.2802
H	-5.2453	-4.8352	-3.4000
H	-5.2829	-3.2839	-2.5198

[revA]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3470	0.0000	0.0000
N	2.1853	1.0391	0.0000
C	1.5089	2.1997	0.0000
C	0.1193	2.3672	0.0000
C	-0.6617	1.1863	0.0000
N	2.0104	3.4839	0.0000
C	0.9249	4.3374	0.0000
N	-0.2299	3.7070	0.0000
N	-2.0032	1.2023	0.0000
H	1.8121	-0.9875	0.0000
H	2.9916	3.7355	0.0000
H	1.0507	5.4146	0.0000
H	-2.4628	2.1034	0.0000
H	-2.5599	0.3227	0.0000
N	-3.5211	-1.2780	0.0000
C	-4.8681	-1.2780	0.0000
N	-5.7064	-2.3171	0.0000
C	-5.0300	-3.4777	0.0000
C	-3.6404	-3.6452	0.0000
C	-2.8594	-2.4643	0.0000
N	-5.5315	-4.7620	0.0000
C	-4.4460	-5.6154	0.0000
N	-3.2912	-4.9850	0.0000
N	-1.5180	-2.4803	0.0000
H	-5.3332	-0.2905	0.0000
H	-6.5127	-5.0135	0.0000
H	-4.5718	-6.6926	0.0000
H	-1.0583	-3.3814	0.0000
H	-0.9612	-1.6007	0.0000
N	0.0000	0.0000	-3.4000
C	1.3483	0.0000	-3.4000
N	2.1732	1.0492	-3.4000
C	1.4868	2.2035	-3.4000
C	0.0948	2.3641	-3.4000
C	-0.6756	1.1770	-3.4000
N	1.9810	3.4905	-3.4000
C	0.8910	4.3384	-3.4000
N	-0.2612	3.7026	-3.4000
N	-2.0181	1.1655	-3.4000
H	1.8056	-0.9899	-3.4000
H	2.9611	3.7465	-3.4000
H	1.0115	5.4160	-3.4000
H	-2.5091	2.0489	-3.4000
H	-2.5352	0.2718	-3.4000
N	-1.3236	-2.4723	-3.4000
C	-0.5098	-3.5872	-3.4000
N	-1.2196	-4.7894	-3.4000

C	-2.5923	-4.8654	-3.4000
C	-3.3788	-3.7587	-3.4000
C	-2.7150	-2.4540	-3.4000
O	-3.3332	-1.3759	-3.4000
O	0.7152	-3.5523	-3.4000
C	-4.8780	-3.8017	-3.4000
H	-0.8200	-1.5313	-3.4000
H	-0.6470	-5.6260	-3.4000
H	-3.0035	-5.8736	-3.4000
H	-5.2829	-3.2839	-4.2802
H	-5.2453	-4.8352	-3.4000
H	-5.2829	-3.2839	-2.5198

[revT]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3486	0.0000	0.0000
N	2.1720	1.0503	0.0000
C	1.4845	2.2035	0.0000
C	0.0927	2.3631	0.0000
C	-0.6754	1.1757	0.0000
N	1.9769	3.4911	0.0000
C	0.8864	4.3378	0.0000
N	-0.2648	3.7010	0.0000
N	-2.0188	1.1660	0.0000
H	1.8048	-0.9909	0.0000
H	2.9568	3.7477	0.0000
H	1.0059	5.4157	0.0000
H	-2.5092	2.0499	0.0000
H	-2.5360	0.2759	0.0000
N	-1.2849	-2.4947	0.0000
C	-2.6521	-2.4481	0.0000
N	-3.2639	-3.6929	0.0000
C	-2.5652	-4.8825	0.0000
C	-1.2109	-4.9231	0.0000
C	-0.4809	-3.6478	0.0000
O	0.7450	-3.5503	0.0000
O	-3.3201	-1.4057	0.0000
C	-0.4144	-6.1930	0.0000
H	-0.7830	-1.5537	0.0000
H	-4.2774	-3.6787	0.0000
H	-3.1798	-5.7813	0.0000
H	0.2426	-6.2376	-0.8795
H	-1.0676	-7.0743	0.0000
H	0.2426	-6.2376	0.8795
N	0.0000	0.0000	-3.4000
C	1.3483	0.0000	-3.4000
N	2.1732	1.0492	-3.4000
C	1.4868	2.2035	-3.4000
C	0.0948	2.3641	-3.4000
C	-0.6756	1.1770	-3.4000
N	1.9810	3.4905	-3.4000
C	0.8910	4.3384	-3.4000
N	-0.2612	3.7026	-3.4000
N	-2.0181	1.1655	-3.4000
H	1.8056	-0.9899	-3.4000
H	2.9611	3.7465	-3.4000
H	1.0115	5.4160	-3.4000
H	-2.5091	2.0489	-3.4000
H	-2.5352	0.2718	-3.4000
N	-1.3236	-2.4723	-3.4000
C	-0.5098	-3.5872	-3.4000
N	-1.2196	-4.7894	-3.4000
C	-2.5923	-4.8654	-3.4000
C	-3.3788	-3.7587	-3.4000
C	-2.7150	-2.4540	-3.4000
O	-3.3332	-1.3759	-3.4000
O	0.7152	-3.5523	-3.4000
C	-4.8780	-3.8017	-3.4000
H	-0.8200	-1.5313	-3.4000
H	-0.6470	-5.6260	-3.4000
H	-3.0035	-5.8736	-3.4000
H	-5.2829	-3.2839	-4.2802
H	-5.2453	-4.8352	-3.4000

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H              -5.2829   -3.2839   -2.5198

[revG]-A/T-A
N               0.0000    0.0000    0.0000
C               1.3405    0.0000    0.0000
N               2.1803    1.0458    0.0000
C               1.5019    2.1986    0.0000
C               0.1097    2.3698    0.0000
C              -0.6601    1.1805    0.0000
N               2.0137    3.4817    0.0000
C               0.9467    4.3440    0.0000
N              -0.2156    3.7205    0.0000
N              -2.0071    1.1511    0.0000
H               1.8087   -0.9855    0.0000
H               2.9977    3.7226    0.0000
H               1.0810    5.4199    0.0000
H              -2.6115    1.9848    0.0000
H              -2.4229    0.2281    0.0000
N              -5.0437    5.4769    0.0000
C              -3.9676    4.6227    0.0000
N              -4.1141    3.3026    0.0000
C              -5.4169    2.9166    0.0000
C              -6.5782    3.6995    0.0000
C              -6.4437    5.1308    0.0000
N              -5.8741    1.6212    0.0000
C              -7.2603    1.6807    0.0000
N              -7.7124    2.9094    0.0000
O              -7.2763    6.0253    0.0000
N              -2.7317    5.1697    0.0000
H              -4.8888    6.4822    0.0000
H              -5.3031    0.7858    0.0000
H              -7.8648    0.7807    0.0000
H              -1.8773    4.5805    0.0000
H              -2.6254    6.1731    0.0000
N               0.0000    0.0000   -3.4000
C               1.3483    0.0000   -3.4000
N               2.1732    1.0492   -3.4000
C               1.4868    2.2035   -3.4000
C               0.0948    2.3641   -3.4000
C              -0.6756    1.1770   -3.4000
N               1.9810    3.4905   -3.4000
C               0.8910    4.3384   -3.4000
N              -0.2612    3.7026   -3.4000
N              -2.0181    1.1655   -3.4000
H               1.8056   -0.9899   -3.4000
H               2.9611    3.7465   -3.4000
H               1.0115    5.4160   -3.4000
H              -2.5091    2.0489   -3.4000
H              -2.5352    0.2718   -3.4000
N              -1.3236   -2.4723   -3.4000
C              -0.5098   -3.5872   -3.4000
N              -1.2196   -4.7894   -3.4000
C              -2.5923   -4.8654   -3.4000
C              -3.3788   -3.7587   -3.4000
C              -2.7150   -2.4540   -3.4000
O              -3.3332   -1.3759   -3.4000
O               0.7152   -3.5523   -3.4000
C              -4.8780   -3.8017   -3.4000
H              -0.8200   -1.5313   -3.4000
H              -0.6470   -5.6260   -3.4000
H              -3.0035   -5.8736   -3.4000
H              -5.2829   -3.2839   -4.2802
H              -5.2453   -4.8352   -3.4000
H              -5.2829   -3.2839   -2.5198

[revC]-A/T-A
N               0.0000    0.0000    0.0000
C               1.3466    0.0000    0.0000
N               2.1876    1.0366    0.0000
C               1.5118    2.1988    0.0000
C               0.1231    2.3687    0.0000
C              -0.6640    1.1895    0.0000
N               2.0164    3.4817    0.0000
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C	0.9324	4.3376	0.0000
N	-0.2230	3.7091	0.0000
N	-2.0008	1.2053	0.0000
H	1.8113	-0.9882	0.0000
H	2.9981	3.7310	0.0000
H	1.0601	5.4147	0.0000
H	-2.4729	2.1000	0.0000
H	-2.5545	0.3246	0.0000
N	-3.4256	-1.3139	0.0000
C	-4.7902	-1.2217	0.0000
N	-5.5033	-2.4568	0.0000
C	-4.8902	-3.6674	0.0000
C	-3.5324	-3.7445	0.0000
C	-2.8074	-2.4986	0.0000
N	-1.4622	-2.4985	0.0000
O	-5.4265	-0.1720	0.0000
H	-6.5147	-2.3725	0.0000
H	-5.5337	-4.5450	0.0000
H	-3.0229	-4.7043	0.0000
H	-0.9276	-1.5980	0.0000
H	-0.9656	-3.3778	0.0000
N	0.0000	0.0000	-3.4000
C	1.3483	0.0000	-3.4000
N	2.1732	1.0492	-3.4000
C	1.4868	2.2035	-3.4000
C	0.0948	2.3641	-3.4000
C	-0.6756	1.1770	-3.4000
N	1.9810	3.4905	-3.4000
C	0.8910	4.3384	-3.4000
N	-0.2612	3.7026	-3.4000
N	-2.0181	1.1655	-3.4000
H	1.8056	-0.9899	-3.4000
H	2.9611	3.7465	-3.4000
H	1.0115	5.4160	-3.4000
H	-2.5091	2.0489	-3.4000
H	-2.5352	0.2718	-3.4000
N	-1.3236	-2.4723	-3.4000
C	-0.5098	-3.5872	-3.4000
N	-1.2196	-4.7894	-3.4000
C	-2.5923	-4.8654	-3.4000
C	-3.3788	-3.7587	-3.4000
C	-2.7150	-2.4540	-3.4000
O	-3.3332	-1.3759	-3.4000
O	0.7152	-3.5523	-3.4000
C	-4.8780	-3.8017	-3.4000
H	-0.8200	-1.5313	-3.4000
H	-0.6470	-5.6260	-3.4000
H	-3.0035	-5.8736	-3.4000
H	-5.2829	-3.2839	-4.2802
H	-5.2453	-4.8352	-3.4000
H	-5.2829	-3.2839	-2.5198

[T]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3861	0.0000	0.0000
N	1.9276	1.2879	0.0000
C	1.1773	2.4392	0.0000
C	-0.1795	2.4186	0.0000
C	-0.8379	1.1139	0.0000
O	-2.0716	0.9794	0.0000
O	2.0838	-1.0019	0.0000
C	-1.0367	3.6492	0.0000
H	-0.4694	-0.9312	0.0000
H	2.9408	1.3222	0.0000
H	1.7465	3.3677	0.0000
H	-1.6946	3.6652	-0.8796
H	-0.4241	4.5591	0.0000
H	-1.6946	3.6652	0.8796
N	-3.5216	-1.4278	0.0000
C	-2.6748	-2.5043	0.0000
N	-3.3152	-3.7322	0.0000
C	-4.6880	-3.8752	0.0000
C	-5.5226	-2.8089	0.0000

C	-4.9338	-1.4614	0.0000
O	-5.5831	-0.4221	0.0000
O	-1.4394	-2.4296	0.0000
C	-7.0175	-2.9189	0.0000
H	-3.0550	-0.4933	0.0000
H	-2.7018	-4.5390	0.0000
H	-5.0467	-4.9032	0.0000
H	-7.4421	-2.4153	0.8794
H	-7.3410	-3.9670	0.0000
H	-7.4421	-2.4153	-0.8794
N	-2.2678	1.0980	-3.4000
C	-0.9202	1.1411	-3.4000
N	-0.1293	2.2161	-3.4000
C	-0.8522	3.3479	-3.4000
C	-2.2486	3.4640	-3.4000
C	-2.9807	2.2528	-3.4000
N	-0.3995	4.6501	-3.4000
C	-1.5160	5.4627	-3.4000
N	-2.6472	4.7904	-3.4000
N	-4.3222	2.1984	-3.4000
H	-0.4315	0.1663	-3.4000
H	0.5720	4.9373	-3.4000
H	-1.4300	6.5436	-3.4000
H	-4.8411	3.0657	-3.4000
H	-4.8104	1.2886	-3.4000
N	-3.5117	-1.4153	-3.4000
C	-2.6627	-2.5036	-3.4000
N	-3.3336	-3.7280	-3.4000
C	-4.7032	-3.8477	-3.4000
C	-5.5248	-2.7668	-3.4000
C	-4.9030	-1.4416	-3.4000
O	-5.5553	-0.3838	-3.4000
O	-1.4394	-2.4296	-3.4000
C	-7.0218	-2.8577	-3.4000
H	-3.0385	-0.4587	-3.4000
H	-2.7346	-4.5458	-3.4000
H	-5.0820	-4.8686	-3.4000
H	-7.4431	-2.3531	-4.2802
H	-7.3559	-3.9024	-3.4000
H	-7.4431	-2.3531	-2.5198

[G]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3681	0.0000	0.0000
N	2.1073	1.0952	0.0000
C	1.3512	2.2156	0.0000
C	-0.0465	2.3447	0.0000
C	-0.8299	1.1459	0.0000
N	1.8197	3.5053	0.0000
C	0.7098	4.3369	0.0000
N	-0.4218	3.6765	0.0000
O	-2.0629	1.0067	0.0000
N	1.9746	-1.2191	0.0000
H	-0.5060	-0.9106	0.0000
H	2.7962	3.7742	0.0000
H	0.8118	5.4164	0.0000
H	2.9833	-1.2486	0.0000
H	1.4388	-2.0748	0.0000
N	-3.3688	-1.4447	0.0000
C	-2.5353	-2.5250	0.0000
N	-3.1736	-3.7502	0.0000
C	-4.5480	-3.8948	0.0000
C	-5.3784	-2.8269	0.0000
C	-4.7858	-1.4796	0.0000
O	-5.4344	-0.4430	0.0000
O	-1.2912	-2.4634	0.0000
C	-6.8733	-2.9305	0.0000
H	-2.9099	-0.4939	0.0000
H	-2.5621	-4.5581	0.0000
H	-4.9058	-4.9230	0.0000
H	-7.2943	-2.4237	0.8791
H	-7.2021	-3.9768	0.0000
H	-7.2943	-2.4237	-0.8791

N	-2.0810	1.0730	-3.4000
C	-0.7330	1.1014	-3.4000
N	0.0697	2.1677	-3.4000
C	-0.6409	3.3073	-3.4000
C	-2.0359	3.4386	-3.4000
C	-2.7812	2.2356	-3.4000
N	-0.1739	4.6045	-3.4000
C	-1.2814	5.4292	-3.4000
N	-2.4200	4.7694	-3.4000
N	-4.1232	2.1958	-3.4000
H	-0.2550	0.1213	-3.4000
H	0.8007	4.8810	-3.4000
H	-1.1836	6.5091	-3.4000
H	-4.6326	3.0688	-3.4000
H	-4.6214	1.2915	-3.4000
N	-3.3523	-1.4265	-3.4000
C	-2.5153	-2.5241	-3.4000
N	-3.1996	-3.7410	-3.4000
C	-4.5704	-3.8457	-3.4000
C	-5.3801	-2.7558	-3.4000
C	-4.7438	-1.4375	-3.4000
O	-5.3845	-0.3727	-3.4000
O	-1.2912	-2.4634	-3.4000
C	-6.8780	-2.8304	-3.4000
H	-2.8687	-0.4751	-3.4000
H	-2.6096	-4.5653	-3.4000
H	-4.9604	-4.8624	-3.4000
H	-7.2937	-2.3212	-4.2802
H	-7.2235	-3.8713	-3.4000
H	-7.2937	-2.3212	-2.5198

[C]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3739	0.0000	0.0000
N	2.0064	1.2835	0.0000
C	1.3241	2.4540	0.0000
C	-0.0350	2.4426	0.0000
C	-0.6793	1.1528	0.0000
N	-2.0226	1.0877	0.0000
O	2.0854	-0.9948	0.0000
H	3.0208	1.2568	0.0000
H	1.9115	3.3701	0.0000
H	-0.6077	3.3660	0.0000
H	-2.5008	0.1670	0.0000
H	-2.5665	1.9380	0.0000
N	-1.4220	-2.6599	0.0000
C	-0.7373	-3.8715	0.0000
N	-1.5938	-4.9810	0.0000
C	-2.9620	-4.9029	0.0000
C	-3.6127	-3.7124	0.0000
C	-2.8047	-2.4951	0.0000
O	-3.3165	-1.3617	0.0000
O	0.4727	-3.9967	0.0000
C	-5.1067	-3.5782	0.0000
H	-0.8372	-1.7887	0.0000
H	-1.1173	-5.8758	0.0000
H	-3.4881	-5.8566	0.0000
H	-5.4490	-3.0171	0.8804
H	-5.5915	-4.5624	0.0000
H	-5.4490	-3.0171	-0.8804
N	0.1793	-0.3577	-3.4000
C	1.5185	-0.5140	-3.4000
N	2.4595	0.4324	-3.4000
C	1.9115	1.6585	-3.4000
C	0.5476	1.9795	-3.4000
C	-0.3553	0.8897	-3.4000
N	2.5516	2.8796	-3.4000
C	1.5673	3.8481	-3.4000
N	0.3491	3.3502	-3.4000
N	-1.6901	1.0338	-3.4000
H	1.8580	-1.5503	-3.4000
H	3.5548	3.0202	-3.4000
H	1.8118	4.9045	-3.4000

H	-2.0753	1.9683	-3.4000
H	-2.3073	0.2061	-3.4000
N	-1.4220	-2.6599	-3.4000
C	-0.7429	-3.8616	-3.4000
N	-1.5873	-4.9735	-3.4000
C	-2.9595	-4.8898	-3.4000
C	-3.6125	-3.6994	-3.4000
C	-2.8019	-2.4805	-3.4000
O	-3.2909	-1.3380	-3.4000
O	0.4779	-3.9690	-3.4000
C	-5.1066	-3.5683	-3.4000
H	-0.8127	-1.7836	-3.4000
H	-1.1155	-5.8708	-3.4000
H	-3.4849	-5.8435	-3.4000
H	-5.4487	-3.0070	-4.2802
H	-5.5911	-4.5522	-3.4000
H	-5.4487	-3.0070	-2.5198

