Supporting Information

The Solvation, Partitioning, Hydrogen Bonding, and Dimerization of Nucleotide Bases: A Multifaceted Challenge for Quantum Chemistry

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Contents:

Solvation Free Energies of Nucleobase Dimers	S2
Components of the Solvation Free Energy for Nucleobase Dimers	S4
Cartesian Coordinates of Gas-Phase Dimer Geometries	S6
Cartesian Coordinates of Liquid-Phase Dimer Geometries	S64

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Solvation Free Energies of Nucleobase Dimers

Table S1. SM*x*/M06-2X/6-31+G** and SM*x*/M06-2X/6-31G** Solvation Free Energies of Nucleobase Dimers Calculated without Nuclear Relaxation [a]

	SM*x*/M06-2X/6-31+G**			SM*x*/M06-2X/6-31G**		
base pair	SM8	SM8AD	SMD	SM8	SM8AD	SMD
			chloroform			
A–T HB	–19.79	–20.73	–23.41	–20.55	–21.19	–21.97
A–U HB	–19.31	–20.19	–23.42	–20.56	–21.16	–21.94
C–G HB	–24.83	–26.24	–28.05	–25.06	–26.16	–26.51
9-HexA–9-HexA HB1	–27.80	–28.42	–34.13	–29.44	–29.66	–32.76
9-HexA–9-HexA HB2	–28.62	–29.05	–34.57	–30.52	–30.67	–36.29
9-HexA–9-HexA HB3	–28.28	–28.85	–34.73	–29.72	–29.98	–33.36
1-HexT–1-HexT HB 1	–23.41	–22.72	–24.72	–22.61	–22.03	–22.77
1-HexT–1-HexT HB 2	–21.23	–21.30	–22.69	–19.67	–19.49	–20.88
1-HexT–1-HexT HB 3	–22.38	–21.81	–24.02	–21.57	–21.05	–22.18
9-EtA–1-cHexU WC	–22.26	–22.81	–25.55	–21.53	–21.82	–24.08
9-EtA–1-cHexU RWC	–22.53	–23.11	–25.89	–21.77	–22.05	–24.39
9-EtA–1-cHexU H	–21.82	–22.44	–24.94	–20.95	–21.34	–23.47
9-EtA–1-cHexU RH	–21.83	–22.44	–24.84	–20.90	–21.24	–23.39
1-cHexU–1-cHexU HB1	–23.43	–22.88	–24.21	–21.03	–20.30	–22.22
1-cHexU–1-cHexU HB2	–22.36	–21.89	–25.01	–21.48	–20.99	–23.01
1-cHexU–1-cHexU HB3	–22.28	–21.85	–24.56	–21.12	–20.65	–22.64
9-HexA–1-HexT WC	–24.26	–24.37	–28.00	–24.63	–24.64	–26.57
9-HexA–1-HexT RWC	–24.43	–24.57	–28.40	–24.86	–24.88	–26.94
9-HexA–1-HexT H	–23.67	–23.91	–27.80	–23.04	–24.39	–26.33
9-HexA–1-HexT RH	–23.99	–24.27	–27.77	–24.23	–24.41	–26.29
A–T S	–15.02	–17.06	–21.89	–17.36	–19.07	–20.30
A–U S	–15.34	–17.31	–22.20	–17.72	–19.42	–20.58
C–G S	–19.92	–22.39	–25.78	–21.72	–23.88	–24.03
			water			
A–T HB	–20.86	–20.50	–23.40	–22.46	–22.24	–21.40
A–U HB	–20.96	–20.34	–24.05	–23.26	–22.79	–22.03
C–G HB	–28.64	–28.61	–30.17	–29.05	–28.81	–27.86
A–T S	–19.48	–22.17	–28.22	–22.33	–25.01	–26.12
A–U S	–20.49	–22.74	–29.21	–23.59	–25.97	–27.10
C–G S	–28.11	–31.11	–35.42	–30.26	–33.25	–33.05

[a] HB refers to hydrogen-bonded structures. S refers to π–π stacked dimers. These solvation free energies were calculated as a difference between the SM*x*/M06-2X/*B* total energy (*x* = 8, 8AD, D; *B* = 6-31G**, 6-31+G**) in solution at the M06-2X/6-31+G** gas-phase geometry and the M06-2X/*B* total energy in the gas phase at the same M06-2X/6-31+G** gas-phase geometry.

Table S2. SM*x*/M06-2X/6-31+G** and SM*x*/M06-2X/6-31G** Solvation Free Energies of Nucleobase Dimers Calculated with Nuclear Relaxation [a]

	SM*x*/M06-2X/6-31+G**			SM*x*/M06-2X/6-31G**		
base pair	SM8	SM8AD	SMD	SM8	SM8AD	SMD
			chloroform			
A–T HB	–19.31	–20.26	–23.77	–19.93	–20.58	–22.09
A–U HB	–18.95	–19.85	–23.76	–20.09	–20.69	–22.08
C–G HB	–24.80	–26.26	–28.59	–24.80	–25.93	–26.83
9-HexA–9-HexA HB1				–27.57	–27.77	–31.68
9-HexA–9-HexA HB2				–28.95	–29.01	–33.83
9-HexA–9-HexA HB3				–27.99	–28.24	–33.62
1-HexT–1-HexT HB1				–20.78	–20.38	–23.31
1-HexT–1-HexT HB2				–18.13	–18.00	–21.16
1-HexT–1-HexT HB3				–19.82	–19.34	–22.42
9-EtA–1-cHexU WC				–20.28	–20.60	–24.25
9-EtA–1-cHexU RWC				–20.48	–20.78	–24.50
9-EtA–1-cHexU H				–19.54	–19.95	–23.55
9-EtA–1-cHexU RH				–19.56	–19.92	–23.49
1-cHexU–1-cHexU HB1				–19.65	–19.02	–22.47
1-cHexU–1-cHexU HB2				–20.02	–19.53	–23.27
1-cHexU–1-cHexU HB3				–19.66	–19.24	–22.68
9-HexA–1-HexT WC				–22.77	–22.93	–26.78
9-HexA–1-HexT RWC				–23.01	–23.06	–27.01
9-HexA–1-HexT H				–22.25	–22.51	–26.42
9-HexA–1-HexT RH				–22.38	–22.58	–26.44
A–T S	–14.91	–16.88	–22.42	–16.58	–18.31	–20.30
A–U S	–15.22	–17.13	–22.83	–17.11	–18.80	–20.68
C–G S	–19.92	–22.47	–27.33	–21.42	–23.73	–24.12
			water			
A–T HB	–21.84	–21.69	–24.46	–23.41	–23.42	–21.96
A–U HB	–22.03	–21.68	–25.21	–24.33	–24.08	–22.65
C–G HB	–30.46	–30.83	–31.76	–30.61	–30.74	–28.98
A–T S	–21.22	–24.27	–29.50	–23.16	–26.33	–26.65
A–U S	–22.12	–24.74	–30.59	–24.45	–27.20	–27.67
C–G S	–31.01	–34.62	–40.69	–33.29	–36.02	–35.91

[a] HB refers to hydrogen-bonded structures. S refers to π-π stacked dimers. These solvation free energies were calculated as a difference between the SM*x*/M06-2X/*B* total energy (*x* = 8, 8AD, D; *B* = 6-31G**, 6-31+G**) in solution at the SM*x*/M06-2X/*B* liquid-phase geometry and the M06-2X/*B* total energy in the gas phase at the M06-2X/*B* gas-phase geometry.

Components of the Solvation Free Energy for Unsubstituted Nucleobase Dimers

Table S3. SM*x*/M06-2X/6-31G** Polarization (G_P), Electronic Relaxation (ΔE_E), and Cavity–Dispersion–Solvent–Structure (G_{CDS}) Components (in kcal/mol) of the Aqueous Solvation Free Energy (ΔG_S) for Nucleobase Dimers Calculated Using the M06-2X/6-31+G** Gas-Phase Geometries

model	G_P	ΔE_E	ΔG_{EP}	G_{CDS}	ΔG_S
		A–T stacking			
SM8	–20.33	2.55	–17.77	–4.56	–22.33
SM8AD	–23.40	3.55	–19.85	–5.16	–25.01
SMD	–33.75	4.90	–28.84	2.72	–26.12
		A–U stacking			
SM8	–21.24	2.76	–18.48	–5.11	–23.59
SM8AD	–23.88	3.60	–20.28	–5.69	–25.97
SMD	–34.22	5.01	–29.21	2.11	–27.10
		C–G stacking			
SM8	–29.23	5.29	–23.94	–6.32	–30.26
SM8AD	–33.19	6.91	–26.28	–6.96	–33.24
SMD	–43.38	7.97	–35.41	2.36	–33.05
		A–T hydrogen bonding			
SM8	–22.66	4.06	–18.60	–3.86	–22.46
SM8AD	–24.04	4.77	–19.27	–2.97	–22.24
SMD	–31.11	5.59	–25.52	4.13	–21.40
		A–U hydrogen bonding			
SM8	–23.45	4.28	–19.17	–4.10	–23.26
SM8AD	–24.62	4.92	–19.70	–3.09	–22.79
SMD	–31.41	5.59	–25.82	3.79	–22.03
		C–G hydrogen bonding			
SM8	–28.50	4.87	–23.63	–5.42	–29.05
SM8AD	–29.55	5.50	–24.05	–4.76	–28.81
SMD	–37.72	6.77	–30.96	3.10	–27.86

Table S4 SM*x*/M06-2X/6-31+G** Polarization (G_P), Electronic Relaxation (ΔE_E), and Cavity–Dispersion–Solvent-structure (G_{CDS}) Components (in kcal/mol) of the Aqueous Solvation Free Energy (ΔG_S) for Nucleobase Dimers Calculated Using the M06-2X/6-31+G** Gas-Phase Geometries

model	G_P	ΔE_E	ΔG_{EP}	G_{CDS}	ΔG_S
		A–T stacking			
SM8AD	–20.35	3.33	–17.02	–5.16	–22.17
SM8	–17.43	2.51	–14.92	–4.56	–19.48
SMD	–36.75	5.81	–30.94	2.72	–28.22
		A–U stacking			
SM8AD	–20.37	3.32	–17.05	–5.69	–22.74
SM8	–18.03	2.65	–15.38	–5.11	–20.49
SMD	–37.23	5.91	–31.32	2.11	–29.21
		C–G stacking			
SM8AD	–31.32	7.18	–24.15	–6.96	–31.11
SM8	–27.64	5.86	–21.79	–6.32	–28.11
SMD	–47.25	9.47	–37.78	2.36	–35.42
		A–T hydrogen bonding			
SM8AD	–22.46	4.94	–17.53	–2.97	–20.50
SM8	–21.35	4.35	–17.00	–3.86	–20.86
SMD	–33.84	6.31	–27.52	4.13	–23.39
		A–U hydrogen bonding			
SM8AD	–22.03	4.78	–17.25	–3.09	–20.34
SM8	–21.15	4.29	–16.86	–4.10	–20.96
SMD	–34.12	6.28	–27.84	3.79	–24.05
		C–G hydrogen bonding			
SM8AD	–30.61	6.76	–23.85	–4.76	–28.61
SM8	–29.26	6.04	–23.22	–5.42	–28.64
SMD	–41.02	7.75	–33.27	3.10	–30.17

Cartesian Coordinates of Gas-Phase Geometries

a) M06-2X/6-31+G** Geometries

9-hexyl– adenine – 9-hexyl– adenine HB1

N	-2.72199700	3.45729000	-0.61763300
C	-4.01777900	3.46131100	-0.28135400
N	-4.73772900	2.48704200	0.26979100
C	-3.98738500	1.39860000	0.48278900
C	-2.63552300	1.23537900	0.19129300
C	-1.98970200	2.35136100	-0.39398000
N	-0.69306900	2.35549700	-0.73293100
N	-4.38858300	0.20883100	1.04139400
C	-3.28337400	-0.59751000	1.04921200
N	-2.21042600	-0.02774900	0.55548400
H	-4.54799900	4.38704400	-0.49005000
H	-0.07146700	1.55604900	-0.59108300
H	-0.33278100	3.20375300	-1.14194300
H	-3.33009600	-1.60509100	1.44280400
N	1.50279700	0.32497900	-0.52607800
C	2.63096500	0.86331800	-1.02079900
N	3.83751500	0.32168700	-1.11757600
C	3.84429800	-0.93174300	-0.63594000
C	2.76668100	-1.62425400	-0.09377400
C	1.53460900	-0.93353100	-0.04864500
N	0.42125600	-1.48742100	0.44726600
N	4.90039300	-1.80431200	-0.57584800
C	4.40826900	-2.95143300	0.00006600
N	3.13560700	-2.89156100	0.30151600
H	2.53378400	1.88233100	-1.38968300
H	0.47236300	-2.43060200	0.79862000
H	-0.45877300	-0.96691100	0.46896200
H	5.04941100	-3.80813700	0.16482000
C	6.26852300	-1.50942900	-0.97418000
C	6.99285600	-0.64149900	0.05145000
H	6.22746000	-1.00008700	-1.94211100
H	6.78376300	-2.46517500	-1.11462500
C	8.42291000	-0.32621700	-0.38102800
H	6.42547600	0.28759900	0.18166700
H	6.99694100	-1.15893300	1.01940500
C	9.16747700	0.54659200	0.62764800
H	8.97886500	-1.26302600	-0.52905600
H	8.40470700	0.18164000	-1.35507300
H	8.61225400	1.48306100	0.77508300
H	9.18482900	0.04134100	1.60344000
C	-5.74580700	-0.11354700	1.45666000

C	-6.65625900	-0.40949800	0.26800300
H	-6.12686200	0.74154100	2.02359200
H	-5.68850800	-0.97280100	2.13278200
C	-8.08128400	-0.73061800	0.71266400
H	-6.65593400	0.46439300	-0.39382800
H	-6.24036000	-1.25052700	-0.30164800
C	-9.01501100	-1.02396700	-0.46021200
H	-8.07062200	-1.59499000	1.39198300
H	-8.48076800	0.11404200	1.29052700
H	-9.02680100	-0.15944200	-1.13797300
H	-8.61556300	-1.86650800	-1.04190600
C	10.59851900	0.86944600	0.20129400
C	11.33040600	1.74368900	1.21739400
H	10.57858900	1.37323100	-0.77353700
H	11.15095600	-0.06753100	0.05373100
H	12.35186400	1.96463200	0.89592500
H	10.80937800	2.69623800	1.35885800
H	11.38492100	1.24714600	2.19181000
C	-10.44383000	-1.34418800	-0.02455000
C	-11.36706300	-1.63191100	-1.20659100
H	-10.83983400	-0.50218400	0.55745200
H	-10.42950700	-2.20814500	0.65242900
H	-12.38437000	-1.85899600	-0.87634800
H	-11.41709300	-0.77048900	-1.88058300
H	-11.00356400	-2.48655500	-1.78667400

9-hexyl– adenine – 9-hexyl– adenine HB2

N	-2.58275	-4.03466	-0.42707
C	-3.81799	-3.59071	-0.69318
N	-4.22205	-2.34398	-0.92184
C	-3.19610	-1.48592	-0.85045
C	-1.86229	-1.78436	-0.57815
C	-1.56937	-3.15325	-0.36834
N	-0.33337	-3.61004	-0.11161
N	-3.23676	-0.12506	-1.02812
C	-1.95275	0.31761	-0.84232
N	-1.09451	-0.63540	-0.57430
H	-4.58871	-4.35660	-0.72677
H	0.48820	-3.00730	-0.09162
H	-0.23745	-4.59930	0.05640
H	-1.71167	1.36999	-0.92656
N	5.68988	-3.21591	0.59414
C	6.12404	-2.02411	1.03500
N	5.44304	-0.88874	1.15682
C	4.16715	-1.04169	0.78247
C	3.56808	-2.21112	0.31929

C	4.41004	-3.33550	0.22564
N	3.95866	-4.54148	-0.20294
N	3.17039	-0.09705	0.77375
C	2.04636	-0.72800	0.30841
N	2.23690	-1.99652	0.02776
H	7.17131	-1.98907	1.32242
H	3.08127	-4.57968	-0.69781
H	4.65221	-5.24669	-0.40043
H	1.09376	-0.22303	0.19085
C	3.33054	1.30595	1.12685
C	4.01804	2.10231	0.02113
H	3.91927	1.34803	2.04855
H	2.33407	1.70559	1.33958
C	4.19571	3.56932	0.40572
H	4.99430	1.64578	-0.18032
H	3.42482	2.02254	-0.89882
C	4.88327	4.38810	-0.68533
H	3.21514	4.01380	0.62835
H	4.78350	3.63414	1.33157
H	5.86352	3.94449	-0.90719
H	4.29795	4.32233	-1.61316
C	-4.43689	0.65866	-1.27746
C	-5.26529	0.86205	-0.01169
H	-5.02343	0.12754	-2.03358
H	-4.12321	1.61817	-1.70152
C	-6.53656	1.66150	-0.28760
H	-5.52103	-0.12300	0.39588
H	-4.65199	1.37643	0.73950
C	-7.37984	1.88384	0.96660
H	-6.27341	2.63560	-0.72417
H	-7.13939	1.13600	-1.04078
H	-7.63927	0.91069	1.40539
H	-6.77904	2.41174	1.72040
C	5.06717	5.85699	-0.30793
C	5.75540	6.66356	-1.40711
H	5.65223	5.92009	0.61843
H	4.08681	6.29745	-0.08472
H	5.87802	7.71145	-1.12008
H	6.74818	6.25678	-1.62549
H	5.17365	6.63505	-2.33434
C	-8.65932	2.67410	0.69780
C	-9.49125	2.89089	1.96007
H	-9.25845	2.14387	-0.05339
H	-8.39800	3.64436	0.25597
H	-10.40233	3.45730	1.74886
H	-9.78584	1.93344	2.40194

H	-8.91996	3.44259	2.71392

9-hexyl– adenine – 9-hexyl– adenine HB3

N	-2.12191	-3.43202	0.23345
C	-3.44098	-3.48835	0.00428
N	-4.25913	-2.51680	-0.39208
C	-3.59695	-1.36270	-0.54439
C	-2.23920	-1.13851	-0.33306
C	-1.48001	-2.26415	0.06243
N	-0.15667	-2.20634	0.28312
N	-4.11066	-0.15038	-0.93721
C	-3.05960	0.72706	-0.92610
N	-1.91980	0.18263	-0.57398
H	-3.89733	-4.46237	0.16125
H	0.40326	-1.39783	0.01260
H	0.30284	-3.07058	0.52485
H	-3.19644	1.76663	-1.19686
N	2.12229	3.43233	0.23398
C	3.44141	3.48853	0.00502
N	4.25948	2.51698	-0.39153
C	3.59714	1.36303	-0.54434
C	2.23932	1.13901	-0.33330
C	1.48024	2.26461	0.06249
N	0.15688	2.20691	0.28306
N	4.11069	0.15076	-0.93752
C	3.05945	-0.72649	-0.92692
N	1.91970	-0.18197	-0.57478
H	3.89788	4.46244	0.16232
H	-0.40322	1.39852	0.01249
H	-0.30251	3.07115	0.52505
H	3.19613	-1.76597	-1.19810
C	5.51292	-0.12254	-1.21666
C	6.34058	-0.24087	0.06022
H	5.88860	0.69588	-1.83861
H	5.55884	-1.04548	-1.80370
C	7.81412	-0.50413	-0.24139
H	6.23329	0.68991	0.62936
H	5.93203	-1.05039	0.67881
C	8.66360	-0.62476	1.02249
H	-7.91190	1.42541	-0.83250
H	-8.20800	-0.30969	-0.86609
H	-8.56509	-0.29665	1.61368
H	-8.27106	1.43678	1.64924
C	10.14095	-0.88215	0.73092
C	10.97790	-0.99949	2.00299
H	10.53119	-0.06935	0.10518

H	10.23702	-1.80144	0.13888
H	12.03145	-1.18350	1.77568
H	10.91749	-0.08063	2.59528
H	10.62084	-1.82290	2.63028
C	-10.14129	0.88114	0.73080
C	-10.97836	0.99825	2.00281
H	-10.53132	0.06831	0.10498
H	-10.23748	1.80045	0.13881
H	-12.03192	1.18206	1.77543
H	-10.91780	0.07936	2.59506
H	-10.62150	1.82169	2.63017

9-hexyl– adenine – 1-hexyl– thymine WC

N	0.66407000	-1.46101600	-0.25904500
C	1.18127400	-0.22001900	-0.34168200
N	2.41435400	0.12622600	-0.68303200
C	3.16431900	-0.95220400	-0.96325500
C	2.76987200	-2.28658000	-0.92065300
C	1.43083200	-2.53051500	-0.54325400
N	0.91121700	-3.76204900	-0.45999200
N	4.47716400	-0.97885500	-1.35736300
C	4.79640400	-2.30641500	-1.51755700
N	3.80514700	-3.12516300	-1.27132500
H	0.48601500	0.57901300	-0.09362400
H	1.49820800	-4.55151800	-0.67759100
H	-0.06229000	-3.89653900	-0.18585900
H	5.78971600	-2.60441700	-1.82842400
N	-3.96708900	-0.53177900	1.17115400
C	-2.63924500	-0.43510800	0.77438300
O	-2.06757500	0.63780500	0.65581400
N	-2.02178500	-1.63896800	0.53259100
C	-2.58955400	-2.89463400	0.60017600
O	-1.92693900	-3.89972800	0.34352500
C	-3.99719900	-2.93115000	0.98925700
C	-4.67357400	-4.26423000	1.08136100
C	-4.60119200	-1.75099900	1.24555500
H	-1.01398200	-1.57896400	0.23685600
H	-5.71854900	-4.15203500	1.38005900
H	-4.16481600	-4.90417100	1.80790500
H	-4.63435700	-4.78275000	0.11918700
H	-5.64625300	-1.69991000	1.53938500
C	-4.70244400	0.71536300	1.38726400
C	-5.25184500	1.29447600	0.08727000
H	-4.01346800	1.42160000	1.85575600
H	-5.51083000	0.50053600	2.09363300
C	-6.00255500	2.60378600	0.31912400

H	-4.41284300	1.45988500	-0.59857500
H	-5.91844800	0.55888400	-0.38313300
C	-6.56843600	3.19813800	-0.96924100
H	-6.82280800	2.43844100	1.03231500
H	-5.32537600	3.33098600	0.78724900
H	-5.74930800	3.35953600	-1.68331500
H	-7.24760200	2.47210000	-1.43783800
C	-7.31218900	4.51405400	-0.74804100
C	-7.87256700	5.09622000	-2.04397700
H	-6.63169500	5.23764100	-0.28142400
H	-8.12836700	4.35139600	-0.03228300
H	-8.40018600	6.03742300	-1.86708900
H	-7.06985900	5.29109200	-2.76264400
H	-8.57581900	4.39984200	-2.51256700
C	5.34525800	0.18164200	-1.48881300
C	5.81511300	0.70492500	-0.13415400
H	4.78201200	0.95522800	-2.02013300
H	6.19465000	-0.11133700	-2.11433200
C	6.70432900	1.93770700	-0.27889200
H	4.93168100	0.94742500	0.46807900
H	6.35776700	-0.09256900	0.38954600
C	7.18630200	2.48012300	1.06536300
H	7.57500500	1.69442600	-0.90449600
H	6.15056200	2.72456400	-0.80910500
H	6.31602900	2.71913700	1.69178400
H	7.74237800	1.69498200	1.59648800
C	8.06826200	3.72027800	0.93142400
C	8.54271400	4.25152200	2.28239900
H	7.51035900	4.50293900	0.40165900
H	8.93574200	3.48010200	0.30318300
H	9.17127400	5.13879800	2.16746300
H	7.69132600	4.52262900	2.91520900
H	9.12543300	3.49390500	2.81670000

9-hexyl– adenine – 1-hexyl– thymine RWC

N	0.67961	0.22417	-1.02414
C	1.76432	0.99044	-0.79717
N	3.03950	0.63794	-0.87873
C	3.16896	-0.64999	-1.23540
C	2.14665	-1.55724	-1.49957
C	0.82905	-1.06477	-1.37992
N	-0.25287	-1.82321	-1.60361
N	4.33005	-1.35441	-1.42284
C	3.94715	-2.62741	-1.77310
N	2.65042	-2.79482	-1.83575

H	1.54354	2.01761	-0.51411
H	-0.12313	-2.78644	-1.86847
H	-1.18817	-1.43366	-1.49406
H	4.68616	-3.39242	-1.97580
N	-4.12061	1.35565	-0.64961
C	-2.91087	0.71839	-0.85368
O	-2.85037	-0.46370	-1.19219
N	-1.80096	1.49023	-0.65815
C	-1.76338	2.81312	-0.23328
O	-0.69615	3.38665	-0.07654
C	-3.07501	3.42581	-0.00098
C	-3.11425	4.85068	0.45729
C	-4.16793	2.66556	-0.21512
H	-0.87645	1.01274	-0.80829
H	-4.14347	5.18769	0.60263
H	-2.62727	5.50237	-0.27389
H	-2.56702	4.96512	1.39735
H	-5.17152	3.05320	-0.06160
C	-5.34438	0.56013	-0.76282
C	-5.66949	-0.17923	0.53139
H	-5.19845	-0.14876	-1.58052
H	-6.15436	1.24350	-1.03817
C	-6.93203	-1.02842	0.40713
H	-4.81455	-0.81523	0.78966
H	-5.78805	0.55121	1.34340
C	-7.27691	-1.76399	1.70081
H	-7.77975	-0.39219	0.11523
H	-6.79915	-1.75981	-0.40171
H	-6.42542	-2.39192	1.99709
H	-7.41550	-1.03172	2.50869
C	-8.52859	-2.63170	1.58680
C	-8.86026	-3.35476	2.89052
H	-8.38644	-3.36577	0.78336
H	-9.37750	-2.00435	1.28570
H	-9.75605	-3.97393	2.79097
H	-8.03414	-4.00527	3.19596
H	-9.03539	-2.63828	3.69995
C	5.67636	-0.84676	-1.20558
C	6.02525	-0.75544	0.27737
H	5.73618	0.14162	-1.67234
H	6.36737	-1.51378	-1.73173
C	7.44448	-0.23689	0.49552
H	5.30159	-0.09040	0.76348
H	5.91307	-1.74789	0.73286
C	7.81282	-0.12649	1.97378
H	8.16131	-0.90190	-0.00743

H	7.54955	0.74886	0.02167
H	7.10278	0.54627	2.47418
H	7.69620	-1.10928	2.45204
C	9.23578	0.37923	2.20248
C	9.58887	0.48611	3.68436
H	9.35131	1.36001	1.72351
H	9.94293	-0.29472	1.70150
H	10.60931	0.85126	3.82965
H	8.90961	1.17450	4.19798
H	9.50748	-0.48906	4.17608

9-hexyl– adenine – 1-hexyl– thymine H

N	-3.65296	-3.97026	0.66015
C	-4.65530	-3.16402	0.28484
N	-4.59313	-1.93416	-0.22100
C	-3.32294	-1.52657	-0.33769
C	-2.18139	-2.24253	0.00650
C	-2.38632	-3.53873	0.53314
N	-1.37879	-4.34221	0.90547
N	-2.86761	-0.32453	-0.83027
C	-1.50331	-0.36914	-0.75586
N	-1.05284	-1.49900	-0.26347
H	-5.65274	-3.57675	0.41340
H	-0.39923	-4.07921	0.81681
H	-1.61778	-5.25500	1.25961
H	-0.86989	0.44763	-1.08218
N	3.74653	-0.84227	-0.69783
C	2.36345	-0.73246	-0.67411
O	1.77541	0.26549	-1.06898
N	1.70797	-1.83164	-0.17821
C	2.27079	-2.98804	0.32133
O	1.56097	-3.89940	0.74254
C	3.73163	-3.03181	0.30598
C	4.41085	-4.25573	0.83855
C	4.37937	-1.95852	-0.19620
H	0.66157	-1.76016	-0.17305
H	5.49734	-4.15828	0.77559
H	4.10224	-5.14189	0.27650
H	4.13065	-4.42754	1.88180
H	5.46462	-1.91976	-0.24034
C	4.51478	0.31830	-1.15187
C	4.71949	1.34402	-0.04180
H	3.96917	0.76504	-1.98616
H	5.47468	-0.05177	-1.52624
C	5.53197	2.54667	-0.51640
H	3.73485	1.67190	0.31168

H	5.22625	0.86209	0.80538
C	5.73893	3.58913	0.58048
H	6.51112	2.20849	-0.88465
H	5.02360	3.01486	-1.37040
H	4.76008	3.93158	0.94341
H	6.23883	3.11922	1.43919
C	6.55661	4.79442	0.11962
C	6.75185	5.82815	1.22652
H	6.05694	5.26182	-0.73867
H	7.53421	4.45016	-0.24196
H	7.33647	6.68433	0.87892
H	5.78738	6.20316	1.58434
H	7.27547	5.38925	2.08230
C	-3.70854	0.77343	-1.28522
C	-4.36841	1.51329	-0.12497
H	-4.47082	0.35061	-1.94748
H	-3.07792	1.44583	-1.87546
C	-5.26156	2.64962	-0.61704
H	-4.95958	0.79372	0.45352
H	-3.58889	1.90610	0.54032
C	-5.95793	3.39242	0.52171
H	-4.66363	3.36229	-1.20296
H	-6.02019	2.24460	-1.30092
H	-6.55716	2.67978	1.10497
H	-5.20239	3.79599	1.21029
C	-6.85587	4.52853	0.03576
C	-7.55272	5.25774	1.18249
H	-7.60640	4.12328	-0.65507
H	-6.25476	5.24051	-0.54452
H	-8.19413	6.06405	0.81608
H	-8.17714	4.56841	1.76039
H	-6.82069	5.69638	1.86868

9-hexyl– adenine – 1-hexyl– thymine RH

N	1.57269	-3.93954	-0.42660
C	2.84664	-3.90716	-0.01045
N	3.54799	-2.87468	0.45182
C	2.80661	-1.75964	0.47140
C	1.47997	-1.63403	0.07413
C	0.84960	-2.80754	-0.39683
N	-0.42771	-2.83152	-0.81014
N	3.18413	-0.50388	0.89027
C	2.09363	0.30336	0.72185
N	1.05317	-0.33488	0.23962
H	3.37324	-4.85697	-0.06046
H	-1.02389	-2.00741	-0.80446

H	-0.79822	-3.71248	-1.12976
H	2.09610	1.35855	0.97070
N	-3.44501	1.45134	-0.81213
C	-2.37227	0.59560	-0.63798
O	-2.44077	-0.60234	-0.90685
N	-1.23634	1.17948	-0.15368
C	-1.05986	2.50583	0.21152
O	0.01810	2.89435	0.64283
C	-2.23949	3.35705	0.03762
C	-2.12942	4.80213	0.41382
C	-3.35564	2.78196	-0.45623
H	-0.40825	0.54838	-0.02509
H	-3.07108	5.32654	0.23453
H	-1.33671	5.28884	-0.16162
H	-1.86244	4.90382	1.46974
H	-4.26863	3.35041	-0.61263
C	-4.71499	0.88371	-1.26831
C	-5.55172	0.33857	-0.11553
H	-4.47957	0.08865	-1.97911
H	-5.25248	1.67491	-1.80126
C	-6.89256	-0.21295	-0.59511
H	-4.97896	-0.44877	0.38893
H	-5.71955	1.13842	0.61865
C	-7.74723	-0.76584	0.54324
H	-7.45038	0.57959	-1.11436
H	-6.71757	-1.00515	-1.33584
H	-7.19833	-1.57057	1.05139
H	-7.90561	0.02086	1.29438
C	-9.10180	-1.29501	0.07531
C	-9.94482	-1.84581	1.22300
H	-8.94301	-2.07884	-0.67637
H	-9.64780	-0.48824	-0.43068
H	-10.91145	-2.21567	0.87028
H	-9.43065	-2.67352	1.72243
H	-10.13456	-1.07177	1.97405
C	4.51453	-0.12717	1.34606
C	5.49795	0.02260	0.18871
H	4.85615	-0.90247	2.03903
H	4.41631	0.81068	1.90208
C	6.88349	0.44087	0.67504
H	5.55663	-0.93380	-0.34434
H	5.10750	0.76632	-0.51763
C	7.89152	0.58755	-0.46327
H	6.80968	1.39424	1.21760
H	7.25691	-0.29915	1.39617
H	7.98058	-0.37035	-0.99400

H	7.50953	1.31204	-1.19601
C	9.27302	1.03318	0.01256
C	10.27312	1.16918	-1.13362
H	9.65068	0.31264	0.74930
H	9.18028	1.99262	0.53780
H	11.25257	1.49836	-0.77589
H	10.40758	0.21252	-1.64910
H	9.92255	1.89798	-1.87197

1-hexyl– thymine – 1-hexyl– thymine HB1

N	4.18977300	-0.76963800	-1.00895700
C	3.26782100	0.27074100	-0.96994400
O	3.60428200	1.43982700	-0.94618100
N	1.94824400	-0.13681300	-0.96614800
C	1.47882700	-1.43726500	-0.95125800
O	0.27273800	-1.67582900	-0.93515800
C	2.50018300	-2.47969700	-0.95639200
C	2.05090300	-3.90842300	-0.94050100
C	3.79084900	-2.08532400	-0.98027400
H	1.23727800	0.60795500	-0.94983500
H	2.90802100	-4.58595000	-0.94630700
H	1.42286100	-4.12388000	-1.80950200
H	1.44444800	-4.11142200	-0.05340400
H	4.60472200	-2.80546100	-0.98570000
N	-4.18987200	0.77073300	-1.00833600
C	-3.26792700	-0.26969300	-0.97047400
O	-3.60439800	-1.43880000	-0.94790500
N	-1.94834300	0.13784300	-0.96636100
C	-1.47891800	1.43827600	-0.95010700
O	-0.27282900	1.67682600	-0.93383100
C	-2.50026500	2.48072000	-0.95407300
C	-2.05097200	3.90942500	-0.93670700
C	-3.79093500	2.08638500	-0.97828200
H	-1.23739100	-0.60695200	-0.95065100
H	-2.90808600	4.58696400	-0.94160700
H	-1.42309800	4.12582900	-1.80559500
H	-1.44434100	4.11144700	-0.04950800
H	-4.60480200	2.80653400	-0.98288100
C	-5.60899400	0.41418300	-0.95688100
C	-6.09695100	0.19031300	0.47098700
H	-5.73737200	-0.49459300	-1.54878500
H	-6.16671600	1.22321100	-1.43956400
C	-7.57507000	-0.19033700	0.51449500
H	-5.49159800	-0.60425500	0.92245900
H	-5.92832800	1.10343900	1.05796900
C	-8.08864700	-0.40917500	1.93636200

H	-8.17329800	0.59503100	0.03061000
H	-7.73049900	-1.10568400	-0.07238900
H	-7.48940300	-1.19211000	2.42093800
H	-7.93375100	0.50630900	2.52448000
C	-9.56506300	-0.79796900	1.98872700
C	-10.06531700	-1.01134800	3.41582300
H	-9.71688600	-1.71339200	1.40281800
H	-10.16152800	-0.01627100	1.50076800
H	-11.12253000	-1.28976000	3.43409300
H	-9.49985100	-1.80680200	3.91209700
H	-9.94778500	-0.09965200	4.01087200
C	5.60889400	-0.41312400	-0.95725200
C	6.09702100	-0.19095200	0.47082300
H	5.73716900	0.49636800	-1.54807900
H	6.16657700	-1.22155300	-1.44098100
C	7.57499700	0.19022400	0.51456100
H	5.49144700	0.60279000	0.92345100
H	5.92885700	-1.10491500	1.05663700
C	8.08894600	0.40666200	1.93666100
H	8.17339900	-0.59400200	0.02904300
H	7.72984200	1.10671100	-0.07069700
H	7.48925500	1.18814100	2.42303500
H	7.93503500	-0.51012100	2.52301200
C	9.56506200	0.79656400	1.98921900
C	10.06581600	1.00710800	3.41656100
H	9.71583800	1.71344900	1.40532800
H	10.16194600	0.01647800	1.49919500
H	11.12277000	1.28649400	3.43495600
H	9.49983300	1.80086500	3.91496200
H	9.94945700	0.09392000	4.00955000

1-hexyl– thymine – 1-hexyl– thymine HB2

N	-4.95523	0.17976	-0.09709
C	-3.99694	-0.44668	-0.88891
O	-4.10593	-1.59419	-1.27926
N	-2.89790	0.33560	-1.18264
C	-2.64194	1.61766	-0.73271
O	-1.57340	2.17205	-0.98141
C	-3.71325	2.23903	0.04084
C	-3.52868	3.65423	0.49499
C	-4.78965	1.47727	0.32998
H	-2.12528	-0.14222	-1.66644
H	-4.38119	3.98494	1.09289
H	-3.41758	4.32412	-0.36260
H	-2.61679	3.74798	1.09132

H	-5.60548	1.85752	0.94001
N	3.17136	0.36024	-0.90424
C	2.12570	1.27671	-0.91541
O	2.27245	2.43810	-0.58420
N	0.91692	0.75947	-1.34047
C	0.64799	-0.55369	-1.67995
O	-0.48540	-0.90743	-1.99990
C	1.78340	-1.46745	-1.62262
C	1.54799	-2.90486	-1.97160
C	2.97230	-0.95996	-1.23341
H	0.11445	1.40225	-1.31242
H	2.47354	-3.48047	-1.89560
H	1.15397	-2.99715	-2.98749
H	0.80158	-3.34313	-1.30161
H	3.85988	-1.58346	-1.16473
C	4.46845	0.82589	-0.40641
C	4.51227	0.86291	1.12215
H	4.62911	1.83117	-0.80343
H	5.22875	0.16397	-0.82860
C	5.84545	1.38623	1.68099
H	3.69755	1.52098	1.44115
H	4.29346	-0.13540	1.52441
C	6.94176	0.34512	1.94386
H	6.23805	2.15611	1.00169
H	5.64403	1.90031	2.62691
H	7.78930	0.87518	2.39317
H	6.58898	-0.36238	2.70762
C	7.43644	-0.44533	0.72119
C	6.68231	-1.75648	0.48709
H	8.49707	-0.68675	0.85278
H	7.38884	0.19292	-0.17123
H	7.00220	-2.24531	-0.43845
H	6.86563	-2.45171	1.31258
H	5.59993	-1.60494	0.43607
C	-5.98180	-0.66239	0.52815
C	-5.56369	-1.18139	1.90914
H	-6.16056	-1.49448	-0.15456
H	-6.89766	-0.06696	0.59639
C	-4.26725	-2.00960	1.89925
H	-5.45998	-0.33665	2.60519
H	-6.39821	-1.78831	2.27931
C	-2.98071	-1.16948	1.99313
H	-4.28584	-2.71354	2.73886
H	-4.24314	-2.61666	0.98658
H	-3.11587	-0.18903	1.51971
H	-2.76812	-0.94812	3.04826

C	-1.76515	-1.84226	1.35482
C	-0.52184	-0.95798	1.42102
H	-1.99451	-2.07348	0.30603
H	-1.57389	-2.80213	1.85292
H	0.34106	-1.44124	0.94975
H	-0.69677	-0.00711	0.90168
H	-0.25333	-0.72560	2.45760

1-hexyl– thymine – 1-hexyl– thymine HB3

N	-4.00324	-0.34539	0.37242
C	-3.00483	0.60248	0.56772
O	-3.21252	1.66355	1.12592
N	-1.76567	0.23360	0.08188
C	-1.45042	-0.92802	-0.59856
O	-0.30662	-1.13911	-0.99709
C	-2.55325	-1.86234	-0.80188
C	-2.27118	-3.13845	-1.53349
C	-3.76126	-1.51428	-0.31067
H	-0.99962	0.90813	0.21707
H	-3.17552	-3.74539	-1.62020
H	-1.50358	-3.71835	-1.01333
H	-1.88606	-2.93047	-2.53567
H	-4.62874	-2.15937	-0.42467
N	4.27206	1.08379	-1.09450
C	3.27268	0.13597	-1.29143
O	3.46969	-0.92484	-1.85328
N	2.03692	0.50268	-0.79320
C	1.72016	1.66637	-0.11775
O	0.57837	1.87406	0.28790
C	2.81913	2.60870	0.06952
C	2.53472	3.89214	0.78704
C	4.02506	2.26030	-0.42577
H	1.27126	-0.17275	-0.92645
H	3.43659	4.50425	0.86198
H	2.15559	3.69408	1.79350
H	1.76176	4.46226	0.26404
H	4.88912	2.91227	-0.32584
C	5.63269	0.77110	-1.54179
C	6.53097	0.29930	-0.39921
H	6.04022	1.67150	-2.01222
H	5.53857	-0.00523	-2.30257
C	6.02476	-0.97426	0.27788
H	7.53153	0.13961	-0.81768
H	6.62833	1.10038	0.34844
C	6.89183	-1.42324	1.45631
H	5.00043	-0.80920	0.63382

H	5.95938	-1.77750	-0.46723
H	6.91016	-0.63264	2.22026
H	6.41922	-2.29389	1.92840
C	8.32807	-1.78998	1.07978
C	9.10369	-2.37492	2.25875
H	8.85611	-0.90442	0.70606
H	8.30912	-2.51274	0.25316
H	10.13222	-2.62238	1.98191
H	9.14163	-1.66373	3.09074
H	8.62460	-3.28856	2.62542
C	-5.35885	0.00132	0.80413
C	-6.09084	0.83848	-0.24540
H	-5.26924	0.56581	1.73516
H	-5.87752	-0.93666	1.01857
C	-7.51453	1.23984	0.17412
H	-5.48270	1.73236	-0.41733
H	-6.12129	0.28323	-1.19369
C	-8.61463	0.29034	-0.31713
H	-7.55975	1.34363	1.26635
H	-7.73158	2.23618	-0.22410
H	-9.58935	0.69317	-0.01236
H	-8.60812	0.29514	-1.41471
C	-8.51063	-1.15719	0.17216
C	-8.63543	-1.29943	1.68899
H	-7.56652	-1.59915	-0.17463
H	-9.30282	-1.74405	-0.30667
H	-8.60168	-2.34898	1.99461
H	-7.83528	-0.77410	2.22003
H	-9.58571	-0.87984	2.03605

9-ethyl– adenine – 1-cyclohexyl – uracil WC

N	1.73760500	0.34479100	0.00439800
C	1.99970900	-0.97652700	0.00296500
N	3.18425800	-1.57170500	0.00077900
C	4.18157700	-0.67272600	-0.00009800
C	4.06528400	0.71348800	0.00106000
C	2.75121300	1.23130500	0.00349900
N	2.48763800	2.54408800	0.00452000
N	5.52982200	-0.92339300	-0.00189900
C	6.14080700	0.31033500	-0.00204800
N	5.30284600	1.31691900	-0.00036800
H	1.11846100	-1.61418800	0.00369000
H	3.25834300	3.19309100	0.00482600
H	1.52390400	2.87927400	0.00851200
H	7.21716600	0.40794700	-0.00338200
N	-3.21275100	0.40358600	-0.00366800

C	-1.86492900	0.03382400	-0.00065300
O	-1.49966900	-1.13036200	0.00080800
N	-0.97566400	1.08133100	-0.00054100
C	-1.26635200	2.43366800	-0.00058000
O	-0.36437600	3.26858900	0.00008800
C	-2.68567400	2.74315900	-0.00140200
C	-3.57359800	1.72718700	-0.00271200
H	0.03926100	0.80582200	0.00118400
H	-2.99593400	3.77815500	-0.00089400
H	-4.64276800	1.91040900	-0.00333400
C	-4.23561800	-0.65749500	-0.00308500
C	-5.08830700	-0.61271800	1.26720300
C	-5.09644700	-0.60683900	-1.26759400
H	-3.66320300	-1.58905400	-0.00706500
C	-6.11195500	-1.75209100	1.26249000
H	-5.62069900	0.34756500	1.32530100
H	-4.43550800	-0.67541100	2.14431100
C	-6.11957400	-1.74673600	-1.26142300
H	-5.63008800	0.35315800	-1.31784200
H	-4.44949400	-0.66499000	-2.14931700
C	-6.98138000	-1.70992900	0.00323100
H	-6.73395600	-1.69574800	2.16147000
H	-5.58055700	-2.71240000	1.30409100
H	-6.74696400	-1.68705800	-2.15642800
H	-5.58801700	-2.70663400	-1.31003100
H	-7.68907000	-2.54533200	0.00361400
H	-7.57883700	-0.78730800	0.00697600
C	6.11575600	-2.26128500	-0.00364700
C	7.63527800	-2.22845200	-0.00222800
H	5.73781400	-2.78724100	-0.88519300
H	5.73618500	-2.78994900	0.87555500
H	8.01396400	-3.25252000	-0.00293500
H	8.02653300	-1.72498600	-0.89060800
H	8.02480700	-1.72674300	0.88790600

9-ethyl– adenine – 1-cyclohexyl – uracil RWC

N	-1.77686	0.39634	-0.00153
C	-2.66336	1.41084	-0.00024
N	-3.98674	1.33267	0.00082
C	-4.40101	0.05595	0.00052
C	-3.60716	-1.08701	-0.00064
C	-2.21138	-0.87666	-0.00178
N	-1.32461	-1.88199	-0.00300
N	-5.69402	-0.40123	0.00130
C	-5.60617	-1.77493	0.00068
N	-4.37741	-2.22843	-0.00052

H	-2.21761	2.40358	-0.00004
H	-1.66495	-2.83002	-0.00335
H	-0.32513	-1.68619	-0.00382
H	-6.49003	-2.39698	0.00102
N	3.17799	0.55371	-0.00232
C	1.84632	0.15332	-0.00448
O	1.52056	-1.03254	-0.00782
N	0.92646	1.16233	-0.00288
C	1.16995	2.53499	0.00220
O	0.24287	3.32789	0.00330
C	2.58610	2.87976	0.00614
C	3.50210	1.89162	0.00388
H	-0.08075	0.86133	-0.00451
H	2.86884	3.92303	0.01080
H	4.56588	2.10372	0.00689
C	4.23455	-0.47413	-0.00382
C	5.09572	-0.38808	-1.26582
C	5.08095	-0.40641	1.26926
H	3.69437	-1.42462	-0.01393
C	6.15854	-1.49086	-1.26175
H	5.59497	0.59047	-1.31097
H	4.45285	-0.46435	-2.14933
C	6.14441	-1.50855	1.26158
H	5.57815	0.57207	1.33438
H	4.42764	-0.49622	2.14383
C	7.01491	-1.42865	0.00527
H	6.78580	-1.40595	-2.15496
H	5.66161	-2.46915	-1.31561
H	6.76148	-1.43610	2.16291
H	5.64717	-2.48760	1.29612
H	7.75253	-2.23789	0.00373
H	7.57843	-0.48494	0.01499
C	-6.87061	0.46430	0.00307
C	-8.16984	-0.32457	-0.00188
H	-6.80547	1.11368	-0.87489
H	-6.80828	1.10715	0.88605
H	-9.01016	0.37259	-0.00131
H	-8.25445	-0.95218	-0.89352
H	-8.25808	-0.95775	0.88545

9-ethyl– adenine – 1-cyclohexyl – uracil H

N	5.24825600	-1.71482900	0.03843700
C	5.95381900	-0.58103400	-0.06965800
N	5.51183400	0.66893900	-0.19219000
C	4.17345700	0.70598800	-0.20124400
C	3.30687500	-0.37654800	-0.09839500

C	3.90540700	-1.65162000	0.02727300
N	3.19459500	-2.78368200	0.13490100
N	3.36477300	1.81396500	-0.31776000
C	2.07685000	1.35755700	-0.27252600
N	1.99842800	0.05382700	-0.14557000
H	7.03373000	-0.70521500	-0.05380500
H	2.17663300	-2.80108300	0.13490900
H	3.70550900	-3.64812700	0.22106700
H	1.21770800	2.01474600	-0.34051400
N	-2.83115000	-0.55768500	-0.02036900
C	-1.51926900	-0.08741500	-0.09805100
O	-1.24578500	1.09810700	-0.21829200
N	-0.55152800	-1.05712200	-0.02917400
C	-0.72642300	-2.42129800	0.12114700
O	0.24424500	-3.17095200	0.17748100
C	-2.11630700	-2.83858200	0.20130300
C	-3.08249400	-1.89914300	0.13128000
H	0.43287800	-0.69916200	-0.07705800
H	-4.13297400	-2.16321100	0.19156500
H	-2.34328500	-3.88839900	0.31978500
C	-3.93621200	0.41656300	-0.05676700
C	-4.87560800	0.16276500	-1.23837100
C	-4.69289800	0.44719700	1.27318500
H	-3.44555100	1.38284700	-0.20223200
C	-5.98468600	1.21854700	-1.27026600
H	-5.33357000	-0.83239100	-1.14552400
H	-4.29927700	0.16958400	-2.16962700
C	-5.80529900	1.49845700	1.23098700
H	-5.13696900	-0.53957500	1.46900500
H	-3.98835400	0.65331000	2.08608000
C	-6.75233900	1.25382300	0.05350800
H	-6.66466600	1.01709800	-2.10413200
H	-5.53720700	2.20432000	-1.45631400
H	-6.35714300	1.49426100	2.17634000
H	-5.35394000	2.49487300	1.13118000
H	-7.52651000	2.02748400	0.02173500
H	-7.26753400	0.29359300	0.19751500
C	3.82834200	3.19290600	-0.40059300
H	4.63978800	3.21940500	-1.13296000
H	2.99779900	3.79010100	-0.78644700
C	4.30712700	3.70660900	0.95213100
H	5.13697100	3.09340200	1.31149900
H	4.65219900	4.73986600	0.86050000
H	3.49756600	3.67250500	1.68633900

