

SUPPLEMENTARY MATERIAL

	Twist	Roll	Rise	Tilt	Slide	Shift
complex						
C1-T2	35.17 (4.49)	12.52 (6.70)	12.52 (6.70)	9.80 (6.17)	-0.65 (0.38)	-0.65 (0.38)
T2-T3	32.11 (3.49)	2.39 (5.40)	2.39 (5.40)	2.53 (5.92)	-0.65 (0.32)	-0.65 (0.32)
T3-T4	40.56 (3.42)	3.61 (4.72)	3.61 (4.72)	6.26 (4.25)	-0.63 (0.30)	-0.63 (0.30)
T4-T5	27.54 (3.44)	3.64 (4.57)	3.64 (4.57)	6.23 (5.01)	-0.88 (0.35)	-0.88 (0.35)
T5-G6	30.80 (4.91)	12.46 (6.64)	12.46 (6.64)	-3.24 (6.26)	-1.34 (0.41)	-1.34 (0.41)
G6-C7	35.04 (4.26)	-1.87 (5.54)	-1.87 (5.54)	2.39 (5.68)	-1.29 (0.50)	-1.29 (0.50)
C7-A8	24.53 (4.29)	13.29 (8.77)	13.29 (8.77)	7.45 (5.63)	-0.93 (0.35)	-0.93 (0.35)
A8-A9	31.07 (3.42)	-2.22 (4.25)	-2.22 (4.25)	6.08 (3.28)	-0.88 (0.27)	-0.88 (0.27)
A9-A10	39.82 (2.93)	-6.72 (4.94)	-6.72 (4.94)	-1.95 (3.25)	-0.39 (0.23)	-0.39 (0.23)
A10-A11	32.65 (3.54)	1.86 (5.03)	1.86 (5.03)	2.29 (4.37)	-1.26 (0.38)	-1.26 (0.38)
A11-G12	34.92 (4.82)	1.26 (4.39)	1.26 (6.37)	1.03 (5.11)	-1.50 (0.44)	-1.5 (0.44)

free						
C1-T2	17.99 (7.75)	20.66 (9.68)	4.59 (0.62)	0.76 (6.89)	0.98 (0.42)	-0.82 (0.88)
T2-T3	26.63 (4.27)	13.03 (4.32)	3.57 (0.48)	6.37 (5.34)	-0.70 (0.31)	0.76 (0.44)
T3-T4	37.33 (4.02)	6.28 (4.68)	3.57 (0.40)	3.92 (5.24)	-1.15 (0.39)	1.13 (0.48)
T4-T5	39.41 (3.82)	3.45 (4.82)	3.20 (0.36)	6.79 (5.38)	-0.73 (0.31)	1.54 (0.54)
T5-G6	20.65 (4.04)	14.70 (4.69)	3.20 (0.32)	6.66 (4.49)	-0.84 (0.34)	0.40 (0.49)
G6-C7	36.57 (3.62)	-12.22 (5.25)	3.43 (0.27)	-0.08 (4.29)	-0.48 (0.31)	0.07 (0.47)
C7-A8	22.56 (4.26)	11.57 (6.12)	2.88 (0.31)	12.63 (4.77)	-0.44 (0.34)	-0.32 (0.40)
A8-A9	40.63 (3.94)	-3.49 (5.96)	3.47 (0.22)	-1.25 (3.72)	0.22 (0.32)	-0.14 (0.44)
A9-A10	34.76 (4.40)	5.54 (4.88)	3.51 (0.23)	-0.42 (4.32)	-1.17 (0.39)	0.63 (0.40)
A10-A11	32.47 (4.51)	3.78 (5.33)	3.37 (0.23)	1.87 (4.60)	-1.41 (0.40)	0.64 (0.37)
A11-G12	38.14 (4.20)	5.37 (7.05)	3.43 (0.26)	2.78 (4.48)	-1.16 (0.46)	1.51 (0.47)