[F]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3824	0.0000	0.0000
N	1.9198	1.2821	0.0000
C	1.1623	2.4348	0.0000
C	-0.1930	2.4166	0.0000
C	-0.8697	1.1141	0.0000
O	-2.0844	0.9504	0.0000
O	2.0784	-1.0087	0.0000
C	-1.0448	3.6507	0.0000
H	-0.4427	-0.9197	0.0000
H	2.9326	1.3218	0.0000
H	1.7329	3.3622	0.0000
H	-1.7025	3.6679	-0.8798
H	-0.4297	4.5588	0.0000
H	-1.7025	3.6679	0.8798
C	1.0511	-4.2605	0.0000
C	1.6938	-5.4935	0.0000
C	1.0011	-6.6973	0.0000
C	-0.3958	-6.6593	0.0000
C	-1.1085	-5.4523	0.0000
C	-0.3358	-4.2887	0.0000
F	-0.9975	-3.0848	0.0000
F	3.0542	-5.5151	0.0000
C	-2.6141	-5.3896	0.0000
H	1.5958	-3.3169	0.0000
H	1.5482	-7.6376	0.0000
H	-0.9539	-7.5963	0.0000
H	-2.9925	-4.8547	0.8822
H	-3.0418	-6.3988	0.0000
H	-2.9925	-4.8547	-0.8822
N	0.0000	0.0000	3.4000
C	1.3803	0.0000	3.4000
N	1.9329	1.2821	3.4000
C	1.1850	2.4356	3.4000
C	-0.1727	2.4185	3.4000
C	-0.8351	1.1131	3.4000
O	-2.0703	0.9768	3.4000
O	2.0744	-1.0101	3.4000
C	-1.0218	3.6548	3.4000
H	-0.4632	-0.9615	3.4000
H	2.9462	1.3129	3.4000
H	1.7568	3.3622	3.4000
H	-1.6788	3.6765	4.2802
H	-0.4036	4.5607	3.4000
H	-1.6788	3.6765	2.5198
N	-1.2166	-2.5267	3.4000
C	-0.4216	-3.6157	3.4000
N	-0.7827	-4.9006	3.4000
C	-2.1198	-5.0267	3.4000
C	-3.0702	-3.9971	3.4000
C	-2.5656	-2.6749	3.4000
N	-2.8680	-6.1846	3.4000
C	-4.1955	-5.8041	3.4000
N	-4.3612	-4.4987	3.4000

N	-3.3478	-1.5837	3.4000
H	0.6476	-3.4015	3.4000
H	-2.4969	-7.1272	3.4000
H	-4.9948	-6.5368	3.4000
H	-4.3508	-1.7080	3.4000
H	-2.9308	-0.6392	3.4000

[A]-G/C-G

N	0.0000	0.0000	0.0000
C	1.3475	0.0000	0.0000
N	2.1960	1.0271	0.0000
C	1.5298	2.1951	0.0000
C	0.1429	2.3705	0.0000
C	-0.6533	1.1974	0.0000
N	2.0408	3.4745	0.0000
C	0.9606	4.3351	0.0000
N	-0.1976	3.7114	0.0000
N	-1.9891	1.2350	0.0000
H	1.8213	-0.9856	0.0000
H	3.0237	3.7200	0.0000
H	1.0931	5.4115	0.0000
H	-2.4341	2.1440	0.0000
H	-2.5693	0.3702	0.0000
N	-1.6981	-2.4111	0.0000
C	-1.0849	-3.6357	0.0000
N	-1.7258	-4.7909	0.0000
C	-3.0665	-4.6283	0.0000
C	-3.8115	-3.4411	0.0000
C	-3.1001	-2.1988	0.0000
N	-4.0045	-5.6297	0.0000
C	-5.2477	-5.0153	0.0000
N	-5.1698	-3.7071	0.0000
O	-3.5502	-1.0435	0.0000
N	0.2770	-3.6396	0.0000
H	-1.1016	-1.5489	0.0000
H	-3.8031	-6.6225	0.0000
H	-6.1647	-5.5940	0.0000
H	0.7494	-4.5313	0.0000
H	0.8088	-2.7834	0.0000
N	0.2684	-3.6440	3.4000
O	-3.5242	-1.0132	3.4000
N	-1.6981	-2.4111	3.4000
C	-1.0825	-3.6406	3.4000
N	-1.7492	-4.7903	3.4000
C	-3.0836	-4.6072	3.4000
C	-3.8189	-3.4100	3.4000
C	-3.0874	-2.1822	3.4000
N	-4.0358	-5.5976	3.4000
C	-5.2730	-4.9694	3.4000
N	-5.1815	-3.6620	3.4000
H	0.8311	-2.7798	3.4000
H	0.7203	-4.5472	3.4000
H	-1.1003	-1.5522	3.4000
H	-3.8449	-6.5922	3.4000
H	-6.1958	-5.5381	3.4000
O	1.8444	-1.2509	3.4000
N	-2.0061	1.2528	3.4000
N	-0.0968	-0.0160	3.4000
C	0.1211	2.4059	3.4000
C	1.2521	-0.1605	3.4000
N	2.0279	1.0203	3.4000
C	1.4721	2.2623	3.4000
C	-0.6703	1.2000	3.4000
H	-0.3385	3.3905	3.4000
H	3.0340	0.8872	3.4000
H	2.1597	3.1046	3.4000
H	-2.5814	0.3690	3.4000
H	-2.4698	2.1507	3.4000

[T]-G/C-G

N	0.0000	0.0000	0.0000
C	1.3645	0.0000	0.0000
N	1.9446	1.2537	0.0000

C	1.2195	2.4302	0.0000
C	-0.1332	2.4353	0.0000
C	-0.8380	1.1432	0.0000
O	-2.0548	1.0235	0.0000
O	2.0757	-1.0226	0.0000
C	-0.9644	3.6821	0.0000
H	-0.4724	-0.9442	0.0000
H	2.9578	1.2631	0.0000
H	1.8150	3.3416	0.0000
H	-1.6228	3.7059	-0.8791
H	-0.3368	4.5817	0.0000
H	-1.6228	3.7059	0.8791
N	0.9140	-3.5498	0.0000
C	1.7498	-4.6330	0.0000
N	1.3341	-5.8872	0.0000
C	-0.0148	-5.9730	0.0000
C	-0.9707	-4.9452	0.0000
C	-0.5002	-3.5926	0.0000
N	-0.7497	-7.1317	0.0000
C	-2.0860	-6.7610	0.0000
N	-2.2545	-5.4616	0.0000
O	-1.1431	-2.5315	0.0000
N	3.0855	-4.3684	0.0000
H	1.3259	-2.5928	0.0000
H	-0.3661	-8.0692	0.0000
H	-2.8784	-7.5012	0.0000
H	3.7250	-5.1491	0.0000
H	3.4357	-3.4215	0.0000
N	3.0904	-4.3706	3.4000
O	-1.1431	-2.5315	3.4000
N	0.9209	-3.5456	3.4000
C	1.7649	-4.6312	3.4000
N	1.3356	-5.8889	3.4000
C	-0.0089	-5.9701	3.4000
C	-0.9638	-4.9397	3.4000
C	-0.4863	-3.5926	3.4000
N	-0.7491	-7.1275	3.4000
C	-2.0852	-6.7531	3.4000
N	-2.2509	-5.4530	3.4000
H	3.4734	-3.4131	3.4000
H	3.7101	-5.1681	3.4000
H	1.3393	-2.5865	3.4000
H	-0.3676	-8.0656	3.4000
H	-2.8792	-7.4912	3.4000
O	4.1685	-1.7157	3.4000
N	-0.0970	-0.0126	3.4000
N	2.0234	-0.8838	3.4000
C	1.7639	1.5339	3.4000
C	3.3745	-0.7620	3.4000
N	3.9047	0.5476	3.4000
C	3.1170	1.6571	3.4000
C	1.2233	0.1967	3.4000
H	1.1208	2.4098	3.4000
H	4.9174	0.6137	3.4000
H	3.6267	2.6175	3.4000
H	-0.4886	-0.9917	3.4000
H	-0.7271	0.7775	3.4000

[G]-G/C-G

N	0.0000	0.0000	0.0000
C	1.3746	0.0000	0.0000
N	2.1003	1.1024	0.0000
C	1.3449	2.2224	0.0000
C	-0.0477	2.3424	0.0000
C	-0.8432	1.1544	0.0000
N	1.8038	3.5171	0.0000
C	0.6957	4.3429	0.0000
N	-0.4325	3.6694	0.0000
O	-2.0621	1.0075	0.0000
N	2.0031	-1.2053	0.0000
H	-0.5191	-0.8760	0.0000
H	2.7779	3.7967	0.0000
H	0.7889	5.4226	0.0000

H	3.0134	-1.2077	0.0000
H	1.5053	-2.0822	0.0000
N	-4.5924	2.4956	0.0000
C	-4.5880	3.8656	0.0000
N	-5.6910	4.6016	0.0000
C	-6.8122	3.8473	0.0000
C	-6.9485	2.4538	0.0000
C	-5.7552	1.6478	0.0000
N	-8.1014	4.3250	0.0000
C	-8.9400	3.2209	0.0000
N	-8.2836	2.0858	0.0000
O	-5.6182	0.4302	0.0000
N	-3.3877	4.5032	0.0000
H	-3.6985	1.9879	0.0000
H	-8.3624	5.3033	0.0000
H	-10.0190	3.3288	0.0000
H	-3.4281	5.5123	0.0000
H	-2.4737	4.0494	0.0000
N	-3.3797	4.4747	-3.4000
O	-5.6059	0.4313	-3.4000
N	-4.5924	2.4956	-3.4000
C	-4.5880	3.8706	-3.4000
N	-5.6966	4.6036	-3.4000
C	-6.8103	3.8460	-3.4000
C	-6.9362	2.4467	-3.4000
C	-5.7348	1.6725	-3.4000
N	-8.1036	4.3094	-3.4000
C	-8.9322	3.1964	-3.4000
N	-8.2686	2.0661	-3.4000
H	-2.4913	3.9510	-3.4000
H	-3.3769	5.4846	-3.4000
H	-3.6749	1.9923	-3.4000
H	-8.3752	5.2851	-3.4000
H	-10.0117	3.2951	-3.4000
O	-0.9036	3.0326	-3.4000
N	-3.2382	-0.9227	-3.4000
N	-2.0927	1.0630	-3.4000
C	-0.8201	-1.0091	-3.4000
C	-0.9490	1.7925	-3.4000
N	0.2711	1.0802	-3.4000
C	0.3260	-0.2794	-3.4000
C	-2.0654	-0.2812	-3.4000
H	-0.7937	-2.0954	-3.4000
H	1.1130	1.6469	-3.4000
H	1.3164	-0.7279	-3.4000
H	-4.1467	-0.3872	-3.4000
H	-3.2540	-1.9332	-3.4000

[C]-G/C-G

N	-0.1956	-3.1483	-1.7000
O	-0.8586	1.4196	-1.7000
N	-0.6354	-0.8692	-1.7000
C	-1.1145	-2.1581	-1.7000
N	-2.4100	-2.4547	-1.7000
C	-3.1863	-1.3539	-1.7000
C	-2.8124	0.0003	-1.7000
C	-1.4156	0.3028	-1.7000
N	-4.5601	-1.3332	-1.7000
C	-4.9445	0.0000	-1.7000
N	-3.9260	0.8249	-1.7000
H	0.8201	-2.9703	-1.7000
H	-0.5479	-4.0948	-1.7000
H	0.4005	-0.7205	-1.7000
H	-5.1572	-2.1512	-1.7000
H	-5.9899	0.2870	-1.7000
O	2.6293	-2.6685	-1.7000
N	1.8339	1.8550	-1.7000
N	2.2083	-0.4066	-1.7000
C	4.1281	1.0860	-1.7000
C	3.0227	-1.4916	-1.7000
N	4.4154	-1.2536	-1.7000
C	4.9445	0.0000	-1.7000
C	2.7064	0.8422	-1.7000

H	4.5346	2.0937	-1.7000
H	5.0043	-2.0800	-1.7000
H	6.0295	0.0718	-1.7000
H	0.7952	1.6730	-1.7000
H	2.1743	2.8065	-1.7000
N	-0.1956	-3.1483	1.7000
O	-0.8586	1.4196	1.7000
N	-0.6354	-0.8692	1.7000
C	-1.1145	-2.1581	1.7000
N	-2.4100	-2.4547	1.7000
C	-3.1863	-1.3539	1.7000
C	-2.8124	0.0003	1.7000
C	-1.4156	0.3028	1.7000
N	-4.5601	-1.3332	1.7000
C	-4.9445	0.0000	1.7000
N	-3.9260	0.8249	1.7000
H	0.8201	-2.9703	1.7000
H	-0.5479	-4.0948	1.7000
H	0.4005	-0.7205	1.7000
H	-5.1572	-2.1512	1.7000
H	-5.9899	0.2870	1.7000
O	2.6293	-2.6685	1.7000
N	1.8339	1.8550	1.7000
N	2.2083	-0.4066	1.7000
C	4.1281	1.0860	1.7000
C	3.0227	-1.4916	1.7000
N	4.4154	-1.2536	1.7000
C	4.9445	0.0000	1.7000
C	2.7064	0.8422	1.7000
H	4.5346	2.0937	1.7000
H	5.0043	-2.0800	1.7000
H	6.0295	0.0718	1.7000
H	0.7952	1.6730	1.7000
H	2.1743	2.8065	1.7000

[F]-G/C-G

N	0.0000	0.0000	0.0000
O	4.6271	0.0000	0.0000
N	2.3312	0.1136	0.0000
C	1.1260	0.7673	0.0000
N	1.0107	2.0805	0.0000
C	2.2134	2.7022	0.0000
C	3.5023	2.1505	0.0000
C	3.6331	0.7204	0.0000
N	2.4147	4.0593	0.0000
C	3.7857	4.2630	0.0000
N	4.4660	3.1426	0.0000
H	0.0327	-1.0080	0.0000
H	-0.8918	0.4731	0.0000
H	2.3507	-0.9061	0.0000
H	1.6833	4.7602	0.0000
H	4.2100	5.2608	0.0000
C	4.5162	-3.3009	0.0000
C	3.2398	-3.8420	0.0000
C	2.9806	-5.2026	0.0000
C	4.0762	-6.0722	0.0000
C	5.3961	-5.6038	0.0000
C	5.5640	-4.2141	0.0000
F	6.8320	-3.7256	0.0000
F	2.1638	-2.9714	0.0000
C	6.5903	-6.5220	0.0000
H	4.6926	-2.2225	0.0000
H	1.9565	-5.5690	0.0000
H	3.9003	-7.1484	0.0000
H	7.2232	-6.3510	-0.8818
H	6.2736	-7.5713	0.0000
H	7.2232	-6.3510	0.8818
N	0.0000	0.0000	3.4000
O	4.6271	0.0000	3.4000
N	2.3300	0.1078	3.4000
C	1.1163	0.7607	3.4000
N	1.0165	2.0860	3.4000
C	2.2208	2.6893	3.4000

C	3.5040	2.1173	3.4000
C	3.6020	0.7116	3.4000
N	2.4464	4.0445	3.4000
C	3.8221	4.2256	3.4000
N	4.4856	3.0953	3.4000
H	0.0243	-1.0310	3.4000
H	-0.8833	0.4897	3.4000
H	2.3284	-0.9386	3.4000
H	1.7267	4.7571	3.4000
H	4.2619	5.2164	3.4000
O	0.0525	-2.8649	3.4000
N	4.6713	-2.7271	3.4000
N	2.3794	-2.7729	3.4000
C	3.5807	-4.8870	3.4000
C	1.1575	-3.4296	3.4000
N	1.1850	-4.8422	3.4000
C	2.3887	-5.5391	3.4000
C	3.5437	-3.4451	3.4000
H	4.5196	-5.4341	3.4000
H	0.2798	-5.3011	3.4000
H	2.3039	-6.6230	3.4000
H	4.6403	-1.6730	3.4000
H	5.5641	-3.2007	3.4000

[revA]-G/C-G

N	0.0000	0.0000	0.0000
O	4.6244	0.0000	0.0000
N	2.3289	0.1258	0.0000
C	1.1134	0.7662	0.0000
N	1.0131	2.0907	0.0000
C	2.2219	2.7110	0.0000
C	3.5081	2.1565	0.0000
C	3.6408	0.7250	0.0000
N	2.4316	4.0686	0.0000
C	3.8049	4.2666	0.0000
N	4.4766	3.1428	0.0000
H	0.0812	-1.0057	0.0000
H	-0.9487	0.4210	0.0000
H	2.3626	-0.8908	0.0000
H	1.7159	4.7839	0.0000
H	4.2325	5.2629	0.0000
N	-3.6410	4.5751	0.0000
C	-4.9583	4.3271	0.0000
N	-5.5902	3.1439	0.0000
C	-4.7102	2.1366	0.0000
C	-3.3103	2.2258	0.0000
C	-2.7739	3.5371	0.0000
N	-4.9758	0.7810	0.0000
C	-3.7676	0.1310	0.0000
N	-2.7408	0.9587	0.0000
N	-1.4556	3.8152	0.0000
H	-5.6008	5.2089	0.0000
H	-5.8983	0.3621	0.0000
H	-3.7006	-0.9512	0.0000
H	-0.7074	3.1076	0.0000
H	-1.2177	4.7991	0.0000
N	0.0000	0.0000	3.4000
O	4.6244	0.0000	3.4000
N	2.3272	0.1078	3.4000
C	1.1128	0.7658	3.4000
N	1.0070	2.0906	3.4000
C	2.2085	2.6993	3.4000
C	3.4943	2.1332	3.4000
C	3.5992	0.7116	3.4000
N	2.4280	4.0556	3.4000
C	3.8028	4.2429	3.4000
N	4.4715	3.1157	3.4000
H	0.0290	-1.0309	3.4000
H	-0.8855	0.4857	3.4000
H	2.3256	-0.9386	3.4000
H	1.7051	4.7649	3.4000
H	4.2382	5.2357	3.4000
O	0.0656	-2.8646	3.4000

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N                4.6685   -2.7271    3.4000
N                2.3766   -2.7729    3.4000
C                3.5780   -4.8870    3.4000
C                1.1731   -3.4243    3.4000
N                1.2070   -4.8368    3.4000
C                2.3860   -5.5391    3.4000
C                3.5410   -3.4451    3.4000
H                4.5168   -5.4341    3.4000
H                0.3039   -5.2998    3.4000
H                2.3012   -6.6230    3.4000
H                4.6376   -1.6730    3.4000
H                5.5613   -3.2007    3.4000

[revT]-G/C-G
N                0.0000    0.0000    0.0000
O                4.6039    0.0000    0.0000
N                2.3142    0.1196    0.0000
C                1.1165    0.7790    0.0000
N                0.9967    2.0954    0.0000
C                2.2001    2.7105    0.0000
C                3.4870    2.1486    0.0000
C                3.5917    0.7205    0.0000
N                2.4127    4.0661    0.0000
C                3.7860    4.2587    0.0000
N                4.4585    3.1341    0.0000
H                0.0638   -1.0081    0.0000
H               -0.9002    0.4558    0.0000
H                2.3134   -0.9262    0.0000
H                1.6870    4.7727    0.0000
H                4.2175    5.2535    0.0000
N                4.4911   -2.7651    0.0000
C                5.7039   -3.4429    0.0000
N                5.5521   -4.8351    0.0000
C                4.3418   -5.4765    0.0000
C                3.1658   -4.7968    0.0000
C                3.2291   -3.3399    0.0000
O                2.2019   -2.6280    0.0000
O                6.8000   -2.9118    0.0000
C                1.8203   -5.4603    0.0000
H                4.5523   -1.7076    0.0000
H                6.4230   -5.3546    0.0000
H                4.3860   -6.5647    0.0000
H                1.2363   -5.1614    0.8814
H                1.9189   -6.5527    0.0000
H                1.2363   -5.1614   -0.8814
N                0.0000    0.0000    3.4000
O                4.6039    0.0000    3.4000
N                2.3068    0.1078    3.4000
C                1.1079    0.7730    3.4000
N                0.9935    2.0970    3.4000
C                2.1911    2.7135    3.4000
C                3.4805    2.1557    3.4000
C                3.5787    0.7116    3.4000
N                2.4018    4.0711    3.4000
C                3.7754    4.2673    3.4000
N                4.4514    3.1444    3.4000
H                0.0356   -1.0306    3.4000
H               -0.8886    0.4799    3.4000
H                2.3051   -0.9386    3.4000
H                1.6744    4.7757    3.4000
H                4.2044    5.2629    3.4000
O                0.0840   -2.8642    3.4000
N                4.6481   -2.7271    3.4000
N                2.3562   -2.7729    3.4000
C                3.5575   -4.8870    3.4000
C                1.1951   -3.4167    3.4000
N                1.2381   -4.8289    3.4000
C                2.3655   -5.5391    3.4000
C                3.5205   -3.4451    3.4000
H                4.4964   -5.4341    3.4000
H                0.3380   -5.2978    3.4000
H                2.2807   -6.6230    3.4000
H                4.6171   -1.6730    3.4000
```

