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SUPPLEMENTARY MATERIAL

Table S1. Sugar–phosphate torsion angles, glycosidic angles (°) and furanose conformations[a]

	α P–O5′	β O5′–C5′	γ C5′–C4′	δ C4′–C3′	ε C3′–O3′	ζ O3′–P	χ C1′–N	*P*	τ_m	Pucker
C1			77	84	–157	–74	–134	16	29	C3′–*endo*
G2	–178	177	–170	143	–178	–84	–111	203	32	C3′–*exo*
T3	–71	–165	40	150	–136	–174	–81	179	42	C2′–*endo*
A4	–59	151	48	140	178	–88	–94	188	29	C3′–*exo*
C5	–79	176	59	135	–145	–154	–92	156	40	C2′–*endo*
G6	67	163	–71	149			–65	201	33	C3′–*exo*
B-DNA[b]	–62	B_I 176 B_{II} 146	48	B_I 128 B_{II} 144	B_I –176 B_{II} –114	B_I –95 B_{II} 174	B_IR –102 B_IY –119 B_{II} –89	160	35	C2′–*endo*

[a] All parameters were calculated using the Curves 5.2 program (19).
[b] Average values for B-DNA taken from Schneider *et al*. (22). *P* is the pseudorotation phase angle, τ_m is the pseudorotation amplitude, B_I and B_{II} are different phosphate conformations.

Table S2. Geometrical properties of base pair steps and base pairs[a]

Base pair	Step	Shift (Å)	Slide (Å)	Rise (Å)	Tilt (°)	Roll (°)	Twist (°)	Propeller twist (°)	Buckle (°)
C1–G6								–12	3.0
	1	0.2	0.1	7.1	–2.2	4.0	26		
G2–C5								–2	–7.5
	2	–0.6	–0.7	3.2	–0.1	3.8	28		
T3–A4								–11	2.6
	3	0.0	0.7	3.3	0.0	–4.2	47		
A4–T3									
B-DNA[b]		0	0	3.4	2	1	36	–11	

[a] All parameters were calculated using the Curves 5.2 program (19).
[b] Average values for B-DNA taken from Neidle (21).