Table 3. Helicoidal parameters for MD ensembles and model structures

	Rise	Prop	Major	Minor	Twist	P-rad
A10.1	3.40 (0.10)	-12.1 (4.0)	19.6 (2.1)	10.9 (1.0)	32.9 (1.4)	10.3 (0.3)
A10.2	3.37 (0.08)	-14.1 (3.7)	20.2 (1.7)	10.9 (1.0)	32.9 (1.5)	10.4 (0.3)
A10.3	3.35 (0.07)	-14.8 (3.2)	20.1 (1.3)	10.5 (0.7)	33.6 (1.0)	10.2 (0.3)
A10.4	3.36 (0.08)	-14.1 (3.4)	19.4 (1.7)	10.6 (1.0)	33.2 (1.6)	10.2 (0.3)
A20.1	3.37 (0.05)	-12.7 (2.4)	20.8 (0.8)	11.1 (0.4)	32.4 (0.8)	10.4 (0.2)
A20.2	3.34 (0.04)	-13.8 (2.2)	20.5 (0.8)	10.9 (0.4)	33.2 (0.7)	10.3 (0.2)
AT10.1	3.32 (0.04)	-11.4 (1.9)	20.2 (0.8)	12.2 (0.6)	33.1 (0.8)	10.6 (0.3)
AT10.2	3.30 (0.04)	-12.6 (1.9)	19.6 (0.7)	11.5 (0.5)	33.4 (0.7)	10.3 (0.2)
CGCAAAAAAGCG duplex, crystal*	3.30 (0.10)	-20.0 (4.2)	17.4 (0.9)	9.9 (0.8)	36.6 (5.6)	---
GGCAAAAAACGG duplex, NMR*	3.07 (0.11)	-15.7 (5.3)	17.0 (0.60	10.3 (1.1)	36.5 (1.3)	---
CGCATATATGCG duplex, crystal*	3.30 (0.24)	-14.6 (5.8)	17.5 (0.5)	10.3 (0.7)	36.3 (4.9)	---
Canonical B-form†	3.36	4.2	16.9	11.7	35.8	8.9
B'-form, Model-18‡	3.23	-22.0	19.4	8.8	35.8	9.4

Helicoidal parameters were calculated using 3DNA. Numbers in parentheses are either standard deviations (SDs) of each base step for model structures or SDs of average values of each conformer for MD ensembles.

*Only the parameters for the central A-T regions were listed for crystallographic structures of duplex CGCAAAAAAGCG [Nelson, H.C., Finch, J.T., Luisi, B.F. & Klug, A. (1987) *Nature* **330**, 221-226; Protein Data Bank (PDB) ID code 1D98] and duplex CGCATATATGCG [Yoon, C., Prive, G.G., Goodsell, D.S. & Dickerson, R.E. (1988) *Proc. Natl. Acad. Sci. USA* **85**, 6332-6336; PDB ID code 1DN9], and solution NMR structure of duplex GGCAAAAAACGG [Macdonald, D., Herbert, K., Zhang, X., Pologruto, T. & Lu, P. (2001) *J.Mol.Biol.* **306**, 1081-1098; PDB ID code 1FZX].

†Canonical B-form structure built from nucgen in AMBER.

‡B'-form structure built from 3DNA with model 18.