Table 1: Comparison of individual pair-wise interaction energies (kcal mol^{-1}) within the set of ten B-DNA base-pair steps. SCS and SCSN energies were evaluated from the parallel- and antiparallel-spin contributions to the DF-LMP2/aug-cc-pVTZ correlation energy.

Individual pair-wise interaction	DF-LMP2	SCS	SCSN	CBS(T)[†]	Individual pair-wise interaction	DF-LMP2	SCS	SCSN	CBS(T)[†]
AA0/3.24					AA20/3.05				
A...A intra	-8.11	-5.05	-6.10	-6.25	A...A intra	-8.07	-4.81	-5.91	-6.06
T...T intra	-4.46	-2.05	-2.85	-3.86	T...T intra	-4.88	-2.62	-3.26	-4.18
A...T inter	-1.74	-1.45	-1.63	-1.71	A...T inter	-2.14	-1.60	-2.04	-2.34
T...A inter	-1.35	-1.10	-1.19	-1.30	T...A inter	-2.12	-1.67	-1.92	-2.16
A...T hbond	-13.65	-12.29	-14.06	—	A...T hbond	-12.45	-11.15	-12.77	—
AG08/3.19					AT10/3.26				
A...G intra	-9.11	-6.59	-7.43	-7.58	A...T intra	-7.74	-5.21	-6.16	-6.64
T...C intra	-6.42	-4.63	-5.50	-6.07	T...T inter	0.75	0.92	1.05	0.88
A...C inter	-0.37	0.25	0.15	-0.47	A...A inter	-0.96	-0.41	-0.67	-0.92
T...G inter	-0.18	0.20	0.03	-0.18	A...T hbond	-13.33	-11.99	-13.71	—
G...C hbond	-26.93	-25.19	-28.47	—					
A...T hbond	-14.06	-12.71	-14.08	—					
CG0/3.19					GA10/3.15				
G...C intra	-8.25	-6.41	-7.52	-7.88	A...G intra	-10.94	-7.49	-8.71	-9.14
G...G inter	-4.33	-2.62	-3.17	-3.19	T...C intra	-5.29	-3.33	-4.00	-4.69
C...C inter	1.14	1.35	1.42	1.24	A...C inter	-0.23	0.17	-0.05	-0.31
G...C hbond	-27.44	-25.68	-29.02	—	T...G inter	0.44	0.68	0.95	0.58
					G...C hbond	-26.65	-24.93	-28.17	—
					A...T hbond	-13.33	-11.99	-13.71	—
GC0/3.25					GG0/3.36				
G...C intra	-11.75	-8.85	-10.26	-10.80	G...G intra	-5.12	-2.35	-2.83	-3.54
G...G inter	1.43	2.14	2.64	1.93	C...C intra	-2.31	-0.51	-0.88	-1.62
C...C inter	2.88	3.02	3.35	3.09	C...G inter	-3.51	-3.12	-3.54	-3.68
G...C hbond	-25.89	-24.09	-27.46		G...C inter	-4.67	-4.50	-4.90	-4.82
					G...C hbond	-27.44	-25.68	-29.02	—
GT10/3.15					TG0/3.19				
T...G intra	-6.03	-3.18	-3.89	-4.96	T...G intra	-6.15	-4.32	-5.10	-5.67
A...C intra	-6.61	-4.01	-4.99	-5.44	A...C intra	-5.74	-3.53	-4.48	-4.96
T...C inter	0.21	0.32	0.40	0.30	A...G inter	-4.58	-3.19	-3.83	-4.22
A...G inter	-4.11	-3.37	-3.63	-4.06	T...C inter	-1.14	-1.02	-1.13	-1.15
T...A hbond	-13.33	-11.99	-13.71	—	T...A hbond	-13.65	-12.29	-14.06	—
G...C hbond	-26.65	-24.93	-28.17	—	G...C hbond	-27.44	-25.68	-29.02	—

[†]CBS(T) values from ref. 16