```
H                5.5409   -3.2007    3.4000

[revG]-G/C-G
N                0.0000    0.0000    0.0000
O                4.5983    0.0000    0.0000
N                2.3072    0.1196    0.0000
C                1.1089    0.7826    0.0000
N                0.9926    2.1018    0.0000
C                2.1947    2.7126    0.0000
C                3.4805    2.1445    0.0000
C                3.5752    0.7209    0.0000
N                2.4160    4.0669    0.0000
C                3.7904    4.2523    0.0000
N                4.4581    3.1250    0.0000
H                0.0738   -1.0098    0.0000
H               -0.9039    0.4486    0.0000
H                2.2674   -0.9358    0.0000
H                1.6945    4.7780    0.0000
H                4.2267    5.2450    0.0000
N                4.2785   -2.6981    0.0000
C                5.4768   -3.3610    0.0000
N                5.5930   -4.6802    0.0000
C                4.3908   -5.2910    0.0000
C                3.1051   -4.7230    0.0000
C                3.0104   -3.2994    0.0000
N                4.1697   -6.6454    0.0000
C                2.7953   -6.8308    0.0000
N                2.1274   -5.7034    0.0000
O                1.9873   -2.5785    0.0000
N                6.5856   -2.5785    0.0000
H                4.3182   -1.6427    0.0000
H                4.8911   -7.3565    0.0000
H                2.3589   -7.8235    0.0000
H                7.4894   -3.0271    0.0000
H                6.5118   -1.5687    0.0000
N                0.0000    0.0000    3.4000
O                4.5983    0.0000    3.4000
N                2.3011    0.1078    3.4000
C                1.1037    0.7789    3.4000
N                0.9822    2.1024    3.4000
C                2.1764    2.7253    3.4000
C                3.4688    2.1745    3.4000
C                3.5731    0.7116    3.4000
N                2.3798    4.0841    3.4000
C                3.7523    4.2876    3.4000
N                4.4343    3.1684    3.4000
H                0.0412   -1.0304    3.4000
H               -0.8912    0.4751    3.4000
H                2.2995   -0.9386    3.4000
H                1.6485    4.7847    3.4000
H                4.1759    5.2855    3.4000
O                0.0995   -2.8637    3.4000
N                4.6424   -2.7271    3.4000
N                2.3505   -2.7729    3.4000
C                3.5519   -4.8870    3.4000
C                1.2136   -3.4102    3.4000
N                1.2642   -4.8221    3.4000
C                2.3599   -5.5391    3.4000
C                3.5148   -3.4451    3.4000
H                4.4907   -5.4341    3.4000
H                0.3667   -5.2958    3.4000
H                2.2751   -6.6230    3.4000
H                4.6115   -1.6730    3.4000
H                5.5352   -3.2007    3.4000

[revC]-G/C-G
N                0.0000    0.0000    0.0000
O                4.6335    0.0000    0.0000
N                2.3311    0.1003    0.0000
C                1.1309    0.7576    0.0000
N                1.0125    2.0768    0.0000
C                2.2153    2.6958    0.0000
C                3.5017    2.1426    0.0000
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C	3.6335	0.7073	0.0000
N	2.4186	4.0553	0.0000
C	3.7902	4.2573	0.0000
N	4.4675	3.1346	0.0000
H	-0.0008	-1.0190	0.0000
H	-0.8732	0.5062	0.0000
H	2.3217	-0.9280	0.0000
H	1.6878	4.7562	0.0000
H	4.2162	5.2544	0.0000
N	-0.3535	-3.1429	0.0000
C	0.9522	-3.5490	0.0000
N	1.1908	-4.9465	0.0000
C	0.1960	-5.8661	0.0000
C	-1.1036	-5.4602	0.0000
C	-1.3334	-4.0427	0.0000
N	-2.6048	-3.5742	0.0000
O	1.9231	-2.7931	0.0000
H	2.1698	-5.2187	0.0000
H	0.4922	-6.9126	0.0000
H	-1.9180	-6.1794	0.0000
H	-2.7586	-2.5745	0.0000
H	-3.3990	-4.1964	0.0000
N	0.0000	0.0000	3.4000
O	4.6335	0.0000	3.4000
N	2.3363	0.1078	3.4000
C	1.1223	0.7518	3.4000
N	1.0331	2.0778	3.4000
C	2.2421	2.6715	3.4000
C	3.5207	2.0893	3.4000
C	3.6083	0.7116	3.4000
N	2.4785	4.0249	3.4000
C	3.8556	4.1950	3.4000
N	4.5101	3.0595	3.4000
H	0.0161	-1.0311	3.4000
H	-0.8794	0.4967	3.4000
H	2.3347	-0.9386	3.4000
H	1.7645	4.7432	3.4000
H	4.3033	5.1823	3.4000
O	0.0297	-2.8652	3.4000
N	4.6776	-2.7271	3.4000
N	2.3857	-2.7729	3.4000
C	3.5871	-4.8870	3.4000
C	1.1302	-3.4387	3.4000
N	1.1464	-4.8515	3.4000
C	2.3951	-5.5391	3.4000
C	3.5501	-3.4451	3.4000
H	4.5259	-5.4341	3.4000
H	0.2376	-5.3032	3.4000
H	2.3103	-6.6230	3.4000
H	4.6467	-1.6730	3.4000
H	5.5704	-3.2007	3.4000

[A]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3553	0.0000	0.0000
N	2.1739	1.0558	0.0000
C	1.4926	2.2078	0.0000
C	0.1005	2.3671	0.0000
C	-0.6555	1.1775	0.0000
N	1.9833	3.4967	0.0000
C	0.8919	4.3415	0.0000
N	-0.2599	3.7051	0.0000
N	-2.0114	1.1952	0.0000
H	1.8114	-0.9924	0.0000
H	2.9632	3.7543	0.0000
H	1.0104	5.4197	0.0000
H	-2.4991	2.0799	0.0000
H	-2.5311	0.3300	0.0000
N	1.4567	-3.3550	0.0000
C	2.5059	-4.2323	0.0000
N	2.1664	-5.6247	0.0000
C	0.8896	-6.0794	0.0000
C	-0.1447	-5.1953	0.0000

C	0.2020	-3.7953	0.0000
N	-0.7838	-2.8682	0.0000
O	3.6939	-3.9282	0.0000
H	2.9572	-6.2608	0.0000
H	0.7484	-7.1586	0.0000
H	-1.1768	-5.5364	0.0000
H	-0.5554	-1.8580	0.0000
H	-1.7482	-3.1661	0.0000
N	4.3294	-1.1341	-3.4000
O	-0.1920	-0.2057	-3.4000
N	2.0799	-0.5621	-3.4000
C	3.3945	-0.1590	-3.4000
N	3.7662	1.1170	-3.4000
C	2.7126	1.9562	-3.4000
C	1.3389	1.6620	-3.4000
C	0.9554	0.2851	-3.4000
N	2.7721	3.3288	-3.4000
C	1.4636	3.7904	-3.4000
N	0.5807	2.8218	-3.4000
H	4.0924	-2.1378	-3.4000
H	5.2949	-0.8376	-3.4000
H	1.8710	-1.5875	-3.4000
H	3.6236	3.8772	-3.4000
H	1.2381	4.8508	-3.4000
O	3.6856	-3.9262	-3.4000
N	-0.7838	-2.8682	-3.4000
N	1.4521	-3.3740	-3.4000
C	-0.1499	-5.2033	-3.4000
C	2.4878	-4.2503	-3.4000
N	2.1689	-5.6267	-3.4000
C	0.8866	-6.0818	-3.4000
C	0.1764	-3.7983	-3.4000
H	-1.1796	-5.5504	-3.4000
H	2.9596	-6.2628	-3.4000
H	0.7516	-7.1607	-3.4000
H	-0.5414	-1.8419	-3.4000
H	-1.7536	-3.1525	-3.4000

[T]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3916	0.0000	0.0000
N	1.9362	1.2914	0.0000
C	1.1951	2.4442	0.0000
C	-0.1615	2.4251	0.0000
C	-0.8237	1.1227	0.0000
O	-2.0623	1.0108	0.0000
O	2.0959	-0.9918	0.0000
C	-1.0133	3.6598	0.0000
H	-0.4708	-0.9377	0.0000
H	2.9497	1.3168	0.0000
H	1.7667	3.3714	0.0000
H	-1.6702	3.6818	-0.8804
H	-0.3949	4.5660	0.0000
H	-1.6702	3.6818	0.8804
N	-1.6162	-2.5465	0.0000
C	-0.9404	-3.7427	0.0000
N	-1.7466	-4.9247	0.0000
C	-3.1013	-4.9066	0.0000
C	-3.7600	-3.7178	0.0000
C	-2.9541	-2.5223	0.0000
N	-3.5582	-1.3207	0.0000
O	0.2758	-3.8727	0.0000
H	-1.2243	-5.7948	0.0000
H	-3.6100	-5.8687	0.0000
H	-4.8457	-3.6734	0.0000
H	-2.9919	-0.4514	0.0000
H	-4.5661	-1.2655	0.0000
N	1.8440	-1.3965	-3.4000
O	-2.1075	0.9890	-3.4000
N	-0.0852	-0.1059	-3.4000
C	1.2886	-0.1651	-3.4000
N	2.0651	0.9134	-3.4000
C	1.3525	2.0564	-3.4000

C	-0.0406	2.2379	-3.4000
C	-0.8621	1.0683	-3.4000
N	1.8671	3.3303	-3.4000
C	0.7879	4.2025	-3.4000
N	-0.3679	3.5844	-3.4000
H	1.2854	-2.2633	-3.4000
H	2.8530	-1.4396	-3.4000
H	-0.6246	-1.0026	-3.4000
H	2.8528	3.5627	-3.4000
H	0.9296	5.2772	-3.4000
O	0.3045	-3.8132	-3.4000
N	-3.5547	-1.3229	-3.4000
N	-1.6162	-2.5465	-3.4000
C	-3.7373	-3.7356	-3.4000
C	-0.9328	-3.7185	-3.4000
N	-1.6932	-4.9092	-3.4000
C	-3.0539	-4.9099	-3.4000
C	-2.9604	-2.5203	-3.4000
H	-4.8238	-3.7188	-3.4000
H	-1.1604	-5.7730	-3.4000
H	-3.5415	-5.8817	-3.4000
H	-2.9834	-0.4365	-3.4000
H	-4.5637	-1.2669	-3.4000

[C]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3679	0.0000	0.0000
N	1.9982	1.2853	0.0000
C	1.3107	2.4567	0.0000
C	-0.0490	2.4476	0.0000
C	-0.6694	1.1489	0.0000
N	-2.0234	1.0683	0.0000
O	2.0883	-0.9951	0.0000
H	3.0127	1.2654	0.0000
H	1.8985	3.3730	0.0000
H	-0.6410	3.3594	0.0000
H	-2.4148	0.1350	0.0000
H	-2.6350	1.8855	0.0000
N	-4.2494	3.2962	0.0000
C	-3.6834	4.5452	0.0000
N	-4.5842	5.6485	0.0000
C	-5.9316	5.5101	0.0000
C	-6.4856	4.2668	0.0000
C	-5.5715	3.1582	0.0000
N	-6.0648	1.8953	0.0000
O	-2.4780	4.7743	0.0000
H	-4.1446	6.5640	0.0000
H	-6.5223	6.4237	0.0000
H	-7.5634	4.1295	0.0000
H	-5.4209	1.1156	0.0000
H	-7.0572	1.7143	0.0000
N	-0.7045	2.4421	3.4000
O	-4.4407	-0.2682	3.4000
N	-2.5179	0.9934	3.4000
C	-1.1541	1.1682	3.4000
N	-0.2893	0.1591	3.4000
C	-0.9030	-1.0399	3.4000
C	-2.2758	-1.3383	3.4000
C	-3.1930	-0.2422	3.4000
N	-0.2828	-2.2659	3.4000
C	-1.2845	-3.2260	3.4000
N	-2.4883	-2.7076	3.4000
H	-1.3342	3.2587	3.4000
H	0.2973	2.5701	3.4000
H	-3.1311	1.8414	3.4000
H	0.7190	-2.4143	3.4000
H	-1.0527	-4.2850	3.4000
O	-2.4423	4.7203	3.4000
N	-6.0777	1.9134	3.4000
N	-4.2494	3.2962	3.4000
C	-6.4632	4.3021	3.4000
C	-3.6672	4.5216	3.4000
N	-4.5253	5.6440	3.4000

C	-5.8812	5.5298	3.4000
C	-5.5866	3.1567	3.4000
H	-7.5444	4.1936	3.4000
H	-4.0673	6.5496	3.4000
H	-6.4491	6.4570	3.4000
H	-5.4337	1.0783	3.4000
H	-7.0785	1.7725	3.4000

[F]-C/G-C

O	0.0000	0.0000	0.0000
N	4.5953	0.0000	0.0000
N	2.3083	0.0411	0.0000
C	3.4424	-2.1198	0.0000
C	1.0830	-0.5721	0.0000
N	1.0946	-2.0044	0.0000
C	2.2312	-2.7412	0.0000
C	3.4226	-0.6803	0.0000
H	4.3685	-2.6884	0.0000
H	0.1784	-2.4416	0.0000
H	2.1197	-3.8236	0.0000
H	4.5727	1.0147	0.0000
H	5.4822	-0.4802	0.0000
C	2.2468	3.5780	0.0000
C	1.2529	4.5521	0.0000
C	1.5386	5.9122	0.0000
C	2.8767	6.3127	0.0000
C	3.9286	5.3864	0.0000
C	3.5536	4.0415	0.0000
F	4.5668	3.1053	0.0000
F	-0.0446	4.1570	0.0000
C	5.3792	5.7953	0.0000
H	2.0184	2.5102	0.0000
H	0.7249	6.6342	0.0000
H	3.1156	7.3768	0.0000
H	5.9060	5.4068	0.8830
H	5.4710	6.8876	0.0000
H	5.9060	5.4068	-0.8830
O	0.0000	0.0000	3.4000
N	4.5953	0.0000	3.4000
N	2.3031	0.0229	3.4000
C	3.4406	-2.1263	3.4000
C	1.0973	-0.5796	3.4000
N	1.1056	-1.9924	3.4000
C	2.2297	-2.7424	3.4000
C	3.4468	-0.6839	3.4000
H	4.3627	-2.7012	3.4000
H	0.1944	-2.4391	3.4000
H	2.1125	-3.8233	3.4000
H	4.5960	1.0546	3.4000
H	5.4736	-0.5000	3.4000
N	-0.0139	2.8654	3.4000
O	4.6328	2.7272	3.4000
N	2.3399	2.9038	3.4000
C	1.1126	3.6110	3.4000
N	1.0307	4.9375	3.4000
C	2.2430	5.5244	3.4000
C	3.5184	4.9352	3.4000
C	3.6294	3.4692	3.4000
N	2.4869	6.8765	3.4000
C	3.8649	7.0390	3.4000
N	4.5131	5.8999	3.4000
H	-0.0035	1.8342	3.4000
H	-0.8905	3.3669	3.4000
H	2.3070	1.8578	3.4000
H	1.7769	7.5987	3.4000
H	4.3181	8.0238	3.4000

Table S5. Cartesian coordinates (in Å) of models 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 BP86/TZ2P (see text).

[A]-A/T-A			
N	0.0000	0.0000	0.0000
C	1.3527	0.0000	0.0000
N	2.1761	1.0527	0.0000
C	1.4952	2.2063	0.0000
C	0.1029	2.3664	0.0000
C	-0.6558	1.1777	0.0000
N	1.9866	3.4948	0.0000
C	0.8954	4.3403	0.0000
N	-0.2563	3.7043	0.0000
N	-2.0101	1.1928	0.0000
H	1.8055	-0.9941	0.0000
H	2.9663	3.7528	0.0000
H	1.0145	5.4184	0.0000
H	-2.5007	2.0759	0.0000
H	-2.5273	0.3256	0.0000
N	1.5699	-3.3792	0.0000
C	2.5486	-4.3006	0.0000
N	2.4506	-5.6368	0.0000
C	1.1652	-6.0203	0.0000
C	0.0369	-5.1907	0.0000
C	0.2835	-3.7973	0.0000
N	0.6503	-7.3008	0.0000
C	-0.7250	-7.1795	0.0000
N	-1.1359	-5.9295	0.0000
N	-0.7138	-2.8907	0.0000
H	3.5637	-3.8997	0.0000
H	1.1929	-8.1558	0.0000
H	-1.3706	-8.0511	0.0000
H	-1.6645	-3.2348	0.0000
H	-0.5205	-1.8771	0.0000
N	1.9287	-2.9508	3.4000
C	3.2701	-3.0866	3.4000
N	3.9852	-4.2135	3.4000
C	3.1860	-5.2928	3.4000
C	1.7849	-5.3124	3.4000
C	1.1380	-4.0538	3.4000
N	3.5480	-6.6231	3.4000
C	2.3783	-7.3569	3.4000
N	1.2960	-6.6083	3.4000
N	-0.1966	-3.9071	3.4000
H	3.8248	-2.1477	3.4000
H	4.4974	-6.9764	3.4000
H	2.3896	-8.4411	3.4000
H	-0.7740	-4.7367	3.4000
H	-0.6211	-2.9659	3.4000
N	0.8608	-0.3578	3.4000
C	1.7827	0.6695	3.4000
N	1.1976	1.9371	3.4000
C	-0.1605	2.1509	3.4000
C	-1.0545	1.1290	3.4000
C	-0.5254	-0.2358	3.4000
O	-1.2490	-1.2462	3.4000
O	2.9980	0.5114	3.4000
C	-2.5418	1.3228	3.4000
H	1.2670	-1.3447	3.4000
H	1.8515	2.7118	3.4000
H	-0.4682	3.1954	3.4000
H	-2.9967	0.8484	4.2802
H	-2.8031	2.3880	3.4000
H	-2.9967	0.8484	2.5198
[T]-A/T-A			
N	-0.5475	-0.7023	0.0000

C	-1.0248	-1.9633	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4092	0.3462	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9232	1.5977	0.0000
H	-0.2608	-2.7414	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5757	2.3696	0.0000
H	0.0957	1.7650	0.0000
N	2.2332	-0.3395	0.0000
C	2.9879	-1.4952	0.0000
N	4.3636	-1.2570	0.0000
C	4.9204	0.0000	0.0000
C	4.1638	1.1274	0.0000
C	2.7087	0.9683	0.0000
O	1.9192	1.9281	0.0000
O	2.5217	-2.6286	0.0000
C	4.7347	2.5143	0.0000
H	1.1749	-0.4774	0.0000
H	4.9433	-2.0886	0.0000
H	6.0089	0.0278	0.0000
H	4.3937	3.0763	0.8802
H	5.8313	2.4920	0.0000
H	4.3937	3.0763	-0.8802
N	-0.0301	-0.8900	3.4000
C	0.3250	-2.1907	3.4000
N	-0.4699	-3.2628	3.4000
C	-1.7642	-2.9046	3.4000
C	-2.2858	-1.6041	3.4000
C	-1.3435	-0.5482	3.4000
N	-2.8757	-3.7203	3.4000
C	-3.9807	-2.8922	3.4000
N	-3.6708	-1.6132	3.4000
N	-1.6860	0.7499	3.4000
H	1.4004	-2.3711	3.4000
H	-2.8645	-4.7333	3.4000
H	-4.9885	-3.2922	3.4000
H	-2.6676	0.9909	3.4000
H	-0.9601	1.4841	3.4000
N	2.0063	1.0380	3.4000
C	3.2961	0.5466	3.4000
N	4.2690	1.5479	3.4000
C	3.9807	2.8922	3.4000
C	2.7059	3.3595	3.4000
C	1.6222	2.3755	3.4000
O	0.4194	2.6879	3.4000
O	3.5851	-0.6444	3.4000
C	2.3526	4.8171	3.4000
H	1.2311	0.3044	3.4000
H	5.2269	1.2159	3.4000
H	4.8450	3.5544	3.4000
H	1.7464	5.0713	4.2802
H	3.2528	5.4436	3.4000
H	1.7464	5.0713	2.5198

