

**SUPPLEMENTARY INFORMATION****A Physical Picture of Atomic Motions within the Dickerson DNA Dodecamer in Solution Derived From Joint Ensemble Refinement Against NMR and Large Angle X-Ray Scattering Data**Charles D. Schwieters<sup>†,\*</sup> and G. Marius Clore<sup>‡,\*</sup>

<sup>†</sup>Division of Computational Bioscience, Center for Information Technology, National Institutes of Health, Building 12A, Bethesda, MD 20892-5624

<sup>‡</sup>Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Building 5, Bethesda, MD 20892-0520

8 Tables detailing helical parameters, and sugar and torsion angle parameters for ensemble sizes  $N_e = 1, 2, 4$  and 8.

## Supplemental Information

Table S1: Helical Parameters for  $N_e = 1$

bases	propeller twist	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
1-24	-14.11(8.76)						
2-23	-17.99(0.57)	0.46(0.17)	0.13(0.12)	3.39(0.08)	-0.47(0.61)	9.97(3.86)	37.211(1.60)
3-22	-21.67(0.90)	-0.67(0.15)	-0.51(0.04)	3.11(0.05)	-2.59(0.98)	-3.93(1.38)	32.782(0.31)
4-21	-14.89(1.71)	0.07(0.17)	0.20(0.10)	3.48(0.08)	5.07(0.48)	2.37(1.17)	36.256(0.63)
5-20	-20.35(0.56)	-0.39(0.06)	0.57(0.11)	3.45(0.09)	-1.49(0.64)	-1.67(1.33)	36.965(0.34)
6-19	-27.86(0.69)	0.46(0.12)	-0.18(0.04)	2.95(0.08)	-1.15(0.44)	-3.80(1.00)	36.232(0.37)
7-18	-27.57(0.89)	0.04(0.05)	-0.70(0.04)	2.85(0.06)	-0.24(0.55)	-2.14(0.85)	39.247(0.56)
8-17	-21.47(0.68)	-0.36(0.06)	-0.16(0.05)	2.89(0.08)	-0.19(0.80)	-2.96(0.70)	36.664(0.48)
9-16	-17.52(2.74)	0.41(0.09)	0.42(0.14)	3.43(0.06)	2.53(1.11)	0.52(1.74)	37.141(0.53)
10-15	-22.27(1.24)	-0.16(0.18)	0.30(0.08)	3.28(0.14)	-5.30(0.75)	2.51(1.22)	36.411(0.62)
11-14	-18.58(0.50)	0.69(0.19)	-0.46(0.04)	3.06(0.05)	2.53(0.76)	-3.47(1.53)	32.772(0.32)
12-13	-14.82(9.33)	-0.50(0.21)	0.16(0.13)	3.44(0.08)	1.93(0.68)	9.78(4.26)	36.711(1.74)

Table S2: Helical Parameters for  $N_e = 2$

bases	propeller twist	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
1-24	-9.69(14.27)						
2-23	-7.59(16.47)	0.40(0.55)	0.20(0.53)	3.72(0.64)	-1.90(5.86)	0.55(14.46)	34.78( 4.85)
3-22	-7.74(8.23)	-0.63(0.53)	-0.68(0.65)	2.99(0.43)	1.05(5.58)	-4.44( 8.73)	32.03( 2.17)
4-21	-10.11(9.18)	0.28(0.40)	0.75(0.77)	3.67(0.43)	2.85(3.92)	2.87( 9.82)	36.00( 2.78)
5-20	-18.62(5.00)	-0.44(0.50)	-0.06(0.71)	3.59(0.26)	-4.08(3.57)	0.49( 8.64)	33.87( 2.33)
6-19	-22.86(6.71)	0.13(0.31)	-0.21(0.35)	3.08(0.22)	-0.24(1.83)	-0.14( 8.49)	37.52( 2.09)
7-18	-23.15(5.74)	-0.01(0.23)	-0.37(0.23)	2.89(0.22)	-0.19(2.20)	-8.71( 8.25)	36.12( 4.03)
8-17	-19.22(5.72)	-0.07(0.32)	-0.20(0.38)	3.04(0.19)	-0.32(2.16)	0.22( 8.03)	37.46( 2.42)
9-16	-10.11(9.73)	0.41(0.49)	-0.09(0.74)	3.60(0.26)	3.72(3.61)	1.57( 7.47)	34.22( 2.36)
10-15	-8.22(8.46)	-0.32(0.42)	0.79(0.88)	3.53(0.43)	-3.22(4.15)	3.82( 9.43)	35.41( 2.63)
11-14	-8.17(14.44)	0.58(0.53)	-0.69(0.73)	2.93(0.36)	-0.78(4.42)	-3.15(11.08)	31.51( 2.06)
12-13	-10.49(13.93)	-0.41(0.54)	0.19(0.56)	3.80(0.77)	2.52(5.68)	2.60(19.35)	33.27(11.47)