9-ethyl– adenine – 1-cyclohexyl – uracil RH

N	3.53996	-3.10951	0.00287
C	4.80138	-2.67819	-0.13644
N	5.24991	-1.42902	-0.23834
C	4.24155	-0.54942	-0.18311
C	2.88963	-0.83995	-0.03771
C	2.54600	-2.20725	0.05364
N	1.27889	-2.63092	0.18817
N	4.31450	0.82257	-0.26858
C	3.03179	1.28458	-0.16487
N	2.14999	0.32208	-0.02752
H	5.55624	-3.45986	-0.17218
H	0.48579	-1.99469	0.19914
H	1.12108	-3.62521	0.23049
H	2.77791	2.33802	-0.20178
N	-2.79976	0.67423	0.05306
C	-1.50168	0.17520	0.09861
O	-1.26124	-1.02628	0.18561
N	-0.51137	1.11314	0.04083
C	-0.64736	2.49157	-0.08974
O	0.34206	3.20700	-0.15045
C	-2.03178	2.94151	-0.14244
C	-3.01967	2.02641	-0.07420
H	0.47020	0.74424	0.04876
H	-4.06416	2.31607	-0.11573
H	-2.23594	3.99821	-0.24147
C	-3.92832	-0.27330	0.07933
C	-4.86543	-0.00782	1.26020
C	-4.68183	-0.27500	-1.25292
H	-3.46216	-1.25244	0.21784
C	-5.99580	-1.04112	1.28014
H	-5.30348	0.99670	1.17365
H	-4.29269	-0.03353	2.19336
C	-5.81657	-1.30235	-1.22332
H	-5.10316	0.72340	-1.44025
H	-3.97964	-0.48917	-2.06579
C	-6.76107	-1.04903	-0.04556
H	-6.67341	-0.83314	2.11431
H	-5.56875	-2.03730	1.45855
H	-6.36580	-1.27726	-2.16986
H	-5.38663	-2.30902	-1.13230
H	-7.55095	-1.80695	-0.02241
H	-7.25621	-0.07721	-0.18191
C	5.54301	1.59747	-0.39046
H	6.14473	1.13121	-1.17540
H	5.25973	2.59903	-0.72449
C	6.31322	1.64155	0.92373

H	6.57972	0.62857	1.23467
H	7.23231	2.22034	0.79969
H	5.71146	2.10705	1.70897

1-cyclohexyl– uracil – 1-cyclohexyl– uracil HB1

N	-3.79718200	0.30299000	0.00077200
C	-2.50123900	0.80085600	-0.00006300
O	-1.52287600	0.05781300	-0.00186000
N	-2.38900400	2.16489800	0.00123600
C	-3.42916400	3.10458300	0.00348900
O	-3.19382300	4.29661400	0.00458300
C	-4.75687700	2.50059100	0.00432300
C	-4.87494100	1.15994800	0.00295100
H	-1.42329700	2.51989800	0.00043000
H	-5.61907700	3.15218600	0.00603200
H	-5.84425500	0.67378100	0.00351100
N	3.57343500	0.28261000	-0.00320500
C	2.27843800	-0.24451900	-0.00249900
O	2.05262700	-1.43969600	-0.00152200
N	1.27359200	0.70077200	-0.00308400
C	1.41071500	2.08119000	-0.00335500
O	0.42458500	2.81076200	-0.00338700
C	2.78557700	2.54682500	-0.00351300
C	3.78228600	1.63807100	-0.00326600
H	0.31117200	0.33997900	-0.00269100
H	2.97394600	3.61062900	-0.00364500
H	4.82383400	1.94116300	-0.00314200
C	4.71102200	-0.65474100	-0.00140700
C	5.56086000	-0.50939800	-1.26607400
C	5.55409600	-0.51190900	1.26806000
H	4.24881800	-1.64552600	-0.00364100
C	6.70208700	-1.53095200	-1.25900600
H	5.98632300	0.50320700	-1.31601100
H	4.92448000	-0.63818700	-2.14799600
C	6.69554800	-1.53320000	1.26516300
H	5.97875900	0.50083700	1.32221800
H	4.91296200	-0.64267200	2.14624600
C	7.55522600	-1.39945300	0.00541300
H	7.31910900	-1.40450400	-2.15424300
H	6.27790200	-2.54296300	-1.30629500
H	7.30790200	-1.40823400	2.16380800
H	6.27126000	-2.54534600	1.30850200
H	8.34888700	-2.15361400	0.00679900
H	8.04972300	-0.41780100	0.00754700
C	-3.99985200	-1.15794600	-0.00055000
C	-4.71950300	-1.62381000	1.26745600

C	-4.72275300	-1.62107300	-1.26770700
H	-2.99041900	-1.57713300	-0.00229300
C	-4.87441100	-3.14773700	1.26042500
H	-5.71578100	-1.16225400	1.32308600
H	-4.15774200	-1.29070500	2.14655600
C	-4.87762200	-3.14501700	-1.26355400
H	-5.71919000	-1.15944400	-1.31979100
H	-4.16326400	-1.28606200	-2.14753000
C	-5.59898400	-3.62419300	-0.00115900
H	-5.41198700	-3.47003600	2.15782900
H	-3.87906200	-3.60991100	1.30327600
H	-5.41747500	-3.46539300	-2.16027800
H	-3.88238500	-3.60709300	-1.30992800
H	-5.67900300	-4.71610900	-0.00223200
H	-6.62517700	-3.23022600	0.00056500

1-cyclohexyl– uracil – 1-cyclohexyl– uracil HB2

N	3.94081	0.29592	0.00006
C	2.59351	0.65165	0.00007
O	1.69789	-0.18293	0.00003
N	2.34480	2.00109	0.00014
C	3.28097	3.04285	0.00019
O	2.92370	4.20482	0.00024
C	4.66506	2.58193	0.00018
C	4.92215	1.26085	0.00013
H	1.35090	2.26393	0.00016
H	5.45435	3.32012	0.00023
H	5.93754	0.87961	0.00013
N	-3.87013	0.41923	-0.00034
C	-3.96649	1.80678	-0.00026
O	-5.02232	2.41140	-0.00022
N	-2.74710	2.45906	-0.00026
C	-1.47140	1.89921	-0.00020
O	-0.49112	2.63247	-0.00018
C	-1.46333	0.44877	-0.00019
C	-2.64333	-0.20409	-0.00024
H	-2.79979	3.47186	-0.00023
H	-0.50626	-0.05828	-0.00014
H	-2.68468	-1.28782	-0.00023
C	-5.11620	-0.37028	-0.00022
C	-5.24066	-1.21932	-1.26760
C	-5.24093	-1.21842	1.26775
H	-5.91477	0.37654	-0.00058
C	-6.56367	-1.99141	-1.26173
H	-4.40783	-1.93485	-1.32079
H	-5.16854	-0.57130	-2.14750

C	-6.56391	-1.99055	1.26215
H	-4.40806	-1.93385	1.32162
H	-5.16903	-0.56974	2.14718
C	-6.69951	-2.84692	0.00049
H	-6.63284	-2.61494	-2.15865
H	-7.39679	-1.27715	-1.30689
H	-6.63325	-2.61346	2.15949

1-cyclohexyl– uracil – 1-cyclohexyl– uracil HB3

N	-4.35554	0.55091	-0.00005
C	-3.96268	1.88441	-0.00009
O	-4.74099	2.81995	-0.00011
N	-2.59207	2.07106	-0.00010
C	-1.59156	1.10179	-0.00006
O	-0.41665	1.44842	-0.00006
C	-2.08892	-0.26031	0.00001
C	-3.42238	-0.46083	0.00000
H	-2.28925	3.03886	-0.00013
H	-1.36945	-1.07055	0.00006
H	-3.83821	-1.46244	0.00005
N	4.30759	-0.40683	-0.00004
C	3.19701	0.44506	-0.00002
O	3.29993	1.65665	-0.00005
N	1.97690	-0.19890	-0.00004
C	1.74082	-1.56988	-0.00001
O	0.59928	-2.01059	-0.00009
C	2.94843	-2.38044	-0.00003
C	4.15012	-1.76915	-0.00003
H	1.15183	0.41541	-0.00006
H	2.85051	-3.45647	-0.00003
H	5.07417	-2.33753	-0.00003
C	5.65213	0.19550	-0.00002
C	6.43008	-0.16767	1.26717
C	6.43020	-0.16782	-1.26710
H	5.46918	1.27340	-0.00009
C	7.80307	0.51138	1.26201
H	6.56912	-1.25710	1.32040
H	5.84898	0.12892	2.14678
C	7.80319	0.51123	-1.26188
H	6.56926	-1.25726	-1.32018
H	5.84919	0.12866	-2.14680
C	8.59261	0.15377	0.00012
H	8.36194	0.22656	2.15916
H	7.66497	1.60007	1.30637
H	8.36215	0.22631	-2.15894
H	7.66510	1.59992	-1.30638

H	9.55961	0.66731	0.00014
H	8.80557	-0.92466	0.00020
C	-5.79848	0.24431	-0.00002
C	-6.21014	-0.50817	-1.26768
C	-6.21013	-0.50796	1.26777
H	-6.28746	1.22227	-0.00010
C	-7.71892	-0.77251	-1.26196
H	-5.67760	-1.46828	-1.32153
H	-5.91751	0.07488	-2.14734
C	-7.71890	-0.77231	1.26212
H	-5.67757	-1.46805	1.32177
H	-5.91749	0.07524	2.14733
C	-8.14367	-1.52765	0.00014
H	-8.00017	-1.33335	-2.15887
H	-8.25211	0.18668	-1.30739
H	-8.00014	-1.33301	2.15912
H	-8.25209	0.18688	1.30740
H	-9.22707	-1.68545	0.00016
H	-7.67751	-2.52299	0.00021

adenine–thymine WC

N	0.95621	0.36878	-0.00032
C	1.56148	1.57188	-0.00019
N	2.86172	1.82860	0.00002
C	3.58264	0.69790	0.00010
C	3.10015	-0.60723	-0.00001
C	1.69580	-0.75566	-0.00023
N	1.09137	-1.95020	-0.00036
N	4.94748	0.55888	0.00032
C	5.20859	-0.79221	0.00034
N	4.12872	-1.52685	0.00013
H	0.88363	2.42279	-0.00028
H	1.65901	-2.78265	-0.00025
H	0.07351	-2.01534	-0.00045
H	6.22070	-1.17250	0.00050
N	-3.81249	1.60184	0.00021
C	-2.42686	1.62977	-0.00012
O	-1.79331	2.66951	-0.00013
N	-1.84846	0.38270	-0.00028
C	-2.50213	-0.83463	-0.00013
O	-1.86507	-1.88607	-0.00023
C	-3.96701	-0.78157	0.00016
C	-4.71849	-2.07685	0.00030
C	-4.54542	0.43687	0.00033
H	-4.26228	2.50588	0.00036
H	-0.79631	0.36727	-0.00040

H	-5.79694	-1.90230	0.00047
H	-4.45623	-2.67299	0.87888
H	-4.45651	-2.67301	-0.87835
H	-5.62297	0.56585	0.00057
H	5.61702	1.31362	0.00045

adenine–uracil WC

N	-0.63216	-0.27969	-0.00300
C	-1.12794	-1.53214	-0.00206
N	-2.39951	-1.90460	-0.00021
C	-3.21896	-0.84294	0.00072
C	-2.85522	0.50014	-0.00008
C	-1.46933	0.77412	-0.00198
N	-0.97585	2.01838	-0.00270
N	-4.59031	-0.82686	0.00257
C	-4.97153	0.49588	0.00290
N	-3.96165	1.32403	0.00147
H	-0.37685	-2.31947	-0.00293
H	-1.61719	2.79540	-0.00156
H	0.03163	2.17621	-0.00356
H	-6.01365	0.78413	0.00426
N	4.23236	-1.09578	0.00208
C	2.84899	-1.24147	-0.00068
O	2.31521	-2.33451	-0.00183
N	2.16149	-0.05243	-0.00203
C	2.70321	1.22334	-0.00035
O	1.97278	2.20956	-0.00133
C	4.16098	1.27750	0.00258
C	4.85798	0.12446	0.00372
H	4.75563	-1.95953	0.00314
H	1.11142	-0.13142	-0.00326
H	4.64273	2.24453	0.00392
H	5.94178	0.09403	0.00598
H	-5.18910	-1.63897	0.00358

cytosine–guanine WC

N	-2.18418	-0.08041	0.00330
C	-2.92223	1.05776	0.00782
O	-2.44390	2.19136	0.01408
N	-4.31802	0.92416	0.00532
C	-4.93671	-0.28539	-0.00190
C	-4.20783	-1.42419	-0.00648
C	-2.77037	-1.27740	-0.00318
N	-1.98588	-2.35363	-0.00654
H	-4.83957	1.78990	0.00888
H	-6.02084	-0.27579	-0.00363

H	-4.67818	-2.39802	-0.01238
H	-2.38829	-3.27630	-0.01130
H	-0.95817	-2.24554	-0.00288
N	3.88315	-1.63847	0.00622
C	4.95144	-0.89490	0.00522
N	4.66445	0.45767	0.00033
C	3.30344	0.57361	-0.00141
N	2.60516	1.72878	-0.00577
C	1.30215	1.52521	-0.00669
N	0.45373	2.57123	-0.01405
N	0.73074	0.27759	-0.00298
C	1.42080	-0.94154	0.00134
O	0.79167	-2.00248	0.00385
C	2.83713	-0.73843	0.00217
H	5.96987	-1.25694	0.00756
H	0.86484	3.48960	-0.00694
H	-0.56034	2.46063	-0.00071
H	-0.29893	0.19741	-0.00235
H	5.31650	1.22709	-0.00171

adenine–adenine hydrogen-bonded structure (global minimum)

N	-3.70999800	-1.94159300	-0.14890300
C	-4.90442700	-1.33968300	-0.09801500
N	-5.17913000	-0.04145300	0.00303400
C	-4.05686300	0.68325300	0.04782600
C	-2.74719800	0.21358900	0.00156400
C	-2.59579300	-1.19082400	-0.09703900
N	-1.40266900	-1.79875300	-0.14404500
N	-3.93686900	2.04945300	0.14661800
C	-2.59658400	2.33183200	0.15226600
N	-1.84745300	1.26289400	0.06633000
H	-5.76223300	-2.00579100	-0.14353800
H	-0.51378300	-1.30144700	-0.05822700
H	-1.40762200	-2.80509900	-0.20637000
H	-2.22848300	3.34620700	0.22166600
H	-4.70250100	2.70426000	0.20122700
N	1.42314400	-0.81480700	0.10498600
C	2.24497400	-1.87263600	0.21518700
N	3.57067600	-1.89930600	0.20898200
C	4.07819000	-0.66641500	0.06971700
C	3.36521700	0.52087900	-0.05428600
C	1.95657000	0.41345300	-0.03002000
N	1.15504100	1.48018400	-0.13686400
N	5.39513000	-0.28445700	0.01973400
C	5.40458300	1.08356900	-0.12835800
N	4.20839100	1.60632400	-0.17639700

H	1.74962200	-2.83513000	0.32513000
H	1.57693200	2.39047500	-0.23129000
H	0.14005700	1.37661800	-0.07524300
H	6.33022500	1.63851600	-0.19404900
H	6.19193000	-0.90010600	0.08331100

uracil–uracil hydrogen-bonded structure (global minimum)

N	4.30054900	0.54665200	0.00006100
C	3.06694900	1.19303700	0.00053200
O	2.97238300	2.39954200	0.00102200
N	1.98837200	0.32748800	0.00017900
C	2.03800700	-1.05685000	-0.00055000
O	1.00465300	-1.72445600	-0.00028000
C	3.37294200	-1.63523800	-0.00067100
C	4.44180700	-0.81427200	-0.00048000
H	5.10167400	1.16209300	0.00026500
H	1.05339300	0.76299300	0.00037000
H	3.46770300	-2.71114800	-0.00101900
H	5.46242400	-1.18007400	-0.00069600
N	1.66521600	-0.83358700	0.00069800
C	1.72516300	0.53716300	-0.00015900
O	-0.72657300	1.24916200	-0.00058300
N	-2.99824300	1.05402900	-0.00065400
C	-4.21104500	0.33978900	-0.00056800
O	-5.26888200	0.93682300	-0.00043600
C	-4.03333800	-1.10756300	0.00068500
C	-2.78702400	-1.62219800	0.00104000
H	-0.71767000	-1.23367800	0.00069400
H	-3.06668400	2.06566000	-0.00127400
H	-4.91609700	-1.73051400	0.00116200
H	-2.59443700	-2.68918200	0.00174500

uracil–uracil hydrogen-bonded structure (used for comparison with experiment)

N	4.24870900	-0.27384000	-0.02918500
C	3.11109700	-1.07623100	-0.01315900
O	3.17862200	-2.28612200	-0.02191700
N	1.93080100	-0.36126300	0.01315700
C	1.79435200	1.02103200	0.02326600
O	0.68429800	1.54096100	0.04616600
C	3.04437600	1.76936700	0.00507000
C	4.21042500	1.09573900	-0.02056000
H	5.12315700	-0.77864500	-0.04952200
H	1.05764800	-0.90602600	0.02729400
H	2.99627400	2.84841200	0.01204500
H	5.17484200	1.59120000	-0.03610200
N	-4.24873000	0.27381600	-0.02920100

C	-3.11113900	1.07625000	-0.01329900
O	-3.17864800	2.28612800	-0.02179000
N	-1.93080800	0.36127000	0.01235100
C	-1.79433700	-1.02099600	0.02296400
O	-0.68426700	-1.54094800	0.04590400
C	-3.04434200	-1.76937900	0.00512300
C	-4.21040700	-1.09576500	-0.02026500
H	-5.12324500	0.77857500	-0.04885500
H	-1.05760400	0.90600700	0.02664300
H	-2.99622800	-2.84842000	0.01232500
H	-5.17483200	-1.59122700	-0.03542700

adenine–thymine stacked structure

N	-1.21942	-2.13718	0.37566
C	-1.20224	-2.23350	-0.99529
N	-0.08621	-1.81419	-1.53226
C	0.67081	-1.41070	-0.45178
C	1.95067	-0.82604	-0.34804
N	2.69917	-0.55045	-1.43894
N	2.43348	-0.55013	0.87145
C	1.66096	-0.79953	1.93870
N	0.42834	-1.30065	1.97682
C	-0.01409	-1.59786	0.74871
N	-1.77007	1.11521	1.23241
C	-2.28948	0.67058	0.03557
O	-3.34835	0.07237	-0.05014
N	-1.48654	0.95991	-1.04670
C	-0.20955	1.53458	-1.03021
O	0.43245	1.63163	-2.06137
C	0.25056	1.98124	0.28842
C	-0.54313	1.73479	1.34928
H	-1.79783	0.59390	-1.93987
H	-2.31236	0.88506	2.05264
H	-0.25939	2.00685	2.36028
C	1.58326	2.65798	0.37327
H	2.36983	1.99663	0.00001
H	1.59368	3.56555	-0.23712
H	1.81845	2.91969	1.40753
H	-2.05385	-2.61700	-1.54055
H	-2.00394	-2.33348	0.98038
H	2.10365	-0.54934	2.90012
H	3.51773	0.02152	-1.29236
H	2.21328	-0.44812	-2.31973

adenine–uracil stacked structure

N	-0.43603	-2.21447	-0.28156

C	-0.37427	-1.88655	-1.61529
N	0.56264	-1.01832	-1.89381
C	1.14785	-0.75620	-0.67201
C	2.17171	0.12968	-0.27359
N	2.79719	0.93934	-1.15524
N	2.53216	0.15397	1.01765
C	1.87153	-0.62691	1.88294
N	0.85648	-1.45726	1.65075
C	0.54295	-1.48839	0.34932
N	-2.01247	0.30001	1.39214
C	-2.35917	0.10705	0.06712
O	-3.18659	-0.71395	-0.28550
N	-1.67425	0.92527	-0.80449
C	-0.61474	1.79702	-0.50547
O	-0.02337	2.36947	-1.40219
C	-0.32685	1.91023	0.92001
C	-1.01336	1.15394	1.79693
H	-2.47002	-0.31300	2.05163
H	-1.85695	0.77048	-1.79009
H	3.36024	1.67771	-0.75942
H	2.30628	1.14663	-2.01469
H	2.20577	-0.56157	2.91574
H	-1.11819	-2.81493	0.15856
H	-1.05920	-2.31963	-2.33131
H	-0.81723	1.16614	2.86264
H	0.47501	2.56508	1.23050

cytosine–guanine stacked structure

N	1.67521	-0.85394	-1.98228
C	2.79226	-0.50534	-1.25352
N	2.60694	-0.60906	0.03447
C	1.30953	-1.05694	0.16157
C	0.51579	-1.30962	1.33766
O	0.81664	-1.20642	2.51469
N	-0.78360	-1.71931	0.96678
C	-1.29407	-1.74660	-0.30161
N	-2.62618	-2.07018	-0.40477
N	-0.57682	-1.51914	-1.37488
C	0.70732	-1.19774	-1.08058
N	-1.39457	1.92314	-1.09990
C	-1.74929	1.30814	0.11671
O	-2.86178	0.79450	0.20531
N	-0.81490	1.30213	1.10499
C	0.39802	1.77858	0.88060
N	1.29822	1.69375	1.88454
C	0.79253	2.37610	-0.37221

C	-0.15479	2.42076	-1.33822
H	-2.10227	1.89856	-1.82086
H	0.01818	2.84370	-2.32173
H	1.78963	2.76405	-0.53011
H	1.05906	1.03502	2.61999
H	2.27652	1.70257	1.63177
H	-1.41530	-1.85733	1.74794
H	-2.93075	-1.99466	-1.36766
H	-3.20548	-1.48582	0.19462
H	3.70843	-0.19132	-1.73343
H	1.56932	-0.85510	-2.98568

b) M06-2X/6-31G** Geometries

9-hexyl–adenine–9-hexyl–adenine HB1

N	-2.70969100	3.41535500	-0.62488100
C	-4.00429000	3.41403200	-0.28944200
N	-4.72490400	2.44187200	0.26347800
C	-3.97011900	1.35748500	0.47739000
C	-2.61899100	1.19378100	0.18687000
C	-1.97488900	2.31120000	-0.39907300
N	-0.68065800	2.32000900	-0.73734500
N	-4.37110800	0.16795600	1.03654800
C	-3.26657500	-0.63811000	1.04521500
N	-2.19484600	-0.06968300	0.55189800
H	-4.53712400	4.33859600	-0.50072700
H	-0.05120400	1.52714200	-0.59228300
H	-0.33020200	3.17185800	-1.14530300
H	-3.31456400	-1.64505000	1.43942700
N	1.51554000	0.31746200	-0.51449800
C	2.65090500	0.85953600	-0.98650600
N	3.85622400	0.31809500	-1.08329200
C	3.85156600	-0.94423600	-0.62619900
C	2.76871600	-1.64417800	-0.10728100
C	1.53806100	-0.95018300	-0.06051100
N	0.42154300	-1.51018300	0.41348300
N	4.90416900	-1.82083900	-0.57192100
C	4.40246500	-2.97677600	-0.02237700
N	3.12885700	-2.91997400	0.26819300
H	2.55920400	1.88660900	-1.33515000
H	0.47372000	-2.45878200	0.74695800
H	-0.45720100	-0.98714500	0.44395200
H	5.04134000	-3.83712500	0.13139300
C	6.27320000	-1.52335000	-0.96096200
C	6.97683600	-0.62374300	0.05095200

H	6.24199200	-1.03724000	-1.94096300
H	6.79919300	-2.47678500	-1.07291100
C	8.40998000	-0.30838200	-0.36917000
H	6.39920100	0.30268600	0.14701200
H	6.96962000	-1.11476800	1.03185200
C	9.13212800	0.59608300	0.62672000
H	8.97504200	-1.24367500	-0.48556100
H	8.40259400	0.17265500	-1.35642700
H	8.56733000	1.53068300	0.74275900
H	9.13862000	0.11709100	1.61524900
C	-5.72718800	-0.14799100	1.45657900
C	-6.65433000	-0.39131400	0.26950000
H	-6.09163000	0.69322900	2.05399400
H	-5.67635200	-1.02849100	2.10499400
C	-8.07801900	-0.71036800	0.71801400
H	-6.64821700	0.50612400	-0.35931900
H	-6.25455800	-1.21537900	-0.33430300
C	-9.02586100	-0.95338800	-0.45409500
H	-8.07103700	-1.59619400	1.36840100
H	-8.46157300	0.11794800	1.32861500
H	-9.03353200	-0.06768500	-1.10317700
H	-8.64187800	-1.77974400	-1.06761900
C	10.56597600	0.91907700	0.21229900
C	11.27613700	1.82329200	1.21587900
H	10.55613000	1.39717900	-0.77506500
H	11.12677300	-0.01669000	0.09495000
H	12.29990200	2.04444800	0.90409200
H	10.74595000	2.77418700	1.32673300
H	11.31992700	1.35185100	2.20258000
C	-10.45319700	-1.27154200	-0.01424700
C	-11.38992000	-1.51218600	-1.19480700
H	-10.83376200	-0.44474800	0.59825100
H	-10.44157300	-2.15540700	0.63583200
H	-12.40608200	-1.73861900	-0.86258900
H	-11.43645800	-0.63035100	-1.84114600
H	-11.04103700	-2.35134300	-1.80462100

9-hexyl–adenine–9-hexyl–adenine HB2

N	-2.61919900	-3.95507600	-0.46322200
C	-3.83630600	-3.48226600	-0.75562000
N	-4.21928500	-2.22425800	-0.95401300
C	-3.18455800	-1.38616300	-0.81413600
C	-1.86536800	-1.70980400	-0.50578100
C	-1.59774600	-3.08996500	-0.33681900
N	-0.37990100	-3.57222500	-0.05257300
N	-3.20377400	-0.01911400	-0.94067900

C	-1.92292400	0.40005300	-0.69195400
N	-1.08606200	-0.57086300	-0.43001300
H	-4.61588900	-4.23593800	-0.84337000
H	0.45061300	-2.98297300	0.00324400
H	-0.30945600	-4.56841500	0.07728700
H	-1.66933700	1.45210700	-0.72697000
N	5.61876600	-3.28844400	0.43435000
C	6.10543400	-2.11174900	0.85802700
N	5.46279900	-0.96272000	1.04019400
C	4.16216900	-1.08561300	0.75209400
C	3.50593600	-2.23429600	0.31838500
C	4.31438300	-3.37498400	0.15460500
N	3.80686800	-4.56386000	-0.25566900
N	3.18934700	-0.11842300	0.81863400
C	2.02298600	-0.71697400	0.42096100
N	2.16450200	-1.98467900	0.11654800
H	7.17123900	-2.10242500	1.07252800
H	2.90416700	-4.56732000	-0.70279100
H	4.47373000	-5.27259400	-0.51807000
H	1.07714800	-0.18973100	0.36436800
C	3.40962500	1.27368100	1.17825500
C	4.09230200	2.05485400	0.05943600
H	4.02773400	1.28811300	2.08116900
H	2.43591700	1.70732400	1.42558300
C	4.33457300	3.51065300	0.44918500
H	5.04426300	1.56370300	-0.17228600
H	3.47108600	2.00306800	-0.84316100
C	5.01728600	4.31226800	-0.65657000
H	3.37889100	3.98829100	0.70630800
H	4.95158800	3.54670500	1.35694000
H	5.97098700	3.83321900	-0.91513600
H	4.40072100	4.27757800	-1.56504900
C	-4.38408100	0.78404900	-1.21419700
C	-5.30459800	0.88777000	-0.00160400
H	-4.91434100	0.31857100	-2.05069800
H	-4.04406300	1.77343100	-1.53677700
C	-6.54760000	1.72075300	-0.30277900
H	-5.59241300	-0.12646700	0.29725300
H	-4.74746600	1.32828400	0.83452200
C	-7.48788000	1.83483900	0.89484700
H	-6.24851500	2.72762600	-0.62609300
H	-7.08912800	1.27370100	-1.14714000
H	-7.78692700	0.82871000	1.21746000
H	-6.94745000	2.28019400	1.74121800
C	5.27001600	5.76850000	-0.27248700
C	5.95060400	6.55849800	-1.38686300

H	5.88719300	5.79959000	0.63394800
H	4.31603100	6.24329000	-0.01092400
H	6.12462100	7.59719800	-1.09529300
H	6.91757600	6.11530600	-1.64392900
H	5.33692700	6.56225600	-2.29304000
C	-8.73579300	2.66394800	0.59960200
C	-9.66738700	2.76988200	1.80380300
H	-9.27284000	2.21693900	-0.24614300
H	-8.43342000	3.66769000	0.27554700
H	-10.55406100	3.36645700	1.57545600
H	-10.00282600	1.77904200	2.12514800
H	-9.15716800	3.23750200	2.65162700

9-hexyl–adenine–9-hexyl–adenine HB3

N	-2.16429400	-3.41011500	0.23181300
C	-3.47485900	-3.43979200	-0.03982600
N	-4.27173300	-2.44838100	-0.42900600
C	-3.59009100	-1.30005200	-0.52115100
C	-2.23855200	-1.09700200	-0.26043200
C	-1.50487000	-2.24456900	0.12133200
N	-0.19135600	-2.20987600	0.38851000
N	-4.07937400	-0.06954700	-0.88823800
C	-3.02148200	0.79540100	-0.81424800
N	-1.89982300	0.22834600	-0.44626000
H	-3.94739600	-4.41331900	0.07036500
H	0.38820200	-1.40599600	0.14590000
H	0.24464100	-3.09193500	0.60484700
H	-3.14091900	1.84461900	-1.05299000
N	2.16476000	3.41029300	0.23181900
C	3.47537200	3.43971000	-0.03962800
N	4.27208100	2.44816600	-0.42880600
C	3.59019100	1.30000200	-0.52117400
C	2.23856400	1.09721800	-0.26072200
C	1.50508200	2.24492300	0.12105900
N	0.19151100	2.21050800	0.38791600
N	4.07925900	0.06941700	-0.88831900
C	3.02118400	-0.79529200	-0.81460100
N	1.89956200	-0.22802500	-0.44677000
H	3.94811300	4.41311300	0.07077500
H	-0.38816600	1.40665900	0.14551000
H	-0.24434800	3.09255300	0.60456900
H	3.14038800	-1.84451700	-1.05342900
C	5.46876300	-0.22319600	-1.20342700
C	6.34557800	-0.25370500	0.04492200
H	5.82011500	0.55018700	-1.89313600
H	5.49457800	-1.18347800	-1.72816800

C	7.80554100	-0.54414800	-0.29273300
H	6.25999100	0.71637500	0.54746300
H	5.95904900	-1.01355300	0.73540000
C	8.70112700	-0.57789000	0.94343500
H	7.87914000	-1.50529500	-0.82038300
H	8.17699200	0.21964900	-0.98888700
H	8.62621400	0.38225200	1.47105300
H	8.32989400	-1.34085100	1.64111600
C	-5.46891600	0.22279400	-1.20337900
C	-6.34569800	0.25359600	0.04499000
H	-5.82018000	-0.55088200	-1.89280300
H	-5.49490100	1.18288800	-1.72845800
C	-7.80569100	0.54382100	-0.29271300
H	-6.26000700	-0.71633100	0.54781200
H	-5.95921200	1.01367200	0.73524200
C	-8.70128800	0.57777600	0.94343700
H	-7.87937400	1.50483600	-0.82059500
H	-8.17707500	-0.22017100	-0.98869000
H	-8.62637900	-0.38227200	1.47122800
H	-8.33007400	1.34086200	1.64099100
C	10.16513400	-0.86275300	0.61552800
C	11.04825600	-0.89413900	1.85978700
H	10.53310400	-0.09912400	-0.08089100
H	10.23628000	-1.82122800	0.08621800
H	12.09158200	-1.09934000	1.60766500
H	11.01226300	0.06401800	2.38722800
H	10.71260600	-1.66833500	2.55670900
C	-10.16529100	0.86256900	0.61544800
C	-11.04846700	0.89407000	1.85966300
H	-10.53321600	0.09885800	-0.08090600
H	-10.23643600	1.82098400	0.08602900
H	-12.09177700	1.09927300	1.60747600
H	-11.01252100	-0.06404400	2.38718300
H	-10.71283600	1.66831400	2.55654300

9-hexyl–adenine–1-hexyl– thymine WC

N	0.65080600	-1.43524800	-0.29726300
C	1.16950900	-0.19568000	-0.37414900
N	2.40130200	0.15249300	-0.71347300
C	3.14718100	-0.92663800	-1.00080000
C	2.75309900	-2.26047500	-0.96688400
C	1.41475500	-2.50461100	-0.58720100
N	0.89489500	-3.73380600	-0.50790100
N	4.46119100	-0.95315000	-1.39042400
C	4.77899000	-2.28045800	-1.55514900
N	3.78802400	-3.09941900	-1.31771700

H	0.47233200	0.60082500	-0.12129900
H	1.48796800	-4.52018300	-0.71552500
H	-0.07011800	-3.86957700	-0.20615800
H	5.77395300	-2.57578400	-1.86345600
N	-3.95451800	-0.53782800	1.17559800
C	-2.63445100	-0.43555500	0.74872700
O	-2.08151400	0.64069700	0.59749800
N	-2.01267600	-1.63845800	0.51668500
C	-2.56464700	-2.89773000	0.62491400
O	-1.90570700	-3.90434900	0.37393000
C	-3.96233500	-2.93736200	1.04867300
C	-4.61610500	-4.27693700	1.18420200
C	-4.57344900	-1.76034600	1.29312800
H	-1.00949500	-1.57210500	0.20393600
H	-5.65618500	-4.17749100	1.50246900
H	-4.08095400	-4.89286700	1.91232900
H	-4.58687500	-4.81577600	0.23317100
H	-5.61135500	-1.71320500	1.61146100
C	-4.68801600	0.70960600	1.38658800
C	-5.24583000	1.28040400	0.08712500
H	-3.99468100	1.41976600	1.84209700
H	-5.49071200	0.50283600	2.10175800
C	-5.98219700	2.59777900	0.31427000
H	-4.41044600	1.43218000	-0.60554000
H	-5.92120400	0.54559200	-0.37077200
C	-6.57448100	3.17581700	-0.96873900
H	-6.78551800	2.45028100	1.04976900
H	-5.28992700	3.32702600	0.75561600
H	-5.77504200	3.30941800	-1.70976300
H	-7.27765200	2.45226100	-1.40349200
C	-7.28967900	4.50720600	-0.75092700
C	-7.88970000	5.06821400	-2.03705300
H	-6.58184900	5.22970900	-0.32612200
H	-8.07958800	4.37373900	-0.00099600
H	-8.39379400	6.02221100	-1.86329700
H	-7.11342200	5.23128400	-2.79106200
H	-8.62168600	4.37359100	-2.46087900
C	5.33169500	0.20594700	-1.50314800
C	5.78439400	0.71777800	-0.13881100
H	4.77757800	0.98516600	-2.03524700
H	6.18928100	-0.08224200	-2.11945300
C	6.69652800	1.93531900	-0.25950900
H	4.89282400	0.97042500	0.44644100
H	6.30263500	-0.09085100	0.39141200
C	7.16097300	2.46032200	1.09697000
H	7.57454100	1.67988900	-0.86906000

H	6.16915000	2.73475100	-0.79690600
H	6.28364100	2.71845900	1.70488300
H	7.68326600	1.65892200	1.63709900
C	8.07770400	3.67649700	0.98834200
C	8.53586400	4.18757800	2.35146100
H	7.55362900	4.47590000	0.44997300
H	8.95135000	3.41598800	0.37760000
H	9.19401000	5.05486300	2.25606600
H	7.67892300	4.48191000	2.96514600
H	9.08122000	3.41015800	2.89565900

9-hexyl–adenine–1-hexyl– thymine RWC

N	0.66872400	0.20292200	-0.97978200
C	1.75789100	0.96592200	-0.77035700
N	3.02998600	0.60965700	-0.86397000
C	3.14728000	-0.68067100	-1.21490500
C	2.12084200	-1.58715900	-1.46130700
C	0.80671200	-1.08839100	-1.32871600
N	-0.28042500	-1.84112400	-1.53296400
N	4.30334100	-1.39001700	-1.41193900
C	3.91175600	-2.66391900	-1.74901800
N	2.61561900	-2.82882900	-1.79563400
H	1.53934800	1.99511200	-0.49180600
H	-0.15572800	-2.80490000	-1.79440100
H	-1.21134700	-1.44392700	-1.41830300
H	4.64769300	-3.43089000	-1.95531100
N	-4.10754600	1.38615000	-0.62848900
C	-2.90768100	0.72158900	-0.81462200
O	-2.87469800	-0.46731500	-1.12569800
N	-1.78693500	1.47732300	-0.62915400
C	-1.72563200	2.81090100	-0.24201800
O	-0.65274400	3.37246900	-0.09666100
C	-3.02791300	3.45006900	-0.03049600
C	-3.03497900	4.88584900	0.39047100
C	-4.13333200	2.70681300	-0.22847300
H	-0.86764000	0.98435200	-0.77056100
H	-4.05431700	5.25941300	0.50946100
H	-2.51441900	5.50161300	-0.34814000
H	-2.49933300	5.00898700	1.33582200
H	-5.12997700	3.11624300	-0.08954000
C	-5.33971200	0.60658500	-0.74543900
C	-5.65542900	-0.16631600	0.53067100
H	-5.21243600	-0.08223800	-1.58316100
H	-6.14690900	1.30369800	-0.99183100
C	-6.93154300	-0.99313800	0.40111600
H	-4.80493200	-0.82097300	0.75190500

H	-5.74874800	0.54048900	1.36575500
C	-7.26705900	-1.76286300	1.67641300
H	-7.77401000	-0.33686100	0.14163400
H	-6.82318100	-1.70025000	-0.43217600
H	-6.42084000	-2.41105300	1.94079100
H	-7.38159100	-1.05455400	2.50846700
C	-8.53297100	-2.60748400	1.55422900
C	-8.85854200	-3.36286200	2.83978900
H	-8.41340000	-3.31853000	0.72723800
H	-9.37525100	-1.95894100	1.28230100
H	-9.76523400	-3.96402500	2.73511500
H	-8.03950800	-4.03467900	3.11463900
H	-9.01031900	-2.66832400	3.67199800
C	5.65108500	-0.88144800	-1.21460700
C	6.00833900	-0.75884600	0.26368500
H	5.71074400	0.09710400	-1.70106100
H	6.33872800	-1.55935600	-1.73076000
C	7.42918900	-0.23957900	0.46518900
H	5.28770900	-0.08181600	0.73673800
H	5.89432600	-1.74031100	0.74064900
C	7.80567100	-0.10952000	1.93907400
H	8.14174300	-0.91211800	-0.03280500
H	7.53371700	0.73832100	-0.02378900
H	7.09808400	0.56821400	2.43520100
H	7.69164100	-1.08550000	2.43059400
C	9.22923400	0.39949800	2.15228300
C	9.59182300	0.52066800	3.62966500
H	9.34076900	1.37483600	1.66239700
H	9.93304100	-0.27801800	1.65235400
H	10.61224000	0.88777300	3.76529100
H	8.91532200	1.21247800	4.14114700
H	9.51402400	-0.44935800	4.13079200

9-hexyl–adenine–1-hexyl– thymine H

N	-3.60079100	-3.97117900	0.67762700
C	-4.60190800	-3.16365900	0.30506300
N	-4.54567000	-1.93524500	-0.20402200
C	-3.27590200	-1.52967300	-0.32490800
C	-2.13335800	-2.24260500	0.01792800
C	-2.33529900	-3.53873200	0.54518300
N	-1.32636800	-4.33954700	0.91373100
N	-2.82207400	-0.32807800	-0.82052300
C	-1.45791100	-0.37073100	-0.74752500
N	-1.00724500	-1.49785300	-0.25447800
H	-5.59952200	-3.57600200	0.43919000
H	-0.34762500	-4.08149000	0.81106600

H	-1.56760100	-5.25251300	1.26315900
H	-0.82413400	0.44487400	-1.07441600
N	3.75918500	-0.82227300	-0.68992700
C	2.37389000	-0.72498300	-0.65405700
O	1.77889900	0.27478200	-1.02701500
N	1.73480200	-1.83803800	-0.16997100
C	2.31070000	-2.99898800	0.30242400
O	1.61944000	-3.92633100	0.71350500
C	3.77191300	-3.02632600	0.27323900
C	4.46043400	-4.25429800	0.78121400
C	4.40638500	-1.94069000	-0.21436700
H	0.68730000	-1.77280000	-0.15901300
H	5.54594800	-4.15438200	0.71388800
H	4.15009100	-5.13261500	0.20849800
H	4.18639900	-4.44366900	1.82278900
H	5.49052500	-1.89151500	-0.26755000
C	4.50501700	0.35269900	-1.13996500
C	4.67341800	1.38823500	-0.03354300
H	3.95710300	0.78431400	-1.98048500
H	5.47684900	0.00505600	-1.50428600
C	5.46471000	2.60566300	-0.50397500
H	3.67597900	1.69332300	0.30224700
H	5.17791500	0.92150200	0.82272700
C	5.64069700	3.65495200	0.59094600
H	6.45330400	2.28665400	-0.86282000
H	4.95616300	3.06043900	-1.36461500
H	4.65277800	3.97894300	0.94476600
H	6.14088400	3.19759000	1.45565800
C	6.43904400	4.87326000	0.13265300
C	6.60983300	5.91144400	1.23800000
H	5.93710100	5.32954400	-0.72976600
H	7.42390200	4.54550700	-0.22332400
H	7.18228900	6.77614500	0.89306300
H	5.63763800	6.27089300	1.58910900
H	7.13430400	5.48289100	2.09778800
C	-3.66752200	0.76213900	-1.28217800
C	-4.37367600	1.47077700	-0.13025100
H	-4.40418300	0.33978200	-1.97275200
H	-3.03303100	1.45503800	-1.84361300
C	-5.27245700	2.59899800	-0.62875300
H	-4.96672700	0.72910800	0.41684700
H	-3.62110600	1.86434700	0.56400300
C	-6.00307300	3.31793200	0.50288600
H	-4.67347800	3.32672700	-1.19393800
H	-6.00940700	2.19182500	-1.33407700
H	-6.59954600	2.58987500	1.06882300

H	-5.26814000	3.72722200	1.20940300
C	-6.91089700	4.44220500	0.00989900
C	-7.63492900	5.15318300	1.14978800
H	-7.64402100	4.02993500	-0.69464000
H	-6.31285200	5.16602000	-0.55797800
H	-8.28418600	5.95053700	0.77941900
H	-8.25514000	4.45080400	1.71535100
H	-6.92000500	5.59915400	1.84829400

9-hexyl–adenine–1-hexyl– thymine RH

N	1.57887600	-3.91417200	-0.41859600
C	2.85559800	-3.86944800	-0.01490600
N	3.55542000	-2.83585100	0.44614200
C	2.80285400	-1.72933400	0.47861600
C	1.47236800	-1.61243700	0.09566800
C	0.84736700	-2.78833400	-0.37588000
N	-0.43182000	-2.81910600	-0.77752900
N	3.17361900	-0.47175500	0.89861600
C	2.07532900	0.32716400	0.74339100
N	1.03771400	-0.31804800	0.26998000
H	3.39057200	-4.81473800	-0.07569500
H	-1.03345800	-2.00011900	-0.76578200
H	-0.79384300	-3.70178800	-1.09900800
H	2.06954100	1.38160000	0.99309900
N	-3.44707300	1.46297200	-0.80156500
C	-2.38352300	0.59515900	-0.61713100
O	-2.47011400	-0.60132800	-0.87814000
N	-1.24613400	1.17142100	-0.13067600
C	-1.05369200	2.49929200	0.22196800
O	0.02397300	2.88346800	0.65145700
C	-2.22570300	3.35885500	0.03826600
C	-2.09615600	4.80319600	0.40740300
C	-3.34542500	2.79432600	-0.45451200
H	-0.42065600	0.53672800	0.00145200
H	-3.02786400	5.34318700	0.22543400
H	-1.29466500	5.27453700	-0.16814400
H	-1.82777900	4.90501000	1.46267500
H	-4.25147100	3.37116000	-0.61842900
C	-4.71515000	0.90053000	-1.26495600
C	-5.54667600	0.32869000	-0.12210600
H	-4.47861200	0.11951500	-1.99041200
H	-5.25760300	1.69824100	-1.78249900
C	-6.88682800	-0.21737500	-0.60794300
H	-4.96745700	-0.46625000	0.36140800
H	-5.71282900	1.11181000	0.62942000
C	-7.73783900	-0.79006300	0.52238800

H	-7.44674600	0.58181400	-1.11368000
H	-6.71240100	-0.99593000	-1.36252400
H	-7.18548300	-1.59869200	1.01954600
H	-7.89835900	-0.01537700	1.28473200
C	-9.08977900	-1.31762100	0.04693400
C	-9.93192600	-1.88273200	1.18686400
H	-8.92797900	-2.09166700	-0.71355000
H	-9.63665800	-0.50734000	-0.45153200
H	-10.89665400	-2.25161800	0.82976600
H	-9.41600200	-2.71334200	1.67842000
H	-10.12424500	-1.11763100	1.94554800
C	4.50484500	-0.09162800	1.34531300
C	5.49021900	0.01617300	0.18553100
H	4.84246800	-0.84822100	2.06028000
H	4.41379100	0.86201300	1.87464000
C	6.87931500	0.43366800	0.66040000
H	5.53723500	-0.95616900	-0.31843900
H	5.10662400	0.74218100	-0.54178300
C	7.88512800	0.55092400	-0.48228400
H	6.81388200	1.39726000	1.18488600
H	7.24867000	-0.29367100	1.39573200
H	7.96173800	-0.41516900	-0.99899200
H	7.50910500	1.26729200	-1.22530000
C	9.27185000	0.98844400	-0.01620800
C	10.26825300	1.10159700	-1.16662000
H	9.64448300	0.27358100	0.72794500
H	9.19002500	1.95383900	0.49894800
H	11.25224400	1.42352100	-0.81661900
H	10.38995200	0.13895200	-1.67287900
H	9.92277100	1.82585200	-1.91097400

1-hexyl– thymine–1-hexyl–thymine HB1

N	4.14656900	-0.85891800	-0.99873600
C	3.24142000	0.19874700	-0.97665000
O	3.59988500	1.35873000	-0.95763200
N	1.91574100	-0.18879500	-0.98057600
C	1.42466400	-1.48070200	-0.96555800
O	0.21789500	-1.70635400	-0.95956900
C	2.43065600	-2.53764600	-0.95524600
C	1.95244200	-3.95589300	-0.93519400
C	3.72666600	-2.16689400	-0.96724700
H	1.21930300	0.57001400	-0.97224100
H	2.79261200	-4.65352700	-0.92777000
H	1.32790300	-4.16254800	-1.80848000
H	1.33170800	-4.13901300	-0.05400500
H	4.52807700	-2.90038800	-0.96058500

N	-4.14704000	0.86194500	-0.99707900
C	-3.24216000	-0.19601000	-0.97854900
O	-3.60089900	-1.35595500	-0.96292700
N	-1.91635700	0.19116500	-0.98183900
C	-1.42492400	1.48289900	-0.96338500
O	-0.21810900	1.70833100	-0.95724700
C	-2.43065000	2.54006300	-0.94989300
C	-1.95204700	3.95812500	-0.92620100
C	-3.72677000	2.16970900	-0.96226600
H	-1.22030800	-0.56797500	-0.97643200
H	-2.79203000	4.65595200	-0.91642200
H	-1.32791100	4.16702500	-1.79924100
H	-1.33080100	4.13864300	-0.04483800
H	-4.52797300	2.90340500	-0.95321900
C	-5.56817400	0.51894500	-0.94159800
C	-6.03629100	0.21884900	0.47841100
H	-5.71671900	-0.35488500	-1.57944300
H	-6.12536400	1.35812800	-1.36970400
C	-7.51838600	-0.14319200	0.52536000
H	-5.43459300	-0.60967300	0.86790700
H	-5.84266900	1.09225700	1.11485500
C	-8.00656300	-0.45464400	1.93815500
H	-8.11398300	0.68146200	0.10934500
H	-7.69999300	-1.01210900	-0.12095800
H	-7.41176300	-1.27945000	2.35262500
H	-7.82225300	0.41258000	2.58691900
C	-9.48798500	-0.82099600	1.99359200
C	-9.96192400	-1.13154800	3.41067500
H	-9.66899400	-1.68653700	1.34431300
H	-10.07943900	0.00426300	1.57753000
H	-11.02318400	-1.39142000	3.43238000
H	-9.40174200	-1.97129400	3.83327400
H	-9.81352800	-0.26997100	4.06909500
C	5.56764300	-0.51575500	-0.94288900
C	6.03634900	-0.21969700	0.47777400
H	5.71568400	0.35997900	-1.57823500
H	6.12483200	-1.35354800	-1.37371500
C	7.51851400	0.14199800	0.52518000
H	5.43490300	0.60782100	0.86977700
H	5.84284200	-1.09483200	1.11187600
C	8.00724100	0.44956200	1.93863400
H	8.11383600	-0.68162200	0.10672500
H	7.70003000	1.01262700	-0.11885300
H	7.41281700	1.27344600	2.35547200
H	7.82288600	-0.41931300	2.58516900
C	9.48878900	0.81533000	1.99456000