[G]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3696	0.0000	0.0000
N	2.1155	1.0903	0.0000
C	1.3698	2.2163	0.0000
C	-0.0253	2.3509	0.0000
C	-0.8176	1.1585	0.0000
N	1.8453	3.5034	0.0000
C	0.7392	4.3399	0.0000
N	-0.3956	3.6845	0.0000
O	-2.0521	1.0437	0.0000
N	1.9828	-1.2160	0.0000
H	-0.5038	-0.9195	0.0000

H	2.8231	3.7679	0.0000
H	0.8460	5.4190	0.0000
H	2.9917	-1.2391	0.0000
H	1.4554	-2.0749	0.0000
N	-1.3956	-2.5980	0.0000
C	-0.7922	-3.8029	0.0000
N	-1.3307	-5.0214	0.0000
C	-2.6734	-4.9487	0.0000
C	-3.4512	-3.7871	0.0000
C	-2.7587	-2.5499	0.0000
N	-3.5885	-5.9785	0.0000
C	-4.8417	-5.3980	0.0000
N	-4.8026	-4.0831	0.0000
N	-3.3905	-1.3724	0.0000
H	0.3012	-3.7852	0.0000
H	-3.3680	-6.9672	0.0000
H	-5.7448	-5.9984	0.0000
H	-4.4025	-1.3815	0.0000
H	-2.8770	-0.4664	0.0000
N	-0.9069	-2.3448	3.4000
C	0.2902	-2.9653	3.4000
N	0.5397	-4.2764	3.4000
C	-0.6009	-4.9853	3.4000
C	-1.9107	-4.4873	3.4000
C	-2.0484	-3.0788	3.4000
N	-0.7545	-6.3554	3.4000
C	-2.1124	-6.6065	3.4000
N	-2.8427	-5.5118	3.4000
N	-3.2350	-2.4507	3.4000
H	1.1517	-2.2969	3.4000
H	-0.0022	-7.0337	3.4000
H	-2.5013	-7.6186	3.4000
H	-4.0774	-3.0092	3.4000
H	-3.2828	-1.4194	3.4000
N	-0.9442	0.4593	3.4000
C	0.2913	1.0746	3.4000
N	0.2145	2.4686	3.4000
C	-0.9693	3.1677	3.4000
C	-2.1769	2.5472	3.4000
C	-2.1879	1.0834	3.4000
O	-3.2329	0.4107	3.4000
O	1.3629	0.4798	3.4000
C	-3.4881	3.2753	3.4000
H	-0.9302	-0.6079	3.4000
H	1.1078	2.9478	3.4000
H	-0.8704	4.2521	3.4000
H	-4.0859	3.0019	4.2802
H	-3.3386	4.3619	3.4000
H	-4.0859	3.0019	2.5198

[C]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3676	0.0000	0.0000
N	2.0004	1.2859	0.0000
C	1.3125	2.4537	0.0000
C	-0.0480	2.4390	0.0000
C	-0.6801	1.1426	0.0000
N	-2.0310	1.0637	0.0000
O	2.0840	-0.9954	0.0000
H	3.0151	1.2666	0.0000
H	1.8965	3.3722	0.0000
H	-0.6210	3.3627	0.0000
H	-2.5038	0.1422	0.0000
H	-2.5799	1.9108	0.0000
N	-3.2696	-1.6394	0.0000
C	-2.2299	-2.5088	0.0000
N	-2.2791	-3.8439	0.0000
C	-3.5408	-4.2906	0.0000
C	-4.7110	-3.5199	0.0000
C	-4.5278	-2.1223	0.0000
N	-3.9912	-5.5942	0.0000
C	-5.3703	-5.5422	0.0000
N	-5.8457	-4.3151	0.0000

N	-5.5793	-1.2661	0.0000
H	-1.2434	-2.0401	0.0000
H	-3.4046	-6.4203	0.0000
H	-5.9710	-6.4453	0.0000
H	-6.5210	-1.6320	0.0000
H	-5.4231	-0.2690	0.0000
N	-2.9171	-1.2169	3.4000
C	-1.5719	-1.3086	3.4000
N	-0.8203	-2.4114	3.4000
C	-1.5836	-3.5164	3.4000
C	-2.9833	-3.5820	3.4000
C	-3.6712	-2.3452	3.4000
N	-1.1782	-4.8341	3.4000
C	-2.3233	-5.6059	3.4000
N	-3.4295	-4.8931	3.4000
N	-5.0098	-2.2423	3.4000
H	-1.0483	-0.3521	3.4000
H	-0.2177	-5.1561	3.4000
H	-2.2764	-6.6891	3.4000
H	-5.5598	-3.0904	3.4000
H	-5.4649	-1.3156	3.4000
N	-4.0694	1.3397	3.4000
C	-3.1817	2.3967	3.4000
N	-3.8080	3.6444	3.4000
C	-5.1724	3.8136	3.4000
C	-6.0324	2.7630	3.4000
C	-5.4589	1.4162	3.4000
O	-6.1489	0.3826	3.4000
O	-1.9618	2.2785	3.4000
C	-7.5252	2.9079	3.4000
H	-3.6311	0.3666	3.4000
H	-3.1799	4.4401	3.4000
H	-5.5141	4.8474	3.4000
H	-7.9644	2.4188	4.2802
H	-7.8213	3.9639	3.4000
H	-7.9644	2.4188	2.5198

[F]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3460	0.0000	0.0000
N	2.1849	1.0427	0.0000
C	1.5116	2.2018	0.0000
C	0.1202	2.3701	0.0000
C	-0.6475	1.1844	0.0000
N	2.0122	3.4871	0.0000
C	0.9265	4.3399	0.0000
N	-0.2290	3.7110	0.0000
N	-1.9985	1.1999	0.0000
H	1.8115	-0.9866	0.0000
H	2.9932	3.7394	0.0000
H	1.0527	5.4172	0.0000
H	-2.4865	2.0844	0.0000
H	-2.5175	0.3300	0.0000
C	-1.7547	-2.9334	0.0000
C	-1.2636	-4.2338	0.0000
C	-2.0924	-5.3480	0.0000
C	-3.4751	-5.1459	0.0000
C	-4.0404	-3.8631	0.0000
C	-3.1348	-2.8002	0.0000
F	-3.6500	-1.5237	0.0000
F	0.0857	-4.4153	0.0000
C	-5.5282	-3.6237	0.0000
H	-1.0985	-2.0589	0.0000
H	-1.6597	-6.3461	0.0000
H	-4.1397	-6.0105	0.0000
H	-5.8416	-3.0490	0.8828
H	-6.0716	-4.5756	0.0000
H	-5.8416	-3.0490	-0.8828
N	-0.0076	-0.5503	-3.4000
C	1.0832	-1.3428	-3.4000
N	2.3673	-0.9789	-3.4000
C	2.4904	0.3584	-3.4000
C	1.4587	1.3066	-3.4000

C	0.1377	0.7990	-3.4000
N	3.6467	1.1092	-3.4000
C	3.2633	2.4358	-3.4000
N	1.9575	2.5987	-3.4000
N	-0.9552	1.5788	-3.4000
H	0.8713	-2.4125	-3.4000
H	4.5901	0.7402	-3.4000
H	3.9942	3.2368	-3.4000
H	-0.8331	2.5821	-3.4000
H	-1.8989	1.1598	-3.4000
N	-2.5316	-1.7724	-3.4000
C	-2.5285	-3.1527	-3.4000
N	-3.8094	-3.7082	-3.4000
C	-4.9646	-2.9628	-3.4000
C	-4.9504	-1.6051	-3.4000
C	-3.6465	-0.9398	-3.4000
O	-3.5129	0.2957	-3.4000
O	-1.5169	-3.8446	-3.4000
C	-6.1886	-0.7587	-3.4000
H	-1.5711	-1.3071	-3.4000
H	-3.8379	-4.7216	-3.4000
H	-5.8899	-3.5367	-3.4000
H	-6.2118	-0.1018	-4.2802
H	-7.0932	-1.3789	-3.4000
H	-6.2118	-0.1018	-2.5198

[revA]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3470	0.0000	0.0000
N	2.1853	1.0391	0.0000
C	1.5089	2.1997	0.0000
C	0.1193	2.3672	0.0000
C	-0.6617	1.1863	0.0000
N	2.0104	3.4839	0.0000
C	0.9249	4.3374	0.0000
N	-0.2299	3.7070	0.0000
N	-2.0032	1.2023	0.0000
H	1.8121	-0.9875	0.0000
H	2.9916	3.7355	0.0000
H	1.0507	5.4146	0.0000
H	-2.4628	2.1034	0.0000
H	-2.5599	0.3227	0.0000
N	-3.5211	-1.2780	0.0000
C	-4.8681	-1.2780	0.0000
N	-5.7064	-2.3171	0.0000
C	-5.0300	-3.4777	0.0000
C	-3.6404	-3.6452	0.0000
C	-2.8594	-2.4643	0.0000
N	-5.5315	-4.7620	0.0000
C	-4.4460	-5.6154	0.0000
N	-3.2912	-4.9850	0.0000
N	-1.5180	-2.4803	0.0000
H	-5.3332	-0.2905	0.0000
H	-6.5127	-5.0135	0.0000
H	-4.5718	-6.6926	0.0000
H	-1.0583	-3.3814	0.0000
H	-0.9612	-1.6007	0.0000
N	-0.0076	-0.5503	-3.4000
C	1.0832	-1.3428	-3.4000
N	2.3673	-0.9789	-3.4000
C	2.4904	0.3584	-3.4000
C	1.4587	1.3066	-3.4000
C	0.1377	0.7990	-3.4000
N	3.6467	1.1092	-3.4000
C	3.2633	2.4358	-3.4000
N	1.9575	2.5987	-3.4000
N	-0.9552	1.5788	-3.4000
H	0.8713	-2.4125	-3.4000
H	4.5901	0.7402	-3.4000
H	3.9942	3.2368	-3.4000
H	-0.8331	2.5821	-3.4000
H	-1.8989	1.1598	-3.4000
N	-2.5316	-1.7724	-3.4000

C	-2.5285	-3.1527	-3.4000
N	-3.8094	-3.7082	-3.4000
C	-4.9646	-2.9628	-3.4000
C	-4.9504	-1.6051	-3.4000
C	-3.6465	-0.9398	-3.4000
O	-3.5129	0.2957	-3.4000
O	-1.5169	-3.8446	-3.4000
C	-6.1886	-0.7587	-3.4000
H	-1.5711	-1.3071	-3.4000
H	-3.8379	-4.7216	-3.4000
H	-5.8899	-3.5367	-3.4000
H	-6.2118	-0.1018	-4.2802
H	-7.0932	-1.3789	-3.4000
H	-6.2118	-0.1018	-2.5198

[revT]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3486	0.0000	0.0000
N	2.1720	1.0503	0.0000
C	1.4845	2.2035	0.0000
C	0.0927	2.3631	0.0000
C	-0.6754	1.1757	0.0000
N	1.9769	3.4911	0.0000
C	0.8864	4.3378	0.0000
N	-0.2648	3.7010	0.0000
N	-2.0188	1.1660	0.0000
H	1.8048	-0.9909	0.0000
H	2.9568	3.7477	0.0000
H	1.0059	5.4157	0.0000
H	-2.5092	2.0499	0.0000
H	-2.5360	0.2759	0.0000
N	-1.2849	-2.4947	0.0000
C	-2.6521	-2.4481	0.0000
N	-3.2639	-3.6929	0.0000
C	-2.5652	-4.8825	0.0000
C	-1.2109	-4.9231	0.0000
C	-0.4809	-3.6478	0.0000
O	0.7450	-3.5503	0.0000
O	-3.3201	-1.4057	0.0000
C	-0.4144	-6.1930	0.0000
H	-0.7830	-1.5537	0.0000
H	-4.2774	-3.6787	0.0000
H	-3.1798	-5.7813	0.0000
H	0.2426	-6.2376	-0.8795
H	-1.0676	-7.0743	0.0000
H	0.2426	-6.2376	0.8795
N	-0.0076	-0.5503	-3.4000
C	1.0832	-1.3428	-3.4000
N	2.3673	-0.9789	-3.4000
C	2.4904	0.3584	-3.4000
C	1.4587	1.3066	-3.4000
C	0.1377	0.7990	-3.4000
N	3.6467	1.1092	-3.4000
C	3.2633	2.4358	-3.4000
N	1.9575	2.5987	-3.4000
N	-0.9552	1.5788	-3.4000
H	0.8713	-2.4125	-3.4000
H	4.5901	0.7402	-3.4000
H	3.9942	3.2368	-3.4000
H	-0.8331	2.5821	-3.4000
H	-1.8989	1.1598	-3.4000
N	-2.5316	-1.7724	-3.4000
C	-2.5285	-3.1527	-3.4000
N	-3.8094	-3.7082	-3.4000
C	-4.9646	-2.9628	-3.4000
C	-4.9504	-1.6051	-3.4000
C	-3.6465	-0.9398	-3.4000
O	-3.5129	0.2957	-3.4000
O	-1.5169	-3.8446	-3.4000
C	-6.1886	-0.7587	-3.4000
H	-1.5711	-1.3071	-3.4000
H	-3.8379	-4.7216	-3.4000
H	-5.8899	-3.5367	-3.4000

H	-6.2118	-0.1018	-4.2802
H	-7.0932	-1.3789	-3.4000
H	-6.2118	-0.1018	-2.5198

[revG]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3405	0.0000	0.0000
N	2.1803	1.0458	0.0000
C	1.5019	2.1986	0.0000
C	0.1097	2.3698	0.0000
C	-0.6601	1.1805	0.0000
N	2.0137	3.4817	0.0000
C	0.9467	4.3440	0.0000
N	-0.2156	3.7205	0.0000
N	-2.0071	1.1511	0.0000
H	1.8087	-0.9855	0.0000
H	2.9977	3.7226	0.0000
H	1.0810	5.4199	0.0000
H	-2.6115	1.9848	0.0000
H	-2.4229	0.2281	0.0000
N	-5.0437	5.4769	0.0000
C	-3.9676	4.6227	0.0000
N	-4.1141	3.3026	0.0000
C	-5.4169	2.9166	0.0000
C	-6.5782	3.6995	0.0000
C	-6.4437	5.1308	0.0000
N	-5.8741	1.6212	0.0000
C	-7.2603	1.6807	0.0000
N	-7.7124	2.9094	0.0000
O	-7.2763	6.0253	0.0000
N	-2.7317	5.1697	0.0000
H	-4.8888	6.4822	0.0000
H	-5.3031	0.7858	0.0000
H	-7.8648	0.7807	0.0000
H	-1.8773	4.5805	0.0000
H	-2.6254	6.1731	0.0000
N	-0.0076	-0.5503	-3.4000
C	1.0832	-1.3428	-3.4000
N	2.3673	-0.9789	-3.4000
C	2.4904	0.3584	-3.4000
C	1.4587	1.3066	-3.4000
C	0.1377	0.7990	-3.4000
N	3.6467	1.1092	-3.4000
C	3.2633	2.4358	-3.4000
N	1.9575	2.5987	-3.4000
N	-0.9552	1.5788	-3.4000
H	0.8713	-2.4125	-3.4000
H	4.5901	0.7402	-3.4000
H	3.9942	3.2368	-3.4000
H	-0.8331	2.5821	-3.4000
H	-1.8989	1.1598	-3.4000
N	-2.5316	-1.7724	-3.4000
C	-2.5285	-3.1527	-3.4000
N	-3.8094	-3.7082	-3.4000
C	-4.9646	-2.9628	-3.4000
C	-4.9504	-1.6051	-3.4000
C	-3.6465	-0.9398	-3.4000
O	-3.5129	0.2957	-3.4000
O	-1.5169	-3.8446	-3.4000
C	-6.1886	-0.7587	-3.4000
H	-1.5711	-1.3071	-3.4000
H	-3.8379	-4.7216	-3.4000
H	-5.8899	-3.5367	-3.4000
H	-6.2118	-0.1018	-4.2802
H	-7.0932	-1.3789	-3.4000
H	-6.2118	-0.1018	-2.5198

[revC]-A/T-A

N	0.0000	0.0000	0.0000
C	1.3466	0.0000	0.0000
N	2.1876	1.0366	0.0000
C	1.5118	2.1988	0.0000
C	0.1231	2.3687	0.0000

C	-0.6640	1.1895	0.0000
N	2.0164	3.4817	0.0000
C	0.9324	4.3376	0.0000
N	-0.2230	3.7091	0.0000
N	-2.0008	1.2053	0.0000
H	1.8113	-0.9882	0.0000
H	2.9981	3.7310	0.0000
H	1.0601	5.4147	0.0000
H	-2.4729	2.1000	0.0000
H	-2.5545	0.3246	0.0000
N	-3.4256	-1.3139	0.0000
C	-4.7902	-1.2217	0.0000
N	-5.5033	-2.4568	0.0000
C	-4.8902	-3.6674	0.0000
C	-3.5324	-3.7445	0.0000
C	-2.8074	-2.4986	0.0000
N	-1.4622	-2.4985	0.0000
O	-5.4265	-0.1720	0.0000
H	-6.5147	-2.3725	0.0000
H	-5.5337	-4.5450	0.0000
H	-3.0229	-4.7043	0.0000
H	-0.9276	-1.5980	0.0000
H	-0.9656	-3.3778	0.0000
N	-0.0076	-0.5503	-3.4000
C	1.0832	-1.3428	-3.4000
N	2.3673	-0.9789	-3.4000
C	2.4904	0.3584	-3.4000
C	1.4587	1.3066	-3.4000
C	0.1377	0.7990	-3.4000
N	3.6467	1.1092	-3.4000
C	3.2633	2.4358	-3.4000
N	1.9575	2.5987	-3.4000
N	-0.9552	1.5788	-3.4000
H	0.8713	-2.4125	-3.4000
H	4.5901	0.7402	-3.4000
H	3.9942	3.2368	-3.4000
H	-0.8331	2.5821	-3.4000
H	-1.8989	1.1598	-3.4000
N	-2.5316	-1.7724	-3.4000
C	-2.5285	-3.1527	-3.4000
N	-3.8094	-3.7082	-3.4000
C	-4.9646	-2.9628	-3.4000
C	-4.9504	-1.6051	-3.4000
C	-3.6465	-0.9398	-3.4000
O	-3.5129	0.2957	-3.4000
O	-1.5169	-3.8446	-3.4000
C	-6.1886	-0.7587	-3.4000
H	-1.5711	-1.3071	-3.4000
H	-3.8379	-4.7216	-3.4000
H	-5.8899	-3.5367	-3.4000
H	-6.2118	-0.1018	-4.2802
H	-7.0932	-1.3789	-3.4000
H	-6.2118	-0.1018	-2.5198

[T]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3861	0.0000	0.0000
N	1.9276	1.2879	0.0000
C	1.1773	2.4392	0.0000
C	-0.1795	2.4186	0.0000
C	-0.8379	1.1139	0.0000
O	-2.0716	0.9794	0.0000
O	2.0838	-1.0019	0.0000
C	-1.0367	3.6492	0.0000
H	-0.4694	-0.9312	0.0000
H	2.9408	1.3222	0.0000
H	1.7465	3.3677	0.0000
H	-1.6946	3.6652	-0.8796
H	-0.4241	4.5591	0.0000
H	-1.6946	3.6652	0.8796
N	-3.5216	-1.4278	0.0000
C	-2.6748	-2.5043	0.0000
N	-3.3152	-3.7322	0.0000

