Table 4. Helicoidal parameters for average structures of MD simulations.

MD	Rise	Prop Twst	Roll	Minor	Major	Incli	Twist	P-Radius
A10.1	3.47 (0.29)	-11.6 (4.3)	2.6 (2.7)	11.3 (0.4)	20.3 (0.5)	4.5 (4.6)	32.8 (2.6)	10.1 (0.6)
A10.2	3.41 (0.06)	-14.0 (2.3)	1.7 (2.0)	11.0 (0.3)	20.5 (0.9)	3.0 (3.6)	33.1 (2.1)	10.2 (0.3)
A10.3	3.36 (0.04)	-14.9 (1.7)	1.1 (1.5)	10.6 (0.2)	20.2 (0.5)	1.9 (2.7)	33.7 (1.2)	10.1 (0.3)
A10.4	3.44 (0.24)	-13.2 (5.0)	1.8 (1.9)	10.6 (0.2)	20.1 (0.8)	3.3 (3.6)	33.2 (3.3)	10.0 (0.2)
A20.1	3.37 (0.08)	-12.5 (1.5)	1.4 (1.3)	11.2 (0.3)	20.9 (0.4)	2.6 (2.6)	32.5 (1.4)	10.2 (0.3)
A20.2	3.34 (0.08)	-13.7 (2.3)	1.6 (1.8)	10.9 (0.2)	20.5 (0.7)	2.8 (3.1)	33.4 (1.8)	10.1 (0.3)
AT10.1	3.28 (0.12)	-11.3 (1.2)	4.2 (4.5)	12.4 (0.3)	20.7 (0.2)	7.1 (7.6)	31.6 (2.6)	10.4 (0.5)
AT10.2	3.28 (0.18)	-12.6 (3.4)	3.1 (4.2)	11.7 (0.3)	20.0 (0.6)	5.3 (7.4)	32.0 (4.1)	10.2 (0.7)
1gip(NMR)*	3.45 (0.08)	-15.0 (4.7)	4.3 (5.4)	13.1 (1.4)	16.8 (0.2)	7.0 (8.9)	35.1 (1.8)	9.5 (0.3)
1gip(MD)†	3.31 (0.14)	-11.1 (5.4)	3.1 (4.7)	11.6 (1.2)	19.5 (0.7)	6.7 (9.6)	32.3 (5.5)	9.9 (0.6)

Helicoidal parameters calculated using 3DNA. Numbers in parentheses are standard deviations.

*NMR structural model of Drew-Dickerson DNA, d(CGCGAATTCGCG)$_2$ [Protein Data Bank entry ID code 1gip; Kuszewski, J., Schwieters, C. & Clore, G. M. (2001) *J. Am. Chem. Soc.* **123**, 3903-3918].

†A 4-ns MD simulation of Drew-Dickerson DNA starting from 1gip structure, with the same condition as simulation A10.3. SXD patterns shown in Fig. 10.