C	9.96326300	1.12207400	3.41229100
H	9.66985900	1.68248800	1.34746100
H	10.07986200	-0.00903200	1.57618500
H	11.02461800	1.38153400	3.43434000
H	9.40349700	1.96092100	3.83722000
H	9.81477700	0.25885900	4.06854200

1-hexyl– thymine–1-hexyl–thymine HB2

N	-4.97038300	0.21910000	-0.17220400
C	-3.98610600	-0.43848000	-0.90734800
O	-4.09494400	-1.59069800	-1.27753500
N	-2.85991100	0.32017400	-1.15511500
C	-2.60860900	1.60928600	-0.72603100
O	-1.52202800	2.14535500	-0.92561800
C	-3.70944500	2.26262300	-0.02430300
C	-3.52232500	3.68569100	0.40029500
C	-4.80878100	1.52420100	0.23023900
H	-2.07210800	-0.18292000	-1.58758900
H	-4.39285100	4.04894500	0.95062400
H	-3.35978900	4.32981100	-0.46841100
H	-2.63556100	3.77906400	1.03283600
H	-5.64810600	1.92980900	0.78971100
N	3.18819100	0.30097900	-0.88725900
C	2.13760200	1.21428100	-0.90736800
O	2.29091100	2.38696000	-0.63356900
N	0.91893500	0.67081900	-1.26803100
C	0.64900800	-0.65505900	-1.54908300
O	-0.48617800	-1.03263600	-1.82827200
C	1.79124300	-1.55887800	-1.48402200
C	1.54816300	-3.00837400	-1.76825300
C	2.98762800	-1.03212500	-1.15194300
H	0.11599500	1.31390100	-1.24858500
H	2.47296200	-3.58412000	-1.69160700
H	1.12921900	-3.13978700	-2.76943100
H	0.81635400	-3.41650200	-1.06475000
H	3.88061900	-1.64782100	-1.08467700
C	4.49438600	0.79952300	-0.45247000
C	4.57995100	0.92032200	1.06954600
H	4.63428200	1.78368800	-0.90529100
H	5.24946900	0.12262100	-0.85927200
C	5.92779100	1.46798400	1.56321400
H	3.77521900	1.59829300	1.37009000
H	4.36891200	-0.05262300	1.53203100
C	7.03168500	0.43941900	1.83867700
H	6.29865300	2.20602700	0.83857700

H	5.75460400	2.02433200	2.49018100
H	7.89427100	0.98828300	2.23234500
H	6.70566500	-0.22953300	2.64686000
C	7.48272900	-0.41022800	0.63962500
C	6.72289100	-1.73075900	0.50049100
H	8.54753900	-0.64479700	0.74314500
H	7.40093400	0.18213100	-0.28088800
H	7.00982600	-2.26773300	-0.40834400
H	6.93624100	-2.38130300	1.35396800
H	5.63909300	-1.58225300	0.48041100
C	-6.02741700	-0.60114500	0.42773700
C	-5.66047500	-1.10452900	1.82843600
H	-6.19020400	-1.44051200	-0.24950600
H	-6.93891900	0.00369600	0.45615400
C	-4.37221100	-1.94406800	1.86880800
H	-5.57051500	-0.24993100	2.51342600
H	-6.51154400	-1.69760400	2.18172700
C	-3.08108600	-1.11588800	1.99734000
H	-4.42498000	-2.64110600	2.71212100
H	-4.32470300	-2.55720500	0.96203700
H	-3.19207800	-0.13572600	1.51744000
H	-2.89691400	-0.89243100	3.05671200
C	-1.85550700	-1.80569300	1.39814800
C	-0.60646900	-0.93398500	1.48715500
H	-2.05728200	-2.04738100	0.34654800
H	-1.68741300	-2.76142600	1.91137700
H	0.27022900	-1.44253600	1.07247100
H	-0.74510600	-0.00090300	0.92726900
H	-0.37979800	-0.66852600	2.52517100

1-hexyl– thymine–1-hexyl–thymine HB3

N	-3.98061600	-0.36416900	0.36736200
C	-2.98711300	0.59294300	0.55386000
O	-3.20593800	1.65975500	1.09107400
N	-1.74454600	0.22041100	0.07948300
C	-1.41910300	-0.95279300	-0.57491600
O	-0.27572700	-1.17224700	-0.96422000
C	-2.51812300	-1.89355700	-0.76718700
C	-2.22089700	-3.17857700	-1.47488000
C	-3.73001400	-1.54366500	-0.29185800
H	-0.98349800	0.90153900	0.21116900
H	-3.11764500	-3.79584200	-1.56103100
H	-1.45255500	-3.74270100	-0.93933000
H	-1.82739400	-2.98303800	-2.47599700
H	-4.59387700	-2.19421700	-0.39997300
N	4.23960400	1.12012800	-1.06249600

C	3.24596500	0.16126400	-1.24711800
O	3.45220900	-0.90275900	-1.79407900
N	2.00916500	0.52805300	-0.75165800
C	1.68472700	1.69908100	-0.09355500
O	0.54531200	1.91179300	0.31046300
C	2.77974300	2.64798900	0.08124600
C	2.48283200	3.93544700	0.78438100
C	3.98677500	2.30247100	-0.40847200
H	1.24952600	-0.15609600	-0.87627600
H	3.37671400	4.55860800	0.85651200
H	2.10207900	3.74344300	1.79109200
H	1.70485700	4.49164200	0.25447200
H	4.84704500	2.96026100	-0.31675300
C	5.59575100	0.80841800	-1.51924300
C	6.50017100	0.31850700	-0.38992100
H	6.00490900	1.71195400	-1.98154900
H	5.49312200	0.04164100	-2.28810200
C	5.99300900	-0.95964600	0.27697100
H	7.49700600	0.15875200	-0.81635400
H	6.60681300	1.11049400	0.36527300
C	6.88192700	-1.43984900	1.42563400
H	4.98073600	-0.78497100	0.65986200
H	5.89686900	-1.74825200	-0.47938500
H	6.93794300	-0.65938500	2.19737000
H	6.40520500	-2.30557300	1.90157200
C	8.29886200	-1.83131000	1.00553600
C	9.09665700	-2.43499800	2.15855700
H	8.83156600	-0.95431800	0.61933500
H	8.24229400	-2.54862900	0.17667400
H	10.11087800	-2.70225100	1.85138300
H	9.17314600	-1.72799600	2.99068900
H	8.61030000	-3.33924600	2.53711600
C	-5.33437800	-0.01338900	0.79708900
C	-6.05565200	0.84421500	-0.24257300
H	-5.24426000	0.53970300	1.73471600
H	-5.86258400	-0.94873500	0.99829400
C	-7.48264100	1.23762800	0.17070200
H	-5.44349100	1.73942300	-0.38736900
H	-6.07566100	0.30831000	-1.20146200
C	-8.57647200	0.29496500	-0.34496300
H	-7.53763400	1.32337100	1.26371800
H	-7.69745400	2.23977800	-0.21277100
H	-9.55422400	0.69125300	-0.04316100
H	-8.56006300	0.31644000	-1.44171800
C	-8.47401600	-1.15908800	0.12275700
C	-8.60994200	-1.32342300	1.63538900

H	-7.52656800	-1.59361600	-0.22338600
H	-9.26070700	-1.74025400	-0.37084800
H	-8.57927600	-2.37662500	1.92622400
H	-7.81318900	-0.80651600	2.17906000
H	-9.56143200	-0.90742800	1.98158400

9-ethyl– adenine–1-cyclohexyl– uracil WC

N	-1.73219700	0.34681600	-0.00444300
C	-1.99290700	-0.97368500	-0.00317700
N	-3.17450000	-1.57206900	-0.00099900
C	-4.17078000	-0.67269900	0.00006100
C	-4.05915300	0.71315300	-0.00088600
C	-2.74536000	1.23240900	-0.00332100
N	-2.48339700	2.54337000	-0.00424900
N	-5.51823100	-0.92530800	0.00195100
C	-6.13127300	0.30720600	0.00228400
N	-5.29746400	1.31511800	0.00073300
H	-1.10820300	-1.60717700	-0.00408400
H	-3.25693700	3.18728300	-0.00418300
H	-1.52039700	2.87897100	-0.00786900
H	-7.20813500	0.40014700	0.00368900
N	3.20531000	0.40557700	0.00257100
C	1.85626400	0.03479200	-0.00050400
O	1.49370700	-1.12799900	-0.00161700
N	0.97117600	1.08451800	-0.00017900
C	1.26072400	2.43719900	0.00073900
O	0.36434900	3.27434900	0.00034700
C	2.68145100	2.74363500	0.00208100
C	3.56715000	1.72849700	0.00285400
H	-0.04250100	0.80790400	-0.00172900
H	2.99270300	3.77778600	0.00252500
H	4.63686800	1.90873100	0.00392700
C	4.22573300	-0.65554400	0.00233500
C	5.08142900	-0.61216100	-1.26592600
C	5.08719200	-0.60791300	1.26652900
H	3.65183300	-1.58564900	0.00522800
C	6.10117800	-1.75459300	-1.26107700
H	5.61702000	0.34614000	-1.31906400
H	4.43081000	-0.66931100	-2.14413100
C	6.10655100	-1.75071200	1.26073000
H	5.62373300	0.35010900	1.31414900
H	4.44071600	-0.66181000	2.14798700
C	6.97016900	-1.71411900	-0.00207800
H	6.72249000	-1.70271400	-2.16013900
H	5.56572100	-2.71210700	-1.29984000

H	6.73169700	-1.69633800	2.15698200
H	5.57100100	-2.70795700	1.30459200
H	7.67777200	-2.54885800	-0.00230000
H	7.56648700	-0.79156100	-0.00475500
C	-6.10067800	-2.26296200	0.00355300
C	-7.61977900	-2.23212200	0.00200200
H	-5.72227500	-2.79004900	0.88407200
H	-5.72048100	-2.79258200	-0.87465000
H	-8.00051100	-3.25491000	0.00254300
H	-8.00904900	-1.72687100	0.88961400
H	-8.00716200	-1.72839500	-0.88730200

9-ethyl– adenine–1-cyclohexyl– uracil RWC

N	1.77117600	0.38896500	-0.00574700
C	2.65392800	1.40538000	-0.00241100
N	3.97644200	1.33296900	-0.00071800
C	4.39141000	0.05691500	-0.00258600
C	3.60358800	-1.08951900	-0.00592500
C	2.20706800	-0.88267700	-0.00759200
N	1.32265300	-1.88738200	-0.01087800
N	5.68542100	-0.39617600	-0.00124000
C	5.60196000	-1.77006900	-0.00409400
N	4.37689600	-2.22883400	-0.00676300
H	2.20023800	2.39483600	-0.00077100
H	1.66693800	-2.83290600	-0.01224800
H	0.32381800	-1.69108300	-0.01228900
H	6.48959800	-2.38689500	-0.00356300
N	-3.17026800	0.55086600	-0.00448900
C	-1.84008300	0.13894600	-0.00649300
O	-1.52851300	-1.04866200	-0.01077100
N	-0.91682600	1.14259100	-0.00338400
C	-1.14803400	2.51788400	0.00409400
O	-0.21787000	3.30358700	0.00609000
C	-2.56272200	2.87094800	0.00961300
C	-3.48443200	1.89076200	0.00557300
H	0.09016300	0.83756400	-0.00547900
H	-2.83835400	3.91560500	0.01695100
H	-4.54704600	2.10873700	0.00998300
C	-4.23260400	-0.46818300	-0.00655500
C	-5.07324200	-0.40365600	1.27070200
C	-5.10246000	-0.36936700	-1.26182200
H	-3.69949200	-1.42198900	-0.02576000
C	-6.14349000	-1.49861400	1.26239900
H	-5.56336300	0.57756200	1.34159700
H	-4.41674500	-0.50073000	2.14131400

C	-6.17141600	-1.46560600	-1.25848100
H	-5.59662800	0.61180600	-1.29473600
H	-4.46672800	-0.44098900	-2.15007500
C	-7.02100100	-1.40418200	0.01259300
H	-6.75344300	-1.43038200	2.16827800
H	-5.65147400	-2.48009900	1.28475900
H	-6.80155600	-1.37421700	-2.14842000
H	-5.67985400	-2.44572700	-1.31744900
H	-7.76580100	-2.20610900	0.01036200
H	-7.57479400	-0.45555900	0.03107000
C	6.85775500	0.47233300	0.00070000
C	8.15820100	-0.31337700	0.01944500
H	6.78520800	1.12722700	0.87385500
H	6.80151600	1.11188900	-0.88499300
H	8.99894500	0.38246300	0.02355500
H	8.23283700	-0.93854500	0.91313100
H	8.25207700	-0.95037700	-0.86403600

9-ethyl– adenine–1-cyclohexyl– uracil H

N	5.23190000	-1.70757400	0.03638500
C	5.93134700	-0.57019100	-0.06276400
N	5.48994100	0.67995200	-0.18194500
C	4.15192000	0.71065000	-0.19708000
C	3.28801300	-0.37347800	-0.10248200
C	3.88922100	-1.64728100	0.01960300
N	3.18055400	-2.77967000	0.11730500
N	3.33973100	1.81645800	-0.31072800
C	2.05329700	1.35620800	-0.27156300
N	1.97943700	0.05367400	-0.15130700
H	7.01225200	-0.69105700	-0.04138100
H	2.16328900	-2.79936300	0.12269000
H	3.69644900	-3.63977200	0.20588100
H	1.19165700	2.00938500	-0.33777200
N	-2.82164800	-0.56140000	-0.01730100
C	-1.50603800	-0.09705400	-0.09904100
O	-1.23001300	1.08532500	-0.22131400
N	-0.54707100	-1.07422300	-0.02990300
C	-0.72772900	-2.43758400	0.12189900
O	0.23408600	-3.19480900	0.17787200
C	-2.12125800	-2.84465300	0.20492200
C	-3.08054100	-1.90086100	0.13566400
H	0.43816700	-0.71854100	-0.08142700
H	-4.13294900	-2.15679300	0.19794600
H	-2.35428000	-3.89245000	0.32506300
C	-3.91900400	0.41880400	-0.05452300
C	-4.86160300	0.17102100	-1.23492000

C	-4.67743600	0.45674100	1.27435500
H	-3.42161600	1.38105200	-0.20090000
C	-5.96290700	1.23430200	-1.26825900
H	-5.32636500	-0.82018200	-1.13805100
H	-4.28626700	0.17008100	-2.16605700
C	-5.78205800	1.51557900	1.23069500
H	-5.12862900	-0.52669600	1.46833100
H	-3.97259800	0.65646800	2.08772800
C	-6.73099900	1.27489100	0.05457000
H	-6.64285400	1.03924300	-2.10301800
H	-5.50741600	2.21626300	-1.45194200
H	-6.33263600	1.51914800	2.17621400
H	-5.32309300	2.50749800	1.12647800
H	-7.50146500	2.05148200	0.02222200
H	-7.24955700	0.31731700	0.19952000
C	3.80336900	3.19418800	-0.39344800
H	4.57351500	3.23528700	-1.16839500
H	2.95560500	3.80152100	-0.72094600
C	4.35982300	3.67776600	0.93972200
H	5.20544000	3.05240200	1.23393800
H	4.70254400	4.71156400	0.85232800
H	3.59381100	3.62720600	1.71746200

9-ethyl– adenine–1-cyclohexyl– uracil RH

N	3.54703200	-3.09871800	0.00052800
C	4.80388900	-2.65741100	-0.14048100
N	5.24878100	-1.40731200	-0.24185300
C	4.23456100	-0.53547600	-0.18259400
C	2.88559200	-0.83243600	-0.03329500
C	2.54925200	-2.20144800	0.05633200
N	1.28601800	-2.63015300	0.19490200
N	4.29943500	0.83720900	-0.26454100
C	3.01498000	1.29226000	-0.15529600
N	2.14116700	0.32536100	-0.01731800
H	5.56358600	-3.43521500	-0.17885600
H	0.48968900	-1.99931200	0.20416100
H	1.13729700	-3.62508200	0.23144500
H	2.75186500	2.34305600	-0.18884900
N	-2.79745500	0.66910900	0.05327800
C	-1.50162100	0.15957100	0.10130800
O	-1.27421700	-1.04253700	0.18628800
N	-0.50882000	1.09277400	0.04627500
C	-0.63286900	2.47333100	-0.07935900
O	0.35851900	3.18227500	-0.13557200
C	-2.01559500	2.93051700	-0.13365300
C	-3.00804100	2.02285000	-0.06999700

H	0.47239500	0.72160000	0.05842900
H	-4.05112500	2.31754200	-0.11243500
H	-2.21339400	3.98821300	-0.22985400
C	-3.93037700	-0.27048200	0.07620100
C	-4.86911300	-0.00374900	1.25556800
C	-4.68463600	-0.26587000	-1.25572300
H	-3.47020900	-1.25219400	0.21291100
C	-6.00290100	-1.03281000	1.27244000
H	-5.30316600	1.00193400	1.16729400
H	-4.29863100	-0.03054500	2.18931000
C	-5.82307200	-1.28860000	-1.22965600
H	-5.10185200	0.73474000	-1.43789700
H	-3.98358200	-0.47844400	-2.06912800
C	-6.76776300	-1.03357700	-0.05301200
H	-6.67917200	-0.82692700	2.10755300
H	-5.57824000	-2.03035400	1.44560200
H	-6.37028200	-1.26150700	-2.17673500
H	-5.39644300	-2.29604200	-1.13786000
H	-7.56189600	-1.78636500	-0.03257800
H	-7.25615100	-0.05876200	-0.18724700
C	5.52541300	1.61293600	-0.39306700
H	6.10064900	1.18171700	-1.21682800
H	5.23724600	2.62952200	-0.67242500
C	6.33850600	1.59223400	0.89505400
H	6.60116400	0.56270000	1.14778500
H	7.25889500	2.16717100	0.76785300
H	5.76659600	2.02572200	1.71910900

1-cyclohexyl-uracil–1-cyclohexyluracil HB1

N	-3.78283500	0.30253300	0.00079900
C	-2.48525900	0.79767000	-0.00023800
O	-1.51503400	0.04818600	-0.00226100
N	-2.37666100	2.16115300	0.00115400
C	-3.41570100	3.10320200	0.00363300
O	-3.18115500	4.29236600	0.00475400
C	-4.74244500	2.49672700	0.00462700
C	-4.86056700	1.15893100	0.00319700
H	-1.41431500	2.52076100	0.00021200
H	-5.60441200	3.14743100	0.00650600
H	-5.82877700	0.67067900	0.00387200
N	3.55994800	0.28891900	-0.00306400
C	2.26390300	-0.23809900	-0.00222700
O	2.03976500	-1.43079800	-0.00098600
N	1.26437500	0.71191100	-0.00294100
C	1.40342400	2.09200000	-0.00356200
O	0.42368900	2.82494600	-0.00372200

C	2.78007700	2.55256800	-0.00385500
C	3.77265700	1.64310600	-0.00344100
H	0.30154500	0.35515600	-0.00247000
H	2.97154000	3.61508000	-0.00423300
H	4.81552400	1.94154200	-0.00342800
C	4.69210900	-0.65201700	-0.00124700
C	5.54401900	-0.51217400	-1.26481000
C	5.53769300	-0.51409200	1.26676400
H	4.22335000	-1.63916900	-0.00317600
C	6.67858500	-1.54053300	-1.25776600
H	5.97561600	0.49734800	-1.31163900
H	4.90766800	-0.63448400	-2.14661900
C	6.67248300	-1.54219100	1.26394200
H	5.96851700	0.49560400	1.31723500
H	4.89686600	-0.63798100	2.14511000
C	7.53307000	-1.41264500	0.00524500
H	7.29497300	-1.42117700	-2.15365100
H	6.24700200	-2.54880100	-1.30102400
H	7.28450800	-1.42389700	2.16295400
H	6.24084200	-2.55057400	1.30383600
H	8.32380400	-2.16893400	0.00666100
H	8.02975700	-0.43304000	0.00706800
C	-3.98486700	-1.15671700	-0.00059400
C	-4.70473500	-1.62478900	1.26617600
C	-4.70830900	-1.62187900	-1.26639800
H	-2.97539300	-1.57429800	-0.00249300
C	-4.85779200	-3.14852900	1.25910400
H	-5.70121000	-1.16473800	1.31857000
H	-4.14590100	-1.28970200	2.14532100
C	-4.86133200	-3.14563600	-1.26238300
H	-5.70494400	-1.16174500	-1.31492200
H	-4.15197300	-1.28476400	-2.14635100
C	-5.58311000	-3.62497900	-0.00117100
H	-5.39195200	-3.47289600	2.15703000
H	-3.86186600	-3.60809700	1.29823300
H	-5.39800800	-3.46795000	-2.15954600
H	-3.86552000	-3.60510800	-1.30536000
H	-5.66500100	-4.71610200	-0.00230700
H	-6.60757400	-3.22890300	0.00071600

1-cyclohexyl-uracil–1-cyclohexyluracil HB2

N	3.91925000	0.29953200	-0.00115900
C	2.56374900	0.63011900	-0.00391500
O	1.68867400	-0.22288900	-0.00578200
N	2.29478900	1.97405300	-0.00444800
C	3.21156300	3.03526700	-0.00234700

O	2.83389300	4.18761600	-0.00324300
C	4.60320800	2.59584200	0.00081000
C	4.88319700	1.28147800	0.00123000
H	1.29804000	2.22524200	-0.00610800
H	5.37955400	3.34701900	0.00269800
H	5.90446900	0.91625800	0.00349400
N	-3.85784600	0.41607500	0.00063000
C	-3.97633500	1.80366700	0.00584900
O	-5.03892600	2.39034800	0.01023300
N	-2.76416100	2.46898600	0.00560700
C	-1.47962500	1.92846300	0.00101000
O	-0.51252100	2.67593200	0.00168800
C	-1.45340700	0.47826100	-0.00419400
C	-2.62303800	-0.18952500	-0.00404200
H	-2.82936400	3.47993800	0.00943800
H	-0.49069700	-0.01783500	-0.00765700
H	-2.65126400	-1.27362700	-0.00768300
C	-5.09204800	-0.38864400	0.00067000
C	-5.20945900	-1.23670900	-1.26810200
C	-5.20438500	-1.24418600	1.26487800
H	-5.89967600	0.34779200	0.00446000
C	-6.52299100	-2.02400500	-1.26218500
H	-4.36856400	-1.94211700	-1.32165600
H	-5.14438100	-0.58703400	-2.14655300
C	-6.51792900	-2.03145900	1.25961300
H	-4.36325200	-1.94984800	1.31087900
H	-5.13576700	-0.59969800	2.14687300
C	-6.64503600	-2.88602700	-0.00356900
H	-6.58893700	-2.64329100	-2.16167700
H	-7.36341600	-1.31868500	-1.29994700
H	-6.58026100	-2.65604100	2.15569400
H	-7.35818800	-1.32638300	1.30490600
H	-7.59789900	-3.42406900	-0.00325100
H	-5.85090300	-3.64501100	-0.00740700
C	4.29876700	-1.12167400	-0.00045100
C	5.07561100	-1.49841200	-1.26471300
C	5.06930800	-1.49886400	1.26752000
H	3.34789700	-1.66007100	-0.00293100
C	5.41364900	-2.99189100	-1.25893900
H	6.00881600	-0.92006400	-1.31306900
H	4.48395800	-1.23217500	-2.14624300
C	5.40743000	-2.99233000	1.26288600
H	6.00222600	-0.92046400	1.32071300
H	4.47325300	-1.23298000	2.14618700
C	6.18693500	-3.37863100	0.00381600
H	5.98668100	-3.24772900	-2.15524200

H	4.48136800	-3.57025200	-1.30238500
H	5.97606400	-3.24845700	2.16190500
H	4.47497600	-3.57075000	1.30155500
H	6.40132600	-4.45182600	0.00416400
H	7.15578000	-2.86087300	0.00630300

1-cyclohexyl-uracil–1-cyclohexyluracil HB3

N	-4.31599200	0.56251100	-0.00031500
C	-3.93430200	1.90112800	-0.00031100
O	-4.71868300	2.82774200	-0.00030700
N	-2.56452900	2.09274600	-0.00036500
C	-1.55618400	1.13106300	-0.00007600
O	-0.38592500	1.48670900	-0.00000100
C	-2.04592200	-0.23365500	0.00004500
C	-3.37642800	-0.44225400	-0.00005900
H	-2.26698000	3.06100300	-0.00034600
H	-1.32244100	-1.04044000	0.00025700
H	-3.78735200	-1.44585500	0.00004500
N	4.26835100	-0.42261500	-0.00006000
C	3.14966400	0.42165000	0.00009000
O	3.24375500	1.63137100	0.00008200
N	1.93734400	-0.23614100	0.00024900
C	1.71228700	-1.60925500	0.00019700
O	0.57915600	-2.06454700	0.00019800
C	2.92911200	-2.40694100	0.00015700
C	4.12346900	-1.78590500	0.00003000
H	1.11048600	0.37572300	0.00023800
H	2.84116500	-3.48335900	0.00019800
H	5.05370000	-2.34418000	-0.00001900
C	5.60482800	0.19281900	-0.00013100
C	6.38860500	-0.16176900	1.26600400
C	6.38877400	-0.16232500	-1.26600400
H	5.40981500	1.26821900	-0.00038100
C	7.75358100	0.53234400	1.26083800
H	6.53972300	-1.24934500	1.31616800
H	5.80467600	0.12560000	2.14600200
C	7.75373700	0.53181900	-1.26095000
H	6.53995200	-1.24991400	-1.31567300
H	5.80496200	0.12463300	-2.14621400
C	8.54713500	0.18185200	0.00006600
H	8.31501500	0.25688600	2.15869600
H	7.60229500	1.61890800	1.30161000
H	8.31528800	0.25599700	-2.15862400
H	7.60244300	1.61836400	-1.30219000
H	9.50934800	0.70320600	0.00001700
H	8.76848400	-0.89425000	0.00030200

C	-5.75544200	0.24802400	-0.00025200
C	-6.16461600	-0.50823400	-1.26649500
C	-6.16472400	-0.50714500	1.26660500
H	-6.24931700	1.22307400	-0.00069400
C	-7.67186100	-0.77888100	-1.26090400
H	-5.62808700	-1.46589900	-1.31627300
H	-5.87288900	0.07299700	-2.14687600
C	-7.67195900	-0.77783600	1.26112800
H	-5.62814100	-1.46473800	1.31724600
H	-5.87309000	0.07486300	2.14650300
C	-8.09271300	-1.53652900	0.00040900
H	-7.95199900	-1.33852900	-2.15828300
H	-8.20781500	0.17832400	-1.30339600
H	-7.95215300	-1.33675000	2.15894700
H	-8.20793500	0.17939300	1.30279300
H	-9.17449800	-1.70161200	0.00043700
H	-7.61955600	-2.52787000	0.00083600

adenine–thymine WC

N	0.94977300	0.37168100	-0.00076200
C	1.55744200	1.57242900	-0.00047100
N	2.85669600	1.82861500	-0.00000800
C	3.57369700	0.69556100	0.00017400
C	3.09033400	-0.60897700	-0.00006400
C	1.68571800	-0.75434800	-0.00056500
N	1.07755500	-1.94475800	-0.00090300
N	4.93779900	0.55305000	0.00072400
C	5.19498000	-0.79824200	0.00070400
N	4.11558100	-1.53153400	0.00028100
H	0.87758900	2.42208100	-0.00061300
H	1.64432800	-2.77656100	-0.00040500
H	0.05947100	-2.00376200	-0.00088400
H	6.20689900	-1.17904200	0.00107400
N	-3.79287300	1.60689100	0.00034800
C	-2.40633100	1.62750100	0.00005800
O	-1.76910800	2.66242700	-0.00032900
N	-1.83776400	0.37550400	-0.00026800
C	-2.49701600	-0.83685000	-0.00009900
O	-1.87484400	-1.89574000	-0.00030900
C	-3.96150800	-0.77238600	0.00034300
C	-4.71530500	-2.06506400	0.00051900
C	-4.53287800	0.44747000	0.00051600
H	-4.23495900	2.51357300	0.00044700
H	-0.78429100	0.35879600	-0.00059100
H	-5.79365600	-1.89265000	0.00073300
H	-4.45183900	-2.66172500	0.87808400

H	-4.45218800	-2.66175100	-0.87713300
H	-5.60945200	0.58251600	0.00078500
H	5.60755400	1.30630800	0.00104700

adenine–uracil WC

N	-0.62590800	-0.28583400	-0.00327200
C	-1.12565300	-1.53532000	-0.00222200
N	-2.39686300	-1.90542600	-0.00021300
C	-3.21121100	-0.84015900	0.00073700
C	-2.84480600	0.50193400	-0.00013200
C	-1.45800800	0.77107400	-0.00219400
N	-0.95922900	2.01102600	-0.00310000
N	-4.58214300	-0.81879600	0.00290500
C	-4.95780900	0.50494400	0.00318400
N	-3.94732500	1.33035500	0.00133800
H	-0.37378000	-2.32223300	-0.00309200
H	-1.59949500	2.78765200	-0.00193400
H	0.04910700	2.16315100	-0.00422500
H	-5.99944500	0.79505200	0.00471700
N	4.21123400	-1.10443700	0.00206100
C	2.82608300	-1.24101700	-0.00069000
O	2.28640700	-2.32874500	-0.00198900
N	2.15116000	-0.04510900	-0.00185000
C	2.69997400	1.22649000	-0.00018000
O	1.98221900	2.21992200	-0.00115600
C	4.15883500	1.26757100	0.00278100
C	4.84543600	0.11030800	0.00380500
H	4.72594300	-1.97218300	0.00300500
H	1.10014600	-0.12084400	-0.00329300
H	4.64847400	2.23009500	0.00419200
H	5.92880000	0.07120300	0.00605500
H	-5.18229600	-1.62871700	0.00413000

cytosine– guanine WC

N	2.17831300	-0.06706900	-0.00254400
C	2.93040500	1.06282000	-0.00850100
O	2.47474800	2.20253900	-0.01531800
N	4.32474800	0.90605300	-0.00691500
C	4.92648300	-0.31105400	0.00061200
C	4.18303900	-1.43830600	0.00643000
C	2.74800700	-1.27119600	0.00401800
N	1.95162500	-2.33633300	0.00842800
H	4.85613600	1.76460800	-0.01157200
H	6.01048300	-0.31600000	0.00152900
H	4.63819200	-2.41887100	0.01256200
H	2.34600400	-3.26164000	0.01270300

H	0.92327300	-2.21953000	0.00409700
N	-3.89684100	-1.62001700	-0.00731700
C	-4.95474000	-0.86372700	-0.00652300
N	-4.65357400	0.48479600	-0.00138800
C	-3.29147100	0.58625400	0.00128400
N	-2.58260400	1.73419100	0.00635500
C	-1.28252700	1.51217000	0.00793300
N	-0.42144100	2.54535400	0.01666400
N	-0.72503000	0.25845300	0.00391900
C	-1.42768600	-0.95261300	-0.00115800
O	-0.81687500	-2.02258700	-0.00385400
C	-2.84166700	-0.73087300	-0.00247500
H	-5.97784000	-1.21257100	-0.00944400
H	-0.82544500	3.46575000	0.00803000
H	0.59110800	2.42510800	0.00154900
H	0.30459800	0.17287300	0.00335100
H	-5.29492400	1.26181300	0.00043400

adenine– adenine hydrogen-bonded structure (global minimum)

N	-3.69854200	-1.94182900	-0.13035500
C	-4.89021600	-1.33905000	-0.06113900
N	-5.16906800	-0.04196100	0.03879100
C	-4.04654400	0.68242300	0.06123500
C	-2.73672900	0.21616000	-0.00527100
C	-2.58484500	-1.18899600	-0.10175400
N	-1.39470800	-1.79607500	-0.17131800
N	-3.92728900	2.04906100	0.15158600
C	-2.58867400	2.33405700	0.13318000
N	-1.83891300	1.26779600	0.03962400
H	-5.74824800	-2.00696500	-0.08913400
H	-0.50267000	-1.30289400	-0.09156700
H	-1.40831900	-2.80228400	-0.22108700
H	-2.22279700	3.34960500	0.19129700
H	-4.69345300	2.70090500	0.21674500
N	1.41585400	-0.82544600	0.06923700
C	2.24278200	-1.87783800	0.18831300
N	3.56727000	-1.90123800	0.20348900
C	4.06967400	-0.66470800	0.07818500
C	3.35393000	0.51972700	-0.05157800
C	1.94495100	0.40582700	-0.05230900
N	1.14424100	1.46891900	-0.17177500
N	5.38451600	-0.27492100	0.05157900
C	5.38762100	1.09372100	-0.08933800
N	4.19125600	1.61087400	-0.15466200
H	1.74782000	-2.84218300	0.28583200
H	1.57122100	2.37801400	-0.24281800

H	0.12849600	1.36606300	-0.11562600
H	6.31178500	1.65266700	-0.13756600
H	6.18214700	-0.88711900	0.12341200

uracil–uracil hydrogen-bonded structure (global minimum)

N	-4.27076500	0.56391700	0.00034200
C	-3.02922600	1.19575800	0.00010100
O	-2.91927900	2.39855700	0.00018600
N	-1.96402200	0.31288400	-0.00028700
C	-2.03030300	-1.07007500	-0.00023600
O	-1.01063600	-1.75518300	-0.00048200
C	-3.37380700	-1.62871900	0.00014400
C	-4.42997600	-0.79434900	0.00044600
H	-5.06189800	1.19080900	0.00080900
H	-1.02603100	0.74160300	-0.00046900
H	-3.48287200	-2.70279200	0.00019100
H	-5.45520200	-1.14615000	0.00074300
N	1.63250100	-0.81449400	-0.00032900
C	1.71010000	0.55525000	-0.00040600
O	0.72489300	1.28261200	-0.00068600
N	2.99124700	1.05098000	-0.00016100
C	4.19701000	0.32339900	0.00028800
O	5.26051700	0.90494300	0.00052200
C	3.99565400	-1.12113800	0.00041200
C	2.74391700	-1.61677400	0.00011300
H	0.68094000	-1.20643500	-0.00043600
H	3.07363500	2.06044800	-0.00024100
H	4.86822900	-1.75744900	0.00075200
H	2.53628400	-2.68059000	0.00018800

uracil–uracil hydrogen-bonded structure (used for comparison with experiment)

N	-4.21258400	0.29802800	-0.01819200
C	-3.06263100	1.08394800	-0.00876700
O	-3.11104600	2.29220500	-0.01330600
N	-1.89520400	0.34652100	0.00724800
C	-1.77954100	-1.03642900	0.01399200
O	-0.68167600	-1.57858100	0.02840700
C	-3.04265300	-1.76289600	0.00320500
C	-4.19616800	-1.07108100	-0.01229600
H	-5.07733300	0.81786900	-0.02923000
H	-1.01532200	0.88144800	0.01609800
H	-3.01255400	-2.84214200	0.00797200
H	-5.16825700	-1.55057000	-0.02093500
N	4.21258700	-0.29802200	-0.01795200
C	3.06264300	-1.08394900	-0.00809500
O	3.11105200	-2.29220100	-0.01359000

N	1.89520700	-0.34652600	0.00752300
C	1.77953700	1.03642200	0.01421000
O	0.68166800	1.57857600	0.02837000
C	3.04264600	1.76289600	0.00354800
C	4.19616400	1.07108800	-0.01205900
H	5.07733700	-0.81785600	-0.02928300
H	1.01532900	-0.88146300	0.01614300
H	3.01254100	2.84214200	0.00825000
H	5.16824900	1.55058200	-0.02086100

adenine–thymine stacked structure

N	-1.41562700	-2.03376500	0.34908300
C	-1.42792800	-2.07195800	-1.02438900
N	-0.28879200	-1.73347500	-1.56654700
C	0.51884300	-1.44843000	-0.48447900
C	1.84002100	-0.96719300	-0.38186500
N	2.58637700	-0.70083400	-1.47775500
N	2.36297200	-0.77524400	0.83697800
C	1.58663900	-1.00006400	1.90553300
N	0.31758900	-1.39920800	1.95070400
C	-0.16166000	-1.61891400	0.72088400
N	-1.64162800	1.23124100	1.26084100
C	-2.20109000	0.86040600	0.05506700
O	-3.29949700	0.34778900	-0.04026800
N	-1.37891500	1.11954300	-1.02199700
C	-0.05163100	1.56274700	-0.99629000
O	0.60177900	1.61322400	-2.02184700
C	0.44437800	1.93606600	0.33186600
C	-0.36472600	1.73395700	1.38867200
H	-1.71291500	0.78422400	-1.91785200
H	-2.19847300	1.02137300	2.07552800
H	-0.05482300	1.95359300	2.40438800
C	1.83662900	2.47654200	0.42730700
H	2.55816100	1.73012300	0.08438900
H	1.94713700	3.36291600	-0.20328400
H	2.08172400	2.73860600	1.45867700
H	-2.32018600	-2.35206700	-1.56698900
H	-2.20608500	-2.17612100	0.95906300
H	2.06070600	-0.81860300	2.86791500
H	3.43871500	-0.18616000	-1.31444000
H	2.07710800	-0.48275200	-2.32347700

adenine–uracil stacked structure

N	-0.50006000	-2.20147100	-0.34880100
C	-0.46855800	-1.80845900	-1.66555200
N	0.47555200	-0.94543900	-1.92991700

C	1.09940600	-0.75627200	-0.71350900
C	2.13919400	0.10219500	-0.29779100
N	2.74766700	0.94974800	-1.15697400
N	2.53128500	0.06554700	0.98317900
C	1.88025400	-0.74743900	1.82505600
N	0.84803000	-1.55284700	1.58383700
C	0.50784000	-1.52311100	0.28940000
N	-1.96669000	0.28854400	1.42188200
C	-2.33330400	0.15610000	0.09361700
O	-3.17192500	-0.63779900	-0.28323500
N	-1.64233100	1.00302100	-0.74683100
C	-0.55126300	1.82744300	-0.42963500
O	0.05234300	2.40992200	-1.30936000
C	-0.24735900	1.87372400	0.99669900
C	-0.94075900	1.09781600	1.84830600
H	-2.42795700	-0.34431100	2.05805700
H	-1.82334700	0.87770700	-1.73578400
H	3.31419600	1.66634000	-0.72823800
H	2.20672000	1.22603000	-1.96540800
H	2.23762800	-0.73086600	2.85273600
H	-1.18500000	-2.80358000	0.08181800
H	-1.18179700	-2.19515600	-2.38031000
H	-0.72940500	1.05694300	2.91008900
H	0.57874000	2.48819800	1.32362600

cytosine–guanine stacked structure

N	1.62599400	-0.85306500	-1.99548000
C	2.75319500	-0.56393700	-1.25951100
N	2.56786700	-0.69958400	0.02478200
C	1.25666400	-1.10849500	0.14015900
C	0.45579400	-1.35567800	1.31316200
O	0.75948500	-1.29247000	2.49015500
N	-0.86019500	-1.69991800	0.93096000
C	-1.37291000	-1.66707800	-0.33604700
N	-2.72211900	-1.91558800	-0.43842800
N	-0.64947900	-1.44525800	-1.40521700
C	0.64730400	-1.18945700	-1.10268700
N	-1.30169600	1.97395500	-1.05981000
C	-1.68673200	1.36735900	0.15346400
O	-2.82107000	0.91081500	0.23619900
N	-0.74936100	1.30879600	1.13896900
C	0.48452600	1.71834700	0.90875200
N	1.39205700	1.56566000	1.90072000
C	0.90459700	2.31266700	-0.33689000
C	-0.04067500	2.41275000	-1.29837200
H	-2.01165500	1.98527300	-1.77743800

H	0.14916000	2.83591500	-2.27857000
H	1.91957800	2.65075200	-0.49193200
H	1.11540700	0.89608800	2.61260900
H	2.35797100	1.48106000	1.61542000
H	-1.49813700	-1.82505100	1.70788700
H	-3.01620600	-1.79842700	-1.40022400
H	-3.25135700	-1.28766900	0.16402300
H	3.67786800	-0.26557700	-1.73306900
H	1.51799600	-0.82297800	-2.99719300

Cartesian Coordinates of Liquid-Phase Geometries

1) Water

1.1) SM8

1.1.1) SM8/M06-2X/6-31G**

adenine–thymine WC

N	0.98012100	0.35795500	-0.00013800
C	1.58088500	1.55774400	-0.00008500
N	2.87731600	1.82721400	0.00000900
C	3.60951400	0.69644700	0.00004100
C	3.13189400	-0.60990300	0.00000000
C	1.72859100	-0.76616100	-0.00009300
N	1.12189400	-1.95098600	-0.00013200
N	4.96581400	0.56835100	0.00016700
C	5.24007200	-0.77314600	0.00008100
N	4.16329700	-1.52421900	0.00007200
H	0.89973200	2.40456100	-0.00011100
H	1.67550600	-2.79950000	-0.00010100
H	0.10631600	-2.00767800	-0.00020400
H	6.25705700	-1.14451500	0.00013200
N	-3.82815000	1.60242200	0.00008200
C	-2.46324900	1.62629600	0.00001400
O	-1.80562300	2.66865500	-0.00010400
N	-1.88200200	0.38109000	-0.00008500
C	-2.54000800	-0.83647800	-0.00004900
O	-1.89373500	-1.89339400	-0.00012700
C	-3.99128800	-0.77987200	0.00007900
C	-4.75683600	-2.06520300	0.00012900
C	-4.56500800	0.44212200	0.00012900
H	-4.29904000	2.50530000	0.00010500
H	-0.84310700	0.36471400	-0.00016600
H	-5.83258700	-1.87491400	0.00021000
H	-4.50885900	-2.66542400	0.87844400
H	-4.50899000	-2.66541500	-0.87822800
H	-5.64261400	0.57830700	0.00020200
H	5.65600700	1.31861900	0.00025500

adenine–uracil WC

N	-0.65444400	-0.27592500	-0.00132800
C	-1.15068400	-1.52262200	-0.00101300
N	-2.41931800	-1.90183600	-0.00027400
C	-3.24528400	-0.83760300	0.00025000
C	-2.88102800	0.50481600	0.00003300

C	-1.49596300	0.78033400	-0.00080400
N	-0.99142200	2.01192200	-0.00111500
N	-4.60760200	-0.82605800	0.00088300
C	-4.99543700	0.48704400	0.00171300
N	-3.98691500	1.32745900	0.00061000
H	-0.39988600	-2.30836700	-0.00147200
H	-1.61375700	2.81130000	-0.00072100
H	0.01589300	2.15419200	-0.00169400
H	-6.04034700	0.77027300	0.00246000
N	4.24135400	-1.10813200	0.00099500
C	2.87905800	-1.23886600	-0.00038500
O	2.31098700	-2.33150600	-0.00057100
N	2.19736000	-0.04644000	-0.00083400
C	2.75120900	1.22587700	-0.00019000
O	2.01434300	2.22163900	-0.00071500
C	4.19472100	1.26617300	0.00105000
C	4.88012100	0.10476700	0.00164000
H	4.78109200	-1.97176300	0.00157000
H	1.16121500	-0.11987300	-0.00153000
H	4.68658900	2.22728600	0.00157300
H	5.96467600	0.06184100	0.00267900
H	-5.23148100	-1.63240700	0.00107600

cytosine–guanine WC

N	-2.20294300	-0.07631900	0.00107300
C	-2.94366600	1.05910600	0.00189400
O	-2.44674600	2.20071200	0.00376100
N	-4.31943400	0.94062300	0.00063000
C	-4.95651600	-0.26265400	-0.00143900
C	-4.23967200	-1.40713100	-0.00226900
C	-2.81309000	-1.27520900	-0.00089900
N	-2.04543100	-2.35985800	-0.00153700
H	-4.85411300	1.80648400	0.00123500
H	-6.04114700	-0.23527200	-0.00231700
H	-4.71677200	-2.37866000	-0.00387500
H	-2.47698200	-3.27933400	-0.00300300
H	-1.03444200	-2.28567100	-0.00028100
N	3.92801600	-1.61720600	0.00157100
C	4.98474600	-0.84314200	-0.00014500
N	4.67280900	0.49402500	-0.00100000
C	3.31640700	0.58931200	-0.00078900
N	2.59493200	1.72639600	-0.00175700
C	1.29021000	1.50035800	-0.00121300
N	0.42963400	2.51718500	-0.00260300
N	0.74293600	0.23547500	0.00029200
C	1.46246600	-0.95551100	0.00129500

O	0.87266300	-2.04803900	0.00255000
C	2.86903800	-0.72777800	0.00074300
H	6.01110200	-1.18794900	-0.00021600
H	0.81674200	3.45377600	-0.00162500
H	-0.58299500	2.38979100	0.00126400
H	-0.29073300	0.14217300	0.00051600
H	5.33884400	1.26692500	-0.00193100

adenine–thymine stacked structure

N	-0.72949000	-2.31215500	0.28051700
C	-0.63770700	-2.39094100	-1.08197400
N	0.40791500	-1.76790300	-1.57431300
C	1.01782900	-1.22982200	-0.45914200
C	2.16783900	-0.42757500	-0.29392300
N	2.92755500	-0.04254600	-1.32677400
N	2.52451200	-0.06768700	0.95153200
C	1.74952900	-0.45439900	1.97413800
N	0.64958000	-1.20006400	1.95872000
C	0.32538200	-1.55419200	0.70554300
N	-1.97880300	0.75190100	1.26590300
C	-2.44375800	0.21692300	0.09659900
O	-3.39238300	-0.56078100	0.03330100
N	-1.75701700	0.65579600	-1.01702100
C	-0.62087700	1.46157200	-1.04494000
O	-0.07539200	1.72289900	-2.11691400
C	-0.18287000	1.95653800	0.25147000
C	-0.87545300	1.56812900	1.34229400
H	-2.04192500	0.23563100	-1.89791900
H	-2.44522100	0.44528500	2.11691400
H	-0.60145100	1.88362000	2.34413200
C	1.01155900	2.85577600	0.29702400
H	1.85411200	2.39959200	-0.22654600
H	0.80136800	3.81090100	-0.19203100
H	1.31357200	3.04743900	1.32905200
H	-1.37155700	-2.93235900	-1.66465300
H	-1.49432900	-2.67502700	0.84536700
H	2.08092200	-0.11791000	2.95376500
H	3.68310000	0.61255000	-1.15955100
H	2.58500700	-0.14010500	-2.27211100

adenine–uracil stacked structure

N	0.30381300	2.20508300	0.09371700
C	0.17168300	2.15516000	-1.26682400
N	-0.77069700	1.33537600	-1.67233100
C	-1.26504100	0.80511700	-0.49797700
C	-2.26421500	-0.15558900	-0.23168900

N	-2.97855900	-0.73420600	-1.20638300
N	-2.52918200	-0.46649700	1.04959300
C	-1.81187000	0.13082800	2.01230200
N	-0.84910000	1.03913600	1.90073600
C	-0.60947800	1.33121300	0.61281800
N	2.17578000	-0.45327900	1.25063500
C	2.43993000	-0.01130400	-0.02006000
O	3.24886100	0.87659400	-0.27124800
N	1.72737400	-0.67762700	-0.99541200
C	0.71732900	-1.62495700	-0.81063400
O	0.11153100	-2.07408400	-1.78256900
C	0.50590800	-1.99958600	0.57114100
C	1.22592400	-1.39811300	1.53877100
H	2.67872400	0.01405300	2.00255700
H	1.85949900	-0.33064500	-1.94164400
H	-3.57099800	-1.51996200	-0.96231900
H	-2.64250400	-0.68749400	-2.15873100
H	-2.06569200	-0.17023900	3.02579600
H	0.99786200	2.74751800	0.60423600
H	0.79880000	2.75353200	-1.91485000
H	1.09655300	-1.62482500	2.59166900
H	-0.25241200	-2.73452900	0.79286000

cytosine–guanine stacked structure

N	0.67022800	-1.34822300	-2.09230300
C	1.67427300	-2.00054200	-1.42277000
N	1.39937200	-2.20346100	-0.15606700
C	0.15233800	-1.63718500	0.00370800
C	-0.66352900	-1.50731500	1.16665800
O	-0.43333200	-1.87917100	2.32279400
N	-1.87757200	-0.88483000	0.85819800
C	-2.23082200	-0.35100200	-0.35834700
N	-3.45444200	0.20749100	-0.43849300
N	-1.47126300	-0.44339200	-1.42707600
C	-0.31004800	-1.09296500	-1.18824000
N	0.45632700	2.33819500	-0.93223800
C	-0.23776400	2.15846200	0.25774100
O	-1.37269500	2.64580400	0.36406700
N	0.38377500	1.47240100	1.25522600
C	1.57795100	0.92238600	1.02689600
N	2.13796700	0.21692200	2.02465500
C	2.29663800	1.07697000	-0.20161300
C	1.68055800	1.79693600	-1.16721200
H	-0.03272400	2.83733300	-1.67242500
H	2.11433000	1.98195900	-2.14606800
H	3.26731300	0.62274000	-0.35541600

H	1.54227000	-0.08285700	2.78049200
H	2.90706700	-0.40538700	1.79680700
H	-2.51245900	-0.76090100	1.64583800
H	-3.61545700	0.74606400	-1.28288300
H	-3.82969700	0.64725700	0.39620100
H	2.58068700	-2.31646700	-1.92421900
H	0.67858200	-1.08300600	-3.07744800