C	-4.6880	-3.8752	0.0000
C	-5.5226	-2.8089	0.0000
C	-4.9338	-1.4614	0.0000
O	-5.5831	-0.4221	0.0000
O	-1.4394	-2.4296	0.0000
C	-7.0175	-2.9189	0.0000
H	-3.0550	-0.4933	0.0000
H	-2.7018	-4.5390	0.0000
H	-5.0467	-4.9032	0.0000
H	-7.4421	-2.4153	0.8794
H	-7.3410	-3.9670	0.0000
H	-7.4421	-2.4153	-0.8794
N	-2.2578	0.5478	-3.4000
C	-1.1422	-0.2095	-3.4000
N	0.1295	0.1953	-3.4000
C	0.2099	1.5359	-3.4000
C	-0.8516	2.4506	-3.4000
C	-2.1558	1.9010	-3.4000
N	1.3416	2.3233	-3.4000
C	0.9159	3.6369	-3.4000
N	-0.3944	3.7580	-3.4000
N	-3.2731	2.6455	-3.4000
H	-1.3198	-1.2854	-3.4000
H	2.2963	1.9846	-3.4000
H	1.6208	4.4608	-3.4000
H	-3.1831	3.6522	-3.4000
H	-4.2028	2.1965	-3.4000
N	-4.7414	-0.7545	-3.4000
C	-4.6943	-2.1339	-3.4000
N	-5.9567	-2.7301	-3.4000
C	-7.1351	-2.0220	-3.4000
C	-7.1644	-0.6645	-3.4000
C	-5.8824	0.0421	-3.4000
O	-5.7884	1.2813	-3.4000
O	-3.6611	-2.7931	-3.4000
C	-8.4290	0.1419	-3.4000
H	-3.7963	-0.2587	-3.4000
H	-5.9528	-3.7438	-3.4000
H	-8.0416	-2.6252	-3.4000
H	-8.4732	0.7977	-4.2802
H	-9.3133	-0.5070	-3.4000
H	-8.4732	0.7977	-2.5198

[G]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3681	0.0000	0.0000
N	2.1073	1.0952	0.0000
C	1.3512	2.2156	0.0000
C	-0.0465	2.3447	0.0000
C	-0.8299	1.1459	0.0000
N	1.8197	3.5053	0.0000
C	0.7098	4.3369	0.0000
N	-0.4218	3.6765	0.0000
O	-2.0629	1.0067	0.0000
N	1.9746	-1.2191	0.0000
H	-0.5060	-0.9106	0.0000
H	2.7962	3.7742	0.0000
H	0.8118	5.4164	0.0000
H	2.9833	-1.2486	0.0000
H	1.4388	-2.0748	0.0000
N	-3.3688	-1.4447	0.0000
C	-2.5353	-2.5250	0.0000
N	-3.1736	-3.7502	0.0000
C	-4.5480	-3.8948	0.0000
C	-5.3784	-2.8269	0.0000
C	-4.7858	-1.4796	0.0000
O	-5.4344	-0.4430	0.0000
O	-1.2912	-2.4634	0.0000
C	-6.8733	-2.9305	0.0000
H	-2.9099	-0.4939	0.0000
H	-2.5621	-4.5581	0.0000
H	-4.9058	-4.9230	0.0000
H	-7.2943	-2.4237	0.8791

H	-7.2021	-3.9768	0.0000
H	-7.2943	-2.4237	-0.8791
N	-2.0770	0.5227	-3.4000
C	-0.9698	-0.2467	-3.4000
N	0.3063	0.1441	-3.4000
C	0.4013	1.4837	-3.4000
C	-0.6501	2.4100	-3.4000
C	-1.9602	1.8748	-3.4000
N	1.5416	2.2587	-3.4000
C	1.1304	3.5769	-3.4000
N	-0.1786	3.7123	-3.4000
N	-3.0692	2.6314	-3.4000
H	-1.1592	-1.3206	-3.4000
H	2.4925	1.9096	-3.4000
H	1.8442	4.3931	-3.4000
H	-2.9683	3.6371	-3.4000
H	-4.0038	2.1926	-3.4000
N	-4.5747	-0.7522	-3.4000
C	-4.5427	-2.1322	-3.4000
N	-5.8116	-2.7144	-3.4000
C	-6.9822	-1.9935	-3.4000
C	-6.9966	-0.6358	-3.4000
C	-5.7070	0.0568	-3.4000
O	-5.5994	1.2948	-3.4000
O	-3.5168	-2.8026	-3.4000
C	-8.2523	0.1844	-3.4000
H	-3.6243	-0.2668	-3.4000
H	-5.8188	-3.7282	-3.4000
H	-7.8952	-2.5867	-3.4000
H	-8.2893	0.8407	-4.2802
H	-9.1436	-0.4547	-3.4000
H	-8.2893	0.8407	-2.5198

[C]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3739	0.0000	0.0000
N	2.0064	1.2835	0.0000
C	1.3241	2.4540	0.0000
C	-0.0350	2.4426	0.0000
C	-0.6793	1.1528	0.0000
N	-2.0226	1.0877	0.0000
O	2.0854	-0.9948	0.0000
H	3.0208	1.2568	0.0000
H	1.9115	3.3701	0.0000
H	-0.6077	3.3660	0.0000
H	-2.5008	0.1670	0.0000
H	-2.5665	1.9380	0.0000
N	-1.4220	-2.6599	0.0000
C	-0.7373	-3.8715	0.0000
N	-1.5938	-4.9810	0.0000
C	-2.9620	-4.9029	0.0000
C	-3.6127	-3.7124	0.0000
C	-2.8047	-2.4951	0.0000
O	-3.3165	-1.3617	0.0000
O	0.4727	-3.9967	0.0000
C	-5.1067	-3.5782	0.0000
H	-0.8372	-1.7887	0.0000
H	-1.1173	-5.8758	0.0000
H	-3.4881	-5.8566	0.0000
H	-5.4490	-3.0171	0.8804
H	-5.5915	-4.5624	0.0000
H	-5.4490	-3.0171	-0.8804
N	0.1080	-0.9035	-3.4000
C	1.0996	-1.8171	-3.4000
N	2.4171	-1.6045	-3.4000
C	2.6945	-0.2904	-3.4000
C	1.7797	0.7709	-3.4000
C	0.4087	0.4199	-3.4000
N	3.9300	0.3213	-3.4000
C	3.7030	1.6834	-3.4000
N	2.4248	1.9965	-3.4000
N	-0.5865	1.3212	-3.4000
H	0.7651	-2.8550	-3.4000

H	4.8243	-0.1547	-3.4000
H	4.5218	2.3942	-3.4000
H	-0.3489	2.3036	-3.4000
H	-1.5723	1.0143	-3.4000
N	-2.5407	-1.8248	-3.4000
C	-2.6976	-3.1961	-3.4000
N	-4.0343	-3.5993	-3.4000
C	-5.0952	-2.7250	-3.4000
C	-4.9238	-1.3781	-3.4000
C	-3.5516	-0.8685	-3.4000
O	-3.2757	0.3432	-3.4000
O	-1.7731	-4.0006	-3.4000
C	-6.0555	-0.3939	-3.4000
H	-1.5327	-1.4739	-3.4000
H	-4.1801	-4.6026	-3.4000
H	-6.0809	-3.1878	-3.4000
H	-6.0024	0.2613	-4.2802
H	-7.0259	-0.9051	-3.4000
H	-6.0024	0.2613	-2.5198

[F]-T/A-T

N	0.0000	0.0000	0.0000
C	1.3824	0.0000	0.0000
N	1.9198	1.2821	0.0000
C	1.1623	2.4348	0.0000
C	-0.1930	2.4166	0.0000
C	-0.8697	1.1141	0.0000
O	-2.0844	0.9504	0.0000
O	2.0784	-1.0087	0.0000
C	-1.0448	3.6507	0.0000
H	-0.4427	-0.9197	0.0000
H	2.9326	1.3218	0.0000
H	1.7329	3.3622	0.0000
H	-1.7025	3.6679	-0.8798
H	-0.4297	4.5588	0.0000
H	-1.7025	3.6679	0.8798
C	1.0511	-4.2605	0.0000
C	1.6938	-5.4935	0.0000
C	1.0011	-6.6973	0.0000
C	-0.3958	-6.6593	0.0000
C	-1.1085	-5.4523	0.0000
C	-0.3358	-4.2887	0.0000
F	-0.9975	-3.0848	0.0000
F	3.0542	-5.5151	0.0000
C	-2.6141	-5.3896	0.0000
H	1.5958	-3.3169	0.0000
H	1.5482	-7.6376	0.0000
H	-0.9539	-7.5963	0.0000
H	-2.9925	-4.8547	0.8822
H	-3.0418	-6.3988	0.0000
H	-2.9925	-4.8547	-0.8822
N	-1.3015	0.5557	3.4000
C	-0.2005	1.3883	3.4000
N	-0.5331	2.7443	3.4000
C	-1.8255	3.2131	3.4000
C	-2.8980	2.3806	3.4000
C	-2.6389	0.9399	3.4000
O	-3.5420	0.0861	3.4000
O	0.9623	1.0014	3.4000
C	-4.3210	2.8545	3.4000
H	-1.0909	-0.4905	3.4000
H	0.2566	3.3800	3.4000
H	-1.9282	4.2971	3.4000
H	-4.8581	2.4755	4.2802
H	-4.3743	3.9499	3.4000
H	-4.8581	2.4755	2.5198
N	-0.7478	-2.1934	3.4000
C	0.5432	-2.5825	3.4000
N	1.0302	-3.8251	3.4000
C	0.0398	-4.7322	3.4000
C	-1.3393	-4.4842	3.4000
C	-1.7343	-3.1253	3.4000
N	0.1415	-6.1071	3.4000

C	-1.1468	-6.6043	3.4000
N	-2.0665	-5.6630	3.4000
N	-3.0164	-2.7267	3.4000
H	1.2667	-1.7667	3.4000
H	1.0060	-6.6350	3.4000
H	-1.3425	-7.6708	3.4000
H	-3.7414	-3.4309	3.4000
H	-3.2535	-1.7219	3.4000

[A]-G/C-G

N	0.0000	0.0000	0.0000
C	1.3475	0.0000	0.0000
N	2.1960	1.0271	0.0000
C	1.5298	2.1951	0.0000
C	0.1429	2.3705	0.0000
C	-0.6533	1.1974	0.0000
N	2.0408	3.4745	0.0000
C	0.9606	4.3351	0.0000
N	-0.1976	3.7114	0.0000
N	-1.9891	1.2350	0.0000
H	1.8213	-0.9856	0.0000
H	3.0237	3.7200	0.0000
H	1.0931	5.4115	0.0000
H	-2.4341	2.1440	0.0000
H	-2.5693	0.3702	0.0000
N	-1.6981	-2.4111	0.0000
C	-1.0849	-3.6357	0.0000
N	-1.7258	-4.7909	0.0000
C	-3.0665	-4.6283	0.0000
C	-3.8115	-3.4411	0.0000
C	-3.1001	-2.1988	0.0000
N	-4.0045	-5.6297	0.0000
C	-5.2477	-5.0153	0.0000
N	-5.1698	-3.7071	0.0000
O	-3.5502	-1.0435	0.0000
N	0.2770	-3.6396	0.0000
H	-1.1016	-1.5489	0.0000
H	-3.8031	-6.6225	0.0000
H	-6.1647	-5.5940	0.0000
H	0.7494	-4.5313	0.0000
H	0.8088	-2.7834	0.0000
N	1.2005	-1.9318	3.4000
O	-3.4141	-2.0326	3.4000
N	-1.1152	-2.0902	3.4000
C	0.1056	-2.7230	3.4000
N	0.2420	-4.0450	3.4000
C	-0.9452	-4.6813	3.4000
C	-2.2437	-4.1450	3.4000
C	-2.3736	-2.7216	3.4000
N	-1.1334	-6.0422	3.4000
C	-2.5035	-6.2612	3.4000
N	-3.1980	-5.1497	3.4000
H	1.1477	-0.9019	3.4000
H	2.0970	-2.3969	3.4000
H	-1.1364	-1.0440	3.4000
H	-0.3943	-6.7347	3.4000
H	-2.9159	-7.2638	3.4000
O	1.0689	0.9306	3.4000
N	-3.5178	0.6929	3.4000
N	-1.2275	0.7887	3.4000
C	-2.4747	2.8761	3.4000
C	-0.0512	1.4646	3.4000
N	-0.1176	2.8759	3.4000
C	-1.2973	3.5540	3.4000
C	-2.4062	1.4353	3.4000
H	-3.4253	3.4025	3.4000
H	0.7745	3.3596	3.4000
H	-1.2362	4.6396	3.4000
H	-3.4639	-0.3603	3.4000
H	-4.4208	1.1468	3.4000

[T]-G/C-G

N	0.0000	0.0000	0.0000

C	1.3645	0.0000	0.0000
N	1.9446	1.2537	0.0000
C	1.2195	2.4302	0.0000
C	-0.1332	2.4353	0.0000
C	-0.8380	1.1432	0.0000
O	-2.0548	1.0235	0.0000
O	2.0757	-1.0226	0.0000
C	-0.9644	3.6821	0.0000
H	-0.4724	-0.9442	0.0000
H	2.9578	1.2631	0.0000
H	1.8150	3.3416	0.0000
H	-1.6228	3.7059	-0.8791
H	-0.3368	4.5817	0.0000
H	-1.6228	3.7059	0.8791
N	0.9140	-3.5498	0.0000
C	1.7498	-4.6330	0.0000
N	1.3341	-5.8872	0.0000
C	-0.0148	-5.9730	0.0000
C	-0.9707	-4.9452	0.0000
C	-0.5002	-3.5926	0.0000
N	-0.7497	-7.1317	0.0000
C	-2.0860	-6.7610	0.0000
N	-2.2545	-5.4616	0.0000
O	-1.1431	-2.5315	0.0000
N	3.0855	-4.3684	0.0000
H	1.3259	-2.5928	0.0000
H	-0.3661	-8.0692	0.0000
H	-2.8784	-7.5012	0.0000
H	3.7250	-5.1491	0.0000
H	3.4357	-3.4215	0.0000
N	3.6700	-2.5092	3.4000
O	-0.8360	-3.5097	3.4000
N	1.4299	-3.1171	3.4000
C	2.7508	-3.4992	3.4000
N	3.1428	-4.7690	3.4000
C	2.1028	-5.6250	3.4000
C	0.7246	-5.3527	3.4000
C	0.3191	-3.9822	3.4000
N	2.1842	-6.9965	3.4000
C	0.8832	-7.4789	3.4000
N	-0.0150	-6.5245	3.4000
H	3.4170	-1.5095	3.4000
H	4.6401	-2.7902	3.4000
H	1.2047	-2.0951	3.4000
H	3.0443	-7.5312	3.4000
H	0.6747	-8.5427	3.4000
O	2.9817	0.2723	3.4000
N	-1.4702	-0.8570	3.4000
N	0.7573	-0.3156	3.4000
C	-0.8738	1.4879	3.4000
C	1.7788	0.5771	3.4000
N	1.4380	1.9483	3.4000
C	0.1485	2.3828	3.4000
C	-0.5251	0.0883	3.4000
H	-1.9089	1.8185	3.4000
H	2.2184	2.5970	3.4000
H	-0.0036	3.4594	3.4000
H	-1.2115	-1.8794	3.4000
H	-2.4444	-0.5883	3.4000

[G]-G/C-G

N	0.0000	0.0000	0.0000
C	1.3746	0.0000	0.0000
N	2.1003	1.1024	0.0000
C	1.3449	2.2224	0.0000
C	-0.0477	2.3424	0.0000
C	-0.8432	1.1544	0.0000
N	1.8038	3.5171	0.0000
C	0.6957	4.3429	0.0000
N	-0.4325	3.6694	0.0000
O	-2.0621	1.0075	0.0000
N	2.0031	-1.2053	0.0000
H	-0.5191	-0.8760	0.0000

H	2.7779	3.7967	0.0000
H	0.7889	5.4226	0.0000
H	3.0134	-1.2077	0.0000
H	1.5053	-2.0822	0.0000
N	-4.5924	2.4956	0.0000
C	-4.5880	3.8656	0.0000
N	-5.6910	4.6016	0.0000
C	-6.8122	3.8473	0.0000
C	-6.9485	2.4538	0.0000
C	-5.7552	1.6478	0.0000
N	-8.1014	4.3250	0.0000
C	-8.9400	3.2209	0.0000
N	-8.2836	2.0858	0.0000
O	-5.6182	0.4302	0.0000
N	-3.3877	4.5032	0.0000
H	-3.6985	1.9879	0.0000
H	-8.3624	5.3033	0.0000
H	-10.0190	3.3288	0.0000
H	-3.4281	5.5123	0.0000
H	-2.4737	4.0494	0.0000
N	-1.7832	3.3559	-3.4000
O	-5.9609	1.3932	-3.4000
N	-3.9276	2.4676	-3.4000
C	-3.1158	3.5774	-3.4000
N	-3.5818	4.8220	-3.4000
C	-4.9281	4.8637	-3.4000
C	-5.8524	3.8057	-3.4000
C	-5.3355	2.4732	-3.4000
N	-5.7021	5.9988	-3.4000
C	-7.0266	5.5854	-3.4000
N	-7.1541	4.2809	-3.4000
H	-1.3723	2.4100	-3.4000
H	-1.1873	4.1713	-3.4000
H	-3.4811	1.5211	-3.4000
H	-5.3482	6.9478	-3.4000
H	-7.8419	6.2998	-3.4000
O	-0.6276	0.7338	-3.4000
N	-4.8412	-1.0939	-3.4000
N	-2.7474	-0.1607	-3.4000
C	-2.9357	-2.5851	-3.4000
C	-1.3932	-0.2428	-3.4000
N	-0.8248	-1.5362	-3.4000
C	-1.5796	-2.6684	-3.4000
C	-3.5153	-1.2642	-3.4000
H	-3.5528	-3.4794	-3.4000
H	0.1894	-1.5726	-3.4000
H	-1.0419	-3.6134	-3.4000
H	-5.2614	-0.1266	-3.4000
H	-5.4479	-1.9021	-3.4000

[C]-G/C-G

N	-0.1956	-3.1483	0.0000
O	-0.8586	1.4196	0.0000
N	-0.6354	-0.8692	0.0000
C	-1.1145	-2.1581	0.0000
N	-2.4100	-2.4547	0.0000
C	-3.1863	-1.3539	0.0000
C	-2.8124	0.0003	0.0000
C	-1.4156	0.3028	0.0000
N	-4.5601	-1.3332	0.0000
C	-4.9445	0.0000	0.0000
N	-3.9260	0.8249	0.0000
H	0.8201	-2.9703	0.0000
H	-0.5479	-4.0948	0.0000
H	0.4005	-0.7205	0.0000
H	-5.1572	-2.1512	0.0000
H	-5.9899	0.2870	0.0000
O	2.6293	-2.6685	0.0000
N	1.8339	1.8550	0.0000
N	2.2083	-0.4066	0.0000
C	4.1281	1.0860	0.0000
C	3.0227	-1.4916	0.0000
N	4.4154	-1.2536	0.0000

C	4.9445	0.0000	0.0000
C	2.7064	0.8422	0.0000
H	4.5346	2.0937	0.0000
H	5.0043	-2.0800	0.0000
H	6.0295	0.0718	0.0000
H	0.7952	1.6730	0.0000
H	2.1743	2.8065	0.0000
N	1.6922	-2.6620	3.4000
O	-1.5290	0.6438	3.4000
N	-0.0031	-1.0767	3.4000
C	0.3668	-2.4010	3.4000
N	-0.5069	-3.4024	3.4000
C	-1.7820	-2.9682	3.4000
C	-2.2755	-1.6529	3.4000
C	-1.3232	-0.5871	3.4000
N	-2.9055	-3.7590	3.4000
C	-4.0002	-2.9063	3.4000
N	-3.6611	-1.6403	3.4000
H	2.4094	-1.9209	3.4000
H	1.9636	-3.6348	3.4000
H	0.7475	-0.3475	3.4000
H	-2.9078	-4.7717	3.4000
H	-5.0146	-3.2886	3.4000
O	3.6957	-0.6134	3.4000
N	0.3933	2.5787	3.4000
N	2.0256	0.9691	3.4000
C	2.7014	3.3050	3.4000
C	3.3222	0.5700	3.4000
N	4.3089	1.5811	3.4000
C	4.0002	2.9063	3.4000
C	1.6945	2.2721	3.4000
H	2.4379	4.3592	3.4000
H	5.2712	1.2587	3.4000
H	4.8357	3.6021	3.4000
H	-0.3400	1.8208	3.4000
H	0.1094	3.5485	3.4000