Table S3: Helical Parameters for  $N_e = 4$ 

bases	propeller twist	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
1-24	-1.05(16.02)						
2-23	-4.83(20.36)	0.24(0.71)	0.188(0.45)	4.21(0.95)	-1.56( 9.57)	-0.24(22.07)	31.26(10.79)
3-22	-6.27(15.18)	-0.47(0.53)	-0.54(0.47)	3.09(0.47)	1.83( 6.51)	-2.22(18.26)	30.88( 3.24)
4-21	-6.69(15.66)	0.00(0.50)	0.48(0.50)	3.61(0.57)	1.12( 7.07)	1.81(10.87)	34.51( 3.59)
5-20	-13.88(28.13)	-0.15(0.60)	0.14(0.77)	3.81(0.43)	-1.71( 5.91)	-0.92( 8.47)	35.86( 3.40)
6-19	-19.44(28.43)	0.14(0.48)	-0.13(0.49)	3.39(0.53)	-2.14( 4.88)	0.73( 9.56)	36.89( 3.45)
7-18	-19.57(28.50)	-0.04(0.31)	-0.49(0.31)	2.94(0.30)	1.00(25.16)	-8.89( 9.71)	36.47( 3.88)
8-17	-15.83(15.73)	-0.04(0.48)	-0.16(0.51)	3.38(0.45)	1.05( 4.60)	1.07( 9.44)	36.90( 3.27)
9-16	-6.34(29.78)	0.19(0.60)	0.01(0.76)	3.70(0.40)	1.22( 5.23)	0.31( 8.73)	35.73( 3.57)
10-15	-9.30(15.59)	0.00(0.59)	0.49(0.49)	3.46(0.59)	-1.12( 7.78)	3.14(10.59)	34.22( 3.53)
11-14	-4.28(31.02)	0.33(0.56)	-0.41(0.53)	3.09(0.60)	-2.97(26.27)	-2.48(14.69)	30.58( 3.22)
12-13	-5.24(22.79)	-0.20(0.61)	0.14(0.52)	4.29(1.05)	2.56(26.21)	0.03(26.78)	31.93( 8.35)

Table S4: Helical Parameters for  $N_e = 8$ 

bases	propeller twist	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
1-24	-0.54(48.02)						
2-23	-7.68(65.57)	-0.144(1.55)	-0.00(1.26)	3.97(2.74)	-2.15(24.16)	2.18(52.35)	25.42(24.97)
3-22	-7.66(75.45)	-0.244(1.31)	-0.22(1.15)	3.16(1.65)	3.71(48.02)	-5.30(43.73)	27.38(14.93)
4-21	7.39(87.93)	0.031(0.91)	0.45(0.79)	3.67(1.01)	-5.86(61.65)	0.80(38.59)	33.20( 8.90)
5-20	2.46(91.39)	-0.119(0.76)	-0.06(0.89)	3.81(0.70)	-0.79(63.30)	-1.45(29.47)	33.54( 8.56)
6-19	4.98(88.96)	0.005(0.54)	0.00(0.63)	3.65(0.69)	-0.42(55.37)	1.69(24.05)	37.70( 4.01)
7-18	4.02(89.77)	-0.008(0.49)	-0.41(0.57)	3.05(0.49)	-2.15(46.73)	-8.78(21.75)	35.69( 5.90)
8-17	10.34(91.78)	-0.032(0.53)	-0.10(0.62)	3.55(0.62)	8.35(66.84)	0.90(16.09)	37.42( 6.00)
9-16	-0.29(89.55)	0.199(0.92)	0.22(1.01)	3.83(0.99)	11.53(73.38)	-0.64(30.06)	32.41(12.96)
10-15	-5.03(90.95)	0.088(0.81)	0.37(0.90)	3.69(1.14)	-8.76(77.09)	6.01(43.40)	32.16(11.97)
11-14	-7.22(93.20)	0.150(0.97)	-0.20(1.02)	3.11(1.59)	-2.35(79.23)	-6.81(44.14)	29.26(11.33)
12-13	-3.19(89.43)	-0.203(1.43)	-0.01(0.97)	3.95(2.51)	-0.37(82.48)	6.86(64.51)	27.80(20.17)