1.1.2) SM8/M06-2X/6-31+G**

adenine–thymine WC

N	-0.94612200	0.32872000	0.00764100
C	-1.53188700	1.54093100	0.03067900
N	-2.82470900	1.81799400	0.03713600
C	-3.56997800	0.69767300	0.01576000
C	-3.10757700	-0.61497800	-0.00860300
C	-1.70777100	-0.78405400	-0.00997200
N	-1.10894400	-1.98119500	-0.02674900
N	-4.93093800	0.58464800	0.01419600
C	-5.21944200	-0.75657300	-0.01072600
N	-4.14849700	-1.51711700	-0.02509500
H	-0.84183200	2.37857300	0.04321300
H	-1.67164400	-2.82600600	-0.04134600
H	-0.09402700	-2.05121900	-0.01685300
H	-6.24581300	-1.11851500	-0.01725300
N	3.76265900	1.62954600	-0.01819000
C	2.39241000	1.61528900	-0.01940400
O	1.70941800	2.63923100	-0.03286100
N	1.84038300	0.35706600	-0.00699900
C	2.53148600	-0.84151200	0.00446900
O	1.90099800	-1.90958400	0.00803600
C	3.98460300	-0.75134400	0.01173900
C	4.78131000	-2.02075800	0.02998200
C	4.53006700	0.48662100	-0.00159500
H	4.21117900	2.54895500	-0.02830500
H	0.79303100	0.32086100	-0.00133000
H	5.85545900	-1.79898300	0.03162200
H	4.55599600	-2.63740000	-0.84483000
H	4.54908500	-2.61646100	0.91741500
H	5.61194500	0.64934900	-0.00008200
H	-5.61284600	1.34827500	0.02879400

adenine–uracil WC

N	0.62510200	-0.24573600	0.00085100
C	1.10360200	-1.50419900	-0.01235600
N	2.36742000	-1.89358000	-0.01839300

C	3.20761300	-0.84254800	-0.00840300
C	2.86134900	0.50527900	0.00484500
C	1.48115400	0.79628500	0.00704700
N	0.99176200	2.04153600	0.01363000
N	4.57354100	-0.84826000	-0.00825000
C	4.97734300	0.46290800	0.00172400
N	3.97678800	1.31366300	0.01200700
H	0.34368700	-2.27938800	-0.01688400
H	1.62702000	2.83294900	0.01825300
H	-0.01252800	2.20239600	0.00982600
H	6.03114600	0.73412600	0.00378600
N	-4.19564600	-1.13355000	0.00683000
C	-2.82412000	-1.23639800	0.01135100
O	-2.23744900	-2.31644700	0.02466500
N	-2.16267600	-0.03230200	-0.00112500
C	-2.74278600	1.22645200	-0.00709300
O	-2.01590700	2.23174400	-0.00321700
C	-4.18929000	1.24507000	-0.01849500
C	-4.85741800	0.06924900	-0.00886900
H	-4.72021800	-2.01189600	0.01576300
H	-1.11682300	-0.08796900	0.00027100
H	-4.70257200	2.19986100	-0.03046400
H	-5.94891300	0.01015800	-0.01309200
H	5.18732100	-1.66759600	-0.01639300

cytosine–guanine WC

N	2.18541300	-0.10221900	-0.00800400
C	2.89906300	1.04848800	-0.00870700
O	2.36857300	2.17671000	-0.01233700
N	4.28012600	0.97033500	-0.00544600
C	4.94830200	-0.21970900	0.00392700
C	4.25650600	-1.38464600	0.00816100
C	2.82460500	-1.28427800	0.00183800
N	2.07312500	-2.38570800	0.00449200
H	4.79351900	1.85278700	-0.00623900
H	6.03943300	-0.16855100	0.00730900
H	4.76209600	-2.34931600	0.01535200
H	2.51886500	-3.30107700	0.01647700
H	1.05936500	-2.32274100	0.00059000
N	-3.89524800	-1.64088700	-0.00352000
C	-4.96227800	-0.88250700	-0.00346400
N	-4.66829300	0.46383500	-0.00044000
C	-3.31106400	0.57516300	0.00201800
N	-2.60138800	1.71861800	0.00456900
C	-1.29503800	1.51661100	0.00667600
N	-0.44830000	2.55061000	0.01144900

N	-0.73267500	0.25868600	0.00763800
C	-1.44120200	-0.94145800	-0.00074300
O	-0.82240900	-2.02149000	-0.00802000
C	-2.84768900	-0.73823500	0.00011700
H	-5.99009600	-1.24053900	-0.00555400
H	-0.85090100	3.48471700	-0.00324600
H	0.56809900	2.43424100	0.00024200
H	0.29912500	0.16545900	0.00297400
H	-5.34537200	1.23379200	0.00084000

adenine–thymine stacked structure

N	-0.60769300	-2.34240400	0.41503000
C	-0.50562000	-2.51540600	-0.94043300
N	0.50367200	-1.86700800	-1.47520000
C	1.08493200	-1.22217000	-0.40247800
C	2.20122900	-0.36306000	-0.29323000
N	2.95200100	-0.02317200	-1.35192600
N	2.53640300	0.09884400	0.92206000
C	1.77870200	-0.24825400	1.97286400
N	0.71437100	-1.04337000	2.00699900
C	0.40846900	-1.50323800	0.78427400
N	-2.08052200	0.71064400	1.19709300
C	-2.45758300	0.09973600	0.02967000
O	-3.35239100	-0.73777400	-0.04178600
N	-1.75554600	0.53877600	-1.07533100
C	-0.67103600	1.41700800	-1.08677800
O	-0.10836000	1.67685700	-2.15084700
C	-0.31402600	1.98570800	0.20615400
C	-1.02945900	1.59599700	1.28559000
H	-1.96184600	0.05229400	-1.94339300
H	-2.56213600	0.40303000	2.04333100
H	-0.81922100	1.97059400	2.28916000
C	0.82462600	2.95970500	0.26343100
H	1.72366200	2.52608800	-0.17953900
H	0.58805400	3.87294200	-0.29027600
H	1.04977600	3.22700100	1.30172600
H	-1.20729800	-3.14132300	-1.48333500
H	-1.33824100	-2.72699400	1.01411400
H	2.09143200	0.17184200	2.92679000
H	3.70868300	0.64201300	-1.23352800
H	2.65293800	-0.25248900	-2.28944800

adenine–uracil stacked structure

N	0.28506200	2.21108300	0.18529900
C	0.13660000	2.22924100	-1.17698000
N	-0.79729000	1.41443200	-1.61136200

C	-1.27602500	0.82126700	-0.46126900
C	-2.26824700	-0.15621100	-0.23002600
N	-2.98847500	-0.69449200	-1.22800000
N	-2.51859600	-0.53009800	1.03476400
C	-1.79735400	0.02231100	2.02198700
N	-0.84251600	0.94231600	1.94148500
C	-0.61661300	1.30149900	0.66859900
N	2.19672200	-0.48659000	1.22223100
C	2.43921300	0.00687900	-0.03832400
O	3.23463200	0.91192000	-0.26654200
N	1.72516000	-0.63044000	-1.03422500
C	0.73000800	-1.59890800	-0.86972800
O	0.12491600	-2.02507100	-1.85398600
C	0.53464800	-2.02772000	0.49911100
C	1.25793800	-1.45355400	1.48557300
H	2.69656800	-0.03359500	1.98959500
H	1.83297500	-0.23547300	-1.96446200
H	-3.58934600	-1.48565400	-1.02166700
H	-2.68402400	-0.57476200	-2.18460300
H	-2.03879100	-0.32938100	3.02290900
H	0.96730900	2.74778000	0.72189200
H	0.74878400	2.87271800	-1.80191800
H	1.14086400	-1.72559300	2.53571300
H	-0.21221100	-2.78313600	0.70177000

cytosine–guanine stacked structure

N	2.18541300	-0.10221900	-0.00800400
C	2.89906300	1.04848800	-0.00870700
O	2.36857300	2.17671000	-0.01233700
N	4.28012600	0.97033500	-0.00544600
C	4.94830200	-0.21970900	0.00392700
C	4.25650600	-1.38464600	0.00816100
C	2.82460500	-1.28427800	0.00183800
N	2.07312500	-2.38570800	0.00449200
H	4.79351900	1.85278700	-0.00623900
H	6.03943300	-0.16855100	0.00730900
H	4.76209600	-2.34931600	0.01535200
H	2.51886500	-3.30107700	0.01647700
H	1.05936500	-2.32274100	0.00059000
N	-3.89524800	-1.64088700	-0.00352000
C	-4.96227800	-0.88250700	-0.00346400
N	-4.66829300	0.46383500	-0.00044000
C	-3.31106400	0.57516300	0.00201800
N	-2.60138800	1.71861800	0.00456900
C	-1.29503800	1.51661100	0.00667600
N	-0.44830000	2.55061000	0.01144900

N	-0.73267500	0.25868600	0.00763800
C	-1.44120200	-0.94145800	-0.00074300
O	-0.82240900	-2.02149000	-0.00802000
C	-2.84768900	-0.73823500	0.00011700
H	-5.99009600	-1.24053900	-0.00555400
H	-0.85090100	3.48471700	-0.00324600
H	0.56809900	2.43424100	0.00024200
H	0.29912500	0.16545900	0.00297400
H	-5.34537200	1.23379200	0.00084000

1.2) SM8AD

1.2.1) SM8AD/M06-2X/6-31G**

adenine–thymine WC

N	0.96431500	0.33441500	-0.00005800
C	1.55563400	1.54068600	-0.00001400
N	2.84825900	1.82310700	0.00002200
C	3.59008100	0.69851100	0.00003300
C	3.12591900	-0.61244700	-0.00000800
C	1.72497200	-0.78180100	-0.00005700
N	1.13063000	-1.97447100	-0.00009300
N	4.94830200	0.58460100	0.00000300
C	5.23425000	-0.75529100	0.00014000
N	4.16608900	-1.51722700	0.00000200
H	0.86647000	2.38097500	-0.00002400
H	1.69545700	-2.81646800	-0.00009300
H	0.11823900	-2.04330500	-0.00012900
H	6.25525400	-1.11629700	0.00018400
N	-3.79319500	1.61699300	0.00002800
C	-2.43083600	1.61842500	0.00008900
O	-1.75505800	2.65352500	-0.00009600
N	-1.86689800	0.36721600	-0.00001200
C	-2.54499000	-0.83785100	-0.00001100
O	-1.91138900	-1.90673600	-0.00005700
C	-3.99291400	-0.76186600	0.00004800
C	-4.77825100	-2.03531000	0.00006100
C	-4.54887800	0.46911300	0.00004100
H	-4.25130600	2.52993300	-0.00002000
H	-0.82297900	0.33536700	-0.00006800
H	-5.85101300	-1.82713300	0.00008200
H	-4.53877900	-2.63873100	0.87871800
H	-4.53881400	-2.63872800	-0.87860800
H	-5.62506300	0.62234900	0.00003300
H	5.63168300	1.34228900	-0.00002700

adenine-uracil WC

N	-0.64133200	-0.25660000	-0.00043800
C	-1.12962200	-1.50815300	-0.00029200
N	-2.39381000	-1.89849200	-0.00003000
C	-3.22753700	-0.84016700	0.00011400
C	-2.87510200	0.50505200	-0.00000400
C	-1.49315500	0.79178400	-0.00030700
N	-1.00159400	2.03011400	-0.00044700
N	-4.59061700	-0.84072900	0.00034200
C	-4.98795800	0.47042700	0.00051000
N	-3.98752300	1.31928900	0.00018600
H	-0.37229800	-2.28773300	-0.00041000
H	-1.63569400	2.82123400	-0.00043800
H	0.00156300	2.18455300	-0.00078600
H	-6.03575000	0.74420700	0.00073700
N	4.21697100	-1.12182500	0.00028100
C	2.85582400	-1.23583600	0.00001300
O	2.27454600	-2.32559500	-0.00035600
N	2.18543100	-0.03914600	-0.00021500
C	2.75492600	1.22524700	0.00000600
O	2.02617600	2.23079200	-0.00015300
C	4.19674600	1.25195600	0.00040000
C	4.87046300	0.08303200	0.00050300
H	4.74780900	-1.99452300	0.00032400
H	1.14355000	-0.10124000	-0.00052600
H	4.69760200	2.20902400	0.00056300
H	5.95534600	0.02760400	0.00074800
H	-5.20809900	-1.65304000	0.00045100

cytosine-guanine WC

N	-2.19952600	-0.07596500	0.00102600
C	-2.94160500	1.05615700	0.00193000
O	-2.44321100	2.20237300	0.00383400
N	-4.31510600	0.94142000	0.00074100
C	-4.95541000	-0.26050800	-0.00137800
C	-4.23923600	-1.40531900	-0.00230700
C	-2.81319000	-1.27471700	-0.00096300
N	-2.04844800	-2.36146200	-0.00165400
H	-4.84838300	1.81047100	0.00142300
H	-6.04057300	-0.23070400	-0.00220900
H	-4.71722900	-2.37701500	-0.00395000
H	-2.48736100	-3.27938700	-0.00312400
H	-1.03875800	-2.29009200	-0.00034800
N	3.92296100	-1.62022200	0.00142900
C	4.97927100	-0.84690700	0.00024500
N	4.67143600	0.49246500	-0.00113300

C	3.31559900	0.58918000	-0.00082200
N	2.59567100	1.72605600	-0.00183600
C	1.29232000	1.50126200	-0.00123900
N	0.43195800	2.51955800	-0.00267400
N	0.74158900	0.23576400	0.00030700
C	1.46338900	-0.95159700	0.00133600
O	0.87142600	-2.04933200	0.00258500
C	2.86623100	-0.72818000	0.00075600
H	6.00568500	-1.19269100	0.00031200
H	0.82386800	3.45566600	-0.00173100
H	-0.57892800	2.39313000	0.00112500
H	-0.29155000	0.14179200	0.00054500
H	5.33955700	1.26499300	-0.00219700

adenine–thymine stacked structure

N	-0.78261500	-2.27700000	0.25968800
C	-0.68914500	-2.34557800	-1.10335000
N	0.37534600	-1.75080800	-1.58942300
C	0.99375200	-1.23200100	-0.46854000
C	2.16379600	-0.46203400	-0.29326700
N	2.94815600	-0.10385600	-1.32078200
N	2.52486000	-0.11795000	0.95481200
C	1.73088600	-0.48502700	1.97026400
N	0.61421000	-1.20568600	1.94834900
C	0.28727000	-1.54277200	0.69177200
N	-1.94002400	0.75192500	1.27872300
C	-2.42956400	0.24609000	0.11040400
O	-3.40163300	-0.50886300	0.04615600
N	-1.74657300	0.68061400	-1.00509600
C	-0.60583400	1.47211700	-1.03464700
O	-0.07306900	1.74982700	-2.11566200
C	-0.14042800	1.94064000	0.25611900
C	-0.82320100	1.54854500	1.35299900
H	-2.06808800	0.29578500	-1.89271100
H	-2.39677100	0.43481500	2.13483800
H	-0.52913600	1.84403400	2.35606700
C	1.06791600	2.82080400	0.29956600
H	1.89614100	2.36014300	-0.24267600
H	0.86576500	3.78680000	-0.17133000
H	1.38558300	2.98997200	1.33115300
H	-1.43657200	-2.86305600	-1.69143300
H	-1.57308800	-2.60172800	0.81570800
H	2.06468200	-0.15879600	2.95308100
H	3.70584200	0.54689100	-1.14234900
H	2.59705400	-0.16796200	-2.26610800

adenine–uracil stacked structure

N	0.34702800	2.18989300	-0.01591900
C	0.22391200	2.06563700	-1.37270000
N	-0.73392100	1.24724100	-1.74175000
C	-1.24265200	0.78596500	-0.54353700
C	-2.26180600	-0.13918700	-0.23224500
N	-2.99618600	-0.74335300	-1.17912800
N	-2.53634200	-0.38105300	1.06167600
C	-1.80792200	0.24946300	1.99424200
N	-0.83167400	1.13760400	1.84261700
C	-0.58129300	1.35555500	0.54247300
N	2.12549400	-0.39207900	1.28655200
C	2.41302300	-0.02252800	0.00122500
O	3.23685500	0.84662900	-0.28529900
N	1.71314800	-0.73219300	-0.94921700
C	0.71242400	-1.67688400	-0.73079100
O	0.13422700	-2.19457800	-1.69168700
C	0.47039400	-1.97427100	0.66105400
C	1.16984600	-1.31930500	1.60986300
H	2.61538000	0.11765900	2.02347900
H	1.87790000	-0.44850200	-1.91402800
H	-3.59591800	-1.50974100	-0.89320300
H	-2.65200200	-0.76015900	-2.12979500
H	-2.06870400	0.00292800	3.02115100
H	1.06924900	2.72380000	0.46713100
H	0.86881600	2.61506200	-2.04677900
H	1.01833300	-1.48623900	2.67172100
H	-0.29008700	-2.70030800	0.90488200

cytosine–guanine stacked structure

N	1.60960800	-1.25349200	-1.79248600
C	2.72370100	-1.00416400	-1.03090800
N	2.47450800	-0.97229500	0.25510900
C	1.11294200	-1.19172800	0.32988400
C	0.23671600	-1.21645900	1.45747100
O	0.50908600	-1.07437300	2.65712900
N	-1.08134700	-1.47559400	1.06145700
C	-1.53398900	-1.57852500	-0.23341000
N	-2.85822500	-1.81294500	-0.39077800
N	-0.73343700	-1.55768000	-1.27425500
C	0.55853100	-1.35551200	-0.93433500
N	-1.16078100	1.81236100	-1.27109900
C	-1.52721400	1.58681300	0.05234100
O	-2.72156600	1.33813500	0.30241800
N	-0.56558200	1.68169300	1.00391100
C	0.70491500	1.85978900	0.63478600

N	1.63202800	1.89665700	1.60576300
C	1.11044000	2.05503000	-0.72678500
C	0.12778400	2.01372100	-1.65500300
H	-1.89732500	1.71759900	-1.96944200
H	0.30359100	2.14076400	-2.72072400
H	2.14937600	2.20327300	-0.99758400
H	1.37887700	1.51081200	2.50368100
H	2.60510400	1.78484300	1.33722000
H	-1.76863200	-1.46577300	1.81459900
H	-3.16739100	-1.73354900	-1.35573400
H	-3.47760900	-1.33558400	0.25825500
H	3.70014800	-0.87508500	-1.48309300
H	1.57334500	-1.30211600	-2.81114300

1.2.2) SM8AD/M06-2X/6-31+G**

adenine–thymine WC

N	-0.93828200	0.31354400	0.00025900
C	-1.51838000	1.52959300	0.00208400
N	-2.80900700	1.81550400	0.00260200
C	-3.55981100	0.69811400	0.00111300
C	-3.10553400	-0.61743400	-0.00075800
C	-1.70722100	-0.79486700	-0.00102800
N	-1.11430100	-1.99574700	-0.00210600
N	-4.92163800	0.59441100	0.00099500
C	-5.21718800	-0.74602300	-0.00065200
N	-4.15213800	-1.51408700	-0.00172700
H	-0.82427400	2.36334900	0.00317200
H	-1.68153400	-2.83800400	-0.00228700
H	-0.10174300	-2.06916500	-0.00112900
H	-6.24612000	-1.10123900	-0.00101500
N	3.73727600	1.64161000	-0.00127300
C	2.36904200	1.60714700	-0.00172700
O	1.67041900	2.62468400	-0.00205400
N	1.83166500	0.34428200	-0.00021000
C	2.53934200	-0.84295500	0.00080500
O	1.92077300	-1.92181300	0.00091800
C	3.99038100	-0.73569100	0.00070600
C	4.80373100	-1.99524700	0.00190800
C	4.52099600	0.50976100	-0.00013100
H	4.17429500	2.56964100	-0.00186300
H	0.78000100	0.29785500	-0.00006000
H	5.87529400	-1.75786400	0.00183600
H	4.58258900	-2.60488000	-0.87930500
H	4.58235300	-2.60329800	0.88415600
H	5.60231600	0.68714600	-0.00012100

H	-5.59989800	1.36248500	0.00200700

adenine–uracil WC

N	0.62106500	-0.24238000	0.00629400
C	1.09973900	-1.50144300	0.00794900
N	2.36241400	-1.89381800	0.00547100
C	3.20267800	-0.84221200	0.00088700
C	2.85835100	0.50602100	-0.00114100
C	1.47890300	0.79878400	0.00170400
N	0.98951400	2.04479700	0.00043700
N	4.56886700	-0.85077300	-0.00275200
C	4.97339700	0.46081700	-0.00658400
N	3.97514900	1.31365800	-0.00595900
H	0.33986700	-2.27639700	0.01156200
H	1.62588900	2.83582800	-0.00225300
H	-0.01364000	2.20309200	0.00322800
H	6.02794600	0.73017400	-0.00980100
N	-4.18785100	-1.13737400	-0.00552100
C	-2.81737800	-1.23405900	-0.00216800
O	-2.22494100	-2.31449500	-0.00219900
N	-2.15868600	-0.02996900	0.00216200
C	-2.74333400	1.22506700	0.00269800
O	-2.01697400	2.23441000	0.00605800
C	-4.18903800	1.24109300	-0.00126700
C	-4.85445300	0.06275400	-0.00518500
H	-4.71048400	-2.02040200	-0.00828100
H	-1.10976000	-0.08582000	0.00445000
H	-4.70540600	2.19569400	-0.00109500
H	-5.94752300	0.00024500	-0.00835300
H	5.18195000	-1.67164900	-0.00261900

cytosine–guanine WC

N	-2.18401500	-0.10323300	0.00587800
C	-2.89678400	1.04568700	0.00758600
O	-2.36259500	2.17707900	0.01371400
N	-4.27654400	0.97350300	0.00356500
C	-4.94903500	-0.21455300	-0.00513900
C	-4.25976300	-1.38102700	-0.00833500
C	-2.82788000	-1.28424200	-0.00216600
N	-2.08045000	-2.38822200	-0.00274100
H	-4.78744900	1.85964100	0.00478600
H	-6.04116500	-0.16010900	-0.00875200
H	-4.76852900	-2.34540100	-0.01482700
H	-2.53319700	-3.30196900	-0.01114200
H	-1.06770500	-2.32806600	0.00014000
N	3.89398600	-1.64371800	0.00321200

C	4.96005800	-0.88481300	0.00283100
N	4.66851400	0.46322500	-0.00052600
C	3.31179700	0.57481200	-0.00211400
N	2.60282300	1.71817000	-0.00498600
C	1.29664500	1.51639400	-0.00512000
N	0.44978700	2.55089400	-0.01196500
N	0.73283500	0.25815400	-0.00291200
C	1.44329200	-0.93859100	0.00219300
O	0.82132800	-2.02288200	0.00646100
C	2.84693700	-0.73899700	0.00077800
H	5.98845100	-1.24270500	0.00440800
H	0.85615800	3.48483400	-0.00316500
H	-0.56514500	2.43503800	-0.00009600
H	-0.29873900	0.16231300	-0.00039900
H	5.34728900	1.23340900	-0.00211500

adenine–thymine stacked structure

N	-0.61597400	-2.32836000	0.44580200
C	-0.51888900	-2.51865300	-0.90818400
N	0.49255300	-1.88471000	-1.45553700
C	1.07852100	-1.22444600	-0.39349700
C	2.20216900	-0.37326800	-0.29888200
N	2.96290000	-0.06578400	-1.36118700
N	2.54322100	0.10403800	0.90920900
C	1.78111100	-0.21944000	1.96420200
N	0.71469700	-1.01189700	2.01560500
C	0.40276800	-1.48486400	0.79954100
N	-2.08351600	0.71166800	1.18510700
C	-2.45846700	0.10490000	0.01677200
O	-3.36497200	-0.72445100	-0.06033700
N	-1.74659800	0.53304400	-1.08493400
C	-0.66370000	1.41005500	-1.09000700
O	-0.09558800	1.67338400	-2.15551600
C	-0.30940100	1.97903000	0.20109700
C	-1.03057200	1.59318000	1.27950700
H	-1.96326600	0.05518700	-1.95775900
H	-2.57091100	0.40454300	2.03245400
H	-0.82259500	1.96877100	2.28572600
C	0.83049600	2.95308900	0.26044100
H	1.72725900	2.52026200	-0.18689600
H	0.59229100	3.86959600	-0.28733000
H	1.05752100	3.21245000	1.30130500
H	-1.22525800	-3.14999900	-1.43996200
H	-1.35157500	-2.69827000	1.05111400
H	2.09600600	0.21635200	2.91065500
H	3.72598400	0.59402000	-1.25139200

H	2.66380600	-0.30788000	-2.29547200

adenine–uracil stacked structure

N	0.28995700	2.21441700	0.14885700
C	0.15916000	2.19834600	-1.21566900
N	-0.77394900	1.37962800	-1.64331600
C	-1.26481400	0.81011000	-0.48522500
C	-2.26670400	-0.15410400	-0.24260600
N	-2.99132500	-0.70083900	-1.23375800
N	-2.53150100	-0.50048600	1.02763600
C	-1.81381900	0.06760000	2.00787600
N	-0.85655200	0.98530900	1.91997500
C	-0.61519400	1.31245500	0.64154800
N	2.18823300	-0.44414100	1.23444700
C	2.43078200	0.00581100	-0.04031900
O	3.23347100	0.90058400	-0.29995200
N	1.71430100	-0.65790900	-1.01530400
C	0.73251500	-1.62981400	-0.81873800
O	0.13937300	-2.10654200	-1.79300200
C	0.53128000	-2.01128100	0.56088900
C	1.25215600	-1.40407100	1.53045100
H	2.68928400	0.03539000	1.98912100
H	1.83959000	-0.30593000	-1.96256500
H	-3.59883200	-1.48288500	-1.01215700
H	-2.67664300	-0.60997100	-2.19021400
H	-2.06525800	-0.26271000	3.01371000
H	0.97778800	2.75396900	0.67846500
H	0.78148000	2.82591700	-1.84758300
H	1.13598200	-1.64369300	2.59051900
H	-0.21246800	-2.76459900	0.78533500

cytosine–guanine stacked structure

N	0.98386800	-1.25532100	-2.06133400
C	2.06885300	-1.72355100	-1.35542000
N	1.80412600	-1.96119400	-0.09444700
C	0.47363200	-1.61191600	0.03562300
C	-0.38749200	-1.60850400	1.17777400
O	-0.11989800	-1.91851500	2.34898200
N	-1.68330300	-1.21169000	0.83430100
C	-2.09194600	-0.75910000	-0.40107100
N	-3.40167200	-0.44208000	-0.52860000
N	-1.29804600	-0.73032000	-1.44638900
C	-0.04377400	-1.16073200	-1.17516600
N	-0.02909600	2.45674300	-0.91624800
C	-0.66370600	2.09968700	0.27165500
O	-1.87688200	2.36544700	0.39616000

N	0.07593600	1.52558300	1.24635600
C	1.34827800	1.21086600	1.00267400
N	2.03517800	0.63293400	2.00585800
C	2.01051300	1.49113400	-0.24043900
C	1.26907600	2.13814800	-1.17873100
H	-0.61352800	2.87719600	-1.64222400
H	1.66112700	2.42950400	-2.16008300
H	3.05067300	1.21836300	-0.41648600
H	1.50927800	0.24409100	2.77349700
H	2.91299600	0.16891000	1.78826700
H	-2.35048300	-1.18911300	1.60542900
H	-3.62996100	0.03602500	-1.39906100
H	-3.87752500	-0.04719100	0.28028600
H	3.03229100	-1.88442500	-1.83678200
H	0.96983100	-0.98760300	-3.05185100

1.3) SMD

1.3.1) SMD/M06-2X/6-31G**

adenine–thymine WC

N	0.97312200	0.37547700	0.02438200
C	1.58827100	1.56944500	0.02411300
N	2.88798300	1.82575400	0.01221700
C	3.60827100	0.68879000	0.00104600
C	3.11577500	-0.61186100	0.00048700
C	1.71230600	-0.75354600	0.00988600
N	1.09323600	-1.93692900	0.00651700
N	4.96796500	0.54664600	-0.01001300
C	5.22414000	-0.79680000	-0.01521200
N	4.14206000	-1.53626900	-0.00849000
H	0.92110100	2.42817500	0.03426600
H	1.63517300	-2.78668000	-0.02765000
H	0.07505900	-1.97136100	0.02330700
H	6.23767300	-1.17106100	-0.02402700
N	-3.80186000	1.61487100	-0.00651100
C	-2.43246300	1.61252700	-0.01108000
O	-1.76107600	2.64219200	-0.01089300
N	-1.86777000	0.36354300	-0.01605200
C	-2.54261300	-0.84032500	-0.00517700
O	-1.91227600	-1.90484300	0.00004300
C	-3.99433200	-0.76292200	-0.00074600
C	-4.77368900	-2.04037700	0.00684700
C	-4.55392200	0.46602600	-0.00080400
H	-4.25554800	2.52095300	-0.00152500
H	-0.82093500	0.33851500	-0.00724600

H	-5.84586700	-1.83689400	0.01459000
H	-4.52566000	-2.64107300	0.88700400
H	-4.53851700	-2.64411400	-0.87475200
H	-5.62695900	0.61942400	0.00469800
H	5.65768000	1.28792500	-0.01236800

adenine–uracil WC

N	-0.64105300	-0.28182800	0.03691700
C	-1.14375200	-1.52689500	0.01380000
N	-2.41367700	-1.90183200	-0.01167200
C	-3.23473400	-0.83523700	-0.01320100
C	-2.86396700	0.50543200	0.01084600
C	-1.47874300	0.77558100	0.03772600
N	-0.96946000	2.00992500	0.07107400
N	-4.60104300	-0.81907100	-0.03966100
C	-4.98033300	0.49530600	-0.03087200
N	-3.97128200	1.33082200	-0.00078000
H	-0.39774700	-2.31833300	0.01715900
H	-1.58653100	2.80639400	0.02988700
H	0.03946600	2.14243200	0.04082400
H	-6.02387300	0.77496000	-0.04791600
N	4.22446100	-1.11322700	-0.00159700
C	2.85534400	-1.23240500	0.00848900
O	2.28610300	-2.32037700	0.02750200
N	2.17822500	-0.04130800	-0.00415300
C	2.73914000	1.22368200	-0.02131400
O	2.00859800	2.22089000	-0.02636600
C	4.18493100	1.25913700	-0.03159800
C	4.86599400	0.09456900	-0.02097100
H	4.75489100	-1.97680200	0.00683800
H	1.13197400	-0.10910200	0.01199200
H	4.68910200	2.21464500	-0.04689800
H	5.94789300	0.04284700	-0.02666000
H	-5.21926000	-1.62053400	-0.06264100

cytosine–guanine WC

N	2.19289400	-0.07524000	0.07844300
C	2.94329300	1.05108600	0.12550800
O	2.45444600	2.18845100	0.24798200
N	4.31992200	0.92849600	0.03460900
C	4.93930200	-0.27350600	-0.10092000
C	4.21080000	-1.41081800	-0.15002000
C	2.78654700	-1.27006300	-0.05188600
N	2.00886800	-2.34920100	-0.08850700
H	4.85983400	1.78526600	0.07109500
H	6.02026900	-0.24987600	-0.16424600

H	4.67004300	-2.38383600	-0.25669000
H	2.42501300	-3.26349100	-0.18574500
H	0.99536700	-2.25332600	-0.00346600
N	-3.93416400	-1.59537900	0.07892800
C	-4.98292000	-0.81874700	0.01096400
N	-4.66352100	0.51453500	-0.06922700
C	-3.30255800	0.59981500	-0.05144100
N	-2.56634000	1.72950200	-0.11131500
C	-1.26694400	1.48630400	-0.07599300
N	-0.38594800	2.49518500	-0.16049200
N	-0.73168700	0.22373600	0.01751100
C	-1.46428000	-0.95713300	0.08075200
O	-0.88614700	-2.05342500	0.16192200
C	-2.86669600	-0.71611200	0.04092900
H	-6.01212600	-1.14658700	0.01425200
H	-0.76018000	3.43059900	-0.10943100
H	0.61097800	2.34690300	0.01188600
H	0.30103900	0.12194000	0.04704300
H	-5.31605200	1.28580600	-0.13093300

adenine–thymine stacked structure

N	-0.95263700	-2.22749200	0.31313900
C	-0.86021100	-2.32049700	-1.04857200
N	0.23649100	-1.79315000	-1.53788500
C	0.88994900	-1.30485600	-0.42278600
C	2.09243600	-0.58577100	-0.25973500
N	2.88306700	-0.26303700	-1.30430400
N	2.47294100	-0.24405600	0.98272300
C	1.66640700	-0.56256000	2.00601600
N	0.50757000	-1.21445700	1.98959600
C	0.16426200	-1.55939500	0.73931000
N	-1.90608200	0.96316300	1.22907600
C	-2.39173000	0.42288900	0.06999800
O	-3.40585000	-0.26480000	0.01592600
N	-1.63913700	0.72643000	-1.04175800
C	-0.43420900	1.42026400	-1.07187500
O	0.17386100	1.54452000	-2.13338000
C	0.00717900	1.96041800	0.20539700
C	-0.74134000	1.69067800	1.29612000
H	-1.93644100	0.28934600	-1.90938400
H	-2.42156400	0.75127000	2.07510800
H	-0.47312400	2.03532100	2.28806400
C	1.26841300	2.76526900	0.23470200
H	2.08264700	2.22625200	-0.25813000
H	1.13718700	3.71430100	-0.29467800
H	1.56356900	2.97727800	1.26406900

H	-1.63757400	-2.79859000	-1.62796500
H	-1.74512000	-2.51198600	0.87640900
H	2.01800200	-0.24705400	2.98488700
H	3.61181200	0.41740700	-1.13608300
H	2.47407700	-0.28173600	-2.22821300

adenine–uracil stacked structure

N	0.40837100	2.18217000	0.02917200
C	0.29050800	2.07259200	-1.32926300
N	-0.67781200	1.27353300	-1.70895200
C	-1.21005500	0.81658800	-0.51879200
C	-2.23670100	-0.10496500	-0.22433700
N	-2.95240000	-0.71114900	-1.19165700
N	-2.52743600	-0.35243300	1.06424400
C	-1.80456000	0.26590000	2.00996500
N	-0.80673800	1.13317600	1.87101500
C	-0.54568800	1.36600600	0.57521100
N	2.12749900	-0.50176700	1.27333100
C	2.39581600	-0.07423900	-0.00281300
O	3.21413200	0.80085600	-0.25909300
N	1.66486400	-0.71929800	-0.97332800
C	0.63314900	-1.63758700	-0.77870400
O	-0.00003400	-2.05592100	-1.74479900
C	0.41973900	-2.01216700	0.60334400
C	1.15891700	-1.42574600	1.56712800
H	2.64242500	-0.04643600	2.01809800
H	1.80011700	-0.38009600	-1.92177900
H	-3.53485500	-1.49039300	-0.91835600
H	-2.56529100	-0.72738200	-2.12481500
H	-2.07945300	0.02104300	3.03251200
H	1.12613500	2.69911100	0.52304200
H	0.95074400	2.61560400	-1.99096100
H	1.03684700	-1.64550500	2.62056300
H	-0.35062500	-2.73334400	0.83563100

cytosine–guanine stacked structure

N	-0.49479700	-1.17625900	-2.13634200
C	-1.04143200	-2.29600800	-1.56294000
N	-1.70235700	-2.04081500	-0.46246200
C	-1.56389600	-0.67621100	-0.30306000
C	-2.03058500	0.18368600	0.73571700
O	-2.68064000	-0.10685200	1.74292800
N	-1.65318300	1.51003400	0.49778700
C	-0.86369300	1.94760700	-0.53525600
N	-0.60081100	3.27819100	-0.56763900
N	-0.43080400	1.16444200	-1.49933300

C	-0.80393700	-0.12474700	-1.32594600
N	2.57947100	-0.08751100	-0.58836400
C	2.07429500	0.85702400	0.30094000
O	2.35658300	2.05048600	0.12152400
N	1.30398900	0.41890000	1.33041100
C	1.03720900	-0.88011600	1.43985600
N	0.26482800	-1.27745200	2.46888700
C	1.55752100	-1.87101100	0.54351100
C	2.32227600	-1.41498700	-0.47533100
H	3.14117200	0.26307200	-1.35512800
H	2.75921500	-2.05526400	-1.23222500
H	1.32251000	-2.91979900	0.66133200
H	-0.27173100	-0.56919500	2.95193800
H	-0.11780000	-2.21222100	2.45124700
H	-1.92827000	2.17726100	1.21369800
H	0.19279500	3.52703900	-1.14380500
H	-0.66341100	3.78150600	0.30824000
H	-0.92676700	-3.26951800	-2.01647400
H	0.09386000	-1.15007900	-2.95999900

1.3.2) SMD/M06-2X/6-31+G**

adenine–thymine WC

N	0.98403000	0.38753600	0.00207300
C	1.60407700	1.57911900	0.04230600
N	2.90675900	1.82823900	0.05708600
C	3.62523100	0.69019200	0.02615800
C	3.12558100	-0.60710400	-0.01719100
C	1.72106300	-0.74341200	-0.02938600
N	1.09888900	-1.92689700	-0.07401900
N	4.98464800	0.54402900	0.03111500
C	5.23813700	-0.79915600	-0.00806900
N	4.15090400	-1.53351200	-0.03820700
H	0.94453000	2.44208300	0.06529800
H	1.63883300	-2.78014200	-0.07819100
H	0.08131700	-1.96717800	-0.04973400
H	6.24978900	-1.17863900	-0.01251300
N	-3.84758200	1.59201400	-0.03027800
C	-2.48118000	1.61893900	-0.02893100
O	-1.83170600	2.66833400	-0.05137100
N	-1.88378700	0.38626200	0.00035400
C	-2.53644700	-0.83094500	0.02099800
O	-1.87538700	-1.88048900	0.04044800
C	-3.98764500	-0.79030200	0.01922600
C	-4.74531000	-2.08104800	0.04445300
C	-4.57459700	0.42724800	-0.00688100

H	-4.32417100	2.48755400	-0.04978900
H	-0.83805700	0.37623200	-0.00165800
H	-5.82032000	-1.89036700	0.04227000
H	-4.49560500	-2.66182000	0.93767500
H	-4.49777000	-2.69566600	-0.82641700
H	-5.65086100	0.55770000	-0.01109300
H	5.67857000	1.28260400	0.05858000

adenine–uracil WC

N	0.66491200	-0.31387000	0.01623900
C	1.18664400	-1.55211700	0.01020800
N	2.46507700	-1.90579600	0.00079900
C	3.27295600	-0.82907500	-0.00298200
C	2.87988800	0.50514400	0.00287600
C	1.49088900	0.75415000	0.01319000
N	0.96362900	1.98365000	0.01998600
N	4.63978900	-0.79353500	-0.01375700
C	5.00104700	0.52535100	-0.01422700
N	3.97686600	1.34575100	-0.00441800
H	0.46000800	-2.35960000	0.01372000
H	1.56689800	2.79316700	0.01859700
H	-0.04838900	2.10062600	0.02344500
H	6.03995500	0.82203200	-0.02242000
N	-4.26249700	-1.10040600	-0.00387800
C	-2.89714400	-1.22828800	-0.00016100
O	-2.33357000	-2.32387600	0.00639300
N	-2.20582500	-0.04544100	-0.00470300
C	-2.76035100	1.22285000	-0.00587500
O	-2.01518900	2.21393800	-0.00325600
C	-4.20329700	1.27260300	-0.00972500
C	-4.89566600	0.11243500	-0.00822500
H	-4.80217300	-1.95986100	-0.00044100
H	-1.16387400	-0.12403100	0.00279400
H	-4.69978000	2.23273800	-0.01235900
H	-5.97815800	0.06939800	-0.00993800
H	5.27214800	-1.58574600	-0.02083300

cytosine–guanine WC

N	2.20239800	-0.08786200	0.12603700
C	2.94574400	1.03948400	0.18366100
O	2.44191000	2.16988000	0.36049900
N	4.31708200	0.93724300	0.04322100
C	4.94109500	-0.25453100	-0.15690700
C	4.21950100	-1.39765500	-0.22139600
C	2.79907600	-1.27357800	-0.06990800
N	2.02249400	-2.35543600	-0.11937700

H	4.85471300	1.79654600	0.08677500
H	6.01909600	-0.21909500	-0.25665200
H	4.68410700	-2.36187000	-0.37810200
H	2.43572000	-3.26556600	-0.26637500
H	1.01216200	-2.26446200	0.00030300
N	-3.93515900	-1.59526900	0.11042700
C	-4.98768600	-0.82369300	0.01216900
N	-4.66882900	0.50672800	-0.10283200
C	-3.30851600	0.59500600	-0.07674100
N	-2.57118700	1.72302600	-0.16210500
C	-1.27153900	1.48737600	-0.10846300
N	-0.39078700	2.49897400	-0.22011800
N	-0.73503900	0.22955900	0.02601900
C	-1.46664100	-0.94865000	0.11588900
O	-0.87878000	-2.04092100	0.23378300
C	-2.86796700	-0.71653900	0.05638300
H	-6.01556900	-1.15548800	0.01669800
H	-0.76679500	3.43537000	-0.16755100
H	0.59498800	2.35722900	0.01195400
H	0.29645700	0.12928300	0.07170900
H	-5.32514100	1.27432200	-0.19004800

adenine–thymine stacked structure

N	-0.86604545	-2.31721658	0.16580829
C	-0.77012936	-2.30711713	-1.19812789
N	0.30009788	-1.69219840	-1.63996107
C	0.93530589	-1.26153153	-0.49116749
C	2.10633376	-0.50572206	-0.27519446
N	2.86796986	-0.05835608	-1.29376403
N	2.47380031	-0.24702750	0.99273140
C	1.68836546	-0.68362120	1.99092804
N	0.56084468	-1.38527389	1.91882091
C	0.22166057	-1.63875036	0.64449183
N	-1.88503984	0.85836525	1.31080781
C	-2.39398051	0.36462902	0.14503785
O	-3.40126770	-0.34247690	0.09221969
N	-1.68876572	0.73353522	-0.97581126
C	-0.51837026	1.48148173	-1.01285129
O	0.03680093	1.69500438	-2.09380116
C	-0.04247247	1.97062521	0.27046621
C	-0.74218986	1.62049151	1.37380434
H	-2.01906291	0.34819308	-1.85836867
H	-2.36653912	0.59544338	2.16393612
H	-0.45172561	1.92711792	2.37250025
C	1.18381281	2.82853048	0.30137394
H	2.01242547	2.34549999	-0.22492700

H	0.99774930	3.78778844	-0.19257802
H	1.48751706	3.01999494	1.33281089
H	-1.52531781	-2.77369307	-1.81553807
H	-1.63587730	-2.69679023	0.70508844
H	2.02932256	-0.43146992	2.99062149
H	3.57045318	0.63842512	-1.08192189
H	2.46674116	-0.03761959	-2.22196273

adenine–uracil stacked structure

N	0.32288177	2.19060564	-0.11336532
C	0.20876502	1.99458801	-1.46283606
N	-0.73985270	1.14594377	-1.78833773
C	-1.25887446	0.74724051	-0.57122109
C	-2.26717526	-0.17373852	-0.21989096
N	-2.97244961	-0.85575991	-1.14526646
N	-2.55296126	-0.34325742	1.08295060
C	-1.84712323	0.34829380	1.99081690
N	-0.87005519	1.22916960	1.79165130
C	-0.60904979	1.38437331	0.48380483
N	2.13299301	-0.36319568	1.32511753
C	2.43114327	-0.01457389	0.03426340
O	3.24590486	0.85846446	-0.25661729
N	1.74863800	-0.73427774	-0.91770621
C	0.74057468	-1.66716636	-0.69199070
O	0.15147249	-2.16929733	-1.65259033
C	0.48977262	-1.96253388	0.70091520
C	1.18098703	-1.29473535	1.64911034
H	2.60988870	0.15318208	2.05728216
H	1.90800241	-0.45185591	-1.88310050
H	-3.53335851	-1.63372073	-0.82357904
H	-2.59252886	-0.91992234	-2.08052243
H	-2.11741968	0.16463693	3.02601973
H	1.02921841	2.75438457	0.34718513
H	0.85276440	2.51226364	-2.15783665
H	1.03120428	-1.45269061	2.71053930
H	-0.26526742	-2.69469828	0.95453630

cytosine–guanine stacked structure

N	-0.70632000	-1.24277000	-2.04483000
C	-1.49431000	-2.18538000	-1.43458000
N	-2.13014000	-1.72133000	-0.38753000
C	-1.71574000	-0.40663000	-0.29942000
C	-2.03693000	0.60544000	0.65150000
O	-2.79964000	0.53642000	1.62554000
N	-1.36398000	1.79579000	0.37386000
C	-0.46278000	1.98990000	-0.64388000

N	0.09391000	3.22165000	-0.72524000
N	-0.18017000	1.07284000	-1.54471000
C	-0.81919000	-0.09719000	-1.31577000
N	2.48506000	-0.75420000	-0.57485000
C	2.29127000	0.40868000	0.15696000
O	2.87411000	1.44820000	-0.21250000
N	1.48987000	0.36040000	1.24798000
C	0.89402000	-0.78984000	1.57362000
N	0.09855000	-0.80078000	2.65307000
C	1.08902000	-2.00681000	0.83940000
C	1.89537000	-1.93325000	-0.24567000
H	3.08603000	-0.69373000	-1.39003000
H	2.11231000	-2.77578000	-0.89171000
H	0.59867000	-2.92635000	1.12995000
H	-0.13859000	0.07133000	3.10686000
H	-0.44939000	-1.62257000	2.86609000
H	-1.51977000	2.55525000	1.03214000
H	0.93632000	3.27607000	-1.28440000
H	0.08291000	3.79975000	0.10611000
H	-1.56322000	-3.19265000	-1.81940000
H	-0.09292000	-1.39909000	-2.83713000

2) Chloroform

2.1) SM8

2.1.1) SM8/M06-2X/6-31G**

9-hexyl–adenine–9-hexyl–adenine HB1

N	-2.722806	3.453306	-0.615973
C	-4.020239	3.449485	-0.290630
N	-4.740193	2.472197	0.250371
C	-3.986724	1.381874	0.464850
C	-2.633103	1.225041	0.182802
C	-1.984495	2.346796	-0.391603
N	-0.692063	2.354789	-0.715870
N	-4.389013	0.191141	1.011617
C	-3.284049	-0.612748	1.026819
N	-2.208099	-0.036408	0.543057
H	-4.553202	4.374966	-0.500217
H	-0.072347	1.554130	-0.573513
H	-0.315694	3.202098	-1.124054
H	-3.331448	-1.623812	1.417082
N	1.507974	0.309961	-0.493123
C	2.636634	0.868304	-0.956589
N	3.846396	0.335041	-1.056073

C	3.852415	-0.934376	-0.612854
C	2.773065	-1.649234	-0.104920
C	1.534508	-0.965053	-0.051753
N	0.420192	-1.527410	0.409240
N	4.911791	-1.800303	-0.567672
C	4.424043	-2.967646	-0.038120
N	3.145983	-2.925956	0.252583
H	2.537478	1.898826	-1.294793
H	0.451511	-2.483005	0.742160
H	-0.456947	-1.002789	0.439721
H	5.071598	-3.825879	0.105076
C	6.286711	-1.503404	-0.958317
C	6.998237	-0.611120	0.054150
H	6.256762	-1.021318	-1.939386
H	6.804910	-2.461725	-1.068795
C	8.435025	-0.316240	-0.371239
H	6.434955	0.322367	0.154443
H	6.989630	-1.103325	1.034060
C	9.174832	0.577005	0.622189
H	8.985136	-1.260063	-0.488091
H	8.431972	0.163886	-1.358498
H	8.625815	1.520152	0.742020
H	9.178144	0.098325	1.610713
C	-5.745548	-0.145763	1.434519
C	-6.675493	-0.394788	0.251142
H	-6.115995	0.681779	2.045372
H	-5.674438	-1.032680	2.072946
C	-8.090200	-0.738003	0.712501
H	-6.689877	0.502785	-0.375237
H	-6.270235	-1.211303	-0.358677
C	-9.047701	-0.984018	-0.451428
H	-8.062692	-1.630097	1.353265
H	-8.478552	0.078222	1.335438
H	-9.074591	-0.094236	-1.093874
H	-8.660163	-1.799821	-1.076484
C	10.612427	0.878081	0.203092
C	11.343044	1.769282	1.202308
H	10.607917	1.356848	-0.783905
H	11.158905	-0.065739	0.082699
H	12.368930	1.973945	0.885106
H	10.833138	2.730649	1.318690
H	11.388171	1.299122	2.189727
C	-10.466306	-1.325364	0.000141
C	-11.414614	-1.566934	-1.169818
H	-10.851948	-0.510788	0.625564
H	-10.437263	-2.215538	0.641003