[F]-G/C-G

N	0.0000	0.0000	0.0000
O	4.6271	0.0000	0.0000
N	2.3312	0.1136	0.0000
C	1.1260	0.7673	0.0000
N	1.0107	2.0805	0.0000
C	2.2134	2.7022	0.0000
C	3.5023	2.1505	0.0000
C	3.6331	0.7204	0.0000
N	2.4147	4.0593	0.0000
C	3.7857	4.2630	0.0000
N	4.4660	3.1426	0.0000
H	0.0327	-1.0080	0.0000
H	-0.8918	0.4731	0.0000
H	2.3507	-0.9061	0.0000
H	1.6833	4.7602	0.0000
H	4.2100	5.2608	0.0000
C	4.5162	-3.3009	0.0000
C	3.2398	-3.8420	0.0000
C	2.9806	-5.2026	0.0000
C	4.0762	-6.0722	0.0000
C	5.3961	-5.6038	0.0000
C	5.5640	-4.2141	0.0000
F	6.8320	-3.7256	0.0000
F	2.1638	-2.9714	0.0000
C	6.5903	-6.5220	0.0000
H	4.6926	-2.2225	0.0000
H	1.9565	-5.5690	0.0000
H	3.9003	-7.1484	0.0000
H	7.2232	-6.3510	-0.8818
H	6.2736	-7.5713	0.0000
H	7.2232	-6.3510	0.8818
N	0.2215	-1.9381	3.4000
O	3.9880	0.7765	3.4000
N	2.0409	-0.4471	3.4000
C	0.6701	-0.6639	3.4000

N	-0.1954	0.3446	3.4000
C	0.4174	1.5440	3.4000
C	1.7901	1.8435	3.4000
C	2.7401	0.7750	3.4000
N	-0.2037	2.7695	3.4000
C	0.7973	3.7304	3.4000
N	2.0015	3.2129	3.4000
H	0.8519	-2.7543	3.4000
H	-0.7802	-2.0669	3.4000
H	2.6373	-1.3070	3.4000
H	-1.2056	2.9172	3.4000
H	0.5647	4.7892	3.4000
O	1.9611	-4.2151	3.4000
N	5.5820	-1.4367	3.4000
N	3.7269	-2.7834	3.4000
C	5.9205	-3.8326	3.4000
C	3.1858	-4.0154	3.4000
N	4.0448	-5.1372	3.4000
C	5.3146	-5.0486	3.4000
C	5.0665	-2.6701	3.4000
H	7.0036	-3.7453	3.4000
H	3.5875	-6.0431	3.4000
H	5.8641	-5.9868	3.4000
H	4.9545	-0.5892	3.4000
H	6.5853	-1.3155	3.4000

[revA]-G/C-G

N	0.0000	0.0000	0.0000
O	4.6244	0.0000	0.0000
N	2.3289	0.1258	0.0000
C	1.1134	0.7662	0.0000
N	1.0131	2.0907	0.0000
C	2.2219	2.7110	0.0000
C	3.5081	2.1565	0.0000
C	3.6408	0.7250	0.0000
N	2.4316	4.0686	0.0000
C	3.8049	4.2666	0.0000
N	4.4766	3.1428	0.0000
H	0.0812	-1.0057	0.0000
H	-0.9487	0.4210	0.0000
H	2.3626	-0.8908	0.0000
H	1.7159	4.7839	0.0000
H	4.2325	5.2629	0.0000
N	-3.6410	4.5751	0.0000
C	-4.9583	4.3271	0.0000
N	-5.5902	3.1439	0.0000
C	-4.7102	2.1366	0.0000
C	-3.3103	2.2258	0.0000
C	-2.7739	3.5371	0.0000
N	-4.9758	0.7810	0.0000
C	-3.7676	0.1310	0.0000
N	-2.7408	0.9587	0.0000
N	-1.4556	3.8152	0.0000
H	-5.6008	5.2089	0.0000
H	-5.8983	0.3621	0.0000
H	-3.7006	-0.9512	0.0000
H	-0.7074	3.1076	0.0000
H	-1.2177	4.7991	0.0000
N	0.2358	-1.9359	3.4000
O	3.9961	0.7782	3.4000
N	2.0392	-0.4297	3.4000
C	0.6749	-0.6584	3.4000
N	-0.1982	0.3436	3.4000
C	0.4057	1.5477	3.4000
C	1.7760	1.8574	3.4000
C	2.7482	0.7868	3.4000
N	-0.2247	2.7684	3.4000
C	0.7691	3.7368	3.4000
N	1.9771	3.2284	3.4000
H	0.8723	-2.7473	3.4000
H	-0.7649	-2.0722	3.4000
H	2.6287	-1.2943	3.4000
H	-1.2277	2.9086	3.4000

H	0.5286	4.7938	3.4000
O	1.9925	-4.1997	3.4000
N	5.5722	-1.4478	3.4000
N	3.7064	-2.7794	3.4000
C	5.8915	-3.8462	3.4000
C	3.2157	-3.9908	3.4000
N	4.0830	-5.1061	3.4000
C	5.2758	-5.0574	3.4000
C	5.0469	-2.6770	3.4000
H	6.9753	-3.7677	3.4000
H	3.6325	-6.0155	3.4000
H	5.8178	-5.9999	3.4000
H	4.9516	-0.5952	3.4000
H	6.5765	-1.3346	3.4000

[revT]-G/C-G

N	0.0000	0.0000	0.0000
O	4.6039	0.0000	0.0000
N	2.3142	0.1196	0.0000
C	1.1165	0.7790	0.0000
N	0.9967	2.0954	0.0000
C	2.2001	2.7105	0.0000
C	3.4870	2.1486	0.0000
C	3.5917	0.7205	0.0000
N	2.4127	4.0661	0.0000
C	3.7860	4.2587	0.0000
N	4.4585	3.1341	0.0000
H	0.0638	-1.0081	0.0000
H	-0.9002	0.4558	0.0000
H	2.3134	-0.9262	0.0000
H	1.6870	4.7727	0.0000
H	4.2175	5.2535	0.0000
N	4.4911	-2.7651	0.0000
C	5.7039	-3.4429	0.0000
N	5.5521	-4.8351	0.0000
C	4.3418	-5.4765	0.0000
C	3.1658	-4.7968	0.0000
C	3.2291	-3.3399	0.0000
O	2.2019	-2.6280	0.0000
O	6.8000	-2.9118	0.0000
C	1.8203	-5.4603	0.0000
H	4.5523	-1.7076	0.0000
H	6.4230	-5.3546	0.0000
H	4.3860	-6.5647	0.0000
H	1.2363	-5.1614	0.8814
H	1.9189	-6.5527	0.0000
H	1.2363	-5.1614	-0.8814
N	0.2162	-1.9372	3.4000
O	3.9462	0.7796	3.4000
N	2.0095	-0.4605	3.4000
C	0.6583	-0.6607	3.4000
N	-0.2124	0.3433	3.4000
C	0.3942	1.5459	3.4000
C	1.7653	1.8524	3.4000
C	2.6983	0.7675	3.4000
N	-0.2332	2.7682	3.4000
C	0.7628	3.7342	3.4000
N	1.9697	3.2229	3.4000
H	0.8508	-2.7501	3.4000
H	-0.7848	-2.0712	3.4000
H	2.6132	-1.3153	3.4000
H	-1.2359	2.9107	3.4000
H	0.5248	4.7918	3.4000
O	1.9675	-4.2052	3.4000
N	5.5589	-1.4200	3.4000
N	3.7153	-2.7824	3.4000
C	5.9178	-3.8129	3.4000
C	3.1912	-3.9992	3.4000
N	4.0559	-5.1165	3.4000
C	5.3222	-5.0340	3.4000
C	5.0539	-2.6577	3.4000
H	7.0001	-3.7164	3.4000
H	3.6033	-6.0248	3.4000

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H                5.8797   -5.9675    3.4000
H                4.9242   -0.5778    3.4000
H                6.5611   -1.2902    3.4000

[revG]-G/C-G
N                0.0000    0.0000    0.0000
O                4.5983    0.0000    0.0000
N                2.3072    0.1196    0.0000
C                1.1089    0.7826    0.0000
N                0.9926    2.1018    0.0000
C                2.1947    2.7126    0.0000
C                3.4805    2.1445    0.0000
C                3.5752    0.7209    0.0000
N                2.4160    4.0669    0.0000
C                3.7904    4.2523    0.0000
N                4.4581    3.1250    0.0000
H                0.0738   -1.0098    0.0000
H               -0.9039    0.4486    0.0000
H                2.2674   -0.9358    0.0000
H                1.6945    4.7780    0.0000
H                4.2267    5.2450    0.0000
N                4.2785   -2.6981    0.0000
C                5.4768   -3.3610    0.0000
N                5.5930   -4.6802    0.0000
C                4.3908   -5.2910    0.0000
C                3.1051   -4.7230    0.0000
C                3.0104   -3.2994    0.0000
N                4.1697   -6.6454    0.0000
C                2.7953   -6.8308    0.0000
N                2.1274   -5.7034    0.0000
O                1.9873   -2.5785    0.0000
N                6.5856   -2.5785    0.0000
H                4.3182   -1.6427    0.0000
H                4.8911   -7.3565    0.0000
H                2.3589   -7.8235    0.0000
H                7.4894   -3.0271    0.0000
H                6.5118   -1.5687    0.0000
N                0.2096   -1.9376    3.4000
O                3.9294    0.7817    3.4000
N                1.9987   -0.4676    3.4000
C                0.6514   -0.6610    3.4000
N               -0.2194    0.3429    3.4000
C                0.3870    1.5456    3.4000
C                1.7580    1.8523    3.4000
C                2.6816    0.7637    3.4000
N               -0.2407    2.7678    3.4000
C                0.7552    3.7339    3.4000
N                1.9621    3.2229    3.4000
H                0.8443   -2.7504    3.4000
H               -0.7914   -2.0717    3.4000
H                2.6064   -1.3195    3.4000
H               -1.2433    2.9102    3.4000
H                0.5170    4.7915    3.4000
O                1.9613   -4.2052    3.4000
N                5.5525   -1.4102    3.4000
N                3.7155   -2.7813    3.4000
C                5.9228   -3.8013    3.4000
C                3.1849   -3.9990    3.4000
N                4.0498   -5.1162    3.4000
C                5.3330   -5.0253    3.4000
C                5.0535   -2.6503    3.4000
H                7.0047   -3.6997    3.4000
H                3.5973   -6.0246    3.4000
H                5.8950   -5.9561    3.4000
H                4.9139   -0.5710    3.4000
H                6.5542   -1.2756    3.4000

[revC]-G/C-G
N                0.0000    0.0000    0.0000
O                4.6335    0.0000    0.0000
N                2.3311    0.1003    0.0000
C                1.1309    0.7576    0.0000
N                1.0125    2.0768    0.0000
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C	2.2153	2.6958	0.0000
C	3.5017	2.1426	0.0000
C	3.6335	0.7073	0.0000
N	2.4186	4.0553	0.0000
C	3.7902	4.2573	0.0000
N	4.4675	3.1346	0.0000
H	-0.0008	-1.0190	0.0000
H	-0.8732	0.5062	0.0000
H	2.3217	-0.9280	0.0000
H	1.6878	4.7562	0.0000
H	4.2162	5.2544	0.0000
N	-0.3535	-3.1429	0.0000
C	0.9522	-3.5490	0.0000
N	1.1908	-4.9465	0.0000
C	0.1960	-5.8661	0.0000
C	-1.1036	-5.4602	0.0000
C	-1.3334	-4.0427	0.0000
N	-2.6048	-3.5742	0.0000
O	1.9231	-2.7931	0.0000
H	2.1698	-5.2187	0.0000
H	0.4922	-6.9126	0.0000
H	-1.9180	-6.1794	0.0000
H	-2.7586	-2.5745	0.0000
H	-3.3990	-4.1964	0.0000
N	0.2156	-1.9383	3.4000
O	3.9878	0.7675	3.4000
N	2.0548	-0.4784	3.4000
C	0.6686	-0.6657	3.4000
N	-0.1934	0.3458	3.4000
C	0.4236	1.5432	3.4000
C	1.7972	1.8378	3.4000
C	2.7399	0.7517	3.4000
N	-0.1933	2.7708	3.4000
C	0.8110	3.7282	3.4000
N	2.0134	3.2065	3.4000
H	0.8431	-2.7567	3.4000
H	-0.7866	-2.0637	3.4000
H	2.6611	-1.3314	3.4000
H	-1.1947	2.9219	3.4000
H	0.5821	4.7878	3.4000
O	1.9472	-4.2213	3.4000
N	5.6070	-1.4273	3.4000
N	3.7675	-2.7951	3.4000
C	5.9731	-3.8190	3.4000
C	3.1727	-4.0258	3.4000
N	4.0277	-5.1506	3.4000
C	5.3812	-5.0420	3.4000
C	5.1058	-2.6665	3.4000
H	7.0551	-3.7193	3.4000
H	3.5673	-6.0549	3.4000
H	5.9415	-5.9738	3.4000
H	4.9698	-0.5870	3.4000
H	6.6089	-1.2945	3.4000

[A]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3553	0.0000	0.0000
N	2.1739	1.0558	0.0000
C	1.4926	2.2078	0.0000
C	0.1005	2.3671	0.0000
C	-0.6555	1.1775	0.0000
N	1.9833	3.4967	0.0000
C	0.8919	4.3415	0.0000
N	-0.2599	3.7051	0.0000
N	-2.0114	1.1952	0.0000
H	1.8114	-0.9924	0.0000
H	2.9632	3.7543	0.0000
H	1.0104	5.4197	0.0000
H	-2.4991	2.0799	0.0000
H	-2.5311	0.3300	0.0000
N	1.4567	-3.3550	0.0000
C	2.5059	-4.2323	0.0000
N	2.1664	-5.6247	0.0000

C	0.8896	-6.0794	0.0000
C	-0.1447	-5.1953	0.0000
C	0.2020	-3.7953	0.0000
N	-0.7838	-2.8682	0.0000
O	3.6939	-3.9282	0.0000
H	2.9572	-6.2608	0.0000
H	0.7484	-7.1586	0.0000
H	-1.1768	-5.5364	0.0000
H	-0.5554	-1.8580	0.0000
H	-1.7482	-3.1661	0.0000
N	3.7338	-2.9904	-3.4000
O	0.6216	0.4183	-3.4000
N	2.2501	-1.2054	-3.4000
C	3.5506	-1.6520	-3.4000
N	4.6013	-0.8381	-3.4000
C	4.2423	0.4601	-3.4000
C	2.9579	1.0294	-3.4000
C	1.8384	0.1410	-3.4000
N	5.0972	1.5356	-3.4000
C	4.3099	2.6781	-3.4000
N	3.0262	2.4134	-3.4000
H	2.9522	-3.6631	-3.4000
H	4.6891	-3.3180	-3.4000
H	1.4784	-1.9122	-3.4000
H	6.1083	1.4787	-3.4000
H	4.7507	3.6685	-3.4000
O	1.5718	-4.8709	-3.4000
N	-1.4221	-1.3879	-3.4000
N	0.0894	-3.1113	-3.4000
C	-2.2819	-3.6496	-3.4000
C	0.4122	-4.4289	-3.4000
N	-0.6548	-5.3550	-3.4000
C	-1.9597	-4.9695	-3.4000
C	-1.1921	-2.7047	-3.4000
H	-3.3189	-3.3251	-3.4000
H	-0.3890	-6.3344	-3.4000
H	-2.7030	-5.7630	-3.4000
H	-0.6228	-0.7000	-3.4000
H	-2.3738	-1.0478	-3.4000

[T]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3916	0.0000	0.0000
N	1.9362	1.2914	0.0000
C	1.1951	2.4442	0.0000
C	-0.1615	2.4251	0.0000
C	-0.8237	1.1227	0.0000
O	-2.0623	1.0108	0.0000
O	2.0959	-0.9918	0.0000
C	-1.0133	3.6598	0.0000
H	-0.4708	-0.9377	0.0000
H	2.9497	1.3168	0.0000
H	1.7667	3.3714	0.0000
H	-1.6702	3.6818	-0.8804
H	-0.3949	4.5660	0.0000
H	-1.6702	3.6818	0.8804
N	-1.6162	-2.5465	0.0000
C	-0.9404	-3.7427	0.0000
N	-1.7466	-4.9247	0.0000
C	-3.1013	-4.9066	0.0000
C	-3.7600	-3.7178	0.0000
C	-2.9541	-2.5223	0.0000
N	-3.5582	-1.3207	0.0000
O	0.2758	-3.8727	0.0000
H	-1.2243	-5.7948	0.0000
H	-3.6100	-5.8687	0.0000
H	-4.8457	-3.6734	0.0000
H	-2.9919	-0.4514	0.0000
H	-4.5661	-1.2655	0.0000
N	0.6625	-2.9472	-3.4000
O	-1.1322	1.3053	-3.4000
N	-0.1396	-0.7691	-3.4000
C	0.9370	-1.6245	-3.4000

N	2.1992	-1.2084	-3.4000
C	2.2944	0.1352	-3.4000
C	1.2741	1.1009	-3.4000
C	-0.0780	0.6375	-3.4000
N	3.4595	0.8633	-3.4000
C	3.0991	2.2032	-3.4000
N	1.8008	2.3826	-3.4000
H	-0.2989	-3.3201	-3.4000
H	1.4535	-3.5751	-3.4000
H	-1.1031	-1.1775	-3.4000
H	4.3936	0.4720	-3.4000
H	3.8454	2.9895	-3.4000
O	-2.0035	-3.9974	-3.4000
N	-3.6619	0.2856	-3.4000
N	-2.8129	-1.8437	-3.4000
C	-5.2278	-1.5589	-3.4000
C	-2.9488	-3.1935	-3.4000
N	-4.2639	-3.7099	-3.4000
C	-5.3650	-2.9106	-3.4000
C	-3.8849	-1.0324	-3.4000
H	-6.0968	-0.9067	-3.4000
H	-4.3406	-4.7219	-3.4000
H	-6.3307	-3.4103	-3.4000
H	-2.6787	0.6670	-3.4000
H	-4.4453	0.9241	-3.4000

[C]-C/G-C

N	0.0000	0.0000	0.0000
C	1.3679	0.0000	0.0000
N	1.9982	1.2853	0.0000
C	1.3107	2.4567	0.0000
C	-0.0490	2.4476	0.0000
C	-0.6694	1.1489	0.0000
N	-2.0234	1.0683	0.0000
O	2.0883	-0.9951	0.0000
H	3.0127	1.2654	0.0000
H	1.8985	3.3730	0.0000
H	-0.6410	3.3594	0.0000
H	-2.4148	0.1350	0.0000
H	-2.6350	1.8855	0.0000
N	-4.2494	3.2962	0.0000
C	-3.6834	4.5452	0.0000
N	-4.5842	5.6485	0.0000
C	-5.9316	5.5101	0.0000
C	-6.4856	4.2668	0.0000
C	-5.5715	3.1582	0.0000
N	-6.0648	1.8953	0.0000
O	-2.4780	4.7743	0.0000
H	-4.1446	6.5640	0.0000
H	-6.5223	6.4237	0.0000
H	-7.5634	4.1295	0.0000
H	-5.4209	1.1156	0.0000
H	-7.0572	1.7143	0.0000
N	-2.0125	3.8876	3.4000
O	-3.4421	-0.5012	3.4000
N	-2.6281	1.6496	3.4000
C	-1.6275	2.5927	3.4000
N	-0.3347	2.2846	3.4000
C	-0.1265	0.9539	3.4000
C	-1.0617	-0.0945	3.4000
C	-2.4480	0.2532	3.4000
N	1.0959	0.3266	3.4000
C	0.8498	-1.0389	3.4000
N	-0.4288	-1.3272	3.4000
H	-3.0020	4.1781	3.4000
H	-1.2773	4.5800	3.4000
H	-3.6226	1.9753	3.4000
H	1.9936	0.7953	3.4000
H	1.6598	-1.7594	3.4000
O	-4.7576	4.7092	3.4000
N	-6.0488	0.3015	3.4000
N	-5.3825	2.4949	3.4000
C	-7.7648	2.0075	3.4000

C	-5.6318	3.8284	3.4000
N	-6.9857	4.2321	3.4000
C	-8.0155	3.3428	3.4000
C	-6.3823	1.5960	3.4000
H	-8.5757	1.2842	3.4000
H	-7.1475	5.2340	3.4000
H	-9.0199	3.7591	3.4000
H	-5.0370	0.0045	3.4000
H	-6.7756	-0.4007	3.4000

[F]-C/G-C

O	0.0000	0.0000	0.0000
N	4.5953	0.0000	0.0000
N	2.3083	0.0411	0.0000
C	3.4424	-2.1198	0.0000
C	1.0830	-0.5721	0.0000
N	1.0946	-2.0044	0.0000
C	2.2312	-2.7412	0.0000
C	3.4226	-0.6803	0.0000
H	4.3685	-2.6884	0.0000
H	0.1784	-2.4416	0.0000
H	2.1197	-3.8236	0.0000
H	4.5727	1.0147	0.0000
H	5.4822	-0.4802	0.0000
C	2.2468	3.5780	0.0000
C	1.2529	4.5521	0.0000
C	1.5386	5.9122	0.0000
C	2.8767	6.3127	0.0000
C	3.9286	5.3864	0.0000
C	3.5536	4.0415	0.0000
F	4.5668	3.1053	0.0000
F	-0.0446	4.1570	0.0000
C	5.3792	5.7953	0.0000
H	2.0184	2.5102	0.0000
H	0.7249	6.6342	0.0000
H	3.1156	7.3768	0.0000
H	5.9060	5.4068	0.8830
H	5.4710	6.8876	0.0000
H	5.9060	5.4068	-0.8830
O	1.8420	-1.3968	3.4000
N	5.5576	1.2935	3.4000
N	3.6897	-0.0354	3.4000
C	5.8732	-1.1055	3.4000
C	3.0700	-1.2182	3.4000
N	3.9096	-2.3545	3.4000
C	5.2556	-2.3156	3.4000
C	5.0303	0.0651	3.4000
H	6.9571	-1.0286	3.4000
H	3.4368	-3.2525	3.4000
H	5.7962	-3.2591	3.4000
H	4.9382	2.1470	3.4000
H	6.5620	1.4052	3.4000
N	0.1416	0.9095	3.4000
O	3.9849	3.5219	3.4000
N	2.0261	2.3170	3.4000
C	0.6120	2.1759	3.4000
N	-0.2361	3.1991	3.4000
C	0.3971	4.3879	3.4000
C	1.7747	4.6637	3.4000
C	2.7370	3.5323	3.4000
N	-0.2029	5.6238	3.4000
C	0.8144	6.5674	3.4000
N	2.0095	6.0294	3.4000
H	0.7579	0.0827	3.4000
H	-0.8622	0.7979	3.4000
H	2.6143	1.4514	3.4000
H	-1.2022	5.7886	3.4000
H	0.5999	7.6300	3.4000

Table S6. Cartesian coordinates (in Å) of the incoming DNA base or mimic X in the gas phase, optimized without any constraint at BP86/TZ2P.