Table S5: Sugar and Torsion angle parameters for  $N_e = 1$ 

base	sugar pucker		$\chi$	backbone torsion angles					
	phase	amplitude		$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$
1	126.7( 3.2)	30.3(3.8)	-127.0(0.8)			60.5(13.4)	126.6( 3.0)	-165.8(0.9)	-101.6( 6.1)
2	164.8( 3.5)	33.8(0.8)	-98.5(0.9)	-68.2( 2.4)	-178.6( 2.0)	48.4( 1.6)	141.1( 1.6)	-167.6(0.5)	-136.6( 2.0)
3	110.2( 2.3)	35.8(0.4)	-127.0(0.4)	-25.5( 2.1)	137.3( 1.9)	43.3( 0.9)	111.3( 1.7)	-165.2(0.8)	-104.3( 0.9)
4	159.3( 2.7)	36.8(1.0)	-98.3(1.4)	-65.7( 4.8)	172.3( 5.4)	54.5( 1.0)	136.5( 0.9)	-163.4(0.8)	-142.9( 1.4)
5	153.7( 1.9)	34.2(0.6)	-112.1(1.0)	-36.4( 1.5)	140.5( 1.6)	49.9( 0.7)	134.7( 0.7)	-172.2(0.6)	-118.6( 0.7)
6	126.1( 2.1)	40.3(1.6)	-124.1(1.3)	-35.9( 2.7)	144.6( 2.3)	51.4( 1.7)	120.2( 1.1)	179.7(0.3)	-99.1( 0.6)
7	110.0( 1.5)	28.1(0.8)	-121.0(0.7)	-58.1( 1.1)	176.9( 1.2)	50.8( 0.7)	113.4( 0.9)	-179.1(0.4)	-96.0( 0.9)
8	143.3( 2.7)	21.2(1.3)	-108.0(0.7)	-41.4( 1.3)	177.9( 1.8)	35.6( 0.8)	126.6( 1.5)	-174.7(0.8)	-98.1( 1.0)
9	151.1( 2.7)	26.4(1.6)	-103.2(1.0)	-53.2( 5.7)	169.4( 3.1)	49.2( 4.9)	131.4( 1.0)	-166.0(0.5)	-125.1( 1.1)
10	150.9( 3.7)	32.2(1.0)	-99.6(1.0)	-24.6( 7.9)	151.8( 4.4)	31.1( 5.3)	134.6( 1.5)	-174.4(0.3)	-123.0( 1.5)
11	107.7( 1.6)	37.1(1.7)	-120.6(0.9)	-21.9( 3.9)	138.8( 2.9)	36.7( 2.1)	112.3( 1.4)	-169.3(0.8)	-105.4(12.6)