H	-12.423700	-1.810599	-0.827314
H	-11.485285	-0.681102	-1.808584
H	-11.066536	-2.395846	-1.794224

9-hexyl–adenine–9-hexyl–adenine HB2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.636104	-3.982041	-0.403925
2	6	0	-3.857538	-3.522226	-0.697626
3	7	0	-4.251514	-2.266933	-0.884080
4	6	0	-3.226904	-1.412987	-0.729679
5	6	0	-1.906421	-1.727490	-0.418133
6	6	0	-1.620146	-3.106496	-0.264003
7	7	0	-0.401666	-3.570502	0.017084
8	7	0	-3.260028	-0.048702	-0.846111
9	6	0	-1.985701	0.383581	-0.593336
10	7	0	-1.139628	-0.584263	-0.333079
11	1	0	-4.627966	-4.284424	-0.798554
12	1	0	0.423224	-2.970617	0.059668
13	1	0	-0.290787	-4.573043	0.114236
14	1	0	-1.740351	1.440144	-0.621316
15	7	0	5.624837	-3.320185	0.324208
16	6	0	6.144080	-2.150982	0.722025
17	7	0	5.525039	-0.993419	0.926202
18	6	0	4.208173	-1.097890	0.688025
19	6	0	3.520212	-2.237517	0.283169
20	6	0	4.303330	-3.397093	0.090333
21	7	0	3.775586	-4.564025	-0.300889
22	7	0	3.256017	-0.117252	0.793880
23	6	0	2.065980	-0.697844	0.451056
24	7	0	2.175969	-1.969092	0.141467
25	1	0	7.218167	-2.156020	0.895777
26	1	0	2.814665	-4.610849	-0.614565
27	1	0	4.391830	-5.338071	-0.514694
28	1	0	1.127290	-0.153544	0.437934
29	6	0	3.493612	1.276394	1.158320
30	6	0	4.185561	2.058740	0.046412
31	1	0	4.103365	1.283020	2.066119
32	1	0	2.520252	1.715164	1.400875
33	6	0	4.419077	3.512934	0.449563
34	1	0	5.139946	1.572669	-0.181027
35	1	0	3.571462	2.013173	-0.860963
36	6	0	5.134224	4.320001	-0.631569
37	1	0	3.456612	3.990086	0.680453

38	1	0	5.009480	3.544442	1.374694
39	1	0	6.097774	3.846008	-0.860460
40	1	0	4.548884	4.285867	-1.560422
41	6	0	-4.435386	0.760191	-1.152115
42	6	0	-5.382349	0.897529	0.036200
43	1	0	-4.948563	0.288245	-1.994494
44	1	0	-4.075717	1.740479	-1.482803
45	6	0	-6.609549	1.729144	-0.329842
46	1	0	-5.685732	-0.103534	0.359176
47	1	0	-4.847190	1.362563	0.873043
48	6	0	-7.586942	1.897253	0.831371
49	1	0	-6.289868	2.720765	-0.679169
50	1	0	-7.128221	1.256967	-1.174352
51	1	0	-7.903678	0.908200	1.187506
52	1	0	-7.072993	2.375976	1.675840
53	6	0	5.368289	5.776427	-0.236068
54	6	0	6.091118	6.571956	-1.318083
55	1	0	5.947928	5.808673	0.694844
56	1	0	4.403803	6.249867	-0.012658
57	1	0	6.250743	7.610613	-1.016430
58	1	0	7.070487	6.135892	-1.538633
59	1	0	5.517162	6.581018	-2.250159
60	6	0	-8.818944	2.719483	0.458865
61	6	0	-9.791293	2.887305	1.621841
62	1	0	-9.330727	2.238824	-0.384019
63	1	0	-8.499283	3.706131	0.100286
64	1	0	-10.664851	3.478649	1.334926
65	1	0	-10.150007	1.917035	1.979214
66	1	0	-9.311576	3.392056	2.466477

9-hexyl–adenine–9-hexyl–adenine HB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.159472	3.440171	0.082944
2	6	0	3.479873	3.468470	-0.132000
3	7	0	4.290142	2.470754	-0.469300
4	6	0	3.613664	1.315967	-0.577042
5	6	0	2.250720	1.118863	-0.376984
6	6	0	1.499726	2.270947	-0.039562
7	7	0	0.183305	2.240825	0.172688
8	7	0	4.118235	0.084352	-0.904298
9	6	0	3.059778	-0.780015	-0.872248
10	7	0	1.919781	-0.205868	-0.564798
11	1	0	3.947489	4.444230	-0.014695

12	1	0	-0.388549	1.421366	-0.035923
13	1	0	-0.281146	3.119826	0.368682
14	1	0	3.189310	-1.834105	-1.094823
15	7	0	-2.159665	-3.440041	0.083234
16	6	0	-3.480092	-3.468251	-0.131565
17	7	0	-4.290304	-2.470520	-0.468959
18	6	0	-3.613715	-1.315828	-0.577009
19	6	0	-2.250735	-1.118812	-0.377127
20	6	0	-1.499816	-2.270903	-0.039563
21	7	0	-0.183371	-2.240873	0.172516
22	7	0	-4.118200	-0.084237	-0.904466
23	6	0	-3.059668	0.780048	-0.872658
24	7	0	-1.919683	0.205848	-0.565254
25	1	0	-3.947793	-4.443940	-0.014006
26	1	0	0.388528	-1.421436	-0.036058
27	1	0	0.281007	-3.119854	0.368772
28	1	0	-3.189129	1.834108	-1.095413
29	6	0	-5.521051	0.233022	-1.158732
30	6	0	-6.351068	0.245925	0.121033
31	1	0	-5.907065	-0.512097	-1.859441
32	1	0	-5.546749	1.209127	-1.654703
33	6	0	-7.814281	0.580200	-0.160732
34	1	0	-6.273630	-0.736855	0.596920
35	1	0	-5.925809	0.978858	0.817371
36	6	0	-8.673955	0.571230	1.101442
37	1	0	-7.882206	1.567431	-0.638152
38	1	0	-8.221099	-0.140608	-0.881914
39	1	0	-8.603758	-0.413863	1.581042
40	1	0	-8.268162	1.291686	1.824446
41	6	0	5.521090	-0.232869	-1.158616
42	6	0	6.351130	-0.246040	0.121136
43	1	0	5.907104	0.512368	-1.859199
44	1	0	5.546773	-1.208886	-1.654761
45	6	0	7.814353	-0.580197	-0.160724
46	1	0	6.273662	0.736627	0.597254
47	1	0	5.925908	-0.979149	0.817310
48	6	0	8.674037	-0.571505	1.101444
49	1	0	7.882304	-1.567310	-0.638384
50	1	0	8.221140	0.140798	-0.881736
51	1	0	8.603745	0.413441	1.581331
52	1	0	8.268322	-1.292212	1.824242
53	6	0	-10.140915	0.899731	0.831889
54	6	0	-10.989847	0.885906	2.099018
55	1	0	-10.545073	0.180306	0.109006
56	1	0	-10.209187	1.884854	0.353295
57	1	0	-12.036057	1.120830	1.886125

58	1	0	-10.961117	-0.096253	2.581228
59	1	0	-10.625419	1.619500	2.825155
60	6	0	10.141028	-0.899780	0.831784
61	6	0	10.989952	-0.886319	2.098923
62	1	0	10.545126	-0.180069	0.109154
63	1	0	10.209392	-1.884731	0.352849
64	1	0	12.036191	-1.121046	1.885950
65	1	0	10.961106	0.095661	2.581491
66	1	0	10.625604	-1.620220	2.824790

1-hexyl–thymine–1-hexyl–thymine HB1

N	4.13310000	-0.83891100	-0.99160500
C	3.22346000	0.20240700	-0.97215400
O	3.56204400	1.37378900	-0.94859500
N	1.90042200	-0.19464600	-0.98478200
C	1.42189200	-1.49221900	-0.98281100
O	0.21062400	-1.71891100	-0.98455600
C	2.43199300	-2.53682400	-0.97846400
C	1.97809100	-3.96288400	-0.97594300
C	3.72596500	-2.15180500	-0.97904000
H	1.19930700	0.55761300	-0.97979100
H	2.83305100	-4.64376000	-0.97155400
H	1.36552800	-4.17776800	-1.85499400
H	1.36021900	-4.17283600	-0.09944600
H	4.53439100	-2.87994800	-0.97508100
N	-4.13372900	0.84849900	-0.98470000
C	-3.22412800	-0.19297900	-0.97403800
O	-3.56275300	-1.36449300	-0.95926900
N	-1.90107500	0.20410600	-0.98393400
C	-1.42248900	1.50160700	-0.97202300
O	-0.21121100	1.72825700	-0.97190200
C	-2.43254200	2.54618100	-0.95878800
C	-1.97857500	3.97215600	-0.94494700
C	-3.72653200	2.16123200	-0.96188400
H	-1.20000800	-0.54820700	-0.98472300
H	-2.83350100	4.65300400	-0.93418600
H	-1.36680200	4.19424500	-1.82275700
H	-1.35989800	4.17486200	-0.06731400
H	-4.53492500	2.88935300	-0.95168900
C	-5.56027600	0.50554600	-0.92859200
C	-6.02688200	0.20980100	0.49231100
H	-5.70906500	-0.36495500	-1.56887000
H	-6.11284700	1.34759200	-1.35737400
C	-7.51008500	-0.15060600	0.53638000
H	-5.42666500	-0.61536300	0.88805300
H	-5.83595400	1.08610800	1.12532400

C	-8.00244100	-0.46054300	1.94833800
H	-8.10288900	0.67547200	0.11981400
H	-7.69252500	-1.01848100	-0.11030200
H	-7.40903100	-1.28386600	2.36699200
H	-7.82055000	0.40704300	2.59710900
C	-9.48424700	-0.82705400	2.00087000
C	-9.96436100	-1.13748300	3.41500100
H	-9.66509900	-1.69237400	1.35139300
H	-10.07559400	-0.00238100	1.58345900
H	-11.02665900	-1.39467600	3.43291200
H	-9.41109900	-1.97955600	3.84226100
H	-9.81915100	-0.27828700	4.07750600
C	5.55965000	-0.49636900	-0.93309600
C	6.02695500	-0.21356800	0.49021200
H	5.70802800	0.37996400	-1.56546200
H	6.11207700	-1.33440400	-1.36984900
C	7.51062000	0.14457800	0.53708200
H	5.42785100	0.60886800	0.89325300
H	5.83505800	-1.09509700	1.11563700
C	8.00324100	0.44339000	1.95134300
H	8.10238300	-0.67916500	0.11445900
H	7.69427200	1.01698400	-0.10312900
H	7.41210600	1.26561600	2.37533800
H	7.81844100	-0.42804800	2.59410300
C	9.48611500	0.80508100	2.00704100
C	9.96636400	1.10499000	3.42339500
H	9.66994400	1.67399500	1.36322300
H	10.07521100	-0.01867800	1.58467200
H	11.02958300	1.35817600	3.44362000
H	9.41589000	1.94642500	3.85548500
H	9.81754800	0.24224900	4.08046900

1-hexyl–thymine–1-hexyl–thymine HB2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.987551	0.219343	-0.286236
2	6	0	-3.966747	-0.470244	-0.920745
3	8	0	-4.054766	-1.640020	-1.254226
4	7	0	-2.819182	0.269391	-1.126186
5	6	0	-2.594124	1.579997	-0.748995
6	8	0	-1.488929	2.100490	-0.912256
7	6	0	-3.730550	2.268811	-0.158274
8	6	0	-3.575307	3.710911	0.209560
9	6	0	-4.847280	1.542166	0.062403

10	1	0	-2.005022	-0.257278	-1.474628
11	1	0	-4.482636	4.091834	0.685049
12	1	0	-3.364700	4.319716	-0.673386
13	1	0	-2.736449	3.845528	0.896381
14	1	0	-5.719033	1.977866	0.547359
15	7	0	3.208470	0.272072	-0.824333
16	6	0	2.145046	1.157936	-0.819780
17	8	0	2.273104	2.340295	-0.552340
18	7	0	0.929199	0.592005	-1.151872
19	6	0	0.682247	-0.737751	-1.440275
20	8	0	-0.456358	-1.126734	-1.709235
21	6	0	1.839124	-1.615947	-1.405905
22	6	0	1.633169	-3.067987	-1.703593
23	6	0	3.031525	-1.063545	-1.095229
24	1	0	0.115606	1.219768	-1.126248
25	1	0	2.573495	-3.619473	-1.625652
26	1	0	1.229378	-3.206900	-2.709454
27	1	0	0.912252	-3.506450	-1.008585
28	1	0	3.939448	-1.661994	-1.052183
29	6	0	4.526280	0.791283	-0.436069
30	6	0	4.669974	0.912978	1.080989
31	1	0	4.637255	1.773882	-0.897750
32	1	0	5.271518	0.121971	-0.873319
33	6	0	6.023782	1.493325	1.519582
34	1	0	3.864249	1.570958	1.416921
35	1	0	4.499565	-0.064075	1.550954
36	6	0	7.169070	0.497148	1.740865
37	1	0	6.341179	2.246695	0.785952
38	1	0	5.874675	2.039237	2.456384
39	1	0	8.029151	1.070543	2.102626
40	1	0	6.899065	-0.186320	2.557150
41	6	0	7.593688	-0.329756	0.516265

1-hexyl–thymine–1-hexyl–thymine HB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.966035	-0.357010	0.346691
2	6	0	-2.969824	0.586505	0.527112
3	8	0	-3.168934	1.660939	1.067678
4	7	0	-1.731413	0.207274	0.047267
5	6	0	-1.417156	-0.970649	-0.605821
6	8	0	-0.269517	-1.189677	-0.996624
7	6	0	-2.517676	-1.902348	-0.790154
8	6	0	-2.242424	-3.194328	-1.493239

9	6	0	-3.725954	-1.541312	-0.308757
10	1	0	-0.966288	0.883114	0.174997
11	1	0	-3.149846	-3.799132	-1.566399
12	1	0	-1.480810	-3.771351	-0.962908
13	1	0	-1.860480	-3.015079	-2.501269
14	1	0	-4.593978	-2.189603	-0.410918
15	7	0	4.221280	1.102740	-1.057837
16	6	0	3.226111	0.157864	-1.240963
17	8	0	3.416180	-0.915344	-1.786232
18	7	0	1.989234	0.534336	-0.751133
19	6	0	1.672758	1.711716	-0.099295
20	8	0	0.526497	1.925965	0.298747
21	6	0	2.768576	2.651173	0.072355
22	6	0	2.489550	3.948072	0.764641
23	6	0	3.975375	2.291978	-0.413580
24	1	0	1.226193	-0.143830	-0.876138
25	1	0	3.393785	4.558864	0.826976
26	1	0	2.114419	3.776238	1.776486
27	1	0	1.721566	4.515728	0.233394
28	1	0	4.839906	2.947190	-0.324432
29	6	0	5.583765	0.791242	-1.512958
30	6	0	6.487695	0.304714	-0.383226
31	1	0	5.990134	1.699003	-1.969782
32	1	0	5.487097	0.031101	-2.287420
33	6	0	6.006629	-0.990135	0.269317
34	1	0	7.487906	0.168798	-0.809914
35	1	0	6.577894	1.090671	0.379911
36	6	0	6.889501	-1.453486	1.430310
37	1	0	4.983825	-0.850233	0.636675
38	1	0	5.945096	-1.777860	-0.491024
39	1	0	6.901275	-0.681362	2.212161
40	1	0	6.434418	-2.340457	1.887322
41	6	0	8.328492	-1.787694	1.035567
42	6	0	9.122411	-2.389128	2.191311
43	1	0	8.839467	-0.884512	0.681404
44	1	0	8.317063	-2.487168	0.189831
45	1	0	10.152820	-2.611137	1.901189
46	1	0	9.157833	-1.702070	3.042907
47	1	0	8.666214	-3.320899	2.539536
48	6	0	-5.323072	-0.007789	0.784330
49	6	0	-6.057973	0.833422	-0.258387
50	1	0	-5.228459	0.549605	1.717648
51	1	0	-5.841053	-0.946818	0.997492
52	6	0	-7.478055	1.237288	0.170685
53	1	0	-5.449233	1.725013	-0.429969
54	1	0	-6.094200	0.282230	-1.207955

55	6	0	-8.585309	0.290718	-0.307804
56	1	0	-7.514949	1.346228	1.262112
57	1	0	-7.694909	2.232316	-0.228978
58	1	0	-9.554945	0.702889	-0.001954
59	1	0	-8.586064	0.288040	-1.404721
60	6	0	-8.489161	-1.153530	0.190304
61	6	0	-8.596210	-1.286943	1.707411
62	1	0	-7.553964	-1.606721	-0.165001
63	1	0	-9.290817	-1.737006	-0.275463
64	1	0	-8.569647	-2.334804	2.018262
65	1	0	-7.784673	-0.770054	2.229148
66	1	0	-9.536148	-0.857471	2.068367

9-ethyl–adenine–1-cyclohexyl–uracil WC

N	1.75004500	0.33465600	-0.02097200
C	2.01668800	-0.98150000	-0.03755400
N	3.20173800	-1.57286900	-0.04875900
C	4.19853900	-0.66962100	-0.04010800
C	4.07719800	0.71599300	-0.02249800
C	2.75925800	1.22980900	-0.01222100
N	2.47906200	2.53146600	0.00499600
N	5.54300800	-0.91757600	-0.04295700
C	6.15324100	0.31251600	-0.02953400
N	5.31272400	1.32107800	-0.01581400
H	1.13648500	-1.62074200	-0.04242600
H	3.23649600	3.20451400	0.01222500
H	1.51056000	2.84993300	0.01211800
H	7.23133900	0.41015100	-0.02496400
N	-3.21524100	0.39711000	0.00426100
C	-1.87505900	0.02943800	-0.00765700
O	-1.50291200	-1.13511200	-0.02370900
N	-0.98736300	1.07885500	0.00058400
C	-1.27874200	2.43270500	0.01989700
O	-0.37345400	3.26695000	0.02573900
C	-2.69262700	2.73720400	0.03194000
C	-3.57886900	1.72072800	0.02392300
H	0.01950300	0.80710300	-0.00802800
H	-3.00692100	3.77093400	0.04749200
H	-4.64903000	1.90487000	0.03295900
C	-4.24659600	-0.66088400	-0.00147500
C	-5.09212000	-0.62612700	1.27386700
C	-5.11668700	-0.58946700	-1.25866100
H	-3.68031300	-1.59385200	-0.02058500
C	-6.11859900	-1.76259200	1.26245000
H	-5.62241000	0.33392600	1.34170400

H	-4.43779800	-0.69684600	2.14774900
C	-6.14275400	-1.72640000	-1.26000400
H	-5.64850300	0.37163100	-1.28861000
H	-4.47950600	-0.63457200	-2.14678900
C	-6.99570500	-1.70480300	0.01006900
H	-6.73357700	-1.71425800	2.16587500
H	-5.58988500	-2.72384200	1.29120600
H	-6.77486100	-1.65266800	-2.14978600
H	-5.61462700	-2.68612500	-1.32626400
H	-7.70459600	-2.53817400	0.00492100
H	-7.59204900	-0.78257700	0.02907000
C	6.15113600	-2.25236800	-0.08017100
C	7.64430700	-2.21387100	0.18834600
H	5.94169800	-2.69338400	-1.05865700
H	5.63202100	-2.85819300	0.66582700
H	8.02619500	-3.23669900	0.19730400
H	8.18282700	-1.66761000	-0.59005700
H	7.86440800	-1.76182000	1.15846600

9-ethyl–adenine–1-cyclohexyl–uracil RWC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.782141	0.386735	-0.001059
2	6	0	2.661643	1.402374	-0.001334
3	7	0	3.984297	1.332377	-0.001467
4	6	0	4.405273	0.055064	-0.001258
5	6	0	3.618167	-1.092315	-0.000940
6	6	0	2.218526	-0.888573	-0.000826
7	7	0	1.332455	-1.884477	-0.000506
8	7	0	5.698734	-0.392068	-0.001184
9	6	0	5.623845	-1.762643	-0.000971
10	7	0	4.396274	-2.227047	-0.000753
11	1	0	2.207265	2.390907	-0.001473
12	1	0	1.659565	-2.842613	-0.000422
13	1	0	0.334908	-1.681179	-0.000683
14	1	0	6.514676	-2.378323	-0.000716
15	7	0	-3.178768	0.550821	0.001712
16	6	0	-1.852960	0.148166	0.000810
17	8	0	-1.524272	-1.036440	0.000950
18	7	0	-0.932165	1.159366	-0.000145
19	6	0	-1.174440	2.530818	-0.000969
20	8	0	-0.242059	3.323263	-0.001975
21	6	0	-2.584192	2.874549	-0.000702
22	6	0	-3.501154	1.888205	0.000527

23	1	0	0.068070	0.858034	-0.000738
24	1	0	-2.867840	3.917525	-0.001554
25	1	0	-4.565273	2.105619	0.000664
26	6	0	-4.243568	-0.473549	0.002071
27	6	0	-5.101910	-0.389296	1.266797
28	6	0	-5.097020	-0.394737	-1.266310
29	1	0	-3.709308	-1.425400	0.005211
30	6	0	-6.165122	-1.491519	1.261694
31	1	0	-5.600881	0.588538	1.312889
32	1	0	-4.460439	-0.466767	2.149547
33	6	0	-6.160562	-1.496628	-1.260681
34	1	0	-5.595257	0.583192	-1.318475
35	1	0	-4.452102	-0.476239	-2.146181
36	6	0	-7.026405	-1.425374	-0.001190
37	1	0	-6.787549	-1.408520	2.157439
38	1	0	-5.668874	-2.469134	1.311371
39	1	0	-6.779737	-1.417001	-2.158982
40	1	0	-5.664399	-2.474555	-1.304741
41	1	0	-7.762634	-2.234695	-0.000887

9-ethyl–adenine–1-cyclohexyl–uracil H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	5.233516	-1.755133	-0.024012
2	6	0	5.955541	-0.632297	-0.127581
3	7	0	5.534759	0.625395	-0.220796
4	6	0	4.194051	0.687658	-0.200494
5	6	0	3.310870	-0.380945	-0.096642
6	6	0	3.888851	-1.669869	-0.005653
7	7	0	3.161649	-2.784039	0.096492
8	7	0	3.406590	1.809155	-0.282315
9	6	0	2.113610	1.376450	-0.218982
10	7	0	2.011281	0.071791	-0.110177
11	1	0	7.034191	-0.775717	-0.136144
12	1	0	2.143417	-2.781208	0.112883
13	1	0	3.652140	-3.668387	0.155989
14	1	0	1.267153	2.052951	-0.260738
15	7	0	-2.845195	-0.536685	0.031240
16	6	0	-1.541192	-0.058475	-0.031563
17	8	0	-1.269927	1.129716	-0.131064
18	7	0	-0.568095	-1.026194	0.026197
19	6	0	-0.739177	-2.394718	0.137554
20	8	0	0.235899	-3.143378	0.178788
21	6	0	-2.122010	-2.817479	0.196185

22	6	0	-3.092303	-1.882618	0.140953
23	1	0	0.409230	-0.668158	-0.020713
24	1	0	-4.142419	-2.157496	0.181597
25	1	0	-2.346797	-3.870925	0.282902
26	6	0	-3.962074	0.428551	-0.022838
27	6	0	-4.830444	0.212843	-1.264731
28	6	0	-4.794752	0.396451	1.261177
29	1	0	-3.476168	1.403023	-0.100315
30	6	0	-5.948148	1.258336	-1.319698
31	1	0	-5.278703	-0.790012	-1.234368
32	1	0	-4.204806	0.260315	-2.160880
33	6	0	-5.911526	1.442243	1.196133
34	1	0	-5.243830	-0.598264	1.388621
35	1	0	-4.143983	0.570330	2.123213
36	6	0	-6.788599	1.240296	-0.041244
37	1	0	-6.577442	1.081015	-2.196751
38	1	0	-5.502444	2.253119	-1.446768
39	1	0	-6.514763	1.395965	2.107514
40	1	0	-5.463960	2.443780	1.164154
41	1	0	-7.563843	2.010948	-0.086456
42	1	0	-7.306816	0.275049	0.036893
43	6	0	3.882397	3.189771	-0.368878
44	1	0	4.631907	3.228087	-1.162577
45	1	0	3.028961	3.800367	-0.676493
46	6	0	4.466111	3.673054	0.950229
47	1	0	5.321266	3.058564	1.235130
48	1	0	4.802747	4.707925	0.845692
49	1	0	3.718411	3.632494	1.745868

9-ethyl–adenine–1-cyclohexyl–uracil RH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.540891	-3.107782	-0.049878
2	6	0	4.808459	-2.676894	-0.089185
3	7	0	5.265024	-1.429299	-0.142002
4	6	0	4.254581	-0.545780	-0.154628
5	6	0	2.895451	-0.834948	-0.117641
6	6	0	2.542678	-2.203791	-0.063079
7	7	0	1.275079	-2.621621	-0.025169
8	7	0	4.337419	0.823551	-0.211189
9	6	0	3.053629	1.287565	-0.199874
10	7	0	2.159834	0.327109	-0.147077
11	1	0	5.563560	-3.460220	-0.075159

12	1	0	0.485800	-1.980097	-0.026332
13	1	0	1.100862	-3.618488	0.017322
14	1	0	2.808860	2.343380	-0.236317
15	7	0	-2.797581	0.666278	-0.033158
16	6	0	-1.500253	0.179769	-0.050337
17	8	0	-1.243621	-1.021396	-0.013241
18	7	0	-0.520180	1.130334	-0.111483
19	6	0	-0.672838	2.512954	-0.153020
20	8	0	0.309861	3.241315	-0.204700
21	6	0	-2.056965	2.946867	-0.127828
22	6	0	-3.033858	2.020969	-0.069330
23	1	0	0.457849	0.770653	-0.123209
24	1	0	-4.081592	2.306074	-0.047290
25	1	0	-2.275675	4.004978	-0.155680
26	6	0	-3.923664	-0.287857	0.037969
27	6	0	-4.713448	-0.123803	1.338867
28	6	0	-4.829700	-0.180123	-1.191101
29	1	0	-3.450086	-1.271364	0.037896
30	6	0	-5.843191	-1.155392	1.408398
31	1	0	-5.145628	0.885481	1.384806
32	1	0	-4.036627	-0.225019	2.192342
33	6	0	-5.957426	-1.213244	-1.110684
34	1	0	-5.270398	0.825052	-1.241979
35	1	0	-4.233917	-0.318531	-2.098093
36	6	0	-6.756912	-1.060204	0.184846
37	1	0	-6.416318	-1.015097	2.329496
38	1	0	-5.407473	-2.161446	1.457769
39	1	0	-6.611860	-1.114550	-1.981631
40	1	0	-5.525051	-2.221045	-1.153037
41	1	0	-7.542266	-1.820017	0.238045
42	1	0	-7.260794	-0.084254	0.185225
43	6	0	5.571066	1.609800	-0.228135
44	1	0	6.217348	1.187728	-1.001102
45	1	0	5.295692	2.623928	-0.530349
46	6	0	6.267789	1.600593	1.124166
47	1	0	6.535921	0.581404	1.406135
48	1	0	7.182218	2.197288	1.070399
49	1	0	5.623880	2.025946	1.897536

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB1

N	-3.76718000	0.30856700	0.00047200
C	-2.46565200	0.77133100	0.00077700
O	-1.50040100	0.00927300	0.00119200
N	-2.32179600	2.13413900	0.00071500
C	-3.33799900	3.09752100	0.00051800

O	-3.06394200	4.28623600	0.00077300
C	-4.67263500	2.52838000	0.00039400
C	-4.82375700	1.19108600	0.00036700
H	-1.34957300	2.46583100	0.00105400
H	-5.52005400	3.19911100	0.00035800
H	-5.80710300	0.73094300	0.00027200
N	3.55946000	0.27135300	-0.00110000
C	2.26454000	-0.23358400	-0.00632600
O	2.01210700	-1.42603900	-0.01143300
N	1.27349100	0.72743800	-0.00564100
C	1.43190600	2.10547400	-0.00036900
O	0.45182900	2.84990300	-0.00037500
C	2.80737100	2.54703400	0.00473500
C	3.79020400	1.62373100	0.00416200
H	0.30958100	0.37649100	-0.00863900
H	3.01463700	3.60726100	0.00896400
H	4.83668600	1.91384700	0.00791700
C	4.69124500	-0.67933800	-0.00115600
C	5.54355600	-0.53810100	-1.26453400
C	5.53667200	-0.54627200	1.26771800
H	4.21978500	-1.66374800	-0.00559100
C	6.67267600	-1.57264700	-1.26017900
H	5.98107900	0.46896300	-1.30721900
H	4.90922900	-0.65337400	-2.14835900
C	6.66578700	-1.58081000	1.26284200
H	5.97397800	0.46046600	1.31929100
H	4.89753000	-0.66722100	2.14730800
C	7.52691000	-1.45659400	0.00405800
H	7.29011700	-1.44969000	-2.15477200
H	6.23711900	-2.57860500	-1.31263000
H	7.27833400	-1.46367400	2.16157000
H	6.22994200	-2.58707100	1.30639400
H	8.31013900	-2.22052100	0.00372000
H	8.03509500	-0.48285500	0.00858900
C	-4.01546000	-1.14943900	0.00034200
C	-4.75237300	-1.59068600	1.26714100
C	-4.75241700	-1.59045900	-1.26651400
H	-3.02063400	-1.59801500	0.00028300
C	-4.95434800	-3.10876200	1.26166500
H	-5.73379300	-1.09921200	1.31697900
H	-4.18652000	-1.27344900	2.14803100
C	-4.95436200	-3.10853800	-1.26130200
H	-5.73385700	-1.09901600	-1.31623300
H	-4.18660700	-1.27305000	-2.14737100
C	-5.68987400	-3.56556500	0.00014500
H	-5.50303800	-3.41147900	2.15831800

H	-3.97476300	-3.60109100	1.30923500
H	-5.50305800	-3.41110300	-2.15800300
H	-3.97477100	-3.60084500	-1.30897200
H	-5.80220600	-4.65387100	0.00004900
H	-6.70379100	-3.14307000	0.00018700

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB2

N	3.93369400	0.30339900	-0.00027500
C	2.57996300	0.60900600	-0.00275900
O	1.71080700	-0.25190500	-0.00476200
N	2.28590900	1.95215000	-0.00281900
C	3.18504500	3.02323300	-0.00102400
O	2.77966900	4.17466300	-0.00153600
C	4.57675500	2.61202700	0.00156400
C	4.88033800	1.30066000	0.00176800
H	1.28504900	2.18181200	-0.00431400
H	5.34101500	3.37597900	0.00321100
H	5.91070200	0.95793700	0.00360600
N	-3.88689100	0.41030700	0.00008800
C	-3.98814100	1.79353800	0.00312100
O	-5.04842300	2.39537700	0.00566900
N	-2.77255100	2.44962900	0.00283300
C	-1.49748300	1.89572400	0.00014500
O	-0.51730300	2.63688000	0.00042800
C	-1.48394800	0.45105300	-0.00271700
C	-2.66005300	-0.20871100	-0.00256500
H	-2.83093000	3.46481500	0.00498100
H	-0.52761400	-0.05418200	-0.00472700
H	-2.69372700	-1.29374300	-0.00460700
C	-5.12867200	-0.39150300	0.00028300
C	-5.24690800	-1.24102500	-1.26735300
C	-5.24421300	-1.24437400	1.26592100
H	-5.93192400	0.34775400	0.00210200
C	-6.56412100	-2.02227300	-1.26164500
H	-4.40977000	-1.95065100	-1.31814200
H	-5.17768000	-0.59550800	-2.14794900
C	-6.56139400	-2.02567100	1.26098700
H	-4.40687800	-1.95403100	1.31302800
H	-5.17314000	-0.60117000	2.14806000
C	-6.69481000	-2.87999800	-0.00133800
H	-6.62859400	-2.64409500	-2.15926800
H	-7.40152300	-1.31433500	-1.30703200
H	-6.62389100	-2.64990900	2.15707300
H	-7.39871600	-1.31788800	1.31010300
H	-7.65213500	-3.40963100	-0.00101600
H	-5.90886200	-3.64721500	-0.00322600

C	4.34692900	-1.11498400	-0.00012900
C	5.13107100	-1.47136100	-1.26551600
C	5.12722500	-1.47229600	1.26736400
H	3.40889500	-1.67334100	-0.00175400
C	5.50277000	-2.95694000	-1.26032600
H	6.05076200	-0.87227200	-1.31363800
H	4.53489800	-1.21881400	-2.14740100
C	5.49888500	-2.95789000	1.26218200
H	6.04681700	-0.87332800	1.31873300
H	4.52840100	-1.22038000	2.14763200
C	6.28330600	-3.32895100	0.00199000
H	6.08261500	-3.19653700	-2.15645400
H	4.58464600	-3.55653200	-1.30842700
H	6.07596500	-3.19818700	2.15990600
H	4.58060800	-3.55750100	1.30699600
H	6.51730900	-4.39779400	0.00194900
H	7.24331200	-2.79536000	0.00368000

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.308611	0.558664	0.006781
2	6	0	3.905608	1.883912	-0.062548
3	8	0	4.674230	2.829554	-0.025873
4	7	0	2.539442	2.054012	-0.177899
5	6	0	1.554583	1.075334	-0.239302
6	8	0	0.376633	1.410701	-0.343454
7	6	0	2.061471	-0.275899	-0.169572
8	6	0	3.392036	-0.463146	-0.052829
9	1	0	2.227812	3.020998	-0.224416
10	1	0	1.355488	-1.094399	-0.218929
11	1	0	3.814758	-1.461737	0.001745
12	7	0	-4.265418	-0.421172	-0.054502
13	6	0	-3.138371	0.392414	-0.107915
14	8	0	-3.195415	1.609374	-0.051963
15	7	0	-1.943825	-0.285013	-0.229835
16	6	0	-1.751197	-1.662941	-0.301111
17	8	0	-0.624773	-2.131851	-0.408137
18	6	0	-2.976850	-2.432795	-0.236464
19	6	0	-4.153941	-1.788129	-0.118085
20	1	0	-1.105508	0.307277	-0.276616
21	1	0	-2.916779	-3.510785	-0.283862
22	1	0	-5.093671	-2.330425	-0.064602
23	6	0	-5.592289	0.213111	0.078986

24	6	0	-6.484925	-0.089813	-1.126830
25	6	0	-6.270261	-0.176220	1.394544
26	1	0	-5.381247	1.283882	0.097623
27	6	0	-7.832954	0.622043	-0.982284
28	1	0	-6.658575	-1.172727	-1.197192
29	1	0	-5.974793	0.216708	-2.044922
30	6	0	-7.618624	0.536305	1.529740
31	1	0	-6.435045	-1.262582	1.419363
32	1	0	-5.610774	0.070486	2.231932
33	6	0	-8.522150	0.244139	0.330193
34	1	0	-8.472008	0.379504	-1.836553
35	1	0	-7.670073	1.707096	-1.007011
36	1	0	-8.105733	0.233814	2.461581
37	1	0	-7.446617	1.618059	1.599151
38	1	0	-9.470142	0.781703	0.429160
39	1	0	-8.766479	-0.826745	0.314700
40	6	0	5.753109	0.263361	0.112507
41	6	0	6.080613	-0.506019	1.394105

adenine–thymine WC

N	0.96835300	0.37361400	-0.00022100
C	1.57452800	1.57159800	-0.00016600
N	2.87312100	1.82901100	-0.00002900
C	3.59833800	0.69612400	0.00006100
C	3.11184100	-0.60853200	0.00001600
C	1.70561900	-0.75543300	-0.00013500
N	1.09314700	-1.93823900	-0.00020700
N	4.95527100	0.55494000	0.00017400
C	5.21990600	-0.78934200	0.00031300
N	4.13691800	-1.52846600	0.00011300
H	0.89560700	2.42163200	-0.00026200
H	1.64775400	-2.78612200	-0.00014900
H	0.07548000	-1.99143700	-0.00029300
H	6.23375900	-1.16946900	0.00044500
N	-3.82580900	1.59453200	0.00018700
C	-2.45234200	1.63416100	-0.00041200
O	-1.81279700	2.67490300	0.00011700
N	-1.86596200	0.38835000	-0.00028300
C	-2.51111900	-0.83456600	-0.00013100
O	-1.86437500	-1.88319500	-0.00017600
C	-3.96866700	-0.78847700	0.00007700
C	-4.71790200	-2.08349500	0.00020800
C	-4.55175900	0.42798300	0.00030800
H	-4.30202000	2.49296500	0.00051700
H	-0.82376200	0.37829100	-0.00034000
H	-5.79678100	-1.91054600	0.00043000

H	-4.46153400	-2.68179200	0.87825000
H	-4.46188700	-2.68176300	-0.87795700
H	-5.63064000	0.55398400	0.00065000
H	5.64545600	1.30425800	0.00021200

adenine–uracil WC

N	-0.64423700	-0.28852700	-0.00169600
C	-1.14387500	-1.53473800	-0.00118300
N	-2.41509700	-1.90414200	-0.00018900
C	-3.23592900	-0.83859500	0.00042700
C	-2.86509100	0.50344900	0.00004000
C	-1.47678100	0.77221800	-0.00109400
N	-0.96888200	2.00340800	-0.00142800
N	-4.60013800	-0.81640400	0.00108500
C	-4.98099200	0.49971900	0.00167400
N	-3.96684300	1.33026200	0.00114400
H	-0.39398600	-2.32277900	-0.00171000
H	-1.59436000	2.80047200	-0.00086000
H	0.04047600	2.14439400	-0.00215200
H	-6.02422400	0.78975100	0.00241100
N	4.23750800	-1.09545900	0.00121200
C	2.86734300	-1.24363300	-0.00025300
O	2.31903800	-2.33414200	-0.00086300
N	2.18033700	-0.05194300	-0.00090000
C	2.71972800	1.22585400	-0.00024300
O	1.98194200	2.21100400	-0.00091000
C	4.16904300	1.27790300	0.00130700
C	4.86337000	0.12277200	0.00195400
H	4.78239100	-1.95427700	0.00172800
H	1.14128600	-0.13210300	-0.00186300
H	4.65436400	2.24270100	0.00190300
H	5.94841600	0.09064400	0.00310500
H	-5.22163800	-1.62377300	0.00127200

cytosine–guanine WC

N	-2.18189400	-0.07563300	0.00114600
C	-2.92339700	1.06215700	0.00229600
O	-2.43798300	2.19804200	0.00435000
N	-4.30521100	0.92998700	0.00106000
C	-4.93186100	-0.27634800	-0.00129700
C	-4.20851000	-1.41705800	-0.00247400
C	-2.77839800	-1.27581300	-0.00109100
N	-2.00185000	-2.35436700	-0.00195400
H	-4.84374600	1.79261200	0.00193600
H	-6.01694000	-0.25807200	-0.00212600
H	-4.68007400	-2.39114600	-0.00430700

H	-2.42172300	-3.27837200	-0.00371600
H	-0.98588500	-2.26639800	-0.00056000
N	3.91352700	-1.61253600	0.00176500
C	4.97008600	-0.84293400	0.00065500
N	4.65551900	0.49543500	-0.00095900
C	3.29772600	0.59041900	-0.00084100
N	2.57509500	1.72829200	-0.00209000
C	1.27134100	1.50252900	-0.00162200
N	0.40969400	2.52277000	-0.00339000
N	0.72530800	0.24021000	0.00000500
C	1.44071300	-0.95898800	0.00127500
O	0.84784100	-2.04008900	0.00249500
C	2.85246900	-0.72851400	0.00086900
H	5.99666000	-1.18681000	0.00091200
H	0.80127000	3.45702200	-0.00215900
H	-0.60464800	2.39589500	0.00140700
H	-0.30897100	0.14578400	0.00019600
H	5.31286400	1.27404800	-0.00204900

adenine–thymine stacked structure

N	-1.05108000	-2.23567200	0.29854200
C	-1.04639000	-2.27266000	-1.07056700
N	0.03276100	-1.75011100	-1.60122800
C	0.77100600	-1.34468000	-0.50977200
C	2.01008100	-0.67753600	-0.39009500
N	2.72359300	-0.29965800	-1.46025000
N	2.48693300	-0.42839500	0.84155700
C	1.74517800	-0.78103200	1.89975800
N	0.55636500	-1.37544300	1.92552400
C	0.11685600	-1.63950000	0.68572400
N	-1.81633400	0.92918300	1.29374200
C	-2.34792600	0.52912200	0.09152700
O	-3.38378600	-0.10658800	-0.01010000
N	-1.58670500	0.92013700	-0.99210500
C	-0.35437200	1.57757700	-0.97789800
O	0.24062400	1.79795500	-2.02140700
C	0.11683100	1.96698800	0.35008100
C	-0.62954000	1.61296200	1.41523100
H	-1.91639000	0.59975000	-1.89741500
H	-2.33173500	0.64964100	2.12336600
H	-0.33440900	1.84877300	2.43267000
C	1.40991200	2.71351100	0.44033500
H	2.21216600	2.15101300	-0.04331000
H	1.33882200	3.68157200	-0.06362900
H	1.69264200	2.88031900	1.48220800
H	-1.87501000	-2.69383800	-1.62468300

H	-1.79943100	-2.56309500	0.90397300
H	2.17927200	-0.54192900	2.86843000
H	3.53944000	0.28340100	-1.31297700
H	2.27139000	-0.25534600	-2.36300700

adenine–uracil stacked structure

N	0.37675000	2.22612000	-0.06974400
C	0.29933600	2.04882400	-1.42579900
N	-0.63126000	1.19847600	-1.78641900
C	-1.18999800	0.79723100	-0.59155600
C	-2.20198100	-0.13657700	-0.27701900
N	-2.84733900	-0.83512300	-1.22341400
N	-2.53662000	-0.30633800	1.01371600
C	-1.86977900	0.38681000	1.94636700
N	-0.87933600	1.25897500	1.78925200
C	-0.57984500	1.42685600	0.49222900
N	2.10187800	-0.36126800	1.30678400
C	2.39404800	-0.07375800	-0.00895200
O	3.21990200	0.75760000	-0.34366200
N	1.65752700	-0.82027100	-0.90539200
C	0.63493700	-1.73659900	-0.62626700
O	0.02355800	-2.26951000	-1.53804800
C	0.41989900	-1.95830300	0.79413200
C	1.14354500	-1.26250000	1.69152300
H	2.61735900	0.16951400	2.00363600
H	1.80630800	-0.59848100	-1.88488100
H	-3.42272600	-1.61268400	-0.91981400
H	-2.41737800	-0.91508100	-2.13541500
H	-2.18194100	0.20055400	2.97194500
H	1.03634600	2.82550000	0.42012100
H	0.96531100	2.57132600	-2.10006100
H	1.00732300	-1.36867700	2.76229200
H	-0.35046300	-2.65258000	1.09442700

cytosine–guanine stacked structure

N	1.24675600	-1.12538400	-2.06321000
C	2.41756600	-1.26272200	-1.35975300
N	2.21987900	-1.46121100	-0.08065000
C	0.84786500	-1.45501500	0.05362500
C	0.02703500	-1.54660400	1.22789400
O	0.36318600	-1.66728600	2.39950100
N	-1.33362000	-1.48229400	0.88094100
C	-1.84300200	-1.22184500	-0.36497100
N	-3.19308300	-1.14161800	-0.46052100
N	-1.09281700	-1.10087800	-1.43718700
C	0.22671400	-1.23555800	-1.16885600

N	-0.60251500	2.37184800	-0.95098800
C	-1.16920000	1.82433800	0.20756400
O	-2.39121200	1.73876100	0.28406000
N	-0.30730500	1.41249900	1.18245700
C	1.00265500	1.47941700	0.98475700
N	1.80332200	0.99698300	1.95946900
C	1.59592600	2.03869500	-0.19762200
C	0.73552500	2.46774300	-1.15055500
H	-1.25354300	2.65775800	-1.67755600
H	1.05715900	2.89771300	-2.09456400
H	2.66887100	2.09548500	-0.32612400
H	1.37002700	0.34259200	2.59787400
H	2.75714900	0.76349800	1.70216700
H	-1.97609000	-1.51297700	1.67008600
H	-3.50530300	-0.77706600	-1.35449500
H	-3.66427900	-0.69213300	0.31854600
H	3.38333600	-1.21420200	-1.84619600
H	1.15607200	-0.95277400	-3.06290200

2.1.2) SM8/M06-2X/6-31+G**

adenine–thymine WC

N	0.95092800	0.35417100	-0.00025600
C	1.54732400	1.56094700	0.00012400
N	2.84373000	1.82298400	0.00041800
C	3.57854600	0.69784300	0.00029000
C	3.10190300	-0.61110600	-0.00008900
C	1.69830200	-0.76697400	-0.00034700
N	1.09254100	-1.95961400	-0.00066900
N	4.93902100	0.56686700	0.00047600
C	5.21324800	-0.77811200	0.00036600
N	4.13346300	-1.52276200	-0.00014800
H	0.86356700	2.40574000	0.00012800
H	1.65327200	-2.80550200	-0.00074900
H	0.07560200	-2.02225500	-0.00062500
H	6.23411500	-1.15248300	0.00049900
N	-3.79141900	1.61110800	0.00007700
C	-2.41546300	1.62666000	-0.00100700
O	-1.75863200	2.65797300	-0.00017000
N	-1.84593100	0.37492400	-0.00063000
C	-2.51132700	-0.83741200	-0.00018200
O	-1.86988200	-1.89117700	-0.00012700
C	-3.96961600	-0.77263700	0.00024800
C	-4.73952400	-2.05771700	0.00073000
C	-4.53603000	0.45427400	0.00051000
H	-4.25462700	2.51998900	0.00055600

H	-0.79912400	0.35232000	-0.00058000
H	-5.81779800	-1.86283800	0.00113900
H	-4.49614000	-2.65999500	0.88083800
H	-4.49684400	-2.66022700	-0.87941300
H	-5.61841000	0.59646100	0.00111900
H	5.62398400	1.32609800	0.00073700

adenine–uracil WC

N	-0.63019600	-0.27092200	-0.00259700
C	-1.11978500	-1.52489800	-0.00199200
N	-2.38831600	-1.89947200	-0.00059200
C	-3.21848500	-0.84273900	0.00044000
C	-2.85784500	0.50256400	0.00007800
C	-1.47270400	0.78076800	-0.00156100
N	-0.97492300	2.02168100	-0.00191100
N	-4.58537000	-0.83074200	0.00167700
C	-4.97553000	0.48524400	0.00272500
N	-3.96485200	1.32094700	0.00165000
H	-0.36582800	-2.30783000	-0.00280000
H	-1.60754900	2.81505600	-0.00087700
H	0.03263100	2.17399800	-0.00285900
H	-6.02501100	0.76934800	0.00406300
N	4.22107400	-1.10531600	0.00189900
C	2.84688400	-1.24141400	-0.00025900
O	2.29024100	-2.32851700	-0.00103900
N	2.16545700	-0.04764900	-0.00147500
C	2.71571900	1.22452300	-0.00046900
O	1.97687200	2.21137700	-0.00149900
C	4.16591400	1.27137400	0.00186500
C	4.85619800	0.11040300	0.00294000
H	4.76158300	-1.97069400	0.00283600
H	1.12106700	-0.12019400	-0.00266300
H	4.65962000	2.23513800	0.00269700
H	5.94652700	0.07387100	0.00468600
H	-5.20226100	-1.64620700	0.00206900

cytosine–guanine WC

N	-2.17454500	-0.09133700	0.00310300
C	-2.90158300	1.05361200	0.00533300
O	-2.39417600	2.18283400	0.01020000
N	-4.28603200	0.94679100	0.00155300
C	-4.93126000	-0.25277900	-0.00296600
C	-4.22137700	-1.40574000	-0.00439800
C	-2.78792100	-1.28238500	-0.00100000
N	-2.01754500	-2.36941400	-0.00255500
H	-4.81355000	1.81887600	0.00258800

H	-6.02141200	-0.22094200	-0.00552500
H	-4.71081200	-2.37655200	-0.00818400
H	-2.44212000	-3.29312700	-0.00601900
H	-0.99970700	-2.28143200	-0.00081700
N	3.88676300	-1.63351700	0.00386300
C	4.95405700	-0.87933000	0.00113200
N	4.65691000	0.46688900	0.00047100
C	3.29907200	0.57819300	-0.00095000
N	2.58784600	1.72199400	-0.00339700
C	1.28276000	1.51866200	-0.00441200
N	0.43525000	2.55530400	-0.00888800
N	0.72144000	0.26248000	-0.00133400
C	1.42572300	-0.94397600	0.00078700
O	0.80918300	-2.01555400	0.00265500
C	2.83770700	-0.73660000	0.00094600
H	5.98031100	-1.23711000	0.00210200
H	0.83910100	3.48756000	-0.00368900
H	-0.58084300	2.44061500	0.00110200
H	-0.31111500	0.17141300	-0.00093800
H	5.32641300	1.24018700	0.00000500

adenine-thymine stacked structure

N	-0.71921300	-2.33276900	0.35530100
C	-0.62402800	-2.47297200	-1.00578800
N	0.40419700	-1.84141700	-1.52031200
C	1.01504000	-1.25880700	-0.43145000
C	2.15946100	-0.43857200	-0.30082900
N	2.89666500	-0.06524700	-1.35723300
N	2.51821000	-0.03324300	0.92773100
C	1.76565000	-0.40075700	1.97457200
N	0.66566600	-1.14645100	1.98469000
C	0.33592200	-1.55500900	0.75031200
N	-2.00069000	0.76209900	1.22985800
C	-2.43539700	0.20345900	0.05190000
O	-3.37234600	-0.57706100	-0.01978100
N	-1.70903200	0.61417700	-1.04766300
C	-0.59714100	1.46198900	-1.06473200
O	-0.03742900	1.71543900	-2.12163200
C	-0.20890400	1.99980100	0.23812700
C	-0.92360700	1.61643300	1.31766600
H	-1.97068800	0.18878700	-1.93133100
H	-2.48856700	0.46659700	2.07268500
H	-0.69093300	1.96704000	2.32245400
C	0.96142300	2.93279100	0.29340800
H	1.85374000	2.45570800	-0.11953900

