Electronic Supplementary Material for PCCP

SUPPORTING INFORMATION

Dependence of A-RNA simulations on the choice of the force field and salt strength.

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Table S1 Average values of twist (in °) of the individual steps in the *CG_Bsc0/LSC* simulation.

Base pair step	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	Start	1-50 ns
3/4	30.35	31.05	31.14	30.64	30.63	**29.69**	30.76
4/5	29.79	29.77	30.42	29.95	29.54	**33.31**	29.89
5/6	29.86	29.98	30.48	30.38	29.36	**29.69**	30.01
6/7	29.22	29.34	29.70	29.48	29.70	**33.30**	29.49
7/8	29.57	29.79	29.82	29.78	27.65	**29.69**	29.32
8/9	29.20	29.88	29.63	29.66	29.42	**33.29**	29.56
9/10	29.69	30.63	29.93	30.42	30.07	**29.69**	30.15
10/11	29.70	30.46	29.72	30.16	30.33	**33.31**	30.07
11/12	30.31	31.20	30.32	30.66	30.55	**29.68**	30.61

Table S2 Average values of twist (in °) of the individual steps in *CG_Bsc0/HSC* simulation.

Base pair step	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	Start	1-50 ns
3/4	30.46	30.25	30.24	30.02	29.41	**29.69**	30.08
4/5	30.55	30.90	31.08	30.48	31.78	**33.31**	30.96
5/6	31.07	30.81	31.22	30.66	31.82	**29.69**	31.12
6/7	31.89	31.40	31.09	30.80	31.92	**33.30**	31.42
7/8	30.96	31.06	30.78	30.62	30.63	**29.69**	30.81
8/9	31.74	30.93	31.31	30.66	31.63	**33.29**	31.25
9/10	31.40	30.98	30.75	30.92	30.78	**29.69**	30.97
10/11	31.98	31.30	31.37	31.39	31.65	**33.31**	31.54
11/12	31.21	31.02	30.93	31.29	30.94	**29.68**	31.08

Table S3 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *CG_ff99/LSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	Start	1-50 ns
P-P (Å)	16.73	17.42	18.81	18.60	16.23	**9.97**	17.56
Twist (°)	29.27	28.61	28.17	28.31	28.82	**31.50**	28.64
Slide (Å)	-1.88	-2.08	-2.18	-2.16	-1.91	**-1.75**	-2.04
Roll (°)	6.39	5.01	4.00	4.46	6.58	**8.91**	5.29
X-displacement (Å)	-4.87	-5.16	-5.30	-5.45	-4.95	**-4.62**	-5.15
Inclination (°)	11.63	9.54	7.63	8.67	12.49	**16.05**	9.99
Helical twist (°)	31.10	30.15	29.58	29.84	30.80	**32.71**	30.29
Helical rise (Å)	2.84	2.91	3.02	2.95	2.80	**2.81**	2.90
Propeller (°)	-10.78	-8.99	-6.69	-7.72	-10.50	**-13.73**	-8.94

Table S4 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *CG_ff99/HSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	Start	1-50 ns
P-P (Å)	10.15	11.24	12.99	12.53	12.68	**9.97**	11.92
Twist (°)	31.1	30.88	30.11	30.23	29.84	**31.5**	30.43
Slide (Å)	-1.49	-1.55	-1.75	-1.71	-1.83	**-1.75**	-1.67
Roll (°)	10.05	9.13	8.28	8.33	7.96	**8.91**	8.75
X-displacement (Å)	-4.07	-4.15	-4.67	-4.57	-4.87	**-4.62**	-4.47
Inclination (°)	17.58	16.17	15.08	15.16	14.84	**16.05**	15.77
Helical twist (°)	33.66	33.21	32.33	32.4	31.99	**32.71**	32.72
Helical rise (Å)	2.6	2.65	2.65	2.64	2.64	**2.81**	2.64
Propeller (°)	-15.67	-15.21	-13.56	-13.7	-13.51	**-13.73**	-14.33

Table S5 Average parameters (calculated and averaged over base pairs 3 to 11) in 10 ns intervals in the *MIX_ff99/LSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	14.30	13.83	14.24	16.67	16.03	**13.73**	15.01
Twist (°)	28.58	29.00	29.38	28.99	29.28	**30.12**	29.05
Slide (Å)	-1.68	-1.65	-1.60	-1.73	-1.74	**-1.74**	-1.68
Roll (°)	7.09	7.37	7.63	6.19	6.55	**6.27**	6.97
X-displacement (Å)	-4.50	-4.49	-4.30	-4.16	-4.27	**-4.06**	-4.34
Inclination (°)	9.50	9.16	10.80	9.61	10.21	**9.00**	9.86
Helical twist (°)	30.02	30.42	30.97	30.43	30.79	**30.76**	30.53
Helical rise (Å)	2.74	2.72	2.72	2.80	2.77	**2.87**	2.75
Propeller (°)	-11.39	-11.79	-12.67	-11.08	-10.93	**-7.07**	-11.57