12	130.6(70.7)	24.3(3.2)	-95.2(4.3)	-81.0(16.6)	-166.2(14.5)	53.4(11.4)	123.2(19.3)		
13	134.5( 4.0)	25.0(3.9)	-126.0(0.6)			61.9( 6.2)	130.5( 2.3)	-166.0(0.7)	-95.3( 6.1)
14	160.3( 3.2)	34.5(0.8)	-99.9(1.0)	-66.0( 2.1)	178.9( 2.2)	47.0( 1.2)	139.0( 1.3)	-167.3(0.6)	-139.0( 2.1)
15	109.2( 1.7)	36.1(0.5)	-127.1(0.3)	-22.4( 1.2)	134.1( 1.3)	42.8( 0.7)	110.4( 1.5)	-165.0(0.5)	-104.8( 0.8)
16	157.3( 2.8)	37.9(1.2)	-97.5(1.2)	-62.3( 4.3)	167.5( 4.7)	53.6( 1.4)	136.4( 1.0)	-163.8(0.7)	-141.8( 1.3)
17	151.7( 1.4)	35.1(0.6)	-113.6(1.2)	-36.6( 1.6)	141.6( 2.0)	49.2( 1.3)	134.1( 0.6)	-171.9(0.7)	-117.6( 0.6)
18	128.3( 3.1)	38.5(2.2)	-122.3(2.0)	-41.0( 2.9)	149.6( 2.7)	51.6( 1.7)	121.7( 1.4)	179.9(0.4)	-98.9( 0.7)
19	109.7( 1.5)	28.4(0.9)	-121.1(0.6)	-57.9( 1.1)	176.6( 1.2)	50.9( 0.7)	113.1( 1.0)	-179.0(0.3)	-94.8( 0.4)
20	141.9( 2.1)	18.6(1.0)	-106.6(0.8)	-44.0( 1.3)	-177.7( 1.8)	35.0( 0.8)	124.9( 0.9)	-173.3(0.5)	-99.3( 0.8)
21	149.6( 2.0)	26.0(1.0)	-103.8(0.5)	-51.1( 5.5)	164.5( 2.6)	51.1( 4.2)	130.6( 1.0)	-165.6(0.7)	-124.4( 0.9)
22	147.5( 3.9)	33.4(1.8)	-101.1(1.2)	-21.9( 4.0)	148.3( 3.1)	30.7( 2.6)	133.3( 1.2)	-174.9(0.4)	-123.6( 1.6)
23	107.3( 1.4)	37.4(1.1)	-120.8(0.6)	-20.1( 1.2)	138.3( 1.3)	35.8( 2.0)	112.1( 1.0)	-169.6(0.6)	-103.3(10.8)
24	128.7(65.8)	24.7(2.9)	-96.0(4.7)	-80.9(16.0)	-166.5(14.1)	53.9(10.9)	123.0(18.0)		