H	0.77015600	3.83685800	-0.29191000
H	1.17717300	3.22290100	1.32653200
H	-1.35133900	-3.05157600	-1.56605300
H	-1.44258400	-2.72978500	0.95179800
H	2.10502700	-0.03471000	2.94135200
H	3.66949800	0.57731800	-1.22338600
H	2.56558600	-0.23633500	-2.29702500

adenine-uracil stacked structure

N	0.29985500	2.23718600	0.08417400
C	0.17361500	2.18209900	-1.28093500
N	-0.74404300	1.33532700	-1.68186100
C	-1.24689600	0.81076100	-0.51095800
C	-2.23580600	-0.16340900	-0.24542700
N	-2.90726800	-0.78485800	-1.22928600
N	-2.51933900	-0.45394200	1.03383100
C	-1.83301600	0.16542500	2.00439700
N	-0.86712700	1.07073400	1.88853100
C	-0.61545300	1.36089500	0.60352400
N	2.16401900	-0.43459100	1.25627800
C	2.42378000	-0.01538500	-0.03171000
O	3.23017500	0.86046700	-0.29941900
N	1.68591300	-0.68316200	-0.98770400
C	0.69796400	-1.65552100	-0.78010900
O	0.09637600	-2.12661300	-1.73384300
C	0.50667000	-2.01574000	0.61464100
C	1.23129800	-1.39346500	1.56738300
H	2.67809000	0.04167600	1.99544800
H	1.81572800	-0.36523700	-1.94296200
H	-3.48540800	-1.58245100	-0.98645200
H	-2.54550000	-0.74177200	-2.17295400
H	-2.10377900	-0.11837000	3.01927200
H	0.95209600	2.82047700	0.60588700
H	0.79602700	2.78950500	-1.93011200
H	1.11987000	-1.61299900	2.62820700
H	-0.23653400	-2.76248700	0.85718900

cytosine-guanine stacked structure

N	1.42001800	-1.07575400	-2.01601400
C	2.58890900	-1.03946600	-1.29014000
N	2.39137300	-1.18873800	-0.00489700
C	1.02547700	-1.33144900	0.11563700
C	0.19742800	-1.46722700	1.28375100
O	0.52955000	-1.49366700	2.46341700
N	-1.15529400	-1.58162300	0.92066300
C	-1.66910300	-1.45432500	-0.34606100

N	-3.02107100	-1.55255900	-0.46609900
N	-0.91731700	-1.29711600	-1.41020800
C	0.40526300	-1.25313900	-1.12395100
N	-0.92619700	2.25461800	-1.01582000
C	-1.39293600	1.68306900	0.17717900
O	-2.59486500	1.44127200	0.28473400
N	-0.47431700	1.42508900	1.14687100
C	0.81329900	1.63695100	0.91680600
N	1.67492900	1.31305100	1.90762700
C	1.31738000	2.19137900	-0.31068900
C	0.39006600	2.48743700	-1.25786900
H	-1.62470000	2.42599100	-1.73752700
H	0.64332000	2.91482000	-2.23036700
H	2.37687000	2.36739400	-0.47122000
H	1.32483000	0.66378800	2.59902800
H	2.64871600	1.17718700	1.65665000
H	-1.80243000	-1.65158300	1.70255400
H	-3.35320000	-1.30096800	-1.39475400
H	-3.56717200	-1.10310400	0.26488100
H	3.55395300	-0.90512100	-1.77007200
H	1.32277500	-0.96739700	-3.02720700

2.2) SM8AD

2.2.1) SM8AD/M06-2X/6-31G**

9-hexyl–adenine–9-hexyl–adenine HB1

N	-2.71983700	3.45398400	-0.61284400
C	-4.01686200	3.44951600	-0.28560700
N	-4.73653300	2.47164400	0.25412300
C	-3.98358500	1.38104000	0.46519700
C	-2.62993700	1.22472300	0.18111700
C	-1.98262900	2.34750800	-0.39165900
N	-0.68899200	2.35577000	-0.71823900
N	-4.38483900	0.18899300	1.01015500
C	-3.27998200	-0.61467200	1.02248300
N	-2.20430700	-0.03750700	0.53855500
H	-4.54946600	4.37558200	-0.49254900
H	-0.06811100	1.55617800	-0.57749600
H	-0.31602600	3.20617700	-1.12404300
H	-3.32751700	-1.62659800	1.41113100
N	1.50201200	0.31964800	-0.50305100
C	2.63181800	0.87638500	-0.96803400
N	3.84069600	0.34268900	-1.06671800
C	3.84704400	-0.92555800	-0.62090900
C	2.76703700	-1.63887600	-0.11136700

C	1.52942900	-0.95405800	-0.05985400
N	0.41378300	-1.51639300	0.40245600
N	4.90570400	-1.79188500	-0.57330100
C	4.41662000	-2.95756500	-0.04046300
N	3.13885600	-2.91453000	0.24958400
H	2.53273500	1.90614400	-1.30806300
H	0.44760500	-2.47146800	0.73804000
H	-0.46278600	-0.99109500	0.43383100
H	5.06420800	-3.81539700	0.10496800
C	6.28128800	-1.49685800	-0.96173000
C	6.99634600	-0.61455900	0.05728700
H	6.25312100	-1.00668900	-1.93874000
H	6.79680200	-2.45577900	-1.07927600
C	8.43416900	-0.32216200	-0.36645700
H	6.43698700	0.32049900	0.16451300
H	6.98634500	-1.11336600	1.03378400
C	9.17665700	0.56526600	0.63023900
H	8.98149100	-1.26714100	-0.48676100
H	8.43294200	0.16157200	-1.35193900
H	8.63161800	1.51049800	0.75181900
H	9.17662800	0.08420300	1.61760900
C	-5.74042900	-0.14946000	1.43405700
C	-6.67140300	-0.39942400	0.25148200
H	-6.11176300	0.67756600	2.04498900
H	-5.66813900	-1.03677000	2.07176600
C	-8.08550800	-0.74248800	0.71515500
H	-6.68711700	0.49752800	-0.37562400
H	-6.26714900	-1.21639700	-0.35828400
C	-9.04541600	-0.98903800	-0.44675300
H	-8.05701500	-1.63423100	1.35632600
H	-8.47284100	0.07395700	1.33842300
H	-9.07298400	-0.09983800	-1.08998900
H	-8.65965400	-1.80561700	-1.07189000
C	10.61618700	0.86120500	0.21382200
C	11.34871900	1.74863700	1.21537000
H	10.61500400	1.34081400	-0.77273700
H	11.15885900	-0.08474300	0.09327800
H	12.37606700	1.94890800	0.90065600
H	10.84224600	2.71177800	1.33101400
H	11.38893100	1.27727300	2.20230700
C	-10.46352500	-1.32898100	0.00779600
C	-11.41447400	-1.57059700	-1.16036100
H	-10.84699200	-0.51361000	0.63346600
H	-10.43371800	-2.21862100	0.64930000
H	-12.42309100	-1.81278400	-0.81590700
H	-11.48462800	-0.68507400	-1.79943100

H -11.06777900 -2.40023700 -1.78437700

9-hexyl–adenine–9-hexyl–adenine HB2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.612470	-3.996904	-0.419617
2	6	0	-3.835260	-3.539581	-0.712036
3	7	0	-4.233904	-2.285426	-0.894339
4	6	0	-3.212937	-1.428363	-0.737091
5	6	0	-1.891452	-1.740247	-0.426224
6	6	0	-1.601101	-3.118237	-0.276167
7	7	0	-0.379234	-3.577379	0.005700
8	7	0	-3.248882	-0.063734	-0.850090
9	6	0	-1.975349	0.370679	-0.596082
10	7	0	-1.127097	-0.595828	-0.338579
11	1	0	-4.602776	-4.303954	-0.816266
12	1	0	0.442716	-2.973872	0.046530
13	1	0	-0.263230	-4.580325	0.093537
14	1	0	-1.732823	1.428077	-0.621878
15	7	0	5.654251	-3.289402	0.352106
16	6	0	6.155003	-2.113003	0.752018
17	7	0	5.520117	-0.962521	0.945992
18	6	0	4.207825	-1.083545	0.694456
19	6	0	3.537234	-2.233219	0.286611
20	6	0	4.337197	-3.382507	0.105309
21	7	0	3.828377	-4.561537	-0.284903
22	7	0	3.243209	-0.113883	0.787061
23	6	0	2.063902	-0.709484	0.433871
24	7	0	2.191202	-1.980553	0.129914
25	1	0	7.227017	-2.104555	0.936968
26	1	0	2.880851	-4.614708	-0.637524
27	1	0	4.465579	-5.315553	-0.509537
28	1	0	1.119288	-0.175474	0.410436
29	6	0	3.460039	1.283797	1.148105
30	6	0	4.149162	2.071681	0.038126
31	1	0	4.064015	1.301650	2.059535
32	1	0	2.479447	1.710975	1.382027
33	6	0	4.362372	3.529588	0.439664
34	1	0	5.110849	1.597245	-0.182731
35	1	0	3.541144	2.017161	-0.872809
36	6	0	5.074410	4.343873	-0.638246
37	1	0	3.392629	3.995209	0.663549
38	1	0	4.946299	3.570135	1.368536
39	1	0	6.045015	3.881294	-0.860617

40	1	0	4.495372	4.301534	-1.570715
41	6	0	-4.425358	0.744888	-1.151410
42	6	0	-5.368281	0.881149	0.040457
43	1	0	-4.942029	0.273800	-1.992080
44	1	0	-4.067428	1.725865	-1.481930
45	6	0	-6.597065	1.712533	-0.321110
46	1	0	-5.670400	-0.120022	0.364130
47	1	0	-4.830929	1.346085	0.875881
48	6	0	-7.572063	1.878222	0.842594
49	1	0	-6.278854	2.704929	-0.669541
50	1	0	-7.117477	1.241617	-1.165244
51	1	0	-7.887519	0.888405	1.197721
52	1	0	-7.056616	2.355658	1.686871
53	6	0	5.288617	5.803657	-0.243278
54	6	0	6.008443	6.606651	-1.322225
55	1	0	5.862088	5.843782	0.691086
56	1	0	4.317135	6.265513	-0.026185
57	1	0	6.154991	7.647033	-1.020494
58	1	0	6.993380	6.180670	-1.537103
59	1	0	5.439057	6.608232	-2.257003
60	6	0	-8.805382	2.700529	0.474249
61	6	0	-9.775666	2.865257	1.639769
62	1	0	-9.318318	2.221356	-0.368728
63	1	0	-8.486861	3.688026	0.117112
64	1	0	-10.650060	3.456577	1.355995
65	1	0	-10.132357	1.893731	1.995387
66	1	0	-9.293902	3.368158	2.484189

9-hexyl–adenine–9-hexyl–adenine HB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.145188	3.450480	0.037833
2	6	0	3.468622	3.478514	-0.158872
3	7	0	4.284862	2.480014	-0.478329
4	6	0	3.612352	1.323607	-0.586151
5	6	0	2.246938	1.126577	-0.402473
6	6	0	1.490256	2.280277	-0.086484
7	7	0	0.168447	2.248214	0.101514
8	7	0	4.121869	0.089472	-0.897360
9	6	0	3.063142	-0.774804	-0.874798
10	7	0	1.918885	-0.199551	-0.585237
11	1	0	3.933066	4.455683	-0.042495
12	1	0	-0.394857	1.423519	-0.106771

13	1	0	-0.299282	3.127698	0.288884
14	1	0	3.197150	-1.830482	-1.088426
15	7	0	-2.145195	-3.450478	0.037743
16	6	0	-3.468631	-3.478505	-0.158954
17	7	0	-4.284870	-2.479995	-0.478382
18	6	0	-3.612358	-1.323588	-0.586189
19	6	0	-2.246941	-1.126568	-0.402521
20	6	0	-1.490260	-2.280276	-0.086561
21	7	0	-0.168449	-2.248219	0.101420
22	7	0	-4.121873	-0.089445	-0.897372
23	6	0	-3.063139	0.774822	-0.874819
24	7	0	-1.918883	0.199561	-0.585270
25	1	0	-3.933079	-4.455672	-0.042578
26	1	0	0.394851	-1.423517	-0.106853
27	1	0	0.299282	-3.127705	0.288773
28	1	0	-3.197143	1.830504	-1.088434
29	6	0	-5.526441	0.227637	-1.139303
30	6	0	-6.347706	0.238076	0.146439
31	1	0	-5.918338	-0.516083	-1.838203
32	1	0	-5.557207	1.205069	-1.632467
33	6	0	-7.812422	0.573466	-0.126290
34	1	0	-6.268117	-0.745640	0.619837
35	1	0	-5.918209	0.969334	0.841839
36	6	0	-8.664184	0.572217	1.141313
37	1	0	-7.882053	1.558378	-0.608225
38	1	0	-8.225381	-0.150058	-0.841230
39	1	0	-8.594127	-0.411210	1.624331
40	1	0	-8.251837	1.294195	1.859059
41	6	0	5.526436	-0.227601	-1.139313
42	6	0	6.347709	-0.238076	0.146423
43	1	0	5.918326	0.516146	-1.838190
44	1	0	5.557201	-1.205015	-1.632511
45	6	0	7.812421	-0.573470	-0.126323
46	1	0	6.268130	0.745629	0.619845
47	1	0	5.918212	-0.969348	0.841810
48	6	0	8.664195	-0.572242	1.141272
49	1	0	7.882043	-1.558374	-0.608273
50	1	0	8.225378	0.150063	-0.841257
51	1	0	8.594153	0.411181	1.624301
52	1	0	8.251847	-1.294223	1.859015
53	6	0	-10.131874	0.904070	0.879286
54	6	0	-10.973618	0.896727	2.151629
55	1	0	-10.541945	0.183443	0.161007
56	1	0	-10.199769	1.887748	0.397783
57	1	0	-12.020086	1.134555	1.944240
58	1	0	-10.944572	-0.084295	2.635848

59	1	0	-10.601685	1.630938	2.873135
60	6	0	10.131878	-0.904108	0.879227
61	6	0	10.973635	-0.896786	2.151563
62	1	0	10.541950	-0.183479	0.160952
63	1	0	10.199759	-1.887782	0.397715
64	1	0	12.020099	-1.134622	1.944161
65	1	0	10.944605	0.084232	2.635791
66	1	0	10.601702	-1.630999	2.873065

9-hexyl–adenine–1-hexyl–thymine WC

N	-0.65827800	-1.76392100	-0.20497600
C	-1.20807900	-0.65696300	-0.73302200
N	-2.49335200	-0.37806500	-0.88154200
C	-3.26736100	-1.37825500	-0.42220300
C	-2.84381200	-2.57542000	0.14813900
C	-1.44578800	-2.75873500	0.25232100
N	-0.88666200	-3.85112700	0.77286400
N	-4.63263700	-1.44108700	-0.41848300
C	-4.95508600	-2.64802900	0.15015900
N	-3.91426300	-3.36378700	0.50309000
H	-0.48872000	0.08536700	-1.07197300
H	-1.48054600	-4.59642600	1.11841200
H	0.12680700	-3.93535600	0.82995600
H	-5.99042100	-2.94648400	0.27163100
N	4.15757200	-0.78451000	-0.62626800
C	2.77813200	-0.73588000	-0.65200500
O	2.15840000	0.22170200	-1.09991500
N	2.15277700	-1.84698900	-0.13851700
C	2.75413300	-2.96052600	0.41426100
O	2.07266200	-3.89207900	0.84982800
C	4.20812600	-2.94056200	0.43950000
C	4.92522100	-4.11490000	1.02822700
C	4.82452300	-1.85540000	-0.07681800
H	1.10636100	-1.82431500	-0.15979100
H	6.00778200	-3.97348500	0.98435600
H	4.67135200	-5.03341500	0.49283700
H	4.63482700	-4.26427700	2.07132200
H	5.90906300	-1.77121800	-0.09194000
C	4.89553800	0.38716100	-1.11491200
C	5.00652800	1.48190000	-0.05939500
H	4.37045500	0.75824900	-1.99625700
H	5.88541300	0.03955300	-1.42596900
C	5.77453700	2.69399700	-0.58157200
H	3.99594000	1.77665100	0.24079600
H	5.50624400	1.07736200	0.83024500
C	5.89397300	3.81140800	0.45246900

H	6.78039500	2.38454500	-0.89721700
H	5.27514900	3.08153200	-1.47895100
H	4.88963900	4.12031700	0.77082200
H	6.39323800	3.42508400	1.35147200
C	6.65801800	5.02884100	-0.06432100
C	6.76951000	6.13979900	0.97513300
H	6.15955100	5.41250200	-0.96301700
H	7.66150600	4.71766100	-0.38068600
H	7.31907700	7.00129700	0.58724500
H	5.77963700	6.48845600	1.28524200
H	7.29058700	5.78882900	1.87140100
C	-5.54628100	-0.39861700	-0.87857000
C	-5.62686700	0.77275700	0.09575500
H	-6.52683000	-0.86588400	-1.01343000
H	-5.19568200	-0.05857100	-1.85675200
C	-6.57646600	1.85728400	-0.40824200
H	-5.96056000	0.40475200	1.07338600
H	-4.62125700	1.18467000	0.22999600
C	-6.67331200	3.04802200	0.54304500
H	-6.24046300	2.20655600	-1.39329400
H	-7.57772800	1.43017200	-0.55654100
H	-7.01074600	2.70081200	1.52897500
H	-5.67252200	3.47291000	0.69596300
C	-7.61623700	4.14074900	0.04327100
C	-7.70454800	5.32578500	0.99985700
H	-8.61554500	3.71384700	-0.10845700
H	-7.27844300	4.48574700	-0.94175400
H	-8.38325500	6.09648500	0.62560200
H	-8.06813500	5.01102900	1.98305100
H	-6.72317000	5.78797200	1.14438700

9-hexyl–adenine–1-hexyl–thymine RWC

N	0.68248000	0.11249000	-0.93565100
C	1.76568000	0.88960000	-0.76178100
N	3.03922000	0.53882000	-0.84502100
C	3.16802000	-0.76662000	-1.14332100
C	2.14568000	-1.68930000	-1.34917100
C	0.82634000	-1.19419000	-1.23328100
N	-0.25841000	-1.95210000	-1.40248100
N	4.32751000	-1.47209000	-1.31476100
C	3.94948000	-2.75912000	-1.60228100
N	2.65092000	-2.93682000	-1.63669100
H	1.54033000	1.92722000	-0.52510100
H	-0.14911000	-2.93347000	-1.62847100
H	-1.18772000	-1.54776000	-1.30792100
H	4.69242000	-3.52816000	-1.78454100

N	-4.09773000	1.33621000	-0.66601100
C	-2.90555000	0.66183000	-0.80725100
O	-2.86348000	-0.54205000	-1.06461100
N	-1.78019000	1.42236000	-0.64440100
C	-1.72059000	2.77223000	-0.32590100
O	-0.63806000	3.33472000	-0.20010100
C	-3.01508000	3.42446000	-0.16093100
C	-3.03080000	4.87964000	0.18701900
C	-4.12244000	2.67432000	-0.33472100
H	-0.86735000	0.92009000	-0.75783100
H	-4.05492000	5.24874000	0.28507900
H	-2.51944000	5.46655000	-0.58008100
H	-2.50296000	5.05816000	1.12710900
H	-5.11923000	3.09725000	-0.22652100
C	-5.34510000	0.56998000	-0.77743100
C	-5.71177000	-0.12987000	0.52676900
H	-5.21073000	-0.15825000	-1.57856100
H	-6.12901000	1.27143000	-1.08003100
C	-7.01291000	-0.91877000	0.39802900
H	-4.89104000	-0.79913000	0.80391900
H	-5.80544000	0.61818000	1.32443900
C	-7.40503000	-1.63095000	1.69083900
H	-7.82511000	-0.24281000	0.09719900
H	-6.91236000	-1.65758000	-0.40753100
H	-6.59330000	-2.30449000	1.99553900
H	-7.50715000	-0.89256000	2.49758900
C	-8.70332000	-2.42633000	1.56854900
C	-9.08649000	-3.13223000	2.86552900
H	-8.59994000	-3.16403000	0.76330900
H	-9.51273000	-1.75164000	1.26279900
H	-10.01675000	-3.69589000	2.75826900
H	-8.30633000	-3.83376000	3.17658900
H	-9.22537000	-2.41277000	3.67853900
C	5.68360000	-0.95399000	-1.16024100
C	6.06432000	-0.75345000	0.30361900
H	5.74069000	-0.00701000	-1.70359100
H	6.35861000	-1.66559000	-1.64716100
C	7.48501000	-0.21101000	0.44376900
H	5.34924000	-0.06088000	0.75909900
H	5.97330000	-1.70988000	0.83240900
C	7.89544000	0.00393000	1.89898900
H	8.19208000	-0.90384000	-0.03288100
H	7.56818000	0.73861000	-0.10059100
H	7.18888000	0.69453000	2.37759900
H	7.81170000	-0.94522000	2.44539900
C	9.31494000	0.54789000	2.04828900

C	9.71473000	0.75893000	3.50532900
H	9.39743000	1.49549000	1.50188900
H	10.01902000	-0.14387000	1.56902900
H	10.73256000	1.14781000	3.59187900
H	9.04381000	1.46942000	3.99787900
H	9.66855000	-0.18019000	4.06554900

9-hexyl–adenine–1-hexyl–thymine H

N	-3.65321300	-3.98128700	0.73640700
C	-4.65989900	-3.17062400	0.38599500
N	-4.60576600	-1.95635100	-0.15180400
C	-3.33520200	-1.56732900	-0.33560000
C	-2.18853000	-2.28967300	-0.02479600
C	-2.38586300	-3.57050500	0.54358500
N	-1.37497700	-4.37292100	0.88912900
N	-2.89020600	-0.38355500	-0.87052600
C	-1.52686900	-0.44072200	-0.85229400
N	-1.06537800	-1.56635600	-0.35673200
H	-5.65658100	-3.56630100	0.57018100
H	-0.39802000	-4.11148700	0.77680500
H	-1.60101100	-5.27247600	1.29677500
H	-0.90124400	0.36620600	-1.21870800
N	3.74341400	-0.86133000	-0.66805800
C	2.36527900	-0.77071100	-0.70425500
O	1.77818500	0.21715600	-1.12932000
N	1.70359700	-1.87674400	-0.22852600
C	2.26360600	-3.02220700	0.29897700
O	1.54859100	-3.94122200	0.70325000
C	3.71804800	-3.04736500	0.33661700
C	4.39336200	-4.25892500	0.89867300
C	4.37159900	-1.96731600	-0.14303000
H	0.66055800	-1.81658600	-0.25710300
H	5.48027200	-4.14836600	0.87168600
H	4.11977300	-5.15349100	0.33355400
H	4.08566200	-4.42961400	1.93332900
H	5.45869200	-1.91681400	-0.14535300
C	4.51940200	0.30283100	-1.11199300
C	4.65290400	1.35794900	-0.01926900
H	4.01310100	0.71807500	-1.98466200
H	5.50174700	-0.06308800	-1.42706000
C	5.46516000	2.56184000	-0.49130300
H	3.64876700	1.67482300	0.27985300
H	5.12878300	0.90803400	0.86154300
C	5.60450300	3.63988000	0.58141000
H	6.46521400	2.23172200	-0.80423600
H	4.99070400	2.99467700	-1.38151300

H	4.60588800	3.97024600	0.89609200
H	6.07761800	3.20793600	1.47367100
C	6.41425300	4.84893400	0.11706900
C	6.54472600	5.92016600	1.19534300
H	5.94190700	5.27858100	-0.77492800
H	7.41214200	4.51686100	-0.19552400
H	7.12634200	6.77653000	0.84470900
H	5.56170200	6.28923300	1.50360200
H	7.04135300	5.52305400	2.08615600
C	-3.72937500	0.72729800	-1.31282500
C	-4.31342500	1.51233200	-0.14230600
H	-4.52876300	0.31008500	-1.93112600
H	-3.10791500	1.36861300	-1.94592000
C	-5.19260600	2.66385200	-0.62540400
H	-4.89713100	0.82780500	0.48162000
H	-3.49386700	1.89841800	0.47545200
C	-5.79274200	3.47229200	0.52287100
H	-4.60326100	3.33159700	-1.26861400
H	-6.00222400	2.26664400	-1.25143900
H	-6.37930400	2.80610100	1.16900900
H	-4.98377100	3.87071100	1.14993200
C	-6.67651400	4.62406800	0.04792700
C	-7.26946800	5.42643500	1.20198700
H	-7.48438800	4.22465400	-0.57753100
H	-6.08846300	5.28725100	-0.59879300
H	-7.89801500	6.24532700	0.84267100
H	-7.88576800	4.79174100	1.84615800
H	-6.48110200	5.86063200	1.82476200

9-hexyl–adenine–1-hexyl–thymine RH

N	1.51176700	-3.87197200	-0.41869500
C	2.79214700	-3.84875400	-0.02602600
N	3.50925300	-2.82391300	0.42365200
C	2.77673200	-1.70063100	0.45711700
C	1.44440800	-1.56373900	0.08403600
C	0.79562600	-2.73341300	-0.37652200
N	-0.48300100	-2.74509400	-0.76558300
N	3.17361200	-0.45127100	0.86658500
C	2.09016800	0.36521000	0.71858100
N	1.03296300	-0.26161600	0.25539000
H	3.31125900	-4.80304600	-0.08645900
H	-1.06985900	-1.91491900	-0.75275800
H	-0.87622300	-3.62249000	-1.08499200
H	2.11135800	1.42088400	0.96710400
N	-3.47148000	1.52721800	-0.77782700
C	-2.39941400	0.68075300	-0.60387600

O	-2.46555700	-0.52119500	-0.86238400
N	-1.26184100	1.27117900	-0.12777300
C	-1.08928200	2.60281300	0.22132000
O	-0.00846500	2.99925900	0.64552400
C	-2.26789200	3.44314600	0.04273400
C	-2.16240700	4.89210600	0.40128000
C	-3.38546500	2.86097000	-0.43936100
H	-0.43630900	0.64332900	0.00049800
H	-3.10743200	5.41065000	0.22146000
H	-1.37944400	5.38009500	-0.18468900
H	-1.89281200	5.01202300	1.45359600
H	-4.29991300	3.42909900	-0.59763200
C	-4.74092600	0.95111000	-1.23867700
C	-5.54436700	0.33632100	-0.09774900
H	-4.50337700	0.19641900	-1.98981500
H	-5.30240900	1.75449600	-1.72580900
C	-6.85792600	-0.26510700	-0.59257500
H	-4.93327600	-0.43594700	0.38022300
H	-5.74681900	1.10600000	0.65803900
C	-7.67972000	-0.89825300	0.52821700
H	-7.45719100	0.51313600	-1.08478500
H	-6.64567900	-1.02168600	-1.35898700
H	-7.07975700	-1.67044200	1.02734200
H	-7.89871500	-0.14086000	1.29300600
C	-8.98947300	-1.51321400	0.03879200
C	-9.80109300	-2.14530100	1.16532500
H	-8.76979200	-2.26791600	-0.72633800
H	-9.58835300	-0.73968400	-0.45804500
H	-10.73304000	-2.58051800	0.79574200
H	-9.23498300	-2.94111600	1.65899100
H	-10.05972300	-1.40377500	1.92767000
C	4.51325200	-0.08078300	1.31641300
C	5.50556800	0.01204300	0.16139700
H	4.83748500	-0.83359100	2.04007500
H	4.42417400	0.87745500	1.83792100
C	6.90221700	0.38535400	0.65379300
H	5.53285100	-0.95334300	-0.35427100
H	5.14923400	0.75750600	-0.55934700
C	7.92443900	0.47333700	-0.47733000
H	6.86107400	1.34861800	1.18026800
H	7.23931600	-0.35560100	1.39042500
H	7.96187300	-0.48670400	-1.00862500
H	7.59068500	1.21670100	-1.21373300
C	9.32612300	0.83836000	0.00777300
C	10.34084000	0.91759200	-1.12856800
H	9.65624300	0.09791000	0.74680600

H	9.28664400	1.79983200	0.53480100
H	11.33687600	1.17912100	-0.76221200
H	10.41964900	-0.03998400	-1.65241400
H	10.04831700	1.67259900	-1.86497100

1-hexyl–thymine–1-hexyl–thymine HB1

N	4.13593400	-0.82573500	-0.99307600
C	3.22330100	0.21006500	-0.97651800
O	3.55589700	1.38512700	-0.95836300
N	1.90181500	-0.19181800	-0.98506000
C	1.42795700	-1.49113500	-0.97451800
O	0.21556800	-1.72154500	-0.97357300
C	2.44122100	-2.53077600	-0.96330200
C	1.99366000	-3.95891200	-0.94904000
C	3.73421200	-2.14017200	-0.96895200
H	1.19867200	0.55757600	-0.98094700
H	2.85178600	-4.63529500	-0.93991100
H	1.38136100	-4.18331500	-1.82598100
H	1.37735100	-4.16441400	-0.07030400
H	4.54602900	-2.86441600	-0.96090100
N	-4.13600800	0.82733000	-0.99188500
C	-3.22341000	-0.20852400	-0.97688300
O	-3.55605900	-1.38359400	-0.96029500
N	-1.90190900	0.19331600	-0.98510800
C	-1.42799600	1.49260000	-0.97290100
O	-0.21559600	1.72296600	-0.97196300
C	-2.44121900	2.53225700	-0.96014100
C	-1.99360000	3.96035700	-0.94404700
C	-3.73422900	2.14171300	-0.96608400
H	-1.19881700	-0.55612200	-0.98198200
H	-2.85169600	4.63676000	-0.93368200
H	-1.38159800	4.18596400	-1.82088800
H	-1.37697800	4.16460400	-0.06524000
H	-4.54600500	2.86598700	-0.95688400
C	-5.56265900	0.48100500	-0.93510500
C	-6.03275400	0.20267200	0.48834000
H	-5.70974500	-0.39730700	-1.56508500
H	-6.11551300	1.31645200	-1.37513000
C	-7.51693400	-0.15375000	0.53300600
H	-5.43559100	-0.61920900	0.89587300
H	-5.84149400	1.08563400	1.11174200
C	-8.01338800	-0.44808800	1.94688500
H	-8.10660300	0.66953300	0.10681500
H	-7.70019900	-1.02762600	-0.10540000
H	-7.42400600	-1.26963500	2.37488400
H	-7.82942100	0.42503800	2.58762200

C	-9.49677100	-0.80822800	2.00004400
C	-9.98105500	-1.10327400	3.41624300
H	-9.67969900	-1.67886000	1.35827800
H	-10.08380100	0.01479500	1.57347800
H	-11.04378700	-1.35803200	3.43422200
H	-9.43026600	-1.94196800	3.85306500
H	-9.83533300	-0.23754800	4.06992100
C	5.56258200	-0.47947600	-0.93589800
C	6.03275900	-0.20329800	0.48793900
H	5.70958100	0.39979800	-1.56454500
H	6.11542400	-1.31423800	-1.37724100
C	7.51700200	0.15278500	0.53311600
H	5.43574000	0.61809300	0.89667700
H	5.84135200	-1.08712300	1.11007100
C	8.01343800	0.44527400	1.94738400
H	8.10652600	-0.67008700	0.10593100
H	7.70047400	1.02741500	-0.10419500
H	7.42433000	1.26654700	2.37628400
H	7.82907200	-0.42852500	2.58709000
C	9.49695300	0.80478100	2.00110000
C	9.98121400	1.09806400	3.41767000
H	9.68028500	1.67605500	1.36032300
H	10.08370600	-0.01799400	1.57367600
H	11.04406400	1.35230800	3.43603600
H	9.43077400	1.93654300	3.85534500
H	9.83501700	0.23169900	4.07039400

1-hexyl–thymine–1-hexyl–thymine HB2

N	-4.97312800	0.19726200	-0.25496400
C	-3.95521700	-0.48293300	-0.90100900
O	-4.03585100	-1.65576500	-1.23154300
N	-2.81866900	0.26698700	-1.12621100
C	-2.60283000	1.58149600	-0.75933200
O	-1.50490600	2.11343100	-0.94411500
C	-3.73593800	2.26015700	-0.15291700
C	-3.58996300	3.70523700	0.20796200
C	-4.84194600	1.52258300	0.08717500
H	-2.00563700	-0.25261000	-1.48716400
H	-4.49338500	4.07731700	0.69754400
H	-3.40080600	4.31281800	-0.68049800
H	-2.74090200	3.85033900	0.87975000
H	-5.71059500	1.95060800	0.58505100
N	3.19215400	0.28007000	-0.83656300
C	2.12995300	1.16524700	-0.83855900
O	2.25467500	2.34720900	-0.56148300
N	0.91771700	0.60324600	-1.18896400

C	0.67358500	-0.72476300	-1.48637100
O	-0.46427100	-1.11227300	-1.76668700
C	1.82920300	-1.60286800	-1.44823400
C	1.62618400	-3.05288400	-1.75881900
C	3.01862500	-1.05314400	-1.12006400
H	0.10474500	1.23122700	-1.16487400
H	2.56698400	-3.60340300	-1.68064300
H	1.22757000	-3.18295000	-2.76776300
H	0.90215200	-3.49755200	-1.07113900
H	3.92615300	-1.65260400	-1.07143000
C	4.50696900	0.79679500	-0.43252000
C	4.63339700	0.91708300	1.08633100
H	4.62561500	1.77942500	-0.89211800
H	5.25545300	0.12530300	-0.86096500
C	5.98559800	1.49173200	1.53799400
H	3.82730200	1.57821900	1.41428700
H	4.45431900	-0.05951500	1.55383700
C	7.12257900	0.48950200	1.77492600
H	6.31534600	2.24060700	0.80526800
H	5.82962800	2.04175800	2.47108200
H	7.98190600	1.05845200	2.14500400
H	6.83903900	-0.19037500	2.58954100
C	7.55675700	-0.34309200	0.55710400
C	6.82250500	-1.67843800	0.43037800
H	8.62914300	-0.55286900	0.62433000
H	7.43292100	0.25382900	-0.35564100
H	7.07742900	-2.19297500	-0.50076400
H	7.08780800	-2.34137800	1.25892800
H	5.73566100	-1.55562100	0.46405200
C	-6.06521200	-0.59316000	0.33575100
C	-5.76320800	-1.02807100	1.77330200
H	-6.21024900	-1.45959700	-0.30826500
H	-6.96999000	0.02140700	0.29811100
C	-4.48183600	-1.86504300	1.92203600
H	-5.70761200	-0.14371000	2.42241500
H	-6.63075700	-1.60582100	2.11058300
C	-3.19436700	-1.03232100	2.06996000
H	-4.57728500	-2.51567500	2.79765200
H	-4.39057100	-2.52553000	1.05417700
H	-3.28543400	-0.07057500	1.55122700
H	-3.05011100	-0.76903800	3.12624100
C	-1.94444700	-1.73978100	1.54463100
C	-0.70234500	-0.85775300	1.62418300
H	-2.11203900	-2.03770500	0.50279400
H	-1.78435000	-2.66640400	2.11098400
H	0.18767100	-1.37863000	1.25677500

H	-0.82786400	0.04948700	1.02164300
H	-0.50121600	-0.54350900	2.65408300

1-hexyl–thymine–1-hexyl–thymine HB3

N	-3.98150400	-0.35301200	0.37145000
C	-2.98171500	0.58589700	0.54421000
O	-3.17973200	1.67530300	1.05803900
N	-1.73936800	0.18727400	0.09109500
C	-1.42499400	-1.00899100	-0.52711000
O	-0.27156200	-1.24645600	-0.89409800
C	-2.52893400	-1.93657700	-0.70578100
C	-2.25355800	-3.24710100	-1.37423200
C	-3.74156300	-1.55503800	-0.25024600
H	-0.97124900	0.85978500	0.21549000
H	-3.16478100	-3.84667000	-1.44448200
H	-1.50293100	-3.81589400	-0.81985800
H	-1.85679900	-3.09427300	-2.38088000
H	-4.61348600	-2.19985200	-0.34785100
N	4.19879400	1.06719600	-1.07903500
C	3.20890600	0.11004500	-1.20853200
O	3.39492300	-0.98075200	-1.72282500
N	1.97969400	0.49258300	-0.70487500
C	1.66841100	1.68660300	-0.08233900
O	0.52746400	1.90376300	0.33365700
C	2.75946100	2.63867600	0.03701600
C	2.48534600	3.95357500	0.69715900
C	3.95789800	2.27421900	-0.46719800
H	1.21855600	-0.19240800	-0.79846300
H	3.38398900	4.57552400	0.71383100
H	2.14169000	3.80828700	1.72434300
H	1.69493700	4.49487400	0.17148200
H	4.81896100	2.93916000	-0.42021800
C	5.55221100	0.75420600	-1.56116700
C	6.49165600	0.31465300	-0.44153100
H	5.93643600	1.65175900	-2.05612800
H	5.44306300	-0.03075400	-2.30881500
C	6.03445500	-0.94982900	0.28428000
H	7.47733000	0.16030400	-0.89493000
H	6.60722100	1.13189200	0.28450600
C	6.96486700	-1.36571900	1.42601700
H	5.02791000	-0.78927900	0.68720400
H	5.93936400	-1.76995800	-0.43739500
H	7.03188100	-0.55012800	2.15973300
H	6.51671500	-2.21461500	1.95628700
C	8.37420200	-1.75528300	0.97893600
C	9.22478900	-2.28286500	2.13025700

H	8.87681900	-0.89132300	0.52784300
H	8.30285200	-2.51612900	0.19103300
H	10.22968500	-2.55569900	1.79747800
H	9.32884700	-1.53049600	2.91865000
H	8.77026600	-3.17069000	2.58063700
C	-5.34027600	0.01149700	0.79267200
C	-6.05368000	0.86338900	-0.25578400
H	-5.25385700	0.56415800	1.72992600
H	-5.87072200	-0.92327500	0.99429900
C	-7.47716600	1.27126200	0.15926200
H	-5.43771500	1.75241300	-0.41431200
H	-6.08063100	0.31714100	-1.20850100
C	-8.58382300	0.34541600	-0.35966700
H	-7.53169600	1.35446900	1.25231000
H	-7.67903900	2.27740100	-0.21972500
H	-9.55524800	0.75126500	-0.05078100
H	-8.57279700	0.37711400	-1.45609000
C	-8.49733100	-1.11423200	0.09325700
C	-8.63263900	-1.29798000	1.60301900
H	-7.55532100	-1.55534600	-0.25986500
H	-9.28996500	-1.68161900	-0.40655300
H	-8.60906300	-2.35558800	1.87908400
H	-7.83232600	-0.79700900	2.15666900
H	-9.58008500	-0.88263900	1.96043600

9-ethyl–adenine–1-cyclohexyl–uracil WC

N	1.73754600	0.34642900	-0.02255800
C	1.99795800	-0.97219600	-0.03951700
N	3.17948300	-1.56859100	-0.05094300
C	4.18104600	-0.67080000	-0.04213100
C	4.06644100	0.71572400	-0.02405900
C	2.75160400	1.23567900	-0.01353300
N	2.47958500	2.54042500	0.00419600
N	5.52405500	-0.92474700	-0.04487000
C	6.13976100	0.30314500	-0.03126100
N	5.30404300	1.31521000	-0.01690000
H	1.11373800	-1.60577700	-0.04441700
H	3.24310900	3.20711300	0.01191800
H	1.51433700	2.86635100	0.01197100
H	7.21849000	0.39495700	-0.02648000
N	-3.20287900	0.39865600	0.00548800
C	-1.86219400	0.03812200	-0.00738900
O	-1.48386700	-1.12605000	-0.02489600
N	-0.97815300	1.09016800	0.00100400
C	-1.27637000	2.44194300	0.02115100
O	-0.37396300	3.28123400	0.02689800

C	-2.69094700	2.74086600	0.03416600
C	-3.57320800	1.72051500	0.02601200
H	0.03295000	0.82070000	-0.00847200
H	-3.00892000	3.77371500	0.05040300
H	-4.64466000	1.89970300	0.03561300
C	-4.23046200	-0.66390200	-0.00085300
C	-5.07647700	-0.63152600	1.27422500
C	-5.10007500	-0.59438200	-1.25848400
H	-3.66109000	-1.59495600	-0.01991900
C	-6.09921400	-1.77152000	1.26208400
H	-5.61008700	0.32673200	1.34127900
H	-4.42228600	-0.69983000	2.14832000
C	-6.12248400	-1.73476000	-1.26056200
H	-5.63501100	0.36500600	-1.28766300
H	-4.46230100	-0.63678500	-2.14624300
C	-6.97618100	-1.71579800	0.00928000
H	-6.71456500	-1.72588600	2.16533900
H	-5.56726400	-2.73099300	1.29010500
H	-6.75432300	-1.66326600	-2.15065900
H	-5.59112700	-2.69273300	-1.32618200
H	-7.68300200	-2.55086600	0.00365700
H	-7.57472600	-0.79496700	0.02828300
C	6.12676200	-2.26167800	-0.08213100
C	7.61851200	-2.22941500	0.19705800
H	5.92300900	-2.69930300	-1.06330200
H	5.60032300	-2.86761600	0.65854400
H	7.99677800	-3.25341100	0.20645200
H	8.16387200	-1.68279100	-0.57622300
H	7.83278900	-1.77952600	1.16939600

9-ethyl–adenine–1-cyclohexyl–uracil RWC

N	1.77507300	0.37934900	-0.00281200
C	2.65245400	1.39829600	-0.00133000
N	3.97445700	1.33155400	-0.00072900
C	4.39949000	0.05571700	-0.00172000
C	3.61538500	-1.09415300	-0.00319100
C	2.21576400	-0.89416400	-0.00372500
N	1.33188500	-1.89379400	-0.00510900
N	5.69373100	-0.38793000	-0.00133500
C	5.62207600	-1.75911700	-0.00264300
N	4.39598200	-2.22663900	-0.00384400
H	2.19435300	2.38501000	-0.00058200
H	1.66220100	-2.85140800	-0.00589800
H	0.33425000	-1.69408200	-0.00576100
H	6.51503300	-2.37192000	-0.00241600
N	-3.17364600	0.54934200	-0.00101900

C	-1.85030400	0.14222500	-0.00221900
O	-1.52563700	-1.04478500	-0.00361700
N	-0.92471200	1.14888600	-0.00180500
C	-1.16255700	2.52042700	0.00052400
O	-0.22597700	3.31009400	0.00080300
C	-2.57016000	2.87053000	0.00219700
C	-3.49147800	1.88778200	0.00149900
H	0.07733600	0.84380600	-0.00263600
H	-2.84878900	3.91514800	0.00408500
H	-4.55527400	2.10939800	0.00284300
C	-4.24309300	-0.47099700	-0.00073200
C	-5.09517500	-0.38801800	1.26834400
C	-5.10212100	-0.38184200	-1.26469600
H	-3.71332900	-1.42531300	-0.00459500
C	-6.16254800	-1.48638900	1.26356300
H	-5.59014400	0.59161200	1.31960800
H	-4.45003200	-0.47102800	2.14780000
C	-6.16928500	-1.48044400	-1.25929600
H	-5.59774300	0.59778500	-1.30862100
H	-4.46182000	-0.46047200	-2.14808800
C	-7.02932500	-1.41178900	0.00460700
H	-6.78068600	-1.40493600	2.16232700
H	-5.66965400	-2.46596000	1.30671600
H	-6.79222500	-1.39489800	-2.15435900
H	-5.67650000	-2.45972500	-1.30964500
H	-7.76832300	-2.21848200	0.00469300
H	-7.59119200	-0.46806000	0.00833200
C	6.87624100	0.47924200	-0.00124100
C	8.17187200	-0.31130800	0.01424900
H	6.80491900	1.13173500	0.87255500
H	6.81738200	1.11714900	-0.88675300
H	9.00937300	0.38895500	0.01668500
H	8.25297500	-0.93362400	0.90884800
H	8.26796900	-0.94452800	-0.87118600

9-ethyl–adenine–1-cyclohexyl–uracil H

N	5.23446100	-1.74604300	-0.01787800
C	5.95140200	-0.61994800	-0.12214400
N	5.52533400	0.63542300	-0.21803200
C	4.18504300	0.69178200	-0.19996700
C	3.30626600	-0.38087500	-0.09611200
C	3.89060000	-1.66648400	-0.00211700
N	3.16798100	-2.78528900	0.10050700
N	3.39252100	1.80959500	-0.28475900
C	2.10154600	1.37196500	-0.22343100
N	2.00442000	0.06657800	-0.11274600

H	7.03060600	-0.75861300	-0.12841100
H	2.15040100	-2.78866700	0.11492300
H	3.66456800	-3.66635000	0.16216600
H	1.25213700	2.04523500	-0.26774600
N	-2.83812600	-0.53908800	0.02793300
C	-1.53408500	-0.06453500	-0.03532900
O	-1.25937700	1.12425900	-0.13491400
N	-0.56208800	-1.03307700	0.02231800
C	-0.73650500	-2.40062100	0.13466400
O	0.23795500	-3.15204800	0.17595900
C	-2.11950700	-2.82101300	0.19431700
C	-3.08847400	-1.88436900	0.13898100
H	0.41772200	-0.67428400	-0.02427200
H	-4.13964400	-2.15708800	0.18071600
H	-2.34535300	-3.87440500	0.28209100
C	-3.95403800	0.42814100	-0.02518500
C	-4.82814700	0.20829200	-1.26239500
C	-4.78091900	0.40058600	1.26273200
H	-3.46763000	1.40185400	-0.10841500
C	-5.94433600	1.25568700	-1.31601000
H	-5.27846600	-0.79338100	-1.22538200
H	-4.20649100	0.25069500	-2.16146900
C	-5.89706600	1.44735300	1.19932500
H	-5.23025100	-0.59348800	1.39444000
H	-4.12612900	0.57620400	2.12125700
C	-6.77971700	1.24242200	-0.03388700
H	-6.57739900	1.07715400	-2.19000500
H	-5.49745600	2.24937500	-1.44722100
H	-6.49640200	1.40463800	2.11335900
H	-5.44858200	2.44826200	1.16199800
H	-7.55454200	2.01347200	-0.07822900
H	-7.29822800	0.27775900	0.04934600
C	3.86217300	3.19204200	-0.37231800
H	4.61223500	3.23333400	-1.16528000
H	3.00595100	3.79832800	-0.68067800
C	4.44289600	3.67901900	0.94721800
H	5.29860300	3.06661600	1.23441100
H	4.77755300	4.71419400	0.84119100
H	3.69386600	3.63811300	1.74138300

9-ethyl–adenine–1-cyclohexyl–uracil RH

N	3.54739700	-3.10712100	-0.04789900
C	4.81348600	-2.67182300	-0.09014500
N	5.26567300	-1.42302700	-0.14444300
C	4.25302900	-0.54314400	-0.15491800
C	2.89456900	-0.83695600	-0.11525100

C	2.54737400	-2.20690500	-0.05945700
N	1.27993800	-2.62986200	-0.01897000
N	4.33081900	0.82663400	-0.21205300
C	3.04612100	1.28665100	-0.19859000
N	2.15502700	0.32314400	-0.14365000
H	5.57109200	-3.45266200	-0.07759800
H	0.48813800	-1.99261900	-0.01893800
H	1.11116300	-3.62789100	0.02440600
H	2.79810200	2.34209200	-0.23521600
N	-2.79476800	0.66238700	-0.03219600
C	-1.49960600	0.17254100	-0.04902900
O	-1.24599600	-1.03039300	-0.01120400
N	-0.51624200	1.11946600	-0.11060400
C	-0.66575200	2.50181700	-0.15384700
O	0.32058300	3.22760400	-0.20550600
C	-2.04761600	2.94055900	-0.13053900
C	-3.02763000	2.01751600	-0.07101800
H	0.46407100	0.75864600	-0.12104900
H	-4.07506200	2.30578300	-0.05020800
H	-2.26255600	3.99965600	-0.16043700
C	-3.92464800	-0.28799300	0.03981900
C	-4.71785000	-0.11408500	1.33739800
C	-4.82607300	-0.18153900	-1.19283600
H	-3.45499700	-1.27330600	0.04578600
C	-5.85206300	-1.14085700	1.40803400
H	-5.14643000	0.89699100	1.37667600
H	-4.04424900	-0.21369400	2.19350700
C	-5.95872100	-1.20937500	-1.11154300
H	-5.26193100	0.82547400	-1.24912400
H	-4.22778100	-0.32652200	-2.09704700
C	-6.76170000	-1.04746700	0.18101400
H	-6.42754400	-0.99395800	2.32654900
H	-5.42071600	-2.14844200	1.46321300
H	-6.61005600	-1.11142600	-1.98481200
H	-5.53071600	-2.21921900	-1.14821500
H	-7.55012300	-1.80394700	0.23508500
H	-7.26174200	-0.06955400	0.17556900
C	5.56100500	1.61802800	-0.23065600
H	6.20825700	1.19908100	-1.00443400
H	5.28040800	2.63102000	-0.53179600
C	6.25981300	1.61203200	1.12106500
H	6.53699300	0.59472500	1.40049500
H	7.16869300	2.21683900	1.06713600
H	5.61295000	2.02991100	1.89584000