Table S6 Average parameters (calculated and averaged over base pairs 3 to 11) in 10 ns intervals in the *MIX_Bsc0/LSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	13.61	12.67	12.61	13.41	12.48	**13.73**	12.96
Twist (°)	29.38	29.45	29.44	29.39	29.23	**30.12**	29.38
Slide (Å)	-1.54	-1.51	-1.52	-1.57	-1.54	**-1.74**	-1.54
Roll (°)	8.36	8.92	8.83	8.2	9.18	**6.27**	8.70
X-displacement (Å)	-4.2	-4.22	-4.25	-4.24	-4.35	**-4.06**	-4.25
Inclination (°)	11.07	11.31	11.24	10.38	11.56	**9.00**	11.11
Helical twist (°)	31.05	31.14	31.14	30.95	30.99	**30.76**	31.05
Helical rise (Å)	2.71	2.69	2.68	2.72	2.65	**2.87**	2.69
Propeller (°)	-12.26	-12.52	-12.74	-12.14	-12.49	**-7.07**	-12.43

Table S7 Average parameters (calculated and averaged over base pairs 3 to 11) in 10 ns intervals in the *MIX_ff99/HSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	11.64	12.43	11.4	10.31	12.61	**13.73**	11.68
Twist (°)	29.78	29.76	29.22	30.09	28.97	**30.12**	29.56
Slide (Å)	-1.55	-1.58	-1.62	-1.48	-1.61	**-1.74**	-1.57
Roll (°)	8.95	8.36	9.07	9.71	8.33	**6.27**	8.88
X-displacement (Å)	-4.37	-4.35	-4.59	-4.29	-4.68	**-4.06**	-4.46
Inclination (°)	11.54	10.85	11.57	12.08	11.01	**9.00**	11.41
Helical twist (°)	31.49	31.32	30.88	31.86	30.59	**30.76**	31.23
Helical rise (Å)	2.64	2.66	2.60	2.60	2.64	**2.87**	2.63
Propeller (°)	-13.08	-12.61	-12.13	-13.8	-12.33	**-7.07**	-12.79

Table S8 Average parameters (calculated and averaged over base pairs 3 to 11) in 10 ns intervals in the *MIX_Bsc0/HSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	10.41	10.5	11.02	10.74	10.76	**13.73**	10.69
Twist (°)	29.73	29.62	29.89	29.79	29.84	**30.12**	29.77
Slide (Å)	-1.47	-1.45	-1.46	-1.46	-1.45	**-1.74**	-1.46
Roll (°)	10.01	10.69	9.95	9.83	9.73	**6.27**	10.04
X-displacement (Å)	-4.32	-4.30	-4.30	-4.27	-4.27	**-4.06**	-4.29
Inclination (°)	12.34	13.86	12.13	12.07	11.85	**9.00**	12.45
Helical twist (°)	31.59	31.79	31.77	31.61	31.61	**30.76**	31.67
Helical rise (Å)	2.58	2.56	2.60	2.60	2.62	**2.87**	2.59
Propeller (°)	-13.43	-12.94	-13.21	-13.42	-13.38	**-7.07**	-13.28

Table S9 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *AU_ff99/LSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	11.97	13.11	11.68	13.13	x	**9.53**	12.47
Twist (°)	28.62	28.27	28.44	27.95	x	**30.55**	28.32
Slide (Å)	-1.27	-1.28	-1.27	-1.28	x	**-1.29**	-1.28
Roll (°)	11.77	11.51	12.20	12.09	x	**9.96**	11.89
X-displacement (Å)	-4.13	-4.15	-4.21	-4.43	x	**-4.07**	-4.23
Inclination (°)	21.33	20.92	22.18	20.65	x	**18.75**	21.27
Helical twist (°)	32.4	32.27	32.46	31.59	x	**32.72**	32.18
Helical rise (Å)	2.44	2.42	2.40	2.36	x	**2.64**	2.41
Propeller (°)	-14.22	-13.85	-14.7	-13.83	x	**-18.82**	-14.15