Table S6: Sugar and Torsion angle parameters for  $N_e = 2$ 

base	sugar pucker		$\chi$	backbone torsion angles					
	phase	amplitude		$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$
1	132.4(39.1)	27.1( 6.1)	-127.6(39.8)			54.8(28.2)	121.5(13.0)	-159.1(46.9)	-100.4(36.2)
2	152.6(13.8)	32.0( 3.8)	-102.3(10.7)	-62.6(25.8)	169.0(32.4)	47.1(16.6)	134.2( 6.7)	-170.0(33.0)	-116.0(38.4)
3	122.3(32.4)	34.3( 6.5)	-116.6(19.3)	-63.6(22.7)	167.7(36.9)	51.0(20.5)	116.4(17.7)	-159.0(29.8)	-113.2(39.5)
4	159.8(14.7)	32.8( 3.5)	-93.1(12.3)	-69.1(31.1)	167.0(34.6)	55.5(16.8)	139.5( 5.8)	-142.5(50.4)	-141.4(45.3)
5	153.1(11.3)	35.6( 2.6)	-110.9(10.6)	-66.5(20.6)	158.6(30.9)	48.3( 9.7)	137.1( 6.3)	-179.0(14.0)	-113.0(24.6)
6	147.5(28.8)	33.1( 5.7)	-112.7(15.6)	-61.1(25.2)	175.0(41.4)	54.0( 5.8)	127.0(12.4)	177.3( 8.1)	-101.3( 9.8)
7	117.0(22.0)	32.1( 7.3)	-117.6( 8.2)	-48.7(15.0)	170.0(19.8)	47.3( 7.2)	116.5(12.2)	180.0( 5.7)	-99.3(12.8)
8	149.5(17.7)	26.8( 4.2)	-107.2( 6.9)	-40.0(18.7)	174.0(18.2)	35.6(10.2)	130.0( 7.7)	-177.4(14.5)	-91.6( 8.6)
9	118.2(29.0)	34.2( 3.7)	-112.5(16.6)	-78.8(22.8)	177.0(23.9)	62.0(13.3)	117.7(16.4)	-145.8(41.2)	-121.7(32.7)
10	155.7(15.6)	31.0( 6.0)	-101.3( 7.9)	-65.7(24.4)	162.5(33.1)	53.8(18.0)	136.0( 7.8)	175.3(24.0)	-101.7(23.2)
11	106.5(32.7)	30.6(10.0)	-117.8(13.8)	-55.1(28.1)	174.3(41.7)	44.1(10.7)	109.3(14.3)	-175.8(31.7)	-94.1(31.1)
12	119.4(43.0)	17.6( 7.5)	-100.7(18.1)	-81.8(24.7)	-168.7(35.6)	57.8(14.5)	115.9( 8.7)		
13	135.9(38.5)	27.3( 6.2)	-124.3(38.9)			59.6(28.1)	122.7(13.3)	-161.6(47.9)	-95.1(36.4)
14	148.4(13.3)	33.1( 3.2)	-104.0(10.3)	-65.0(24.3)	170.4(29.6)	47.8(17.4)	132.0( 6.6)	-174.5(31.6)	-111.6(37.2)
15	122.0(32.9)	34.2( 6.4)	-116.7(18.5)	-64.5(19.3)	172.2(40.6)	50.1(19.1)	116.0(18.4)	-162.1(23.5)	-109.7(37.8)
16	159.9(16.0)	33.0( 3.9)	-92.8(13.1)	-65.5(26.8)	167.1(35.1)	53.2(15.7)	139.4( 5.9)	-142.6(51.3)	-140.1(46.4)
17	152.4(12.0)	36.0( 2.6)	-111.2(10.5)	-67.4(20.6)	159.6(31.3)	48.1(10.3)	137.0( 6.7)	-179.3(14.3)	-114.5(25.6)
18	147.6(28.9)	32.7( 5.4)	-112.3(15.3)	-60.8(26.5)	175.3(42.5)	53.6( 5.3)	127.2(12.5)	177.4( 8.6)	-101.7( 9.6)
19	117.1(22.1)	32.3( 6.7)	-117.8( 8.4)	-47.0(16.5)	168.6(20.0)	47.0( 7.5)	116.3(12.2)	179.8( 6.7)	-98.4(13.8)
20	149.5(18.7)	26.0( 4.7)	-107.1( 5.9)	-42.3(18.9)	176.5(20.4)	35.9( 9.8)	129.3( 7.6)	-175.8(13.4)	-92.6(11.3)
21	115.7(27.8)	34.6( 4.1)	-112.1(16.2)	-75.1(27.0)	172.6(25.2)	60.6(15.5)	116.3(16.0)	-144.4(42.9)	-121.0(37.6)
22	152.9(17.7)	31.3( 5.0)	-101.9( 8.9)	-69.9(22.4)	163.1(34.0)	56.5(17.5)	135.0( 8.5)	174.7(24.4)	-101.2(21.5)
23	111.3(33.2)	30.4(10.0)	-118.1(13.8)	-53.8(26.2)	174.1(40.0)	44.7(10.9)	110.5(15.8)	-172.4(35.0)	-97.2(31.8)
24	125.5(52.4)	17.9( 7.5)	-99.9(15.6)	-79.7(24.0)	-171.7(37.6)	56.8(16.4)	115.6(10.1)		