=== A			
N	-0.5366	-0.6983	0.0000
C	-1.0218	-1.9520	0.0000
N	-2.2984	-2.3596	0.0000
C	-3.1368	-1.3147	0.0000
C	-2.7920	0.0445	0.0000
C	-1.4091	0.3278	0.0000
N	-4.5165	-1.3178	0.0000
C	-4.9202	0.0023	0.0000
N	-3.9173	0.8537	0.0000
N	-0.9298	1.5943	0.0000
H	-0.2699	-2.7425	0.0000
H	-5.1060	-2.1416	0.0000
H	-5.9705	0.2730	0.0000
H	-1.5666	2.3782	0.0000
H	0.0700	1.7417	0.0000
=== T			
N	2.2453	-0.3407	0.0000
C	2.9912	-1.5087	0.0000
N	4.3612	-1.2608	0.0000
C	4.9164	0.0012	0.0000
C	4.1668	1.1311	0.0000
C	2.7066	0.9937	0.0000
O	1.9069	1.9233	0.0000
O	2.5154	-2.6341	0.0000
C	4.7416	2.5157	0.0000
H	1.2347	-0.4636	0.0000
H	4.9457	-2.0887	0.0000
H	6.0050	0.0260	0.0000
H	4.3994	3.0774	0.8799
H	5.8381	2.4914	0.0000
H	4.3994	3.0774	-0.8799
=== G			
N	0.1937	0.6606	-3.2835
C	-0.5509	1.8105	-3.2754
N	-1.9157	1.6785	-3.4241
N	-0.0259	3.0123	-3.1841
C	1.3283	2.9822	-3.1114
C	2.1944	1.8817	-3.0950
C	1.6328	0.5599	-3.1910
O	2.1534	-0.5449	-3.2112
N	3.5108	2.2897	-2.9938
C	3.4482	3.5989	-2.9493
N	2.1501	4.0764	-3.0167
H	-0.2613	-0.2397	-3.4172
H	-2.3515	0.8534	-3.0271
H	-2.4172	2.5416	-3.2397
H	4.2957	4.2699	-2.8676
H	1.8427	5.0416	-3.0011
=== C			
O	2.6348	-2.6682	0.0000
N	1.8396	1.8583	0.0000
N	2.1934	-0.3985	0.0000
C	4.1289	1.0900	0.0000
C	3.0058	-1.5017	0.0000
N	4.4176	-1.2422	0.0000
C	4.9491	0.0027	0.0000
C	2.7160	0.8179	0.0000
H	4.5301	2.1000	0.0000
H	5.0058	-2.0697	0.0000
H	6.0348	0.0785	0.0000
H	0.8502	1.6459	0.0000
H	2.1487	2.8182	0.0000

=== F

C	-1.7601	-2.9385	0.0000
C	-1.2628	-4.2364	0.0000
C	-2.0918	-5.3498	0.0000
C	-3.4744	-5.1449	0.0000
C	-4.0403	-3.8630	0.0000
C	-3.1410	-2.7923	0.0000
F	-3.6453	-1.5263	0.0000
F	0.0865	-4.4116	0.0000
C	-5.5276	-3.6238	0.0000
H	-1.1007	-2.0742	0.0000
H	-1.6599	-6.3479	0.0000
H	-4.1389	-6.0096	0.0000
H	-5.8394	-3.0476	0.8822
H	-6.0720	-4.5750	0.0000
H	-5.8394	-3.0476	-0.8822

Table S7. Cartesian coordinates (in Å) of the incoming DNA base or mimic X in water, optimized without any constraint at COSMO-BP86/TZ2P.

=== A			
N	-0.5339	-0.7016	0.0000
C	-1.0196	-1.9555	0.0000
N	-2.2980	-2.3589	0.0000
C	-3.1437	-1.3105	0.0000
C	-2.7899	0.0460	0.0000
C	-1.4063	0.3369	0.0000
N	-4.5176	-1.3153	0.0000
C	-4.9261	-0.0070	0.0000
N	-3.9199	0.8519	0.0000
N	-0.9245	1.5935	0.0000
H	-0.2693	-2.7469	0.0000
H	-5.1199	-2.1317	0.0000
H	-5.9766	0.2579	0.0000
H	-1.5510	2.3873	0.0000
H	0.0748	1.7554	0.0000
=== T			
N	2.2492	-0.3389	0.0000
C	3.0041	-1.4938	0.0000
N	4.3596	-1.2575	0.0000
C	4.9126	-0.0019	0.0000
C	4.1588	1.1303	0.0000
C	2.7128	0.9823	0.0000
O	1.8961	1.9177	0.0000
O	2.5108	-2.6270	0.0000
C	4.7472	2.5102	0.0000
H	1.2385	-0.4676	0.0000
H	4.9605	-2.0761	0.0000
H	5.9992	0.0204	0.0000
H	4.4196	3.0770	0.8826
H	5.8422	2.4663	0.0000
H	4.4196	3.0770	-0.8826
=== G			
N	1.4832	0.7813	0.0196
C	1.7109	-0.5749	0.0254
N	3.0013	-0.9853	-0.0120
N	0.7309	-1.4701	0.0236
C	-0.4968	-0.9052	0.0068
C	-0.8310	0.4557	-0.0022
C	0.2222	1.4173	0.0047
O	0.1547	2.6595	-0.0003
N	-2.2085	0.6236	-0.0174
C	-2.6874	-0.6057	-0.0175
N	-1.6988	-1.5615	-0.0032
H	2.2834	1.4111	0.0187
H	3.7431	-0.3402	0.2317
H	3.1735	-1.9658	0.1780
H	-3.7361	-0.8762	-0.0273
H	-1.8339	-2.5672	-0.0003
=== C			
O	2.6265	-2.6707	0.0000
N	1.8436	1.8579	0.0000
N	2.1986	-0.4122	0.0000
C	4.1212	1.0877	0.0000
C	3.0312	-1.4873	0.0000
N	4.4119	-1.2478	0.0000
C	4.9421	0.0026	0.0000
C	2.7116	0.8300	0.0000
H	4.5174	2.0989	0.0000
H	5.0199	-2.0620	0.0000
H	6.0258	0.0700	0.0000
H	0.8471	1.6765	0.0000
H	2.1661	2.8162	0.0000

=== F

C	-1.7582	-2.9363	0.0000
C	-1.2666	-4.2358	0.0000
C	-2.0918	-5.3512	0.0000
C	-3.4759	-5.1462	0.0000
C	-4.0420	-3.8624	0.0000
C	-3.1396	-2.7948	0.0000
F	-3.6442	-1.5226	0.0000
F	0.0895	-4.4118	0.0000
C	-5.5299	-3.6265	0.0000
H	-1.0985	-2.0720	0.0000
H	-1.6628	-6.3507	0.0000
H	-4.1396	-6.0108	0.0000
H	-5.8424	-3.0514	0.8826
H	-6.0700	-4.5794	0.0000
H	-5.8424	-3.0514	-0.8826

Table S8. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 0º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in the gas phase and at BP86/TZ2P (see text).

A/T-A			
N	-0.5382	-0.7005	0.0000
C	-1.0221	-1.9553	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4081	0.3258	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9232	1.5960	-0.0640
H	-0.2693	-2.7450	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5616	2.3546	0.1394
H	0.0560	1.7227	0.1626
N	-0.5475	-0.7023	3.4000
C	-1.0248	-1.9633	3.4000
N	-2.2980	-2.3635	3.4000
C	-3.1346	-1.3129	3.4000
C	-2.7921	0.0458	3.4000
C	-1.4092	0.3462	3.4000
N	-4.5132	-1.3195	3.4000
C	-4.9204	0.0000	3.4000
N	-3.9180	0.8525	3.4000
N	-0.9232	1.5977	3.4000
H	-0.2608	-2.7414	3.4000
H	-5.0996	-2.1456	3.4000
H	-5.9709	0.2687	3.4000
H	-1.5757	2.3696	3.4000
H	0.0957	1.7650	3.4000
N	2.2332	-0.3395	3.4000
C	2.9879	-1.4952	3.4000
N	4.3636	-1.2570	3.4000
C	4.9204	0.0000	3.4000
C	4.1638	1.1274	3.4000
C	2.7087	0.9683	3.4000
O	1.9192	1.9281	3.4000
O	2.5217	-2.6286	3.4000
C	4.7347	2.5143	3.4000
H	1.1749	-0.4774	3.4000
H	4.9433	-2.0886	3.4000
H	6.0089	0.0278	3.4000
H	4.3937	3.0763	4.2802
H	5.8313	2.4920	3.4000
H	4.3937	3.0763	2.5198
T/A-T			
N	2.2416	-0.3443	0.0000
C	2.9904	-1.5099	0.0000
N	4.3636	-1.2570	0.0000
C	4.9204	0.0000	0.0000
C	4.1638	1.1274	0.0000
C	2.7031	0.9899	0.0000
O	1.9084	1.9225	0.0000
O	2.5256	-2.6378	0.0000
C	4.7347	2.5143	0.0000
H	1.2308	-0.4689	0.0000
H	4.9433	-2.0886	0.0000
H	6.0089	0.0278	0.0000
H	4.3937	3.0763	0.8802
H	5.8313	2.4920	0.0000

H	4.3937	3.0763	-0.8802
N	-0.5475	-0.7023	3.4000
C	-1.0248	-1.9633	3.4000
N	-2.2980	-2.3635	3.4000
C	-3.1346	-1.3129	3.4000
C	-2.7921	0.0458	3.4000
C	-1.4092	0.3462	3.4000
N	-4.5132	-1.3195	3.4000
C	-4.9204	0.0000	3.4000
N	-3.9180	0.8525	3.4000
N	-0.9232	1.5977	3.4000
H	-0.2608	-2.7414	3.4000
H	-5.0996	-2.1456	3.4000
H	-5.9709	0.2687	3.4000
H	-1.5757	2.3696	3.4000
H	0.0957	1.7650	3.4000
N	2.2332	-0.3395	3.4000
C	2.9879	-1.4952	3.4000
N	4.3636	-1.2570	3.4000
C	4.9204	0.0000	3.4000
C	4.1638	1.1274	3.4000
C	2.7087	0.9683	3.4000
O	1.9192	1.9281	3.4000
O	2.5217	-2.6286	3.4000
C	4.7347	2.5143	3.4000
H	1.1749	-0.4774	3.4000
H	4.9433	-2.0886	3.4000
H	6.0089	0.0278	3.4000
H	4.3937	3.0763	4.2802
H	5.8313	2.4920	3.4000
H	4.3937	3.0763	2.5198

G/C-G

N	-0.2036	-3.2008	-0.0773
O	-0.8229	1.3996	0.0000
N	-0.6393	-0.8941	0.0000
C	-1.1267	-2.1726	0.0000
N	-2.4100	-2.4547	0.0000
C	-3.1863	-1.3539	0.0000
C	-2.8124	0.0003	0.0000
C	-1.4105	0.3286	0.0000
N	-4.5601	-1.3332	0.0000
C	-4.9445	0.0000	0.0000
N	-3.9260	0.8249	0.0000
H	0.6465	-3.0728	0.4647
H	-0.6422	-4.1002	0.1002
H	0.3654	-0.7338	0.0000
H	-5.1572	-2.1512	0.0000
H	-5.9899	0.2870	0.0000
N	-0.1956	-3.1483	3.4000
O	-0.8586	1.4196	3.4000
N	-0.6354	-0.8692	3.4000
C	-1.1145	-2.1581	3.4000
N	-2.4100	-2.4547	3.4000
C	-3.1863	-1.3539	3.4000
C	-2.8124	0.0003	3.4000
C	-1.4156	0.3028	3.4000
N	-4.5601	-1.3332	3.4000
C	-4.9445	0.0000	3.4000
N	-3.9260	0.8249	3.4000
H	0.8201	-2.9703	3.4000
H	-0.5479	-4.0948	3.4000
H	0.4005	-0.7205	3.4000
H	-5.1572	-2.1512	3.4000
H	-5.9899	0.2870	3.4000
O	2.6293	-2.6685	3.4000
N	1.8339	1.8550	3.4000
N	2.2083	-0.4066	3.4000
C	4.1281	1.0860	3.4000
C	3.0227	-1.4916	3.4000
N	4.4154	-1.2536	3.4000
C	4.9445	0.0000	3.4000

C	2.7064	0.8422	3.4000
H	4.5346	2.0937	3.4000
H	5.0043	-2.0800	3.4000
H	6.0295	0.0718	3.4000
H	0.7952	1.6730	3.4000
H	2.1743	2.8065	3.4000

C/G-C

O	2.6336	-2.6790	0.0000
N	1.8291	1.8467	-0.0612
N	2.1938	-0.4074	0.0000
C	4.1281	1.0860	0.0000
C	3.0025	-1.5132	0.0000
N	4.4154	-1.2536	0.0000
C	4.9445	0.0000	0.0000
C	2.7115	0.8098	0.0000
H	4.5346	2.0937	0.0000
H	5.0043	-2.0800	0.0000
H	6.0295	0.0718	0.0000
H	0.8520	1.6223	0.0936
H	2.1343	2.7922	0.1185
N	-0.1956	-3.1483	3.4000
O	-0.8586	1.4196	3.4000
N	-0.6354	-0.8692	3.4000
C	-1.1145	-2.1581	3.4000
N	-2.4100	-2.4547	3.4000
C	-3.1863	-1.3539	3.4000
C	-2.8124	0.0003	3.4000
C	-1.4156	0.3028	3.4000
N	-4.5601	-1.3332	3.4000
C	-4.9445	0.0000	3.4000
N	-3.9260	0.8249	3.4000
H	0.8201	-2.9703	3.4000
H	-0.5479	-4.0948	3.4000
H	0.4005	-0.7205	3.4000
H	-5.1572	-2.1512	3.4000
H	-5.9899	0.2870	3.4000
O	2.6293	-2.6685	3.4000
N	1.8339	1.8550	3.4000
N	2.2083	-0.4066	3.4000
C	4.1281	1.0860	3.4000
C	3.0227	-1.4916	3.4000
N	4.4154	-1.2536	3.4000
C	4.9445	0.0000	3.4000
C	2.7064	0.8422	3.4000
H	4.5346	2.0937	3.4000
H	5.0043	-2.0800	3.4000
H	6.0295	0.0718	3.4000
H	0.7952	1.6730	3.4000
H	2.1743	2.8065	3.4000

Table S9. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 0º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1 in water at COSMO-BP86/TZ2P (see text).

A/T-A			
N	-0.5367	-0.7062	0.0000
C	-1.0185	-1.9599	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4074	0.3314	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9164	1.5892	-0.0695
H	-0.2678	-2.7514	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5341	2.3754	0.0889
H	0.0745	1.7308	0.0877
N	-0.5475	-0.7023	3.4000
C	-1.0248	-1.9633	3.4000
N	-2.2980	-2.3635	3.4000
C	-3.1346	-1.3129	3.4000
C	-2.7921	0.0458	3.4000
C	-1.4092	0.3462	3.4000
N	-4.5132	-1.3195	3.4000
C	-4.9204	0.0000	3.4000
N	-3.9180	0.8525	3.4000
N	-0.9232	1.5977	3.4000
H	-0.2608	-2.7414	3.4000
H	-5.0996	-2.1456	3.4000
H	-5.9709	0.2687	3.4000
H	-1.5757	2.3696	3.4000
H	0.0957	1.7650	3.4000
N	2.2332	-0.3395	3.4000
C	2.9879	-1.4952	3.4000
N	4.3636	-1.2570	3.4000
C	4.9204	0.0000	3.4000
C	4.1638	1.1274	3.4000
C	2.7087	0.9683	3.4000
O	1.9192	1.9281	3.4000
O	2.5217	-2.6286	3.4000
C	4.7347	2.5143	3.4000
H	1.1749	-0.4774	3.4000
H	4.9433	-2.0886	3.4000
H	6.0089	0.0278	3.4000
H	4.3937	3.0763	4.2802
H	5.8313	2.4920	3.4000
H	4.3937	3.0763	2.5198
T/A-T			
N	-1.4335	-2.6815	0.0000
C	-0.7575	-3.8842	0.0000
N	-1.5938	-4.9810	0.0000
C	-2.9620	-4.9029	0.0000
C	-3.6127	-3.7124	0.0000
C	-2.8218	-2.4906	0.0000
O	-3.2833	-1.3410	0.0000
O	0.4729	-3.9740	0.0000
C	-5.1067	-3.5782	0.0000
H	-0.8554	-1.8424	0.0000
H	-1.1173	-5.8758	0.0000
H	-3.4881	-5.8566	0.0000
H	-5.4490	-3.0171	0.8804
H	-5.5915	-4.5624	0.0000

H	-5.4490	-3.0171	-0.8804
N	0.1793	-0.3577	-3.4000
C	1.5185	-0.5140	-3.4000
N	2.4595	0.4324	-3.4000
C	1.9115	1.6585	-3.4000
C	0.5476	1.9795	-3.4000
C	-0.3553	0.8897	-3.4000
N	2.5516	2.8796	-3.4000
C	1.5673	3.8481	-3.4000
N	0.3491	3.3502	-3.4000
N	-1.6901	1.0338	-3.4000
H	1.8580	-1.5503	-3.4000
H	3.5548	3.0202	-3.4000
H	1.8118	4.9045	-3.4000
H	-2.0753	1.9683	-3.4000
H	-2.3073	0.2061	-3.4000
N	-1.4219	-2.6599	-3.4000
C	-0.7429	-3.8616	-3.4000
N	-1.5872	-4.9735	-3.4000
C	-2.9595	-4.8898	-3.4000
C	-3.6125	-3.6994	-3.4000
C	-2.8019	-2.4805	-3.4000
O	-3.2909	-1.3380	-3.4000
O	0.4779	-3.9690	-3.4000
C	-5.1066	-3.5683	-3.4000
H	-0.8127	-1.7836	-3.4000
H	-1.1155	-5.8708	-3.4000
H	-3.4849	-5.8435	-3.4000
H	-5.4487	-3.0070	-4.2802
H	-5.5911	-4.5522	-3.4000
H	-5.4487	-3.0070	-2.5198