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB1

N	-3.76787800	0.30913400	0.00066900
C	-2.46723500	0.77008000	0.00095000
O	-1.50097600	0.00701600	0.00141100
N	-2.32117700	2.13271900	0.00080100
C	-3.33609800	3.09669400	0.00063200
O	-3.05978000	4.28638000	0.00075300
C	-4.67099200	2.53004100	0.00049500
C	-4.82390100	1.19262000	0.00052800
H	-1.34896300	2.46332400	0.00106300
H	-5.51720200	3.20266200	0.00042100
H	-5.80803200	0.73312000	0.00045200
N	3.56177800	0.26848100	-0.00129600
C	2.26815300	-0.23539800	-0.00695000
O	2.01403700	-1.42899700	-0.01239700
N	1.27679500	0.72515300	-0.00631900
C	1.43561500	2.10281600	-0.00066200
O	0.45405000	2.84759600	-0.00071400
C	2.81018300	2.54440100	0.00486000
C	3.79330000	1.62078500	0.00430000
H	0.31300500	0.37451100	-0.00952000
H	3.01688700	3.60496800	0.00938700
H	4.84034100	1.91074700	0.00834200
C	4.69450200	-0.68205200	-0.00126800
C	5.54652500	-0.53881200	-1.26462200
C	5.53919300	-0.54730200	1.26792700
H	4.22432400	-1.66700300	-0.00590700
C	6.67700700	-1.57203100	-1.26016200
H	5.98285300	0.46880500	-1.30636000
H	4.91233000	-0.65443400	-2.14840900
C	6.66966200	-1.58051700	1.26309600
H	5.97529600	0.45997800	1.31896100
H	4.89986600	-0.66881900	2.14721600
C	7.53098700	-1.45448600	0.00436900
H	7.29436600	-1.44865700	-2.15467700
H	6.24267700	-2.57852200	-1.31205200
H	7.28180600	-1.46319400	2.16199800
H	6.23502900	-2.58731700	1.30568200
H	8.31583800	-2.21664600	0.00408500
H	8.03691800	-0.47955600	0.00911200
C	-4.01922400	-1.14897300	0.00053500
C	-4.75774200	-1.58744600	1.26741200
C	-4.75775400	-1.58721200	-1.26641800
H	-3.02566400	-1.60024800	0.00049400
C	-4.96427700	-3.10504800	1.26190500
H	-5.73774500	-1.09309400	1.31649700
H	-4.19113300	-1.27162500	2.14822600

C	-4.96426700	-3.10481800	-1.26118800
H	-5.73777200	-1.09288400	-1.31540300
H	-4.19116700	-1.27122000	-2.14718400
C	-5.70164200	-3.55940200	0.00031400
H	-5.51343400	-3.40640500	2.15865800
H	-3.98611800	-3.60023200	1.30866300
H	-5.51341400	-3.40601600	-2.15800100
H	-3.98610200	-3.59998100	-1.30803300
H	-5.81806600	-4.64722400	0.00021400
H	-6.71397700	-3.13305500	0.00034700

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB2

N	3.92713100	0.30378600	0.00922600
C	2.57614300	0.60943200	-0.07372800
O	1.71010700	-0.25188100	-0.16246500
N	2.27863300	1.95089500	-0.04950600
C	3.17429200	3.02074700	0.03697800
O	2.76756800	4.17240500	0.05088400
C	4.56503700	2.61147200	0.10227100
C	4.87081300	1.30057700	0.08674600
H	1.27845100	2.18251800	-0.09165000
H	5.32655700	3.37627200	0.16668100
H	5.90125500	0.95853200	0.13636700
N	-3.87842900	0.40801400	-0.01038900
C	-3.97645900	1.78910800	0.07073300
O	-5.03332100	2.38945900	0.17204900
N	-2.76193100	2.44638800	0.02689200
C	-1.49132200	1.89389500	-0.08008200
O	-0.51073900	2.63573100	-0.09970300
C	-1.48097300	0.45155900	-0.15967800
C	-2.65668400	-0.20873700	-0.12244100
H	-2.81718200	3.46221100	0.08790200
H	-0.52753300	-0.05285000	-0.23977900
H	-2.69290600	-1.29317900	-0.18038000
C	-5.12052200	-0.39246100	0.03384900
C	-5.33220700	-1.17050400	-1.26663100
C	-5.14736400	-1.31442900	1.25516200
H	-5.91795900	0.34622800	0.13439500
C	-6.65000600	-1.94862800	-1.20942400
H	-4.50383800	-1.87708000	-1.41542200
H	-5.32279700	-0.47776200	-2.11326800
C	-6.46560500	-2.09216400	1.30252100
H	-4.31270500	-2.02704600	1.20056400
H	-5.00844800	-0.72190500	2.16440200
C	-6.69492200	-2.87470400	0.00788100
H	-6.78247600	-2.51930800	-2.13329300

H	-7.48423100	-1.23753500	-1.15494200
H	-6.46635200	-2.76515700	2.16488100
H	-7.29310900	-1.38683500	1.45185500
H	-7.65286700	-3.40179400	0.04828900
H	-5.91578500	-3.64220300	-0.09382200
C	4.34059400	-1.11473300	0.00341600
C	5.14507800	-1.45813400	-1.25284500
C	5.10243400	-1.48271600	1.27947500
H	3.40338100	-1.67410500	-0.01747400
C	5.51846800	-2.94336500	-1.25550900
H	6.06338700	-0.85518100	-1.27828100
H	4.56237100	-1.19779900	-2.14124800
C	5.47197900	-2.96886400	1.26592600
H	6.02370600	-0.88837700	1.34795300
H	4.49254900	-1.23607100	2.15355100
C	6.27918000	-3.32601500	0.01586700
H	6.11189200	-3.17549900	-2.14468700
H	4.60140100	-3.54285600	-1.32195600
H	6.03242400	-3.21942100	2.17137600
H	4.55270900	-3.56809600	1.28665400
H	6.51661400	-4.39406100	0.00945900
H	7.23701100	-2.78895100	0.03927200

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB3

N	4.30181000	0.55947600	0.00040000
C	3.89552200	1.88344600	-0.07034600
O	4.66170200	2.83193400	-0.03953700
N	2.52833300	2.05029100	-0.18033100
C	1.54631800	1.06902900	-0.23245500
O	0.36610500	1.40267100	-0.32963700
C	2.05613900	-0.28045000	-0.16220300
C	3.38809500	-0.46428000	-0.05118800
H	2.21275300	3.01842500	-0.22765900
H	1.35208600	-1.10085500	-0.20603700
H	3.81310900	-1.46275900	0.00450900
N	-4.25871900	-0.42332300	-0.05758300
C	-3.12965200	0.38766900	-0.10928000
O	-3.18436000	1.60579300	-0.05587800
N	-1.93577300	-0.29148100	-0.22599000
C	-1.74667400	-1.66914200	-0.29069600
O	-0.61998800	-2.14180800	-0.39115300
C	-2.97333000	-2.43715300	-0.22813700
C	-4.14995600	-1.79017200	-0.11581000
H	-1.09594800	0.29996300	-0.27004000
H	-2.91418300	-3.51577100	-0.27154900
H	-5.09122200	-2.33180200	-0.06338200

C	-5.58414200	0.21522000	0.07363200
C	-6.47850500	-0.09365100	-1.12957200
C	-6.26087000	-0.16665700	1.39225800
H	-5.37067700	1.28545200	0.08602300
C	-7.82529900	0.62129300	-0.98694100
H	-6.65436000	-1.17673200	-1.19278000
H	-5.96908400	0.20655900	-2.04994400
C	-7.60826200	0.54838800	1.52525000
H	-6.42702700	-1.25281700	1.42207500
H	-5.59988100	0.08330400	2.22729400
C	-8.51355000	0.25031900	0.32821800
H	-8.46574100	0.37608400	-1.83939400
H	-7.66054300	1.70581000	-1.01637400
H	-8.09465100	0.25204500	2.45941700
H	-7.43484300	1.63019200	1.58769200
H	-9.46127100	0.78855500	0.42541200
H	-8.75795500	-0.82060700	0.31840000
C	5.74765600	0.26806800	0.10471100
C	6.07791200	-0.48859500	1.39336300
C	6.25505800	-0.47513500	-1.13291600
H	6.22218500	1.25057100	0.14468100
C	7.58753600	-0.72758900	1.49203300
H	5.56123600	-1.45802300	1.39964500
H	5.71362800	0.07879400	2.25502900
C	7.76312600	-0.71771200	-1.02462400
H	5.74007000	-1.44204700	-1.22008500
H	6.01385700	0.10198500	-2.03044600
C	8.11294400	-1.46952800	0.26142000
H	7.81462200	-1.28609600	2.40478900
H	8.09851400	0.23993900	1.57810000
H	8.11231700	-1.27092300	-1.90144300
H	8.28310500	0.24873800	-1.03270500
H	9.19555100	-1.60905800	0.33654400
H	7.66673100	-2.47260900	0.22609600

adenine–thymine WC

N	0.96261200	0.36803100	-0.00015500
C	1.56684400	1.56818000	-0.00009700
N	2.86437900	1.82740200	0.00000800
C	3.59115100	0.69628900	0.00005700
C	3.10780300	-0.60971200	0.00000700
C	1.70228900	-0.75891100	-0.00010500
N	1.09189000	-1.94431300	-0.00015700
N	4.94903300	0.55776200	0.00013500
C	5.21585900	-0.78740900	0.00017100
N	4.13480600	-1.52734800	0.00009500

H	0.88533400	2.41609300	-0.00015000
H	1.64926700	-2.79093200	-0.00011900
H	0.07513000	-1.99969800	-0.00022100
H	6.23099800	-1.16462100	0.00024300
N	-3.81125500	1.60000200	0.00011600
C	-2.43779600	1.63057100	-0.00021800
O	-1.79268000	2.66918200	0.00001900
N	-1.85846800	0.38249600	-0.00018400
C	-2.51208700	-0.83580400	-0.00008500
O	-1.87138000	-1.88934700	-0.00013000
C	-3.96891400	-0.78111100	0.00006800
C	-4.72526000	-2.07234500	0.00016100
C	-4.54537800	0.43884200	0.00020000
H	-4.27884000	2.50549500	0.00029600
H	-0.81319000	0.36837100	-0.00023400
H	-5.80302700	-1.89303400	0.00030000
H	-4.47123700	-2.67139600	0.87825400
H	-4.47146000	-2.67139000	-0.87800100
H	-5.62389300	0.57103700	0.00040300
H	5.63535500	1.31162900	0.00017100

adenine–uracil WC

N	-0.63426300	-0.28249500	-0.00132900
C	-1.13143300	-1.53106800	-0.00098100
N	-2.40120100	-1.90255700	-0.00019800
C	-3.22406200	-0.83931900	0.00028000
C	-2.85681700	0.50388200	0.00003800
C	-1.46966500	0.77553300	-0.00081500
N	-0.96514300	2.00966300	-0.00106800
N	-4.58900000	-0.82006200	0.00108100
C	-4.97220400	0.49682200	0.00114700
N	-3.95997200	1.32820600	0.00083300
H	-0.37849300	-2.31614300	-0.00137300
H	-1.59462900	2.80413500	-0.00061300
H	0.04298200	2.15361500	-0.00164900
H	-6.01644000	0.78368200	0.00170900
N	4.21837700	-1.10358900	0.00094500
C	2.84765100	-1.24151500	-0.00013700
O	2.29274600	-2.33023800	-0.00074700
N	2.16785800	-0.04668700	-0.00074900
C	2.71741900	1.22632500	-0.00018600
O	1.98623500	2.21812100	-0.00072200
C	4.16663100	1.26923200	0.00106400
C	4.85398800	0.10955400	0.00155400
H	4.75513000	-1.97023000	0.00132900
H	1.12458600	-0.12258700	-0.00148900

H	4.65721100	2.23172000	0.00154500
H	5.93918400	0.06953400	0.00244800
H	-5.20703000	-1.63082100	0.00146000

cytosine–guanine WC

N	-2.18012300	-0.07603300	0.00109000
C	-2.92168400	1.06109900	0.00215300
O	-2.43649200	2.19857600	0.00414300
N	-4.30293400	0.92955600	0.00092400
C	-4.93099300	-0.27620300	-0.00130600
C	-4.20751100	-1.41714300	-0.00234800
C	-2.77739900	-1.27579700	-0.00100200
N	-2.00030900	-2.35472400	-0.00178600
H	-4.83945300	1.79559800	0.00170500
H	-6.01645700	-0.25702000	-0.00213400
H	-4.67940300	-2.39136900	-0.00407500
H	-2.42075400	-3.27974200	-0.00337600
H	-0.98448500	-2.26633700	-0.00045500
N	3.91108600	-1.61276600	0.00155600
C	4.96793700	-0.84470300	0.00054200
N	4.65453900	0.49519600	-0.00093100
C	3.29647100	0.59099900	-0.00077800
N	2.57405400	1.72846100	-0.00188500
C	1.27155600	1.50309600	-0.00148000
N	0.40864500	2.52398800	-0.00324300
N	0.72435500	0.24052600	0.00005800
C	1.44053100	-0.95824300	0.00123100
O	0.84681900	-2.04074300	0.00243600
C	2.85108800	-0.72830300	0.00078200
H	5.99456400	-1.18863400	0.00075000
H	0.80155600	3.45841000	-0.00192200
H	-0.60525400	2.39768700	0.00133400
H	-0.30943900	0.14577300	0.00023600
H	5.31135300	1.27473400	-0.00194300

adenine–thymine stacked structure

N	-1.08695900	-2.20472000	0.28589400
C	-1.06045300	-2.24993900	-1.08334400
N	0.03504100	-1.74780600	-1.59924900
C	0.76141800	-1.34597100	-0.49861800
C	2.00804200	-0.69680700	-0.36253800
N	2.74575800	-0.33796800	-1.42543700
N	2.47078700	-0.44982600	0.87396400
C	1.70636800	-0.78368500	1.92233700
N	0.50729800	-1.35777900	1.93302200
C	0.08336600	-1.62175600	0.68840300

N	-1.80028800	0.95855400	1.28809200
C	-2.34042000	0.55181600	0.09292100
O	-3.38801600	-0.06919400	0.00264500
N	-1.57537600	0.91380300	-0.99699400
C	-0.33392600	1.55263700	-0.99325900
O	0.26341000	1.74864200	-2.04192400
C	0.14395900	1.95730000	0.32702600
C	-0.60483000	1.62923800	1.39899200
H	-1.91841500	0.59638900	-1.90097600
H	-2.31618200	0.68994200	2.12361400
H	-0.30508200	1.87638400	2.41267900
C	1.44538200	2.69104000	0.40404600
H	2.24074300	2.11170000	-0.07062500
H	1.38414700	3.65104000	-0.11622400
H	1.73004000	2.87174000	1.44301000
H	-1.88693000	-2.66210400	-1.64793500
H	-1.85634200	-2.50605700	0.88079400
H	2.12932400	-0.54657300	2.89644600
H	3.56550300	0.23690100	-1.26506200
H	2.30277300	-0.27800100	-2.33232200

adenine–uracil stacked structure

N	-0.40733700	-2.20766800	-0.15793100
C	-0.33000600	-1.97349300	-1.50602300
N	0.61128500	-1.12151200	-1.83241100
C	1.17728600	-0.77825300	-0.62308900
C	2.19901100	0.13080500	-0.27127900
N	2.84869700	0.86504200	-1.19044700
N	2.54136600	0.23984100	1.02308500
C	1.86810400	-0.48417700	1.92740100
N	0.86512900	-1.33526600	1.73693400
C	0.56059000	-1.44420700	0.43535700
N	-2.06993700	0.33212700	1.33637300
C	-2.38860000	0.09080900	0.01843600
O	-3.22948200	-0.72315200	-0.32704400
N	-1.66135800	0.85737400	-0.86732400
C	-0.62288900	1.75077800	-0.57731400
O	-0.01739800	2.30252600	-1.48363800
C	-0.38278200	1.92929800	0.84490500
C	-1.09688900	1.21248400	1.73367300
H	-2.57339400	-0.22553200	2.02389000
H	-1.83861400	0.67631500	-1.85269800
H	3.42502300	1.62703700	-0.85052700
H	2.40661300	0.99869000	-2.09067400
H	2.18627800	-0.34654500	2.95882200
H	-1.08113000	-2.81220000	0.30847000

H	-1.00517300	-2.45785100	-2.19977200
H	-0.94166800	1.28380700	2.80501200
H	0.39924600	2.60745200	1.15257000

cytosine–guanine stacked structure

N	1.11062800	-1.21693200	-2.05534100
C	2.26607800	-1.46055900	-1.35372200
N	2.05443300	-1.63186100	-0.07322300
C	0.69013500	-1.49462400	0.06476200
C	-0.13090700	-1.50058200	1.24178900
O	0.19570600	-1.65201100	2.41357300
N	-1.48005800	-1.30702900	0.89915900
C	-1.96859000	-1.01406900	-0.34855000
N	-3.30901300	-0.81523900	-0.43942200
N	-1.21535700	-0.97337600	-1.42327200
C	0.08777500	-1.22397100	-1.15690300
N	-0.36741400	2.30795300	-0.99330900
C	-0.96477000	1.89780500	0.20464700
O	-2.18989500	1.94402600	0.29974600
N	-0.13447400	1.46200800	1.19462100
C	1.17059400	1.37129000	0.97376400
N	1.93280600	0.85278600	1.96050500
C	1.79837200	1.79822000	-0.24567000
C	0.96994100	2.25361600	-1.21452400
H	-1.00234300	2.60420600	-1.73172900
H	1.31652100	2.58853600	-2.18811100
H	2.86913800	1.73494300	-0.38976300
H	1.44127000	0.28909300	2.64043000
H	2.84494000	0.49144000	1.69796100
H	-2.12031600	-1.27463700	1.69252300
H	-3.58599300	-0.43447000	-1.33926800
H	-3.72436500	-0.29609400	0.33031000
H	3.23052900	-1.50536500	-1.84349400
H	1.03151300	-1.04470800	-3.05700200

2.2.2) SM8AD/M06-2X/6-31+G**

adenine–thymine WC

N	0.95338700	0.35357200	0.00820200
C	1.55007800	1.56050700	0.02219600
N	2.84652400	1.82240600	0.02448200
C	3.58061200	0.69730000	0.00980200
C	3.10409000	-0.61171600	-0.00590500
C	1.70070000	-0.76716400	-0.00540200
N	1.09358600	-1.95998600	-0.01741000
N	4.94140200	0.56623900	0.00684500

C	5.21540200	-0.77956200	-0.01000600
N	4.13588000	-1.52330400	-0.01795800
H	0.86650200	2.40524600	0.03130200
H	1.65260200	-2.80664200	-0.02726700
H	0.07727500	-2.02053200	-0.00922000
H	6.23658000	-1.15365600	-0.01568100
N	-3.78818900	1.61375400	-0.01393600
C	-2.41259400	1.62418400	-0.01335100
O	-1.75261300	2.65458200	-0.01973800
N	-1.84711500	0.37118700	-0.00385800
C	-2.51703600	-0.83848100	0.00494600
O	-1.87919900	-1.89533300	0.01012100
C	-3.97517400	-0.76869600	0.00652600
C	-4.74905800	-2.05164500	0.01794800
C	-4.53787700	0.46008800	-0.00354200
H	-4.24585400	2.52721700	-0.02088200
H	-0.79941100	0.34707800	0.00046900
H	-5.82666200	-1.85267400	0.01749000
H	-4.50612100	-2.64703300	0.90293300
H	-4.50800300	-2.66166600	-0.85753700
H	-5.62056600	0.60587000	-0.00399900
H	5.62497200	1.32683400	0.01548000

adenine–uracil WC

N	-0.62476000	-0.26682900	-0.00017700
C	-1.11255600	-1.52208000	0.00016100
N	-2.38045800	-1.89824600	0.00033400
C	-3.21171000	-0.84270200	0.00013600
C	-2.85316500	0.50318800	-0.00020600
C	-1.46881600	0.78330400	-0.00038000
N	-0.97300700	2.02591700	-0.00077200
N	-4.57891200	-0.83264000	0.00019900
C	-4.97078800	0.48376800	-0.00006600
N	-3.96142400	1.32006700	-0.00033600
H	-0.35680800	-2.30299800	0.00029400
H	-1.60764000	2.81746500	-0.00074400
H	0.03337200	2.18027300	-0.00087300
H	-6.02091800	0.76600500	-0.00006800
N	4.20670500	-1.11376200	0.00043100
C	2.83165300	-1.23939000	0.00015200
O	2.26835700	-2.32427900	-0.00000100
N	2.15810200	-0.04200500	-0.00012800
C	2.71821800	1.22544200	0.00001600
O	1.98666100	2.21889500	-0.00006000
C	4.16897400	1.26251500	0.00027800
C	4.85165500	0.09682400	0.00047800

H	4.73854700	-1.98634000	0.00063800
H	1.11052100	-0.10976500	-0.00043600
H	4.66862300	2.22394900	0.00031900
H	5.94247900	0.05204900	0.00067000
H	-5.19283600	-1.65030600	0.00041700

cytosine–guanine WC

N	-1.13962300	-0.20715400	0.00797400
C	-1.81297000	1.00659800	-0.01078600
O	-1.14305100	2.05465400	-0.02354700
N	-3.16745100	0.99424000	-0.01457800
C	-3.80963000	-0.17019800	0.00200200
N	-5.15335500	-0.12720700	-0.00335700
C	-3.14183700	-1.44102500	0.02323400
C	-1.78238700	-1.39655700	0.02414000
H	-5.71406600	-0.97516300	0.00746200
H	-5.62811700	0.76762100	-0.01910600
H	-3.68406900	-2.38401200	0.03631400
H	-1.13952400	-2.27488500	0.03575200
H	-0.09594800	-0.16012300	0.00359500
N	3.60480600	-1.32372900	-0.01062900
C	2.21097700	-1.27182500	-0.01259100
O	1.55767100	-2.31687700	-0.02170200
N	1.64119400	-0.03874800	-0.00439800
C	2.38049900	1.07273100	0.00882600
N	1.72785900	2.23623900	0.01541200
C	3.81919300	1.02612000	0.01482800
C	4.38400200	-0.20609500	0.00397100
H	2.24264200	3.11345900	0.02618600
H	0.70514100	2.24332300	0.00255600
H	4.42353900	1.93051400	0.02618100
H	5.46400200	-0.36519900	0.00601400
H	4.02833900	-2.25173600	-0.01766700

adenine–thymine stacked structure

N	-0.91450700	-2.26406000	0.38763100
C	-0.86526300	-2.39895600	-0.97687900
N	0.19595400	-1.84593100	-1.51353300
C	0.87838200	-1.32194300	-0.43690000
C	2.08144100	-0.58775600	-0.33134900
N	2.81348400	-0.25368700	-1.40826000
N	2.50890500	-0.23292000	0.89005700
C	1.75857400	-0.55178800	1.95436000
N	0.60094500	-1.20452100	1.98785100
C	0.20749900	-1.57273000	0.76021400
N	-1.93255400	0.90775300	1.22110300

C	-2.39416900	0.39062800	0.03464700
O	-3.39136300	-0.31156600	-0.05250200
N	-1.62149000	0.74302700	-1.05262200
C	-0.43633100	1.48387100	-1.04681700
O	0.17073000	1.67623300	-2.09187300
C	-0.03174100	1.99652200	0.26097700
C	-0.79331200	1.67467200	1.32881500
H	-1.90465800	0.34414700	-1.94304700
H	-2.45860100	0.65071600	2.05564300
H	-0.55035400	2.00714400	2.33820200
C	1.20795200	2.83438100	0.33404100
H	2.06586500	2.28534600	-0.06117600
H	1.09828600	3.74836900	-0.25664100
H	1.42789900	3.10999600	1.37038100
H	-1.65147000	-2.91248000	-1.52167900
H	-1.65779900	-2.59924900	0.99947100
H	2.15337000	-0.22789400	2.91488200
H	3.60709300	0.36530500	-1.28388700
H	2.40209900	-0.31775200	-2.32939900

adenine–uracil stacked structure

N	0.33383300	2.22238900	0.07715700
C	0.21772900	2.16036600	-1.28905800
N	-0.70930100	1.32508500	-1.69173600
C	-1.22909500	0.81492100	-0.52163100
C	-2.23503600	-0.14168500	-0.25807500
N	-2.91217100	-0.75653600	-1.24391200
N	-2.53379000	-0.41988900	1.02019200
C	-1.84570300	0.19484300	1.99244100
N	-0.86481500	1.08469900	1.87935000
C	-0.59810500	1.36210200	0.59492000
N	2.15293700	-0.42145100	1.25741000
C	2.41422300	-0.03200700	-0.03923000
O	3.22724400	0.83381900	-0.32489700
N	1.67153900	-0.71358800	-0.98034900
C	0.67798800	-1.67447000	-0.75029800
O	0.06998600	-2.16108600	-1.69346500
C	0.48823800	-2.00733300	0.65127800
C	1.21717500	-1.36983800	1.59069500
H	2.67136600	0.07067100	1.98515100
H	1.81157600	-0.42510800	-1.94464300
H	-3.49726100	-1.54791000	-0.99850800
H	-2.54156900	-0.72739600	-2.18460200
H	-2.12918600	-0.07844000	3.00650200
H	0.99198100	2.79872000	0.60065500
H	0.85601600	2.75339500	-1.93671800

H	1.10560900	-1.56633600	2.65666500
H	-0.25849700	-2.74582000	0.90935500

cytosine–guanine stacked structure

N	1.35590400	-1.12141000	-2.02082500
C	2.52603700	-1.15135000	-1.29592400
N	2.32210700	-1.29939100	-0.01183800
C	0.95087100	-1.37252800	0.10944000
C	0.11782900	-1.47588400	1.27655700
O	0.44973500	-1.53178300	2.45665400
N	-1.23896100	-1.51713200	0.91511200
C	-1.74693000	-1.35204700	-0.34981200
N	-3.10229400	-1.37997100	-0.46873100
N	-0.98916000	-1.22493000	-1.41343600
C	0.33414700	-1.25210500	-1.12876900
N	-0.80346900	2.27673400	-1.01032500
C	-1.29665800	1.73801400	0.18641400
O	-2.51122300	1.55886800	0.29659000
N	-0.39288200	1.43983300	1.15713600
C	0.90403400	1.58076600	0.92349000
N	1.74910900	1.21720600	1.91461300
C	1.43464200	2.09945600	-0.30835500
C	0.52269800	2.43908300	-1.25580100
H	-1.49393000	2.47967200	-1.73266500
H	0.79665300	2.84742000	-2.23121200
H	2.50186400	2.21759300	-0.47169600
H	1.36636200	0.59231800	2.61031600
H	2.71323200	1.02624900	1.66182300
H	-1.88838500	-1.56044300	1.69793700
H	-3.42179600	-1.10360300	-1.39501900
H	-3.62423500	-0.90839500	0.26687100
H	3.49631300	-1.06394100	-1.77648400
H	1.26333900	-1.00055700	-3.03119100

2.3) SMD

2.3.1) SMD/M06-2X/6-31G**

9-hexyl–adenine–9-hexyl–adenine HB1

N	-3.33575600	3.57297000	-0.36978800
C	-4.60590500	3.35796900	-0.00461000
N	-5.16253000	2.23935100	0.44798200
C	-4.26807300	1.24144200	0.50340400
C	-2.92389700	1.30155600	0.14811500
C	-2.45258000	2.55945700	-0.29886200
N	-1.18127500	2.77199500	-0.66022100

N	-4.48004100	-0.04839600	0.91901900
C	-3.28298200	-0.69335200	0.78595900
N	-2.32160800	0.07269100	0.32793200
H	-5.26451000	4.21974900	-0.08618300
H	-0.44271300	2.09029800	-0.46613700
H	-0.92169600	3.71719300	-0.90296800
H	-3.18359400	-1.73836100	1.04922200
N	1.26174600	1.14914500	-0.13462100
C	2.33368800	1.94583200	0.00226600
N	3.61670900	1.62165400	-0.06365700
C	3.77690800	0.30886900	-0.29969800
C	2.77071000	-0.63901000	-0.46049800
C	1.44134700	-0.16598500	-0.36582100
N	0.37301100	-0.95754300	-0.50997000
N	4.95227500	-0.38308700	-0.42513700
C	4.59823300	-1.68870700	-0.65586100
N	3.30293900	-1.88984700	-0.68100200
H	2.10602400	2.99307500	0.18930200
H	0.51633600	-1.95142400	-0.60757800
H	-0.55653400	-0.59753600	-0.27849300
H	5.34866000	-2.45485200	-0.79039800
C	6.28527000	0.21702600	-0.37288300
C	7.38294700	-0.79871600	-0.09032100
H	6.25721400	0.97923700	0.41147300
H	6.47403200	0.72913300	-1.32274300
C	8.74280000	-0.11293900	0.03359100
H	7.15160500	-1.33953600	0.83556600
H	7.42641000	-1.53871600	-0.89875100
C	9.87883300	-1.09790600	0.30087900
H	8.95435400	0.44460700	-0.88866300
H	8.70390100	0.62767000	0.84332600
H	9.66922400	-1.65260900	1.22580200
H	9.91307900	-1.84344300	-0.50552900
C	-5.75308400	-0.60281500	1.36593100
C	-6.70552100	-0.87539800	0.20632000
H	-6.19514100	0.11318400	2.06523000
H	-5.53193100	-1.52176500	1.91613800
C	-8.03500900	-1.44525800	0.69495300
H	-6.87823100	0.06113100	-0.33677200
H	-6.23027700	-1.57473800	-0.49238900
C	-9.01453000	-1.71669300	-0.44445600
H	-7.85316800	-2.37649500	1.24893800
H	-8.49080100	-0.74344400	1.40622300
H	-9.19320500	-0.78492100	-0.99808900
H	-8.55947700	-2.41754300	-1.15781700
C	11.24203100	-0.41871200	0.41705100

C	12.37013800	-1.40851900	0.69068300
H	11.20442600	0.32963800	1.21888500
H	11.45092600	0.13152200	-0.50932400
H	13.33676900	-0.90341000	0.77299000
H	12.19720400	-1.95200400	1.62560400
H	12.44696100	-2.14845300	-0.11306000
C	-10.34984400	-2.28152400	0.03550900
C	-11.32259900	-2.54082700	-1.11059900
H	-10.80000400	-1.58124600	0.75048000
H	-10.17083500	-3.21383300	0.58643200
H	-12.27453900	-2.93895100	-0.74772100
H	-11.53426900	-1.61799200	-1.66068900
H	-10.90777600	-3.26243000	-1.82238300

9-hexyl–adenine–9-hexyl–adenine HB2

N	-2.67539600	-3.92291100	-0.24422200
C	-3.89453600	-3.46631300	-0.55921200
N	-4.27574100	-2.21830600	-0.80924100
C	-3.24439300	-1.36598300	-0.70392200
C	-1.92630100	-1.67988100	-0.38150500
C	-1.65353500	-3.05080200	-0.15553200
N	-0.43021900	-3.50440300	0.14335900
N	-3.26131900	-0.00740100	-0.88321500
C	-1.98086700	0.42115200	-0.65407900
N	-1.14515700	-0.54191600	-0.35167000
H	-4.67220500	-4.22460000	-0.61963900
H	0.37760600	-2.87864100	0.18643800
H	-0.32506600	-4.48875900	0.33888500
H	-1.73086900	1.47149800	-0.73356400
N	5.27622400	-3.55085000	0.17160000
C	5.94070900	-2.45904400	0.58042300
N	5.46213900	-1.24733300	0.84084700
C	4.13561600	-1.19536600	0.65957300
C	3.31228200	-2.24004400	0.25044300
C	3.94987000	-3.47043100	-0.00911500
N	3.26795200	-4.56494700	-0.40611200
N	3.29908900	-0.12233200	0.83741600
C	2.04135700	-0.56070300	0.52900700
N	2.00108200	-1.82307000	0.17485700
H	7.01285800	-2.58826200	0.70699700
H	2.32739200	-4.45589600	-0.75654900
H	3.80146000	-5.36107600	-0.72422100
H	1.17399300	0.08483100	0.57839200
C	3.70604400	1.22028900	1.23556200
C	4.29864700	2.01346000	0.07579400
H	4.43986000	1.11351300	2.03980800

H	2.82341400	1.71965500	1.64486600
C	4.75700400	3.39870000	0.52530600
H	5.14678900	1.45461700	-0.33800000
H	3.54787100	2.10193900	-0.71920600
C	5.33526100	4.23330100	-0.61463000
H	3.91084400	3.93585200	0.97590900
H	5.51209600	3.29033500	1.31542000
H	6.17218600	3.69068300	-1.07506000
H	4.57598700	4.35337700	-1.39962100
C	-4.42960900	0.79900100	-1.21313200
C	-5.36546600	0.98507100	-0.02279300
H	-4.95356600	0.30286700	-2.03563800
H	-4.06403400	1.76296100	-1.57835400
C	-6.57766600	1.83553900	-0.39440900
H	-5.69337700	-0.00102900	0.32646900
H	-4.81265900	1.45528700	0.79968500
C	-7.54165300	2.03591500	0.77282300
H	-6.23894100	2.81506900	-0.75913400
H	-7.11126700	1.36053000	-1.22851000
H	-7.87627800	1.05614400	1.13974800
H	-7.00965300	2.51308400	1.60727400
C	5.81533000	5.61043700	-0.16063600
C	6.37740700	6.44562400	-1.30646500
H	6.58090600	5.48615300	0.61563400
H	4.98124000	6.14525300	0.31165300
H	6.72216000	7.42394000	-0.95938500
H	7.22608400	5.94106700	-1.78024300
H	5.61939700	6.61296700	-2.07892300
C	-8.76050400	2.87907500	0.40390100
C	-9.71271300	3.07745200	1.57913500
H	-9.29263100	2.39728700	-0.42598700
H	-8.42467500	3.85523300	0.03116500
H	-10.58036500	3.68106700	1.29784900
H	-10.08135000	2.11574800	1.95113800
H	-9.20949500	3.58289200	2.41013700

9-hexyl–adenine–9-hexyl–adenine HB3

N	-2.15965100	-3.40196300	0.17337400
C	-3.48162500	-3.43877800	-0.03976200
N	-4.29313800	-2.45084500	-0.40153200
C	-3.62197700	-1.29788900	-0.54206100
C	-2.25930100	-1.09578900	-0.34511700
C	-1.50596500	-2.23550900	0.02299500
N	-0.18528700	-2.19166100	0.24190100
N	-4.12413400	-0.07430200	-0.90719700
C	-3.06465500	0.78885400	-0.90098600

N	-1.92712400	0.22350000	-0.57318800
H	-3.94742000	-4.41133200	0.10090100
H	0.37822900	-1.38295300	-0.02299700
H	0.28108500	-3.06661900	0.43190300
H	-3.19784000	1.83251200	-1.15544600
N	2.15929300	3.40236600	0.17426300
C	3.48126800	3.43943700	-0.03883500
N	4.29292600	2.45170900	-0.40082800
C	3.62196600	1.29866600	-0.54150900
C	2.25935100	1.09624900	-0.34437400
C	1.50582400	2.23580200	0.02378800
N	0.18515400	2.19152700	0.24300200
N	4.12430200	0.07530600	-0.90709300
C	3.06500900	-0.78809400	-0.90082400
N	1.92741000	-0.22306900	-0.57276400
H	3.94688800	4.41207200	0.10184600
H	-0.37806100	1.38308800	-0.02343600
H	-0.28152600	3.06658600	0.43184500
H	3.19841100	-1.83167500	-1.15548600
C	5.52333100	-0.22727100	-1.19058000
C	6.37297300	-0.25032200	0.07611200
H	5.89289900	0.53115200	-1.88735700
H	5.54780400	-1.19526200	-1.69898600
C	7.83481200	-0.57405800	-0.22285200
H	6.30186800	0.72903600	0.56331500
H	5.95831900	-0.98995000	0.77184800
C	8.70049200	-0.57084600	1.03539900
H	7.90295200	-1.55575900	-0.71137300
H	8.23100500	0.15821600	-0.93891200
H	8.62442100	0.41083700	1.52234000
H	8.30180800	-1.30129200	1.75268300
C	-5.52311800	0.22857800	-1.19062800
C	-6.37294300	0.25021100	0.07596300
H	-5.89257200	-0.52897800	-1.88840200
H	-5.54748300	1.19718500	-1.69786700
C	-7.83484800	0.57379800	-0.22282700
H	-6.30163800	-0.72956800	0.56226700
H	-5.95853300	0.98932900	0.77238400
C	-8.70043500	0.56977800	1.03549700
H	-7.90326400	1.55571200	-0.71087800
H	-8.23090300	-0.15823800	-0.93920000
H	-8.62381300	-0.41201600	1.52213100
H	-8.30202700	1.30020000	1.75296000
C	10.16985800	-0.88435300	0.76118200
C	11.01678900	-0.86734200	2.03018200
H	10.56676800	-0.15556900	0.04320700

H	10.24756400	-1.86717900	0.27882900
H	12.06619700	-1.08965300	1.81685800
H	10.97392300	0.11309300	2.51607600
H	10.65755200	-1.60912200	2.75125900
C	-10.16999100	0.88261300	0.76159600
C	-11.01663800	0.86482100	2.03079200
H	-10.56669000	0.15379800	0.04353800
H	-10.24831400	1.86551700	0.27950600
H	-12.06620700	1.08666200	1.81779500
H	-10.97312000	-0.11573300	2.51638900
H	-10.65760100	1.60658100	2.75199000

9-hexyl–adenine–1-hexyl–thymine WC

N	-0.69309300	-1.73127700	-0.22697700
C	-1.25195900	-0.62956500	-0.75567000
N	-2.53969800	-0.35779100	-0.89806800
C	-3.30686700	-1.35835600	-0.43197200
C	-2.87329200	-2.55278800	0.13662800
C	-1.47368200	-2.72723900	0.23652800
N	-0.90622400	-3.81703900	0.75991600
N	-4.67419000	-1.42638300	-0.41401300
C	-4.98662500	-2.63186800	0.15941300
N	-3.94093500	-3.34233200	0.50353500
H	-0.54033400	0.11667200	-1.10202300
H	-1.49045300	-4.56013800	1.11098100
H	0.10963700	-3.89033500	0.81750300
H	-6.01993300	-2.92719400	0.28883800
N	4.15558400	-0.79845700	-0.63393700
C	2.77311100	-0.73866400	-0.66846000
O	2.16538500	0.21833900	-1.12689200
N	2.13655300	-1.84039800	-0.14917600
C	2.72404800	-2.94924100	0.42327700
O	2.03432800	-3.87164900	0.86164000
C	4.17949600	-2.93587900	0.46587600
C	4.88428400	-4.10528500	1.07951600
C	4.80904200	-1.86367200	-0.06170700
H	1.09016600	-1.80790300	-0.17779200
H	5.96648400	-3.95915500	1.06278200
H	4.64897300	-5.02891600	0.54185000
H	4.56786900	-4.24978600	2.11697900
H	5.89243700	-1.78554600	-0.06926600
C	4.90547300	0.35913000	-1.13145300
C	5.04292700	1.45193100	-0.07768100
H	4.37897600	0.73708200	-2.01016500
H	5.88664100	-0.00515700	-1.44857300
C	5.84857900	2.64180800	-0.59332600

H	4.03969800	1.77853100	0.21971400
H	5.52584100	1.03027900	0.81353000
C	5.99418400	3.75155700	0.44557500
H	6.84586300	2.30132400	-0.90466700
H	5.36450100	3.04690600	-1.49213700
H	4.99651400	4.09609500	0.74985000
H	6.46806400	3.34403400	1.34939400
C	6.80784600	4.94209500	-0.05743200
C	6.93530900	6.04867700	0.98459200
H	6.33815500	5.34267500	-0.96485200
H	7.80712400	4.59805400	-0.35368300
H	7.51676100	6.89370500	0.60471600
H	5.95044800	6.42633600	1.27881700
H	7.43185700	5.68067000	1.88872700
C	-5.58924500	-0.38706400	-0.87161200
C	-5.65616400	0.78800400	0.09850600
H	-6.57143900	-0.85176000	-0.99525000
H	-5.24620100	-0.05186500	-1.85509400
C	-6.60454800	1.87646200	-0.39872600
H	-5.98178600	0.42312100	1.08030800
H	-4.64773900	1.19988300	0.22192500
C	-6.68093900	3.07050900	0.55007200
H	-6.27564400	2.21959400	-1.38880000
H	-7.60952700	1.45360900	-0.53345000
H	-7.00977000	2.72750600	1.54065900
H	-5.67514500	3.49013900	0.68665900
C	-7.62287600	4.16777300	0.05830700
C	-7.70047300	5.34993000	1.01942200
H	-8.62497600	3.74466900	-0.08743900
H	-7.28759400	4.51527900	-0.92711600
H	-8.38241200	6.12210500	0.65181900
H	-8.05622300	5.03171900	2.00506500
H	-6.71629500	5.81045500	1.15520100

9-hexyl–adenine–1-hexyl–thymine RWC

N	0.65554800	0.30100500	-0.99716100
C	1.74441000	1.06979000	-0.82409500
N	3.01562300	0.70927700	-0.90822300
C	3.13765000	-0.59699000	-1.20003400
C	2.10736500	-1.51260100	-1.39751000
C	0.79191500	-1.00696800	-1.28784100
N	-0.29865700	-1.76078400	-1.45476000
N	4.29186200	-1.31380300	-1.36755000
C	3.90411200	-2.59929500	-1.64568800
N	2.60510600	-2.76644400	-1.67702700

H	1.53006100	2.10839800	-0.58226300
H	-0.19654600	-2.73728200	-1.68420900
H	-1.22584600	-1.34670900	-1.37125200
H	4.64383800	-3.37005300	-1.81914000
N	-4.16504900	1.41395400	-0.54873800
C	-2.96245100	0.78107100	-0.78021800
O	-2.90451100	-0.39094400	-1.15311300
N	-1.84887800	1.54544200	-0.57185800
C	-1.80452500	2.85686600	-0.12037700
O	-0.73111500	3.42573200	0.03146800
C	-3.10826000	3.46087100	0.14229600
C	-3.14176900	4.87250400	0.63816500
C	-4.20675500	2.71114300	-0.08420100
H	-0.92917900	1.07705300	-0.74867500
H	-4.16880700	5.20477500	0.80470700
H	-2.66782400	5.54774700	-0.08072400
H	-2.58759200	4.96582000	1.57712600
H	-5.20753000	3.09878300	0.08367000
C	-5.39583100	0.63196000	-0.70724400
C	-5.70687400	-0.20927200	0.52524800
H	-5.26836800	-0.00643500	-1.58392100
H	-6.20383100	1.33918000	-0.91277500
C	-6.97462000	-1.03902000	0.33970700
H	-4.85408200	-0.86952700	0.72172200
H	-5.81343600	0.45267100	1.39446400
C	-7.30845100	-1.89070100	1.56234100
H	-7.82040400	-0.37367000	0.11763700
H	-6.85522700	-1.69157000	-0.53576300
H	-6.46009900	-2.55207000	1.78526500
H	-7.42929100	-1.23879200	2.43861100
C	-8.57020700	-2.73145300	1.38059600
C	-8.88781400	-3.58676100	2.60320700
H	-8.44988600	-3.37570900	0.50027500
H	-9.41763500	-2.06845200	1.16384900
H	-9.79692300	-4.17680200	2.45573100
H	-8.06929800	-4.28136800	2.81938900
H	-9.03507100	-2.96235500	3.49094100
C	5.65145700	-0.80992500	-1.21479100
C	6.08308300	-0.73934600	0.24658800
H	5.68937700	0.18124300	-1.67595100
H	6.30839400	-1.47346800	-1.78470300
C	7.52828000	-0.26745800	0.38317400
H	5.41113000	-0.05805900	0.78233300
H	5.96839300	-1.73148800	0.70041200
C	7.99622500	-0.20432300	1.83537500
H	8.18622600	-0.94343500	-0.18043000

H	7.63430300	0.72394400	-0.07729300
H	7.34811500	0.48186200	2.39720000
H	7.87401100	-1.19287500	2.29925000
C	9.44982700	0.24162100	1.97639900
C	9.90975200	0.29736100	3.42990200
H	9.57121300	1.22888700	1.51297300
H	10.09351800	-0.44507800	1.41181200
H	10.95306900	0.61595700	3.50982000
H	9.30026600	1.00029100	4.00745200
H	9.82196000	-0.68470000	3.90686700

9-hexyl–adenine–1-hexyl–thymine H

N	-3.59476700	-4.04135600	0.57374700
C	-4.61197100	-3.23673300	0.23800200
N	-4.57204900	-1.98793200	-0.21607200
C	-3.30913700	-1.54947000	-0.31756300
C	-2.15501600	-2.25892900	-0.00335500
C	-2.33450900	-3.58238900	0.46173600
N	-1.31184900	-4.38356900	0.78135000
N	-2.87645700	-0.32539000	-0.76681900
C	-1.51372200	-0.35133400	-0.70080400
N	-1.03991900	-1.48860600	-0.25064700
H	-5.60214400	-3.67137300	0.35251400
H	-0.34122100	-4.08093700	0.72495200
H	-1.52060200	-5.31455200	1.10990300
H	-0.90560300	0.49091500	-1.00487200
N	3.78967400	-0.82952700	-0.64607100
C	2.41018600	-0.72483500	-0.63854700
O	1.82110300	0.27354000	-1.03119800
N	1.75235800	-1.83033400	-0.15754000
C	2.31411000	-2.99069900	0.33176400
O	1.60262500	-3.91113100	0.73558800
C	3.77023200	-3.02789600	0.32935700
C	4.44940500	-4.25328300	0.85648700
C	4.42152900	-1.94851800	-0.15614000
H	0.71069000	-1.75977100	-0.15975000
H	5.53556600	-4.15189500	0.80190700
H	4.15280600	-5.13870400	0.28598800
H	4.16845100	-4.43526600	1.89836100
H	5.50637600	-1.90685700	-0.19248800
C	4.56011400	0.32909300	-1.10931600
C	4.71851700	1.38730700	-0.02364800
H	4.03905600	0.74476000	-1.97455100
H	5.53343200	-0.04246200	-1.44115700
C	5.52910000	2.58571000	-0.51154200
H	3.72080100	1.71348200	0.29184000

H	5.20587600	0.93479800	0.84966200
C	5.68266600	3.66865200	0.55414800
H	6.52363000	2.24850800	-0.83476600
H	5.04410500	3.01582900	-1.39827600
H	4.68724300	4.00822100	0.87126800
H	6.15926700	3.23758300	1.44548400
C	6.49693400	4.86963200	0.07733800
C	6.62822500	5.95138900	1.14466900
H	6.02547400	5.29196900	-0.81930100
H	7.49493500	4.53130300	-0.22942500
H	7.21052000	6.80399900	0.78361100
H	5.64454200	6.32387000	1.44928600
H	7.12567000	5.56162300	2.03909100
C	-3.72631000	0.76812500	-1.22545900
C	-4.42725800	1.48644900	-0.07720200
H	-4.46235300	0.34581400	-1.91616400
H	-3.08951700	1.45599600	-1.78854700
C	-5.30789800	2.62273800	-0.59088400
H	-5.03552500	0.76082100	0.47552200
H	-3.67383300	1.87687200	0.61743900
C	-6.04167500	3.35849900	0.52783000
H	-4.69088300	3.33753200	-1.15256100
H	-6.04141700	2.22000700	-1.30218700
H	-6.66373300	2.64442100	1.08430900
H	-5.30994600	3.75453800	1.24523500
C	-6.91714700	4.50097400	0.01766000
C	-7.65401300	5.22277500	1.14164400
H	-7.64210100	4.10483000	-0.70476900
H	-6.29245200	5.21608700	-0.53265400
H	-8.27347100	6.03854400	0.75815500
H	-8.30828000	4.53443300	1.68680200
H	-6.94830500	5.64924300	1.86233200

9-hexyl–adenine–1-hexyl–thymine RH

N	1.59400600	-3.90121600	-0.52738200
C	2.87773000	-3.87917500	-0.14249700
N	3.57890300	-2.86797800	0.35984500
C	2.82787900	-1.76205500	0.46774300
C	1.48766500	-1.63218200	0.12143600
C	0.85853100	-2.78109800	-0.41060200
N	-0.42220000	-2.78990000	-0.79997400
N	3.20755800	-0.52671500	0.93451700
C	2.10505900	0.27353600	0.84589100
N	1.05383700	-0.34912900	0.36815000
H	3.41228000	-4.81858000	-0.26314200
H	-1.02048500	-1.97043000	-0.72656700

H	-0.80160700	-3.64764700	-1.17237100
H	2.11980200	1.31402400	1.14470400
N	-3.45198100	1.43091100	-0.80004200
C	-2.39500900	0.57542000	-0.57204600
O	-2.47030000	-0.63285800	-0.79168500
N	-1.26190900	1.16728000	-0.08946700
C	-1.07652300	2.50689500	0.21739800
O	-0.00214700	2.90072500	0.65564800
C	-2.23833300	3.35779000	-0.02352400
C	-2.12001100	4.81778900	0.28311300
C	-3.35300600	2.77500600	-0.51196900
H	-0.44351100	0.53965400	0.07396700
H	-3.05007600	5.34250300	0.05358100
H	-1.31034400	5.27222800	-0.29607800
H	-1.88245000	4.97438500	1.33978600
H	-4.25358700	3.34653700	-0.71772200
C	-4.72000700	0.85836500	-1.26308000
C	-5.56553900	0.32679100	-0.11150600
H	-4.48134500	0.05870400	-1.96698700
H	-5.24941200	1.64651100	-1.80529400
C	-6.90731000	-0.21675200	-0.59656000
H	-5.00392400	-0.46227000	0.40231000
H	-5.73013400	1.13347000	0.61476000
C	-7.76829400	-0.76474900	0.53888300
H	-7.45616800	0.58008400	-1.11727700
H	-6.73439900	-1.00911300	-1.33716100
H	-7.22538200	-1.57185400	1.04925800
H	-7.92541500	0.02275900	1.28891100
C	-9.12302000	-1.28764600	0.06553500
C	-9.97461500	-1.83157000	1.20816300
H	-8.96474600	-2.07379200	-0.68355600
H	-9.66260500	-0.47952900	-0.44472900
H	-10.93941700	-2.20196800	0.84991800
H	-9.46697700	-2.65791300	1.71669600
H	-10.17113400	-1.05496600	1.95493000
C	4.54701300	-0.15112600	1.37484900
C	5.51512000	0.00925700	0.20708100
H	4.90115700	-0.92535800	2.06196700
H	4.45201100	0.78325600	1.93499200
C	6.90090100	0.43655300	0.68364500
H	5.58175700	-0.94308000	-0.33185400
H	5.11386800	0.75228800	-0.49259500
C	7.89583000	0.59010500	-0.46430400
H	6.82268200	1.38846300	1.22655300
H	7.28440500	-0.30074600	1.40160800
H	7.98322400	-0.36549800	-0.99891100