Table S7: Sugar and Torsion angle parameters for  $N_e = 4$ 

base	sugar pucker		$\chi$	backbone torsion angles					
	phase	amplitude		$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$
1	119.7(47.3)	26.2(6.4)	-119.5(51.8)			58.7(24.4)	119.6(13.0)	-129.1(47.1)	-130.7(65.9)
2	148.6(12.6)	32.7(3.1)	-102.6(12.7)	-68.1(39.3)	161.0(27.5)	47.8(20.7)	134.7( 6.8)	-149.2(46.8)	-129.9(46.1)
3	123.3(29.0)	33.6(6.4)	-114.8(22.2)	-74.8(22.7)	165.7(34.8)	54.8(20.9)	118.7(15.8)	-146.8(37.2)	-118.7(46.2)
4	159.0(12.4)	33.0(2.8)	-93.3(17.7)	-83.8(25.5)	170.5(32.0)	58.5(18.7)	140.2( 4.5)	-139.9(53.0)	-145.8(50.6)
5	161.6(12.5)	31.9(4.5)	-102.0(17.6)	-81.7(27.7)	168.6(35.0)	55.5(19.9)	140.9( 4.0)	-152.6(49.7)	-125.9(48.1)
6	145.3(32.5)	34.1(6.7)	-115.1(20.5)	-70.5(18.3)	168.4(35.0)	53.8(11.6)	124.5(15.6)	177.2(13.7)	-100.6(12.9)
7	117.4(25.2)	32.3(6.8)	-118.2( 9.3)	-49.8(20.2)	169.9(23.2)	49.2(12.8)	115.4(13.0)	-178.4(22.0)	-96.7(19.1)
8	146.6(21.1)	28.6(4.2)	-110.9( 8.5)	-56.5(29.8)	174.5(22.4)	50.1(23.1)	130.2( 9.5)	-169.2(33.0)	-97.2(16.4)
9	114.0(36.4)	33.2(4.5)	-115.9(20.7)	-77.4(18.4)	172.6(28.5)	64.0(13.7)	116.2(17.0)	-140.6(40.6)	-117.9(48.5)
10	146.0(15.9)	30.8(4.9)	-98.8(12.8)	-69.1(18.4)	165.7(21.9)	51.5(21.2)	132.7( 8.5)	-147.8(48.8)	-124.6(40.4)
11	108.6(24.2)	35.1(5.1)	-114.9(18.8)	-55.8(29.1)	152.2(27.7)	43.4(15.6)	110.0(14.7)	-148.1(42.8)	-112.5(51.3)
12	87.4(42.6)	25.1(6.6)	-99.6(28.2)	-87.6(21.7)	-179.4(35.1)	55.6(23.1)	106.7(11.1)		
13	119.5(49.4)	26.2(5.9)	-120.7(49.2)			60.8(24.8)	119.3(14.0)	-131.1(49.8)	-109.1(77.5)
14	147.6(13.9)	33.5(3.1)	-103.4(13.6)	-69.4(37.3)	162.6(24.8)	47.0(20.9)	134.1( 7.2)	-147.8(48.4)	-129.8(47.0)
15	120.8(27.5)	34.0(6.5)	-115.4(25.4)	-74.3(22.5)	163.9(35.7)	55.1(21.5)	117.4(15.4)	-146.9(37.2)	-117.7(46.2)
16	157.3(11.2)	33.6(3.3)	-93.5(18.4)	-80.5(23.9)	168.0(32.3)	56.8(17.6)	139.6( 4.3)	-138.5(54.8)	-147.0(53.3)
17	158.3(12.7)	32.7(4.8)	-103.7(16.8)	-80.9(28.3)	168.6(32.2)	53.1(18.6)	139.7( 4.7)	-152.0(50.3)	-126.6(47.1)
18	144.7(31.6)	34.0(6.5)	-114.8(20.8)	-70.2(19.3)	169.1(35.8)	53.1(11.6)	124.7(15.2)	179.8(23.2)	-102.0(21.1)
19	116.4(25.0)	31.7(6.6)	-118.2( 9.1)	-51.2(21.8)	169.6(24.5)	49.1(13.2)	114.4(12.3)	179.9(11.4)	-95.3(14.8)
20	144.8(22.3)	27.8(4.7)	-110.1( 7.9)	-57.3(30.6)	176.4(23.3)	50.6(22.9)	129.6( 9.9)	-164.0(36.4)	-98.4(20.6)
21	113.3(34.2)	33.3(4.4)	-116.0(22.2)	-80.9(17.1)	168.0(26.9)	68.1(12.4)	115.4(16.5)	-139.4(41.6)	-118.8(48.2)
22	144.9(17.3)	31.8(4.0)	-100.1(12.1)	-70.8(18.9)	164.9(24.4)	54.3(22.7)	132.6( 9.3)	-157.4(48.1)	-118.5(38.5)
23	110.3(26.9)	34.2(6.0)	-116.3(19.4)	-55.0(27.5)	158.1(33.0)	43.5(14.8)	110.8(15.4)	-144.9(40.4)	-111.9(49.3)
24	83.5(43.8)	25.0(6.4)	-98.3(27.2)	-85.1(23.4)	177.5(35.1)	52.9(22.5)	105.7(11.5)		