	Propeller	Buckle	Inclination	X-disp
complex				
C1-G24	-22.71 (7.67)	16.64 (9.29)	2.29 (3.24)	-1.65 (0.60)
T2-A23	-21.66 (5.77)	14.19 (7.87)	2.83 (3.36)	-1.59 (0.50)
T3-A22	-26.38 (5.60)	4.17 (6.43)	2.90 (3.17)	-1.65 (0.44)
T4-A21	-13.55 (5.24)	-4.34 (6.06)	2.86 (3.01)	-1.51 (0.30)
T5-A20	-10.32 (6.05)	2.68 (5.98)	0.96 (3.32)	-1.74 (0.32)
G6-C19	-13.68 (6.94)	-7.76 (9.06)	-1.18 (3.67)	-1.53 (0.35)
C7-G18	-3.30 (6.83)	-10.95 (7.59)	0.38 (3.91)	-1.53 (0.41)
A8-T17	-4.66 (5.06)	0.17 (5.92)	2.23 (3.93)	-1.91 (0.35)
A9-T16	-13.95 (5.27)	4.59 (5.97)	3.93 (3.37)	-1.63 (0.39)
A10-T15	-23.57 (5.20)	-5.08 (5.76)	3.25 (3.33)	-1.80 (0.60)
A11-T14	-20.44 (6.05)	-12.51 (6.80)	3.27 (3.66)	-1.79 (0.70)
G12-C13	-25.19 (7.62)	-18.48 (9.20)	2.94 (3.80)	-1.80 (0.86)
free				
C1-G24	-41.71 (13.35)	33.16 (8.89)	7.85 (5.18)	-1.32 (0.44)
T2-A23	-33.75 (7.12)	15.47 (7.64)	8.68 (4.31)	-1.91 (0.37)
T3-A22	-29.38 (6.67)	6.94 (7.44)	8.00 (3.59)	-1.88 (0.32)
T4-A21	-28.54 (5.67)	-7.63 (7.85)	6.93 (3.35)	-1.82 (0.31)
T5-A20	-11.52 (5.95)	-16.09 (6.48)	6.08 (2.88)	-1.49 (0.32)
G6-C19	-3.07 (6.49)	1.00 (6.38)	2.81 (2.67)	-1.41 (0.30)
C7-G18	-4.49 (6.12)	-1.57 (6.41)	3.32 (2.60)	-1.42 (0.32)
A8-T17	-10.21 (5.89)	13.55 (6.42)	7.49 (2.85)	-1.58 (0.30)
A9-T16	-27.15 (5.59)	6.15 (8.10)	8.11 (3.49)	-1.81 (0.34)
A10-T15	-25.68 (5.22)	-8.94 (6.77)	9.05 (3.77)	-1.91 (0.34)
A11-T14	-30.16 (6.89)	-16.01 (6.90)	10.16 (4.64)	-1.98 (0.39)
G12-C13	-36.63 (10.88)	-32.72 (10.5)	10.19 (5.78)	-1.44 (0.46)

	Minor grooove width	Minor grooove width
	complex	free
G24-T5	10.44 (0.45)	9.85 (0.63)
A23-G6	10.72 (0.51)	10.10 (0.60)
A22-C7	12.95 (0.84)	12.36 (1.05)
A21-A8	14.06 (0.99)	12.42 (0.84)
A20-A9	13.81 (1.04)	12.55 (0.70)
C19-A10	13.93 (0.63)	12.48 (1.03)
G18-A11	10.71 (0.55)	10.03 (1.00)
T17-G12	10.47 (0.44)	9.91 (1.04)
	Pucker	Pucker
	complex	free
C1	53.31 (17.6)	37.54 (50.26)
T2	125.9 (16.07)	36.71 (9.86)
T3	137.1 (12.75)	157.58 (7.82)
T4	120.21 (17.04)	134.51 (9.40)
T5	125.29 (10.63)	117.38 (25.61)
G6	114.97 (27.27)	142.69 (8.41)
C7	55.15 (37.89)	110.45 (17.55)
A8	157.35 (17.05)	151.34 (10.09)
A9	147.38 (8.64)	159.57 (14.93)
A10	111.29 (23.15)	140.08 (15.47)
A11	114.79 (13.90)	128.41 (16.25)
G12	129.19 (28.84)	136.36 (9.94)

Figure S1. Supplementary data on helical parameters for free DNA (free) and 2:1 complex (complex) of H33258 with d(CTTTTGCAAAG)₂. Mean values are given with one standard deviation in parentheses.