Table S10 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *AU_Bsc0/LSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-50 ns	x-ray	1-50 ns
P-P (Å)	10.13	10.92	11.05	10.76	11.48	**9.53**	10.87
Twist (°)	29.09	29.06	29.75	30.47	30.74	**30.55**	29.82
Slide (Å)	-1.3	-1.13	-1.21	-1.13	-1.12	**-1.29**	-1.18
Roll (°)	13.17	12.38	11.36	9.89	9.28	**9.96**	11.22
X-displacement (Å)	-4.24	-3.93	-3.84	-3.38	-3.30	**-4.07**	-3.74
Inclination (°)	23.22	21.82	20.03	16.85	15.72	**18.75**	19.53
Helical twist (°)	33.22	33.86	33.44	35.3	35.73	**32.72**	34.31
Helical rise (Å)	2.41	2.46	2.52	2.58	2.63	**2.64**	2.52
Propeller (°)	-15.53	-14.1	-16.15	-15.79	-15.93	**-18.82**	-15.50

Table S11 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *AU_ff99/HSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-48 ns	x-ray	1-50 ns
P-P (Å)	9.23	9.79	11.48	9.82	11.72	**9.53**	10.41
Twist (°)	29.63	29.24	28.11	29.5	29.25	**30.55**	29.15
Slide (Å)	-1.4	-1.29	-1.07	-1.19	-1.29	**-1.29**	-1.25
Roll (°)	13.28	12.84	13.2	14.66	13.6	**9.96**	13.52
X-displacement (Å)	-4.37	-4.22	-3.94	-4.09	-4.23	**-4.07**	-4.17
Inclination (°)	23.02	23.02	23.85	25.38	23.75	**18.75**	23.80
Helical twist (°)	33.67	33.41	32.61	34.16	33.6	**32.72**	33.49
Helical rise (Å)	2.39	2.34	2.35	2.35	2.37	**2.64**	2.36
Propeller (°)	-17.04	-15.87	-14.43	-16.26	-16.08	**-18.82**	-15.94

Table S12 Average parameters (calculated and averaged over base pairs 3 to 12) in 10 ns intervals in the *AU_Bsc0/HSC* simulation.

Parameter	1-10 ns	10-20 ns	20-30 ns	30-40 ns	40-47 ns	x-ray	1-50 ns
P-P (Å)	8.59	8.65	8.59	9.29	9.08	**9.53**	8.84
Twist (°)	29.77	29.68	29.68	28.64	28.93	**30.55**	29.34
Slide (Å)	-1.27	-1.29	-1.28	-1.07	-1.06	**-1.29**	-1.19
Roll (°)	13.93	13.87	13.92	13.88	13.95	**9.96**	13.91
X-displacement (Å)	-4.14	-4.19	-4.17	-3.91	-3.89	**-4.07**	-4.06
Inclination (°)	24.04	23.94	24.07	24.61	24.68	**18.75**	24.27
Helical twist (°)	33.98	33.9	33.89	33.45	33.45	**32.72**	33.73
Helical rise (Å)	2.38	2.38	2.38	2.36	2.39	**2.64**	2.38
Propeller (°)	-17.23	-17.49	-17.11	-15.03	-15.33	**-18.82**	-16.44

Table S13 Zero point vibrational energies (ZPVE, in kcal/mol), Schlitter entropies (S, in cal/K.mol) and corresponding -TS energies (at T = 300 K).

Structure		ff99/LSC	ff99/HSC	Bsc0/LSC	Bsc0/HSC	ff99/ LSC-HSC	Bsc0/ LSC-HSC	ff99-Bsc0/ LSC	ff99-Bsc0/ HSC
CG	ZPVE	1421.5	1474.1	1515.6	1510.6	-52.6	5.0	-94.1	-36.5
	S	2958.4	2752.5	2597.3	2651.1	205.9	-53.8	361.1	101.4
	-TS	-887.5	-825.8	-779.2	-795.3	-61.7	16.1	-108.3	-30.5
AU	ZPVE	1335.1	1385.0	1417.2	1441.6	-49.9	-24.4	-82.1	-56.6
	S	3082.4	2892.6	2802.6	2685.5	189.8	117.1	279.8	207.1
	-TS	-924.7	-867.8	-840.8	-805.6	-56.9	-35.2	-83.9	-62.2
MIX	ZPVE	1361.0	1379.1	1444.4	1402.0	-18.1	42.4	-83.4	-22.9
	S	2524.4	2463.1	2390.6	2388.0	61.3	2.6	133.8	75.1
	-TS	-757.3	-738.9	-717.2	-716.4	-18.4	-0.8	-40.1	-22.5
Average	ZPVE					-40.2	7.7	-86.5	-38.7
	S					152.3	22.0	258.2	127.9
	-TS					-45.7	-6.6	-77.4	-38.4
Average	ZPVE						-16.3		-62.6
	S						87.2		193.1
	-TS						-26.2		-57.9