Table S8: Sugar and Torsion angle parameters for  $N_e = 8$ 

base	sugar pucker		$\chi$	backbone torsion angles					
	phase	amplitude		$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$
1	121.7(60.1)	26.0(5.7)	-99.0(67.0)			57.7(26.1)	121.7(13.7)	-131.5(50.4)	-123.5(82.9)
2	142.3(32.6)	33.5(4.2)	-103.5(22.0)	-69.6(33.8)	157.2(25.8)	49.7(23.9)	131.6(14.8)	-143.8(51.5)	-132.1(47.2)
3	124.2(33.2)	32.8(6.5)	-115.8(34.4)	-78.1(26.3)	161.1(35.0)	59.6(21.6)	119.3(16.7)	-143.5(39.7)	-121.5(45.0)
4	153.0(31.3)	32.1(3.7)	-93.5(24.0)	-78.8(26.9)	164.0(33.7)	59.5(18.9)	137.3(11.1)	-137.9(52.6)	-144.0(54.2)
5	153.6(19.0)	32.7(4.8)	-104.7(21.0)	-77.1(27.7)	160.9(32.2)	55.0(20.3)	137.5( 8.7)	-155.7(48.0)	-123.6(46.8)
6	150.0(31.4)	31.6(4.8)	-109.0(25.9)	-76.5(22.9)	175.5(37.9)	56.1(11.4)	129.8(13.6)	-164.7(44.9)	-113.5(46.2)
7	115.0(25.0)	32.8(6.4)	-117.7(15.1)	-60.0(24.2)	167.8(23.0)	51.6(16.2)	114.0(13.0)	-176.0(25.4)	-96.9(24.7)
8	140.7(36.5)	26.9(5.1)	-111.3(11.2)	-66.0(30.8)	175.2(24.3)	56.9(24.2)	129.3( 9.8)	-160.9(38.4)	-100.4(33.8)
9	110.5(38.3)	32.1(4.7)	-123.6(43.9)	-81.2(18.5)	169.1(24.7)	64.5(18.4)	114.8(16.8)	-139.2(42.3)	-120.6(47.5)
10	144.6(29.1)	30.3(5.3)	-99.5(17.5)	-71.2(24.3)	162.4(28.1)	58.5(21.4)	132.0(12.1)	-150.7(49.7)	-122.4(42.7)
11	107.3(30.1)	34.3(6.5)	-111.4(39.0)	-57.5(30.3)	155.2(30.1)	44.8(20.1)	110.6(15.1)	-140.1(52.6)	-121.4(61.3)
12	87.3(44.6)	25.8(7.7)	-106.5(40.6)	-86.4(24.7)	178.9(32.2)	56.9(23.8)	105.6(12.5)		
13	121.5(53.7)	25.3(5.2)	-105.4(63.7)			58.7(26.0)	121.9(13.6)	-131.1(47.5)	-122.1(77.8)
14	145.0(25.7)	33.9(3.8)	-104.3(18.2)	-66.5(33.6)	157.7(26.5)	48.3(23.5)	133.0(13.0)	-144.0(52.0)	-130.3(46.8)
15	122.3(31.8)	33.6(6.6)	-117.1(32.7)	-77.3(24.6)	162.4(35.7)	58.3(22.2)	118.2(16.5)	-143.1(39.8)	-121.4(43.1)
16	152.2(35.8)	31.7(3.6)	-94.1(23.0)	-80.2(25.8)	164.4(33.7)	60.7(18.5)	137.3(11.2)	-136.4(53.1)	-143.7(52.0)
17	153.5(22.3)	32.7(4.8)	-105.0(21.8)	-78.9(27.4)	159.8(32.6)	57.7(21.8)	137.9( 8.2)	-156.3(47.9)	-123.4(46.9)
18	147.9(30.6)	32.1(4.5)	-108.6(26.9)	-75.3(22.8)	174.8(38.0)	55.7(12.3)	129.3(13.2)	-165.4(44.2)	-112.4(45.8)
19	114.4(24.1)	32.6(6.1)	-117.7(12.7)	-60.9(24.8)	168.4(22.7)	51.8(16.2)	114.1(12.5)	-173.7(29.4)	-98.0(28.6)
20	141.0(32.5)	26.8(4.9)	-111.7( 9.7)	-69.0(29.8)	175.8(25.2)	58.6(24.4)	129.2( 9.7)	-159.4(40.1)	-101.6(33.1)
21	111.5(35.6)	32.8(4.5)	-119.1(31.8)	-80.9(18.5)	167.4(24.5)	65.9(17.0)	114.9(16.6)	-140.2(42.6)	-120.3(47.3)
22	145.0(27.5)	31.0(5.1)	-100.1(17.3)	-74.2(24.4)	164.4(28.2)	58.8(22.1)	132.4(12.4)	-150.0(49.8)	-124.3(42.2)
23	110.2(33.6)	34.0(6.7)	-107.4(49.8)	-58.1(30.2)	155.3(30.9)	45.2(21.6)	111.7(16.8)	-141.8(51.1)	-118.0(64.1)
24	83.8(47.2)	25.9(8.2)	-108.2(49.7)	-85.1(26.3)	-178.7(33.9)	56.6(24.3)	105.6(12.8)		