H	7.50332900	1.31505800	-1.19051800
C	9.28015000	1.03920500	-0.00212700
C	10.26127400	1.19376100	-1.16003500
H	9.67282800	0.31311000	0.72093800
H	9.18880100	1.99211500	0.53461200
H	11.24553200	1.52192400	-0.81379300
H	10.39229300	0.24474400	-1.69059600
H	9.89832300	1.93050800	-1.88449900

1-hexyl–thymine–1-hexyl–thymine HB1

N	-4.12312800	0.98695800	-0.85853300
C	-3.20233300	-0.04126800	-0.97202900
O	-3.52960400	-1.20813000	-1.10418700
N	-1.88444000	0.36361700	-0.92556000
C	-1.41420300	1.64994800	-0.75082500
O	-0.20448800	1.88207300	-0.72033000
C	-2.43368900	2.67675400	-0.60741300
C	-1.99020600	4.09206800	-0.40374900
C	-3.72561400	2.28737100	-0.66446300
H	-1.17977500	-0.38411900	-1.00402100
H	-2.84964200	4.76168400	-0.32717300
H	-1.36052700	4.42562000	-1.23384400
H	-1.39256900	4.18493900	0.50818300
H	-4.53802400	3.00140000	-0.56443200
N	4.10650000	-0.68945900	-1.08309600
C	3.18740100	0.33630500	-0.93886300
O	3.51579700	1.50196500	-0.79971700
N	1.86911400	-0.06958900	-0.96897000
C	1.39857300	-1.36214200	-1.08834900
O	0.18894800	-1.59661200	-1.09508000
C	2.41749500	-2.39347800	-1.20281900
C	1.97437200	-3.81781100	-1.32695600
C	3.70904700	-1.99974800	-1.19060300
H	1.16520200	0.67713200	-0.87610000
H	2.83473100	-4.48627400	-1.40331300
H	1.34488400	-3.95466600	-2.21136400
H	1.37672100	-4.11568300	-0.46032200
H	4.52215400	-2.71522000	-1.27457500
C	5.52946000	-0.34241300	-1.01103300
C	6.02999200	-0.27202900	0.42737100
H	5.65511600	0.62078400	-1.50932500
H	6.07709200	-1.09936600	-1.57938200
C	7.51063600	0.09251000	0.49722900
H	5.43539700	0.47276600	0.96928000
H	5.85914100	-1.24145600	0.91353500
C	8.03756000	0.15204700	1.92926000

H	8.09594200	-0.64049700	-0.07514200
H	7.66839400	1.06446700	0.01096800
H	7.45076700	0.88325600	2.50171800
H	7.87844700	-0.82023300	2.41588000
C	9.51774000	0.51915100	2.00829400
C	10.03384700	0.57691000	3.44277700
H	9.67479600	1.48975000	1.52091800
H	10.10164200	-0.21246000	1.43518600
H	11.09613200	0.83552500	3.47720900
H	9.48857700	1.32668900	4.02566100
H	9.90818700	-0.38865200	3.94423700
C	-5.54498700	0.62637500	-0.86433400
C	-6.02507600	0.14791200	0.50118900
H	-5.68073000	-0.15673700	-1.61309400
H	-6.10153400	1.51033500	-1.18757000
C	-7.50285300	-0.23486100	0.47745000
H	-5.41976000	-0.71523400	0.80072600
H	-5.85382900	0.94073400	1.24072000
C	-8.00814200	-0.73084200	1.83056100
H	-8.10107100	0.63061400	0.16083800
H	-7.66199400	-1.01621100	-0.27767600
H	-7.40914900	-1.59612500	2.14505000
H	-7.84721000	0.04831200	2.58830100
C	-9.48496400	-1.11972800	1.81295600
C	-9.97402400	-1.62515100	3.16667900
H	-9.64442000	-1.89289300	1.05075600
H	-10.08336800	-0.25302300	1.50458300
H	-11.03263800	-1.89873900	3.13619300
H	-9.40944300	-2.50912000	3.48111700
H	-9.84938700	-0.85963300	3.93990400

1-hexyl–thymine–1-hexyl–thymine HB2

N	-4.94845400	0.21359700	-0.22107600
C	-3.94864500	-0.45557700	-0.91031100
O	-4.03786100	-1.62002700	-1.26163000
N	-2.81344400	0.29315400	-1.13962600
C	-2.58606300	1.60179800	-0.76429900
O	-1.49257000	2.13311600	-0.96593400
C	-3.70653400	2.27241100	-0.12132600
C	-3.54913100	3.71212800	0.25646600
C	-4.80934300	1.53471400	0.13309400
H	-2.01712100	-0.22658800	-1.53733600
H	-4.44897800	4.08526400	0.75025000
H	-3.35448700	4.32809500	-0.62659100
H	-2.69804800	3.84295200	0.93144600
H	-5.66646500	1.95587600	0.65207000

N	3.16584900	0.25022300	-0.86814500
C	2.09828200	1.13125100	-0.91271200
O	2.21614000	2.32224100	-0.68194200
N	0.89163500	0.55071400	-1.24555400
C	0.65076000	-0.78743400	-1.48869900
O	-0.48438100	-1.18684800	-1.75509600
C	1.81057600	-1.66025800	-1.40410600
C	1.61264300	-3.12411800	-1.64726500
C	2.99754600	-1.09356100	-1.09539300
H	0.07887600	1.18270400	-1.24987500
H	2.55563200	-3.66574000	-1.54555500
H	1.21226500	-3.30247300	-2.64973500
H	0.89126800	-3.53944700	-0.93654000
H	3.90695000	-1.68282500	-1.01544700
C	4.47327700	0.78571300	-0.47091600
C	4.58077000	0.94761400	1.04512500
H	4.59140500	1.75615900	-0.95806100
H	5.22799300	0.10726100	-0.87376600
C	5.91975000	1.54516800	1.50303500
H	3.76368700	1.61012400	1.34830700
H	4.40502800	-0.01970400	1.53315700
C	7.05767900	0.55606400	1.78284800
H	6.25694300	2.27786700	0.75676000
H	5.74358000	2.11451700	2.42196500
H	7.90784200	1.14040800	2.15262500
H	6.76256700	-0.10543200	2.60915700
C	7.51805300	-0.30410200	0.59499300
C	6.80609800	-1.65398700	0.50077900
H	8.59285300	-0.49700400	0.68392700
H	7.39488900	0.26190000	-0.33758100
H	7.10056000	-2.20266800	-0.39937600
H	7.05598300	-2.27585500	1.36656300
H	5.71660600	-1.54843800	0.48977600
C	-6.03195600	-0.58450000	0.36955600
C	-5.71012800	-1.04168000	1.79575200
H	-6.18253200	-1.44398500	-0.28451800
H	-6.93710100	0.02770300	0.35077100
C	-4.41879400	-1.86892100	1.90822700
H	-5.65259800	-0.16511500	2.45547900
H	-6.56936800	-1.63157600	2.13341900
C	-3.13817900	-1.02831000	2.06015000
H	-4.49740900	-2.54428500	2.76705200
H	-4.33379600	-2.50695200	1.02086200
H	-3.24243000	-0.05971700	1.55590000
H	-2.98875800	-0.78204100	3.11981100
C	-1.88842400	-1.71886300	1.51447200

C	-0.65143800	-0.83112200	1.60684300
H	-2.06066100	-1.99269900	0.46523100
H	-1.72091600	-2.65783600	2.05820800
H	0.24057500	-1.33860100	1.22438200
H	-0.78714000	0.08869400	1.02388900
H	-0.44820200	-0.53878800	2.64313100

1-hexyl–thymine–1-hexyl–thymine HB3

N	-3.94657300	-0.39500000	0.36949500
C	-2.93035900	0.52255400	0.57761400
O	-3.09942800	1.56922100	1.17932400
N	-1.71116200	0.15592900	0.04557400
C	-1.42417200	-0.99327700	-0.66381100
O	-0.28844800	-1.20493900	-1.09208300
C	-2.53927300	-1.90628700	-0.85938900
C	-2.29572000	-3.16861100	-1.62623300
C	-3.73452700	-1.55196600	-0.34006600
H	-0.94216300	0.83026400	0.17023400
H	-3.21050600	-3.76089300	-1.69893300
H	-1.52387800	-3.77486000	-1.14282400
H	-1.94165000	-2.94675500	-2.63740200
H	-4.61205000	-2.18292300	-0.45168100
N	4.20414700	1.04895200	-1.08682800
C	3.20106000	0.10325300	-1.22396100
O	3.38123600	-0.99767300	-1.71504200
N	1.96852000	0.51080700	-0.75484500
C	1.65687200	1.71646900	-0.15992200
O	0.51214600	1.95123000	0.23057600
C	2.75765600	2.65987100	-0.03931300
C	2.48362400	3.99242800	0.58430000
C	3.96285100	2.27207700	-0.50871000
H	1.19861900	-0.16391700	-0.87043400
H	3.38891200	4.60281500	0.61229200
H	2.11038300	3.87373000	1.60601300
H	1.71411900	4.53289600	0.02486200
H	4.82886800	2.92629000	-0.45944900
C	5.56107000	0.71025300	-1.53497100
C	6.47404000	0.29011700	-0.38654300
H	5.96299600	1.58946600	-2.04563200
H	5.45893600	-0.09492800	-2.26341000
C	5.98845500	-0.95249900	0.35859700
H	7.46742200	0.11655400	-0.81527700
H	6.57822800	1.12537500	0.32018500
C	6.89507300	-1.35734900	1.52291000
H	4.97787600	-0.76729800	0.74314700
H	5.90019000	-1.78759300	-0.34805600

H	6.96666200	-0.52595100	2.23832000
H	6.42388200	-2.18765100	2.06385900
C	8.30170800	-1.78334300	1.10259300
C	9.12655100	-2.30270300	2.27633700
H	8.82583200	-0.93938200	0.63862800
H	8.22329300	-2.56130600	0.33168400
H	10.13036900	-2.60267200	1.96185600
H	9.23511500	-1.53521600	3.05018000
H	8.64725700	-3.17204600	2.73882700
C	-5.28617900	-0.04668200	0.85644700
C	-6.00836600	0.89983100	-0.10048500
H	-5.16778100	0.42665800	1.83362700
H	-5.82915200	-0.98418700	0.99535800
C	-7.41615900	1.28981100	0.37882900
H	-5.38312400	1.79282300	-0.19804900
H	-6.06212400	0.43499300	-1.09412700
C	-8.54483900	0.43619100	-0.21051800
H	-7.45064300	1.26096300	1.47597300
H	-7.60699200	2.33224100	0.10437800
H	-9.50585300	0.82667100	0.14828300
H	-8.54357000	0.56977300	-1.29971700
C	-8.47690600	-1.05980800	0.10521700
C	-8.60889700	-1.37479400	1.59329800
H	-7.54124800	-1.47974000	-0.28817200
H	-9.28173600	-1.56789500	-0.43828700
H	-8.59437800	-2.45362000	1.77414400
H	-7.79972600	-0.93066400	2.18192800
H	-9.55232400	-0.98273900	1.98837800

9-ethyl–adenine–1-cyclohexyl–uracil WC

N	-1.74873500	0.30795900	0.01167900
C	-2.03025500	-1.00646400	0.01921800
N	-3.22096000	-1.58488000	0.03536300
C	-4.20912000	-0.67389500	0.04230700
C	-4.07151100	0.71061000	0.03523900
C	-2.74942100	1.21062600	0.01895500
N	-2.46118300	2.51458300	0.01209400
N	-5.55896800	-0.90449300	0.05246200
C	-6.15311300	0.33241500	0.05566800
N	-5.30103200	1.32878200	0.04362000
H	-1.15724200	-1.65490300	0.01313200
H	-3.21217200	3.18752000	0.00900000
H	-1.49000900	2.82626900	-0.01593300
H	-7.22892600	0.43632100	0.06295500
N	3.22253700	0.39629800	0.00552500
C	1.88072800	0.02474100	0.01584100

O	1.51189200	-1.13937900	0.04598100
N	0.98916300	1.07014100	-0.00967900
C	1.27665700	2.42153800	-0.05515000
O	0.37046300	3.25487300	-0.07340200
C	2.69019400	2.73138800	-0.08013000
C	3.58073600	1.71789800	-0.04957100
H	-0.01945700	0.79149400	0.00019300
H	3.00464800	3.76452000	-0.12193100
H	4.64896900	1.90532600	-0.06835000
C	4.25610200	-0.65920500	0.03469200
C	5.04848800	-0.69781200	-1.27353100
C	5.17141100	-0.51131800	1.25158500
H	3.69668800	-1.59258500	0.13146000
C	6.08367600	-1.82553700	-1.23384000
H	5.56332000	0.26158900	-1.41978800
H	4.35726900	-0.82973400	-2.11240000
C	6.20132900	-1.64409200	1.27837500
H	5.70112600	0.44981200	1.20436100
H	4.56702200	-0.50802200	2.16453600
C	7.00666700	-1.68711600	-0.02181100
H	6.66371700	-1.82821900	-2.16199400
H	5.56099300	-2.78986500	-1.18113700
H	6.86582300	-1.51910300	2.13896800
H	5.68030100	-2.60101200	1.41336300
H	7.72420700	-2.51364600	0.00424700
H	7.58932300	-0.76040000	-0.11553700
C	-6.17891600	-2.23037300	0.08024200
C	-7.67274400	-2.17759000	-0.18571200
H	-5.97682500	-2.68316700	1.05539700
H	-5.67262800	-2.83623000	-0.67550900
H	-8.06174700	-3.19772700	-0.20479600
H	-8.20483900	-1.63301200	0.59868000
H	-7.88960500	-1.71279600	-1.15125300

9-ethyl–adenine–1-cyclohexyl–uracil RWC

N	1.78707300	0.39343800	-0.03527300
C	2.66921100	1.40651300	-0.01038300
N	3.99097200	1.33301200	0.01128600
C	4.41109300	0.05632200	0.00362500
C	3.61922700	-1.08853200	-0.02431200
C	2.22139300	-0.88116600	-0.04263700
N	1.32983000	-1.87664500	-0.06266100
N	5.70291700	-0.39676200	0.02753200
C	5.62315900	-1.76642100	0.01247500
N	4.39527700	-2.22546800	-0.01992000
H	2.21677400	2.39614000	-0.00663600

H	1.65045400	-2.83255700	-0.06258300
H	0.33337700	-1.66749500	-0.06484400
H	6.51403300	-2.37826400	0.02315800
N	-3.18202000	0.54713900	-0.01481700
C	-1.85620000	0.14122900	-0.03566600
O	-1.52981400	-1.04423200	-0.05879000
N	-0.93294800	1.14818500	-0.02837900
C	-1.16899600	2.51858400	0.00618700
O	-0.23265700	3.30585900	0.01054000
C	-2.57765300	2.86798900	0.03728600
C	-3.49866800	1.88381000	0.02712700
H	0.06989800	0.84583800	-0.03975600
H	-2.86243600	3.91036400	0.06946500
H	-4.56033700	2.10369600	0.05340500
C	-4.25043300	-0.47369500	-0.02189400
C	-5.04452500	-0.45721000	1.28591500
C	-5.16052900	-0.32148700	-1.24236300
H	-3.72439900	-1.42790500	-0.09773900
C	-6.11523900	-1.55175600	1.26973200
H	-5.52966300	0.52034600	1.41029400
H	-4.35867700	-0.59189000	2.12873800
C	-6.22806500	-1.41915300	-1.24553400
H	-5.65708700	0.65800400	-1.21646900
H	-4.55677700	-0.35835500	-2.15499900
C	-7.03393200	-1.40893500	0.05494400
H	-6.69429400	-1.51628200	2.19780000
H	-5.62371700	-2.53328700	1.23728200
H	-6.88837900	-1.28971100	-2.10865700
H	-5.73950800	-2.39555100	-1.36101800
H	-7.77775300	-2.21232000	0.04602200
H	-7.58615200	-0.46211400	0.12940300
C	6.88351400	0.46641800	0.09406200
C	8.18017900	-0.31333600	-0.02166300
H	6.84494800	1.01415900	1.04012300
H	6.79753700	1.19884300	-0.71285600
H	9.01534000	0.38926400	0.01130700
H	8.30211100	-1.01819700	0.80513200
H	8.23555200	-0.86108100	-0.96634600

9-ethyl–adenine–1-cyclohexyl–uracil H

N	5.22687000	-1.73494900	0.01612600
C	5.94569300	-0.60783100	-0.07714900
N	5.51872200	0.64615100	-0.18885300
C	4.17907900	0.70263800	-0.20561800
C	3.30182300	-0.37192600	-0.11961400
C	3.88339300	-1.65578900	0.00027000

N	3.15487000	-2.77343200	0.10044000
N	3.38410400	1.81844500	-0.30787600
C	2.09357200	1.37553200	-0.27629600
N	1.99900400	0.07165000	-0.16787400
H	7.02451600	-0.74340600	-0.05604500
H	2.13671700	-2.76324600	0.11670500
H	3.64097600	-3.65267900	0.19421700
H	1.24940600	2.05011000	-0.34118000
N	-2.83139900	-0.55536900	-0.01019000
C	-1.52219000	-0.09566500	-0.11188900
O	-1.23677000	1.08396500	-0.26106500
N	-0.55946000	-1.07067400	-0.03376300
C	-0.74064100	-2.42810000	0.15016800
O	0.22891200	-3.18297300	0.21398900
C	-2.12735100	-2.83291800	0.25335700
C	-3.08949600	-1.88979900	0.17112900
H	0.42115400	-0.71542300	-0.09326900
H	-4.14054200	-2.14797700	0.24640900
H	-2.36567500	-3.87723200	0.39726200
C	-3.93683200	0.42277900	-0.06031900
C	-4.87889100	0.15082400	-1.23541400
C	-4.68973300	0.47583600	1.27033000
H	-3.44747500	1.38575100	-0.22287700
C	-5.98312300	1.21055700	-1.28213300
H	-5.33786700	-0.84056800	-1.12103100
H	-4.30531500	0.14093600	-2.16799400
C	-5.79652200	1.53157400	1.21198000
H	-5.13731200	-0.50562300	1.47872200
H	-3.98437200	0.69244700	2.07934400
C	-6.74761500	1.27239400	0.04165600
H	-6.66494500	0.99666100	-2.11103300
H	-5.53134900	2.19064900	-1.48472900
H	-6.34527700	1.54577200	2.15885300
H	-5.33959900	2.52283600	1.09257300
H	-7.51637800	2.05074000	-0.00175600
H	-7.26694300	0.31786900	0.20285600
C	3.85258600	3.20006700	-0.37051800
H	4.64657800	3.24472700	-1.12026800
H	3.01524400	3.80573000	-0.72398500
C	4.35701100	3.68298100	0.98140900
H	5.19768900	3.07014100	1.31575900
H	4.69646600	4.71888700	0.90199100
H	3.56362300	3.63327500	1.73191400

9-ethyl–adenine–1-cyclohexyl–uracil RH

N	3.52292300	-3.10226300	0.02177900

C	4.78926500	-2.68616900	-0.11581200
N	5.25113300	-1.44507400	-0.22955600
C	4.25299000	-0.55011600	-0.19029300
C	2.89743800	-0.82525000	-0.05093100
C	2.53662700	-2.18820000	0.05546700
N	1.26716500	-2.59081900	0.19098100
N	4.34281100	0.81853500	-0.27342700
C	3.06710400	1.29431600	-0.17831100
N	2.17134700	0.34470900	-0.04643800
H	5.53640400	-3.47646100	-0.13763200
H	0.48740500	-1.93819000	0.18699200
H	1.08286900	-3.58113700	0.24903900
H	2.83915900	2.35196100	-0.21841700
N	-2.80724700	0.66722700	0.03312700
C	-1.51141600	0.17585700	0.08355100
O	-1.26108700	-1.02555200	0.14935300
N	-0.52604400	1.12131800	0.05239900
C	-0.66928300	2.50077300	-0.04589100
O	0.31944600	3.22159600	-0.08113000
C	-2.05149300	2.94067600	-0.09959300
C	-3.03490700	2.01900000	-0.06035800
H	0.45371400	0.76091100	0.05664300
H	-4.08012600	2.30513600	-0.10296300
H	-2.26787800	3.99717400	-0.17400400
C	-3.93876300	-0.28207200	0.05177600
C	-4.84726700	-0.05139100	1.26160400
C	-4.72230500	-0.23823400	-1.26185600
H	-3.47516300	-1.26630500	0.14852100
C	-5.97929400	-1.08214300	1.27539700
H	-5.28137300	0.95654300	1.21298800
H	-4.25434800	-0.10827400	2.18031300
C	-5.85478700	-1.26776900	-1.23650300
H	-5.14816400	0.76452700	-1.40333100
H	-4.04068500	-0.42629000	-2.09791300
C	-6.77338000	-1.05103600	-0.03215800
H	-6.63725900	-0.89546300	2.12978200
H	-5.55093600	-2.08332600	1.41486600
H	-6.42370500	-1.21516200	-2.16998700
H	-5.42132800	-2.27529000	-1.18299100
H	-7.56096700	-1.81138600	-0.01453400
H	-7.27097800	-0.07638700	-0.12886500
C	5.57726700	1.58837000	-0.40586000
H	6.14974800	1.15338300	-1.22911600
H	5.29042100	2.60342900	-0.68891300
C	6.38920700	1.57988400	0.88087300
H	6.66232800	0.55717900	1.15203300

H	7.30698500	2.15677200	0.74116400
H	5.82038100	2.02390600	1.70185500

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB1

N	-3.75711500	0.30765100	0.00078600
C	-2.44963600	0.76009200	0.00212200
O	-1.49029700	-0.00900100	0.00308700
N	-2.29449200	2.11946000	0.00268900
C	-3.29894700	3.09137500	0.00391800
O	-3.01266900	4.27623100	0.00613800
C	-4.64094200	2.53581300	0.00216600
C	-4.80362900	1.19909300	0.00083500
H	-1.31895600	2.44945400	0.00227800
H	-5.48605400	3.20965900	0.00229900
H	-5.78956400	0.74792700	-0.00031300
N	3.55528600	0.27461000	-0.00319500
C	2.25266400	-0.21661800	-0.00628700
O	1.98620800	-1.40503200	-0.00783800
N	1.27294400	0.75359900	-0.00772300
C	1.44359000	2.12724500	-0.00596400
O	0.47049800	2.87995500	-0.00726300
C	2.82434100	2.55665300	-0.00303600
C	3.79811600	1.62275500	-0.00159000
H	0.30470300	0.40790300	-0.01084800
H	3.04728200	3.61386900	-0.00217300
H	4.84655900	1.90077600	-0.00066500
C	4.67562500	-0.68837300	-0.00021000
C	5.52704400	-0.56132800	-1.26538300
C	5.52161300	-0.55777100	1.26818400
H	4.19666100	-1.66995700	-0.00007900
C	6.64505600	-1.60776500	-1.25586500
H	5.97366900	0.44118900	-1.31351700
H	4.88909400	-0.67799100	-2.14740600
C	6.64017200	-1.60356100	1.26652500
H	5.96656200	0.44552800	1.31485100
H	4.87992800	-0.67230200	2.14778500
C	7.50187100	-1.49186400	0.00681200
H	7.26290300	-1.49618500	-2.15220100
H	6.19835400	-2.60978300	-1.29876200
H	7.25448600	-1.48869600	2.16487200
H	6.19353300	-2.60553400	1.31127100
H	8.27785000	-2.26394800	0.00962400
H	8.01671900	-0.52142700	0.00623300
C	-4.01710500	-1.14754300	0.00055000
C	-4.75853400	-1.58052800	1.26716900
C	-4.75631000	-1.58062900	-1.26734000

H	-3.02754200	-1.60907300	0.00148000
C	-4.97356300	-3.09673600	1.26097500
H	-5.73452200	-1.07875800	1.31545000
H	-4.18716900	-1.26987700	2.14783500
C	-4.97124600	-3.09685400	-1.26136500
H	-5.73225800	-1.07893100	-1.31740700
H	-4.18341900	-1.27004500	-2.14703500
C	-5.71331600	-3.54627700	-0.00085300
H	-5.52537000	-3.39478100	2.15781200
H	-3.99747300	-3.59726800	1.30567400
H	-5.52136200	-3.39505400	-2.15918900
H	-3.99503400	-3.59731600	-1.30419400
H	-5.83433400	-4.63424300	-0.00091100
H	-6.72270700	-3.11267700	-0.00183300

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB2

N	-3.92531000	0.30592100	0.00735500
C	-2.56290900	0.58066200	0.04050600
O	-1.71237200	-0.29911300	0.06763700
N	-2.23853100	1.91392700	0.03973400
C	-3.10778000	3.00584200	0.01099100
O	-2.67154900	4.14503300	0.01457200
C	-4.51044800	2.63030200	-0.02145700
C	-4.84544100	1.32568000	-0.02172400
H	-1.23234600	2.12909600	0.05595700
H	-5.26058400	3.40846200	-0.04546700
H	-5.88265700	1.00896500	-0.04495200
N	3.88377200	0.39596300	-0.04210700
C	3.99670400	1.77912300	-0.08777900
O	5.05908900	2.37045700	-0.15240800
N	2.78850900	2.44807600	-0.05712500
C	1.51172700	1.90713300	0.01545600
O	0.53809000	2.65599800	0.02971400
C	1.48602200	0.46340400	0.06995400
C	2.65568300	-0.20922200	0.04100800
H	2.85464900	3.46021500	-0.09751600
H	0.52790200	-0.03808900	0.12759500
H	2.68271900	-1.29280900	0.08069000
C	5.11987100	-0.41368300	-0.05216600
C	5.31790800	-1.14113500	1.27892300
C	5.14777200	-1.38309900	-1.23516400
H	5.92593200	0.31278600	-0.17732100
C	6.63188100	-1.92694100	1.26122600
H	4.48029400	-1.83254000	1.44575300
H	5.31005900	-0.41368600	2.09729200
C	6.46610700	-2.16197300	-1.24469400

H	4.31391400	-2.09363300	-1.15411900
H	5.01475400	-0.82589000	-2.16836000
C	6.68401200	-2.89716000	0.07925100
H	6.75377600	-2.46449600	2.20678100
H	7.46890100	-1.22017100	1.18590900
H	6.47112100	-2.86720700	-2.08155700
H	7.29564800	-1.46227100	-1.41189900
H	7.64281700	-3.42543200	0.06546700
H	5.90150100	-3.65828700	0.20202700
C	-4.37128800	-1.10196800	0.00271300
C	-5.17652800	-1.43707500	1.26021500
C	-5.14580600	-1.43999500	-1.27331900
H	-3.44923200	-1.68725900	0.01398400
C	-5.58652100	-2.91226100	1.25029400
H	-6.07926200	-0.81273200	1.29714200
H	-4.58004300	-1.20210600	2.14784000
C	-5.55568700	-2.91524900	-1.27033500
H	-6.04851100	-0.81764300	-1.33299800
H	-4.52888500	-1.20594300	-2.14709400
C	-6.36591600	-3.26126300	-0.01928500
H	-6.18039200	-3.13774800	2.14157900
H	-4.68397900	-3.53553400	1.30173900
H	-6.12804700	-3.14189400	-2.17534200
H	-4.65236900	-3.53874000	-1.29902600
H	-6.63170100	-4.32333600	-0.02134400
H	-7.30731800	-2.69503900	-0.03153900

1-cyclohexyl–uracil–1-cyclohexyl–uracil HB3

N	-3.92531000	0.30592100	0.00735500
C	-2.56290900	0.58066200	0.04050600
O	-1.71237200	-0.29911300	0.06763700
N	-2.23853100	1.91392700	0.03973400
C	-3.10778000	3.00584200	0.01099100
O	-2.67154900	4.14503300	0.01457200
C	-4.51044800	2.63030200	-0.02145700
C	-4.84544100	1.32568000	-0.02172400
H	-1.23234600	2.12909600	0.05595700
H	-5.26058400	3.40846200	-0.04546700
H	-5.88265700	1.00896500	-0.04495200
N	3.88377200	0.39596300	-0.04210700
C	3.99670400	1.77912300	-0.08777900
O	5.05908900	2.37045700	-0.15240800
N	2.78850900	2.44807600	-0.05712500
C	1.51172700	1.90713300	0.01545600
O	0.53809000	2.65599800	0.02971400
C	1.48602200	0.46340400	0.06995400

C	2.65568300	-0.20922200	0.04100800
H	2.85464900	3.46021500	-0.09751600
H	0.52790200	-0.03808900	0.12759500
H	2.68271900	-1.29280900	0.08069000
C	5.11987100	-0.41368300	-0.05216600
C	5.31790800	-1.14113500	1.27892300
C	5.14777200	-1.38309900	-1.23516400
H	5.92593200	0.31278600	-0.17732100
C	6.63188100	-1.92694100	1.26122600
H	4.48029400	-1.83254000	1.44575300
H	5.31005900	-0.41368600	2.09729200
C	6.46610700	-2.16197300	-1.24469400
H	4.31391400	-2.09363300	-1.15411900
H	5.01475400	-0.82589000	-2.16836000
C	6.68401200	-2.89716000	0.07925100
H	6.75377600	-2.46449600	2.20678100
H	7.46890100	-1.22017100	1.18590900
H	6.47112100	-2.86720700	-2.08155700
H	7.29564800	-1.46227100	-1.41189900
H	7.64281700	-3.42543200	0.06546700
H	5.90150100	-3.65828700	0.20202700
C	-4.37128800	-1.10196800	0.00271300
C	-5.17652800	-1.43707500	1.26021500
C	-5.14580600	-1.43999500	-1.27331900
H	-3.44923200	-1.68725900	0.01398400
C	-5.58652100	-2.91226100	1.25029400
H	-6.07926200	-0.81273200	1.29714200
H	-4.58004300	-1.20210600	2.14784000
C	-5.55568700	-2.91524900	-1.27033500
H	-6.04851100	-0.81764300	-1.33299800
H	-4.52888500	-1.20594300	-2.14709400
C	-6.36591600	-3.26126300	-0.01928500
H	-6.18039200	-3.13774800	2.14157900
H	-4.68397900	-3.53553400	1.30173900
H	-6.12804700	-3.14189400	-2.17534200
H	-4.65236900	-3.53874000	-1.29902600
H	-6.63170100	-4.32333600	-0.02134400
H	-7.30731800	-2.69503900	-0.03153900

adenine–thymine WC

N	0.96496100	0.37937500	-0.01328500
C	1.57555300	1.57593800	-0.00688600
N	2.87532700	1.82728600	0.00176900
C	3.59650500	0.69372600	0.00445300
C	3.10439900	-0.60887500	-0.00131800
C	1.69821200	-0.75056600	-0.01132500

N	1.08227000	-1.93516700	-0.01855900
N	4.95664500	0.54665500	0.01448700
C	5.21345300	-0.79901400	0.01468200
N	4.12914200	-1.53123400	0.00547900
H	0.89974700	2.42816200	-0.00897200
H	1.63271600	-2.78017600	-0.02035400
H	0.06363100	-1.98369000	-0.01960100
H	6.22553600	-1.17798700	0.02186800
N	-3.81413500	1.60064300	0.00719400
C	-2.43621000	1.62750600	-0.00383700
O	-1.79202100	2.66402100	-0.00757700
N	-1.85881200	0.38026100	-0.01030400
C	-2.51142500	-0.83654800	-0.00360200
O	-1.87253200	-1.88907600	-0.00806300
C	-3.97084900	-0.78016000	0.00791600
C	-4.72688600	-2.07182600	0.01380500
C	-4.54778100	0.43969300	0.01276900
H	-4.27719400	2.50011600	0.01198000
H	-0.81098200	0.36670900	-0.01534500
H	-5.80420200	-1.89281400	0.01958200
H	-4.46774700	-2.67010900	0.89246000
H	-4.47727900	-2.67191800	-0.86635400
H	-5.62401000	0.57444900	0.02148800
H	5.63859000	1.29371900	0.02097200

adenine–uracil WC

N	0.64030900	-0.29439000	0.00161200
C	1.14454500	-1.53962300	-0.00032200
N	2.41715600	-1.90366200	-0.00176800
C	3.23444700	-0.83725200	-0.00114800
C	2.85804200	0.50350100	0.00103000
C	1.46900600	0.76749800	0.00232000
N	0.95807200	2.00099400	0.00442200
N	4.60183300	-0.80992100	-0.00251600
C	4.97559800	0.50853100	-0.00136600
N	3.95945200	1.33262800	0.00094100
H	0.39691300	-2.32995700	-0.00046900
H	1.57870600	2.79567000	0.00372300
H	-0.05259700	2.13711400	0.00223300
H	6.01696000	0.79776000	-0.00236400
N	-4.23093000	-1.09980900	-0.00015700
C	-2.85518300	-1.23970900	0.00123400
O	-2.30580500	-2.32807900	0.00327200
N	-2.17296400	-0.04772500	0.00024000
C	-2.71764100	1.22540500	-0.00149100
O	-1.98633200	2.21432900	-0.00204200

C	-4.16976100	1.27239200	-0.00241300
C	-4.86063600	0.11475000	-0.00169100
H	-4.76502600	-1.95922300	0.00105100
H	-1.12779200	-0.12652900	0.00085500
H	-4.66261600	2.23398700	-0.00371200
H	-5.94374900	0.07540400	-0.00229600
H	5.21531000	-1.61399600	-0.00519300

cytosine–guanine WC

N	-2.18416400	-0.07365100	0.02521400
C	-2.92954300	1.06021400	0.04069600
O	-2.44993400	2.19722100	0.07977200
N	-4.31490700	0.92323000	0.01115800
C	-4.93322800	-0.28436400	-0.03435200
C	-4.20337100	-1.42197800	-0.05044100
C	-2.77195200	-1.27291900	-0.01669800
N	-1.98978800	-2.34935800	-0.02678600
H	-4.85106800	1.78171100	0.02269100
H	-6.01662600	-0.26955300	-0.05591700
H	-4.66681100	-2.39828900	-0.08687800
H	-2.39655000	-3.27141400	-0.05814800
H	-0.96970700	-2.24684000	0.00459400
N	3.91842500	-1.60506300	0.02528800
C	4.97350700	-0.83839500	0.00233400
N	4.65880400	0.50074600	-0.02363400
C	3.29785700	0.59408100	-0.01673900
N	2.57023600	1.73037500	-0.03560900
C	1.26900100	1.49874700	-0.02386000
N	0.39978700	2.51970000	-0.05211400
N	0.72605600	0.23763900	0.00686500
C	1.44455400	-0.95996300	0.02712200
O	0.85333500	-2.04285500	0.05259700
C	2.85499600	-0.72470000	0.01387200
H	6.00015100	-1.17518300	0.00267700
H	0.78455900	3.45108600	-0.03640200
H	-0.61199400	2.38397400	0.01312200
H	-0.30673000	0.14230500	0.01616000
H	5.30550200	1.27761200	-0.04512700

adenine–thymine stacked structure

N	-1.13847300	-2.18803800	0.29233400
C	-1.10048200	-2.24227500	-1.07643900
N	0.00464500	-1.75719100	-1.58432900
C	0.73428900	-1.36822200	-0.48086400
C	1.98656900	-0.73258600	-0.33991500
N	2.72818100	-0.37577300	-1.40744600

N	2.44429500	-0.48447900	0.89684900
C	1.67455800	-0.81309000	1.94398900
N	0.46392900	-1.36336600	1.94650200
C	0.04364900	-1.63027900	0.70188400
N	-1.78753300	1.03804400	1.27416800
C	-2.32626100	0.61074800	0.08368800
O	-3.38460300	0.01120800	0.00086100
N	-1.53793500	0.91106500	-1.00702400
C	-0.28401300	1.52488800	-1.01045600
O	0.33223000	1.66097600	-2.05566700
C	0.18910100	1.96318600	0.30209800
C	-0.57867800	1.68759300	1.37570700
H	-1.87277500	0.57108900	-1.90231400
H	-2.31934600	0.81988800	2.10638000
H	-0.28851000	1.96100900	2.38414800
C	1.50567500	2.67136400	0.36871700
H	2.28680900	2.07277600	-0.10821200
H	1.46089900	3.62935400	-0.15901800
H	1.79612300	2.85532300	1.40533200
H	-1.92766500	-2.64621800	-1.64303600
H	-1.90390300	-2.48254400	0.88443500
H	2.09620000	-0.58447700	2.91994200
H	3.52738600	0.21955800	-1.24010000
H	2.25756000	-0.28302600	-2.29693700

adenine–uracil stacked structure

N	0.41642200	2.21468000	-0.06317500
C	0.31019700	2.04981200	-1.41982100
N	-0.63505200	1.21312800	-1.76744500
C	-1.18430100	0.81401700	-0.56731100
C	-2.19679000	-0.11489700	-0.24280800
N	-2.85054600	-0.81599700	-1.19091800
N	-2.51525900	-0.28927100	1.04899900
C	-1.83172300	0.39443600	1.97735200
N	-0.82631300	1.24840500	1.80941200
C	-0.54770600	1.42814400	0.51029700
N	2.08578200	-0.45220700	1.31113700
C	2.38683500	-0.10190600	0.01160700
O	3.22523900	0.73368200	-0.27557400
N	1.63297000	-0.77491000	-0.92446000
C	0.59756300	-1.68996800	-0.69701000
O	-0.02953800	-2.14887500	-1.63727700
C	0.37985900	-1.99345500	0.70883700
C	1.11474500	-1.36159100	1.64437900
H	2.60906000	0.02720700	2.03217900
H	1.78615900	-0.50475100	-1.89041700

H	-3.40041600	-1.60286600	-0.87517500
H	-2.39484900	-0.91031100	-2.08839200
H	-2.13318000	0.20985900	3.00572400
H	1.08585700	2.79853200	0.42089800
H	0.96920500	2.57113300	-2.09991200
H	0.98254500	-1.52602600	2.70709300
H	-0.39808800	-2.69558600	0.97282000

cytosine–guanine stacked structure

N	-1.11969755	-1.43259993	-1.80909741
C	-2.13913658	-2.01504447	-1.09534437
N	-2.60572769	-1.23658118	-0.15578874
C	-1.85782188	-0.08357938	-0.26317025
C	-1.89600253	1.12635809	0.50959365
O	-2.62432444	1.43646543	1.43903556
N	-0.89420655	2.01629064	0.06570580
C	0.03020789	1.77804042	-0.91853368
N	0.97100662	2.73950679	-1.12499220
N	0.03938691	0.68883489	-1.65102308
C	-0.91951749	-0.19139416	-1.28181205
N	2.30989082	-1.37330841	-0.35861357
C	2.41455448	-0.04637842	0.08255050
O	3.19901547	0.70324931	-0.49093505
N	1.60995729	0.33068499	1.11906818
C	0.76197340	-0.54040138	1.64559603
N	-0.02767069	-0.11621006	2.65067938
C	0.64302064	-1.90481101	1.20396030
C	1.45140297	-2.27164734	0.18354644
H	2.90853115	-1.62876186	-1.13292130
H	1.45704983	-3.26701837	-0.24590084
H	-0.06154036	-2.58906205	1.65612736
H	-0.02588467	0.86974403	2.86767569
H	-0.83542310	-0.65474442	2.92441126
H	-0.84452491	2.88807818	0.58202246
H	1.80892515	2.35909610	-1.55164235
H	1.18080964	3.32779892	-0.32889725
H	-2.49002167	-3.01116173	-1.32295627
H	-0.60810867	-1.83486484	-2.58261078

2.3.2) SMD/M06-2X/6-31+G**

adenine–thymine WC

N	-0.98068600	0.39122200	0.02346800
C	-1.59755700	1.58598400	0.02852400
N	-2.90027400	1.82957600	0.02067400
C	-3.61908500	0.69435600	0.00498900

C	-3.11901500	-0.60525200	-0.00284500
C	-1.71197000	-0.74092300	0.00717500
N	-1.09378300	-1.92700300	0.00054200
N	-4.97881600	0.54212000	-0.00762200
C	-5.23116700	-0.80449900	-0.02237000
N	-4.14115700	-1.53117500	-0.02004700
H	-0.93176400	2.44520300	0.03897200
H	-1.64141500	-2.77524800	-0.01097000
H	-0.07502600	-1.97640000	0.01037200
H	-6.24086300	-1.18962900	-0.03423500
N	3.85324600	1.58631800	-0.01434200
C	2.47810700	1.63062300	-0.01087300
O	1.84519000	2.67813700	-0.01645400
N	1.87956500	0.39397400	-0.00055800
C	2.51836100	-0.83188600	0.00440300
O	1.85703900	-1.87321500	0.01254900
C	3.97722600	-0.79853000	-0.00050900
C	4.72166500	-2.09774000	0.00507200
C	4.57105300	0.41481600	-0.00927000
H	4.33156000	2.47915900	-0.02067500
H	0.83415800	0.39158500	0.00646600
H	5.80022400	-1.92376400	0.00252100
H	4.46341900	-2.69918100	-0.87191100
H	4.46586100	-2.68984700	0.88910400
H	5.64915600	0.53535500	-0.01280700
H	-5.66551200	1.28645000	-0.00617100

adenine–uracil WC

N	-0.64977100	-0.29172100	0.00467800
C	-1.15166200	-1.53895300	0.00810300
N	-2.42580400	-1.90299600	0.00729900
C	-3.24709900	-0.83941500	0.00190700
C	-2.87082200	0.50149700	-0.00273600
C	-1.48252700	0.76806400	-0.00071000
N	-0.97525300	2.00544900	-0.00357300
N	-4.61479000	-0.81525100	-0.00019000
C	-4.99243900	0.50197700	-0.00555500
N	-3.97537700	1.32749700	-0.00735800
H	-0.40711400	-2.33163300	0.01196800
H	-1.59637400	2.80119300	-0.00821800
H	0.03475800	2.14642700	-0.00043100
H	-6.03394700	0.79099200	-0.00789600
N	4.25766600	-1.08821300	-0.00643300
C	2.88513600	-1.23894900	-0.00308700
O	2.34277200	-2.33469000	-0.00524700
N	2.18763600	-0.05623100	0.00291100

C	2.72354100	1.22128900	0.00489700
O	1.97614100	2.20170500	0.00932600
C	4.17335900	1.28461000	0.00123600
C	4.87687700	0.13241700	-0.00438700
H	4.80211500	-1.94246800	-0.01137800
H	1.14388200	-0.14003000	0.00462000
H	4.65710800	2.25145700	0.00271900
H	5.96054800	0.10350200	-0.00756400
H	-5.22862400	-1.62052100	0.00419800

cytosine–guanine WC

N	2.19372300	-0.08526300	0.00114700
C	2.92569200	1.05536100	-0.00224500
O	2.42243500	2.18778000	-0.00360100
N	4.31119500	0.94074000	-0.00427700
C	4.94646900	-0.26019100	-0.00284000
C	4.23091800	-1.40894200	0.00032100
C	2.79730600	-1.27869000	0.00227100
N	2.02603700	-2.36535900	0.00547000
H	4.83906600	1.80579600	-0.00615100
H	6.02994000	-0.23137400	-0.00446600
H	4.70924000	-2.37923300	0.00150200
H	2.44134400	-3.28529100	0.00459800
H	1.00536800	-2.27173800	0.00529200
N	-3.90715100	-1.62360700	-0.00355500
C	-4.97328600	-0.86931200	-0.00342800
N	-4.67235200	0.47347100	-0.00153700
C	-3.31266400	0.58143700	-0.00017000
N	-2.59540400	1.72513600	0.00208800
C	-1.29089100	1.51189400	0.00303100
N	-0.43352300	2.54510300	0.00673700
N	-0.73422500	0.25619100	0.00173500
C	-1.44016000	-0.94839100	-0.00002800
O	-0.82980700	-2.02396500	-0.00003800
C	-2.85257000	-0.73247500	-0.00156800
H	-5.99533400	-1.21952900	-0.00461200
H	-0.82303700	3.47594900	0.00294300
H	0.58129800	2.41582200	0.00013500
H	0.29801700	0.16683300	0.00283200
H	-5.32990100	1.24322300	0.00031200

adenine–thymine stacked structure

N	-0.99066600	-2.28469300	0.26731200
C	-0.94997900	-2.32640400	-1.10180300
N	0.11938300	-1.75761100	-1.60344900
C	0.81994300	-1.32544100	-0.49712400

C	2.03712700	-0.62487300	-0.35124000
N	2.75859500	-0.21965200	-1.41229100
N	2.47777400	-0.36260100	0.89003800
C	1.73119500	-0.74638700	1.93605900
N	0.55784400	-1.37290300	1.92937000
C	0.14978200	-1.64963800	0.68182300
N	-1.83880900	0.92123800	1.29511000
C	-2.36342400	0.48786000	0.10330200
O	-3.39630400	-0.16343400	0.01979100
N	-1.60671700	0.84212600	-0.99126400
C	-0.40371100	1.55119100	-0.99627800
O	0.17486100	1.76713700	-2.05303400
C	0.06844600	1.98350500	0.31820900
C	-0.66786600	1.63817800	1.39577500
H	-1.94169900	0.51119500	-1.89149300
H	-2.34994600	0.66279000	2.13019800
H	-0.38170100	1.90696300	2.40715500
C	1.33979400	2.77090500	0.38926000
H	2.14726500	2.24498200	-0.12910800
H	1.22290500	3.74699800	-0.09317100
H	1.63945200	2.92696600	1.42855900
H	-1.74471400	-2.78537200	-1.67341600
H	-1.72931000	-2.64757700	0.85745600
H	2.13928800	-0.50364000	2.91390800
H	3.54259800	0.39832400	-1.25384500
H	2.31773200	-0.20594300	-2.32197600

adenine–uracil stacked structure

N	0.32170100	2.23087900	-0.12969900
C	0.21119400	2.03556100	-1.48181300
N	-0.70473800	1.15435600	-1.80190500
C	-1.22954600	0.75817200	-0.58967100
C	-2.22365300	-0.18146900	-0.23873100
N	-2.87460400	-0.91261100	-1.16316300
N	-2.52814900	-0.33162900	1.06063900
C	-1.85836100	0.38961700	1.97128500
N	-0.87979700	1.26852300	1.77233000
C	-0.60836800	1.42179400	0.46761400
N	2.09700500	-0.34164500	1.33385500
C	2.41340100	-0.03075200	0.03037100
O	3.24484500	0.81325800	-0.27053100
N	1.69493500	-0.74626000	-0.90079000
C	0.70721600	-1.70779200	-0.65910700
O	0.13869400	-2.24803300	-1.59765900
C	0.45809900	-1.96356300	0.74970100
C	1.15035400	-1.27333700	1.67915300

H	2.59040000	0.17599000	2.05122300
H	1.88569400	-0.52619100	-1.87425000
H	-3.43691800	-1.68814100	-0.84012100
H	-2.47578600	-0.97954300	-2.08970000
H	-2.14922600	0.22171200	3.00501500
H	0.96057000	2.86438600	0.33576300
H	0.84166800	2.56862100	-2.18008000
H	1.00304900	-1.40794600	2.74466300
H	-0.29425500	-2.69135400	1.02132500

cytosine–guanine stacked structure

N	-1.15107500	-1.44373000	-1.79897700
C	-2.17012800	-2.01686500	-1.07582900
N	-2.62195400	-1.22939300	-0.13431800
C	-1.86840400	-0.08099100	-0.25215000
C	-1.88465800	1.12987400	0.51638200
O	-2.60193400	1.44492200	1.45898700
N	-0.88800700	2.01544200	0.06101900
C	0.02384500	1.77036300	-0.93474100
N	0.96424100	2.72712600	-1.16243200
N	0.02090700	0.67398000	-1.65727700
C	-0.93922700	-0.20123200	-1.27913500
N	2.29546000	-1.39505700	-0.36574200
C	2.42064600	-0.06740800	0.05746000
O	3.21001200	0.67118200	-0.53512700
N	1.63859100	0.33590700	1.09789600
C	0.78622200	-0.51554500	1.65554600
N	0.02079100	-0.05946500	2.66406300
C	0.64582600	-1.88392800	1.23319200
C	1.43585900	-2.27579300	0.20497900
H	2.88096200	-1.67403300	-1.14371800
H	1.42413900	-3.27849700	-0.20817500
H	-0.05899100	-2.55529300	1.70578900
H	0.03731600	0.92966200	2.87240300
H	-0.77083800	-0.59589300	2.98932200
H	-0.82423200	2.88918900	0.57520700
H	1.79892500	2.35431400	-1.60415700
H	1.17850000	3.34198700	-0.38688400
H	-2.53120400	-3.01135600	-1.29599200
H	-0.65175400	-1.85342500	-2.57853500