G/C-G

N	-1.7080	-2.4169	0.0000
C	-1.0712	-3.6374	0.0000
N	-1.7258	-4.7909	0.0000
C	-3.0665	-4.6283	0.0000
C	-3.8115	-3.4411	0.0000
C	-3.1090	-2.1997	0.0000
N	-4.0045	-5.6297	0.0000
C	-5.2477	-5.0153	0.0000
N	-5.1698	-3.7071	0.0000
O	-3.5534	-1.0403	0.0000
N	0.2827	-3.6309	-0.0773
H	-1.1457	-1.5676	0.0000
H	-3.8031	-6.6225	0.0000
H	-6.1647	-5.5940	0.0000
H	0.7528	-4.5097	0.1059
H	0.8016	-2.7906	0.1451
N	0.2684	-3.6440	3.4000
O	-3.5242	-1.0132	3.4000
N	-1.6981	-2.4111	3.4000
C	-1.0825	-3.6406	3.4000
N	-1.7492	-4.7903	3.4000
C	-3.0836	-4.6072	3.4000
C	-3.8189	-3.4100	3.4000
C	-3.0874	-2.1822	3.4000
N	-4.0358	-5.5976	3.4000
C	-5.2730	-4.9694	3.4000
N	-5.1815	-3.6620	3.4000
H	0.8311	-2.7798	3.4000
H	0.7203	-4.5472	3.4000
H	-1.1003	-1.5522	3.4000
H	-3.8449	-6.5922	3.4000
H	-6.1959	-5.5381	3.4000
O	1.8444	-1.2509	3.4000
N	-2.0061	1.2528	3.4000
N	-0.0968	-0.0160	3.4000
C	0.1211	2.4059	3.4000
C	1.2521	-0.1605	3.4000
N	2.0279	1.0203	3.4000
C	1.4721	2.2623	3.4000

C	-0.6703	1.2000	3.4000
H	-0.3385	3.3905	3.4000
H	3.0340	0.8872	3.4000
H	2.1597	3.1046	3.4000
H	-2.5814	0.3690	3.4000
H	-2.4698	2.1507	3.4000

C/G-C

O	2.6282	-2.6712	0.0000
N	1.8484	1.8573	-0.0560
N	2.2028	-0.4102	0.0000
C	4.1281	1.0860	0.0000
C	3.0296	-1.4893	0.0000
N	4.4154	-1.2536	0.0000
C	4.9445	0.0000	0.0000
C	2.7173	0.8280	0.0000
H	4.5346	2.0937	0.0000
H	5.0043	-2.0800	0.0000
H	6.0295	0.0718	0.0000
H	0.8559	1.6716	0.0238
H	2.1663	2.8137	0.0243
N	-0.1956	-3.1483	3.4000
O	-0.8586	1.4196	3.4000
N	-0.6354	-0.8692	3.4000
C	-1.1145	-2.1581	3.4000
N	-2.4100	-2.4547	3.4000
C	-3.1863	-1.3539	3.4000
C	-2.8124	0.0003	3.4000
C	-1.4156	0.3028	3.4000
N	-4.5601	-1.3332	3.4000
C	-4.9445	0.0000	3.4000
N	-3.9260	0.8249	3.4000
H	0.8201	-2.9703	3.4000
H	-0.5479	-4.0948	3.4000
H	0.4005	-0.7205	3.4000
H	-5.1572	-2.1512	3.4000
H	-5.9899	0.2870	3.4000
O	2.6293	-2.6685	3.4000
N	1.8339	1.8550	3.4000
N	2.2083	-0.4066	3.4000
C	4.1281	1.0860	3.4000
C	3.0227	-1.4916	3.4000
N	4.4154	-1.2536	3.4000
C	4.9445	0.0000	3.4000
C	2.7064	0.8422	3.4000
H	4.5346	2.0937	3.4000
H	5.0043	-2.0800	3.4000
H	6.0295	0.0718	3.4000
H	0.7952	1.6730	3.4000
H	2.1743	2.8065	3.4000

Table S10. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1, again in the gas phase and at BP86/TZ2P (see text).

A/T-A			
N	-0.5385	-0.7004	0.0000
C	-1.0206	-1.9553	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4087	0.3261	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9213	1.5961	-0.0366
H	-0.2680	-2.7451	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5553	2.3527	0.1872
H	0.0566	1.7138	0.1999
N	-0.0301	-0.8900	3.4000
C	0.3250	-2.1907	3.4000
N	-0.4699	-3.2628	3.4000
C	-1.7642	-2.9046	3.4000
C	-2.2858	-1.6041	3.4000
C	-1.3435	-0.5482	3.4000
N	-2.8757	-3.7203	3.4000
C	-3.9807	-2.8922	3.4000
N	-3.6708	-1.6132	3.4000
N	-1.6860	0.7499	3.4000
H	1.4004	-2.3711	3.4000
H	-2.8645	-4.7333	3.4000
H	-4.9885	-3.2922	3.4000
H	-2.6676	0.9909	3.4000
H	-0.9601	1.4841	3.4000
N	2.0063	1.0380	3.4000
C	3.2961	0.5466	3.4000
N	4.2690	1.5479	3.4000
C	3.9807	2.8922	3.4000
C	2.7059	3.3595	3.4000
C	1.6222	2.3755	3.4000
O	0.4194	2.6879	3.4000
O	3.5851	-0.6444	3.4000
C	2.3526	4.8171	3.4000
H	1.2311	0.3044	3.4000
H	5.2269	1.2159	3.4000
H	4.8450	3.5544	3.4000
H	1.7464	5.0713	4.2802
H	3.2528	5.4436	3.4000
H	1.7464	5.0713	2.5198
T/A-T			
N	2.2432	-0.3418	0.0000
C	2.9934	-1.5071	0.0000
N	4.3636	-1.2570	0.0000
C	4.9204	0.0000	0.0000
C	4.1638	1.1274	0.0000
C	2.7041	0.9893	0.0000
O	1.9090	1.9242	0.0000
O	2.5240	-2.6339	0.0000
C	4.7347	2.5143	0.0000
H	1.2327	-0.4674	0.0000
H	4.9433	-2.0886	0.0000
H	6.0089	0.0278	0.0000
H	4.3937	3.0763	0.8802
H	5.8313	2.4920	0.0000

H	4.3937	3.0763	-0.8802
N	-0.0301	-0.8900	3.4000
C	0.3250	-2.1907	3.4000
N	-0.4699	-3.2628	3.4000
C	-1.7642	-2.9046	3.4000
C	-2.2858	-1.6041	3.4000
C	-1.3435	-0.5482	3.4000
N	-2.8757	-3.7203	3.4000
C	-3.9807	-2.8922	3.4000
N	-3.6708	-1.6132	3.4000
N	-1.6860	0.7499	3.4000
H	1.4004	-2.3711	3.4000
H	-2.8645	-4.7333	3.4000
H	-4.9885	-3.2922	3.4000
H	-2.6676	0.9909	3.4000
H	-0.9601	1.4841	3.4000
N	2.0063	1.0380	3.4000
C	3.2961	0.5466	3.4000
N	4.2690	1.5479	3.4000
C	3.9807	2.8922	3.4000
C	2.7059	3.3595	3.4000
C	1.6222	2.3755	3.4000
O	0.4194	2.6879	3.4000
O	3.5851	-0.6444	3.4000
C	2.3526	4.8171	3.4000
H	1.2311	0.3044	3.4000
H	5.2269	1.2159	3.4000
H	4.8450	3.5544	3.4000
H	1.7464	5.0713	4.2802
H	3.2528	5.4436	3.4000
H	1.7464	5.0713	2.5198

G/C-G

N	-0.1984	-3.1913	-0.0646
O	-0.8304	1.4067	0.0000
N	-0.6415	-0.8872	0.0000
C	-1.1257	-2.1680	0.0000
N	-2.4100	-2.4547	0.0000
C	-3.1863	-1.3539	0.0000
C	-2.8124	0.0003	0.0000
C	-1.4148	0.3314	0.0000
N	-4.5601	-1.3332	0.0000
C	-4.9445	0.0000	0.0000
N	-3.9260	0.8249	0.0000
H	0.6706	-3.0320	0.4384
H	-0.6171	-4.0868	0.1704
H	0.3631	-0.7247	0.0000
H	-5.1572	-2.1512	0.0000
H	-5.9899	0.2870	0.0000
N	1.6922	-2.6620	3.4000
O	-1.5290	0.6438	3.4000
N	-0.0031	-1.0767	3.4000
C	0.3668	-2.4010	3.4000
N	-0.5069	-3.4024	3.4000
C	-1.7820	-2.9682	3.4000
C	-2.2755	-1.6529	3.4000
C	-1.3232	-0.5871	3.4000
N	-2.9055	-3.7590	3.4000
C	-4.0002	-2.9063	3.4000
N	-3.6611	-1.6403	3.4000
H	2.4094	-1.9209	3.4000
H	1.9636	-3.6348	3.4000
H	0.7475	-0.3475	3.4000
H	-2.9078	-4.7717	3.4000
H	-5.0146	-3.2886	3.4000
O	3.6957	-0.6134	3.4000
N	0.3933	2.5787	3.4000
N	2.0256	0.9691	3.4000
C	2.7014	3.3050	3.4000
C	3.3222	0.5700	3.4000
N	4.3089	1.5811	3.4000
C	4.0002	2.9063	3.4000

C	1.6945	2.2721	3.4000
H	2.4379	4.3592	3.4000
H	5.2712	1.2587	3.4000
H	4.8357	3.6021	3.4000
H	-0.3400	1.8208	3.4000
H	0.1094	3.5485	3.4000

C/G-C

O	2.6393	-2.6812	0.0000
N	1.8281	1.8447	-0.0624
N	2.1958	-0.4102	0.0000
C	4.1281	1.0860	0.0000
C	3.0084	-1.5145	0.0000
N	4.4154	-1.2536	0.0000
C	4.9445	0.0000	0.0000
C	2.7123	0.8067	0.0000
H	4.5346	2.0937	0.0000
H	5.0043	-2.0800	0.0000
H	6.0295	0.0718	0.0000
H	0.8534	1.6098	0.0932
H	2.1320	2.7814	0.1646
N	1.6922	-2.6620	3.4000
O	-1.5290	0.6438	3.4000
N	-0.0031	-1.0767	3.4000
C	0.3668	-2.4010	3.4000
N	-0.5069	-3.4024	3.4000
C	-1.7820	-2.9682	3.4000
C	-2.2755	-1.6529	3.4000
C	-1.3232	-0.5871	3.4000
N	-2.9055	-3.7590	3.4000
C	-4.0002	-2.9063	3.4000
N	-3.6611	-1.6403	3.4000
H	2.4094	-1.9209	3.4000
H	1.9636	-3.6348	3.4000
H	0.7475	-0.3475	3.4000
H	-2.9078	-4.7717	3.4000
H	-5.0146	-3.2886	3.4000
O	3.6957	-0.6134	3.4000
N	0.3933	2.5787	3.4000
N	2.0256	0.9691	3.4000
C	2.7014	3.3050	3.4000
C	3.3222	0.5700	3.4000
N	4.3089	1.5811	3.4000
C	4.0002	2.9063	3.4000
C	1.6945	2.2721	3.4000
H	2.4379	4.3592	3.4000
H	5.2712	1.2587	3.4000
H	4.8357	3.6021	3.4000
H	-0.3400	1.8208	3.4000
H	0.1094	3.5485	3.4000

Table S11. Cartesian coordinates (in Å) of models of template-primer complexes Y_1/Z-Y_2 with 3.4 Å stacking distance and a twist angle of 36º, based on DNA base pairs in the gas phase that were optimized in C_s symmetry at BP86/TZ2P, followed by a constrained optimization of the front atoms in the unpaired base Y_1 in water at COSMO-BP86/TZ2P (see text).

A/T-A			
N	-0.5368	-0.7047	0.0000
C	-1.0186	-1.9593	0.0000
N	-2.2980	-2.3635	0.0000
C	-3.1346	-1.3129	0.0000
C	-2.7921	0.0458	0.0000
C	-1.4080	0.3324	0.0000
N	-4.5132	-1.3195	0.0000
C	-4.9204	0.0000	0.0000
N	-3.9180	0.8525	0.0000
N	-0.9182	1.5908	-0.0454
H	-0.2671	-2.7502	0.0000
H	-5.0996	-2.1456	0.0000
H	-5.9709	0.2687	0.0000
H	-1.5392	2.3775	0.0947
H	0.0739	1.7333	0.1004
N	-0.0301	-0.8900	3.4000
C	0.3250	-2.1907	3.4000
N	-0.4699	-3.2628	3.4000
C	-1.7642	-2.9046	3.4000
C	-2.2858	-1.6041	3.4000
C	-1.3435	-0.5482	3.4000
N	-2.8757	-3.7203	3.4000
C	-3.9807	-2.8922	3.4000
N	-3.6708	-1.6132	3.4000
N	-1.6860	0.7499	3.4000
H	1.4004	-2.3711	3.4000
H	-2.8645	-4.7333	3.4000
H	-4.9885	-3.2922	3.4000
H	-2.6676	0.9909	3.4000
H	-0.9601	1.4841	3.4000
N	2.0063	1.0380	3.4000
C	3.2961	0.5466	3.4000
N	4.2690	1.5479	3.4000
C	3.9807	2.8922	3.4000
C	2.7059	3.3595	3.4000
C	1.6222	2.3755	3.4000
O	0.4194	2.6879	3.4000
O	3.5851	-0.6444	3.4000
C	2.3526	4.8171	3.4000
H	1.2311	0.3044	3.4000
H	5.2269	1.2159	3.4000
H	4.8450	3.5544	3.4000
H	1.7464	5.0713	4.2802
H	3.2528	5.4436	3.4000
H	1.7464	5.0713	2.5198
T/A-T			
N	2.2498	-0.3410	0.0000
C	3.0077	-1.4935	0.0000
N	4.3636	-1.2570	0.0000
C	4.9204	0.0000	0.0000
C	4.1638	1.1274	0.0000
C	2.7140	0.9816	0.0000
O	1.9016	1.9167	0.0000
O	2.5194	-2.6278	0.0000
C	4.7347	2.5143	0.0000
H	1.2394	-0.4707	0.0000
H	4.9433	-2.0886	0.0000
H	6.0089	0.0278	0.0000
H	4.3937	3.0763	0.8802
H	5.8313	2.4920	0.0000

H	4.3937	3.0763	-0.8802
N	-0.0301	-0.8900	3.4000
C	0.3250	-2.1907	3.4000
N	-0.4699	-3.2628	3.4000
C	-1.7642	-2.9046	3.4000
C	-2.2858	-1.6041	3.4000
C	-1.3435	-0.5482	3.4000
N	-2.8757	-3.7203	3.4000
C	-3.9807	-2.8922	3.4000
N	-3.6708	-1.6132	3.4000
N	-1.6860	0.7499	3.4000
H	1.4004	-2.3711	3.4000
H	-2.8645	-4.7333	3.4000
H	-4.9885	-3.2922	3.4000
H	-2.6676	0.9909	3.4000
H	-0.9601	1.4841	3.4000
N	2.0063	1.0380	3.4000
C	3.2961	0.5466	3.4000
N	4.2690	1.5479	3.4000
C	3.9807	2.8922	3.4000
C	2.7059	3.3595	3.4000
C	1.6222	2.3755	3.4000
O	0.4194	2.6879	3.4000
O	3.5851	-0.6444	3.4000
C	2.3526	4.8171	3.4000
H	1.2311	0.3044	3.4000
H	5.2269	1.2159	3.4000
H	4.8450	3.5544	3.4000
H	1.7464	5.0713	4.2802
H	3.2528	5.4436	3.4000
H	1.7464	5.0713	2.5198

G/C-G

N	-0.1980	-3.1572	-0.0749
O	-0.8621	1.4236	0.0000
N	-0.6424	-0.8684	0.0000
C	-1.1156	-2.1609	0.0000
N	-2.4100	-2.4547	0.0000
C	-3.1863	-1.3539	0.0000
C	-2.8124	0.0003	0.0000
C	-1.4227	0.3165	0.0000
N	-4.5601	-1.3332	0.0000
C	-4.9445	0.0000	0.0000
N	-3.9260	0.8249	0.0000
H	0.7738	-2.9692	0.1390
H	-0.5289	-4.0933	0.1285
H	0.3640	-0.7132	0.0000
H	-5.1572	-2.1512	0.0000
H	-5.9899	0.2870	0.0000
N	1.6922	-2.6620	3.4000
O	-1.5290	0.6438	3.4000
N	-0.0031	-1.0767	3.4000
C	0.3668	-2.4010	3.4000
N	-0.5069	-3.4024	3.4000
C	-1.7820	-2.9682	3.4000
C	-2.2755	-1.6529	3.4000
C	-1.3232	-0.5871	3.4000
N	-2.9055	-3.7590	3.4000
C	-4.0002	-2.9063	3.4000
N	-3.6611	-1.6403	3.4000
H	2.4094	-1.9209	3.4000
H	1.9636	-3.6348	3.4000
H	0.7475	-0.3475	3.4000
H	-2.9078	-4.7717	3.4000
H	-5.0146	-3.2886	3.4000
O	3.6957	-0.6134	3.4000
N	0.3933	2.5787	3.4000
N	2.0256	0.9691	3.4000
C	2.7014	3.3050	3.4000
C	3.3222	0.5700	3.4000
N	4.3089	1.5811	3.4000
C	4.0002	2.9063	3.4000
C	1.6945	2.2721	3.4000

H	2.4379	4.3592	3.4000
H	5.2712	1.2587	3.4000
H	4.8357	3.6021	3.4000
H	-0.3400	1.8208	3.4000
H	0.1094	3.5485	3.4000

C/G-C

O	2.6328	-2.6731	0.0000
N	1.8481	1.8550	-0.0478
N	2.2031	-0.4126	0.0000
C	4.1281	1.0860	0.0000
C	3.0320	-1.4902	0.0000
N	4.4154	-1.2536	0.0000
C	4.9445	0.0000	0.0000
C	2.7165	0.8261	0.0000
H	4.5346	2.0937	0.0000
H	5.0043	-2.0800	0.0000
H	6.0295	0.0718	0.0000
H	0.8536	1.6703	0.0020
H	2.1679	2.8130	-0.0077
N	1.6922	-2.6620	3.4000
O	-1.5290	0.6438	3.4000
N	-0.0031	-1.0767	3.4000
C	0.3668	-2.4010	3.4000
N	-0.5069	-3.4024	3.4000
C	-1.7820	-2.9682	3.4000
C	-2.2755	-1.6529	3.4000
C	-1.3232	-0.5871	3.4000
N	-2.9055	-3.7590	3.4000
C	-4.0002	-2.9063	3.4000
N	-3.6611	-1.6403	3.4000
H	2.4094	-1.9209	3.4000
H	1.9636	-3.6348	3.4000
H	0.7475	-0.3475	3.4000
H	-2.9078	-4.7717	3.4000
H	-5.0146	-3.2886	3.4000
O	3.6957	-0.6134	3.4000
N	0.3933	2.5787	3.4000
N	2.0256	0.9691	3.4000
C	2.7014	3.3050	3.4000
C	3.3222	0.5700	3.4000
N	4.3089	1.5811	3.4000
C	4.0002	2.9063	3.4000
C	1.6945	2.2721	3.4000
H	2.4379	4.3592	3.4000
H	5.2712	1.2587	3.4000
H	4.8357	3.6021	3.4000
H	-0.3400	1.8208	3.4000
H	0.1094	3.5485	3.4000