Supplementary Table 1

Deviations (Å) between the current model and selected models of d(CGCGCG)$_2$ in the PDB. The pairwise superpositions were calculated for all non-H atoms of the Z-DNA molecule ("All") or only for selected subsets in the indicated chemical moieties.

PDB code	1D48	1DCG	2DCG	1I0T	1ICK
Crystal form	B	A	A	B	A
All 240 atoms					
Rmsd	0.604	0.323	0.124	0.790	0.094
Average	0.498	0.263	0.115	0.603	0.084
Maximum	3.067	1.545	0.272	4.543	0.219
at	OP1_5	OP1_9	C5_7	OP1_9	O6_6
Nucleobases only, 114 atoms					
Rmsd	0.393	0.231	0.134	0.435	0.099
Average	0.375	0.213	0.127	0.415	0.088
Maximum	0.747	0.462	0.263	0.808	0.206
at	N4_7	C8_6	C5_7	N7_10	C5_7
Phosphate groups only, 50 atoms					
Rmsd	0.964	0.500	0.113	1.326	0.078
Average	0.813	0.400	0.103	1.039	0.072
Maximum	2.964	1.394	0.197	4.175	0.144
at	OP1_5	OP1_9	OP1_4	OP1_9	O3'_1
Sugars only (including O3' and O5'), 96 atoms					
Rmsd	0.516	0.270	0.105	0.642	0.087
Average	0.475	0.250	0.097	0.581	0.078
Maximum	1.184	0.616	0.223	2.412	0.186
at	O3'_12	O3'_7	C2'_1	C3'_7	C5'_7

Supplementary Table 2

Average values of bond lengths (Å) and angles (º) in the current structure and in representative structures of d(CGCGCG)$_2$ from the PDB. Values in parentheses are root-mean-square deviations (rmsd) from each average over the bonds (or angles) of the same type in the same moiety. Rmsd values calculated for deviations of all bonds (or angles) within entire moieties from the respective mean values of their individual types are also given. The corresponding targets (with their standard uncertainties) from the stereochemical restraint library of Parkinson *et al.* (1996) are given in the last column. Bold-face numbers highlight library standards that do not agree with the present results and likely need adjustment.

Bonds

	current	1D48	1DCG	2DCG	1I0T	1ICK	Parkinson
Cytosine (average of 6 bonds)							
N1-C2	1.391(3)	1.366(8)	1.387(13)	1.401(17)	1.403(14)	1.399(13)	1.397(10)
N1-C6	1.367(4)	1.378(10)	1.376(11)	1.373(19)	1.366(19)	1.356(10)	1.367(6)
N1-C1'	1.467(2)	1.494(6)	1.515(30)	1.491(31)	1.453(9)	1.473(4)	1.470(12)
C2-N3	1.351(3)	1.364(9)	1.364(16)	1.364(8)	1.358(8)	1.363(11)	1.353(8)
C2-O2	1.248(3)	1.210(4)	1.234(10)	1.237(11)	1.239(10)	1.245(13)	1.240(9)
N3-C4	1.343(2)	1.377(7)	1.357(14)	1.357(20)	1.333(8)	1.338(19)	1.335 (7)
C4-C5	1.431(4)	1.423(10)	1.419(19)	1.450(20)	1.429(5)	1.429(11)	1.425(8)
C4-N4	1.327(1)	1.353(4)	1.364(9)	1.342(16)	1.338(21)	1.342(8)	1.335(9)
C5-C6	1.345(5)	1.327(5)	1.334(11)	1.334(14)	1.357(22)	1.345(10)	1.339(8)
rmsd (54 bonds)	0.0033	0.0077	0.0157	0.0194	0.0137	0.0120	
Guanine (average of 6 bonds)							
N1-C2	1.374(2)	1.344(7)	1.354(18)	1.367(10)	1.369(16)	1.361(12)	1.373(8)
N1-C6	1.384(4)	1.338(7)	1.353(18)	1.374(12)	1.389(17)	1.394(16)	1.391(7)
N9-C1'	1.449(4)	1.413(13)	1.416(23)	1.429(30)	1.450(11)	1.456(7)	1.459(9)
C2-N3	1.329(1)	1.354(7)	1.341(15)	1.342(19)	1.334(7)	1.339(12)	1.323(8)
C2-N2	1.342(3)	1.255(7)	1.294(13)	1.302(14)	1.345(16)	1.349(9)	1.341(10)
N3-C4	1.347(1)	1.351(9)	1.359(17)	1.346(22)	1.346(14)	1.349(10)	1.350(7)
C4-C5	1.383(3)	1.367(8)	1.364(15)	1.358(18)	1.386(5)	1.381(13)	1.379(7)
C4-N9	1.380(1)	1.397(10)	1.403(18)	1.399(8)	1.374(11)	1.386(12)	1.375(8)
C5-C6	1.416(5)	1.430(6)	1.425(9)	1.426(23)	1.416(15)	1.415(9)	1.419(10)
C5-N7	1.390(5)	1.371(12)	1.378(19)	1.382(25)	1.388(7)	1.399(14)	1.388(6)

C6-O6	1.249(3)	1.272(15)	1.267(7)	1.261(16)	1.245(14)	1.256(9)	1.237(9)
N7-C8	1.308(6)	1.329(12)	1.334(17)	1.317(26)	1.298(20)	1.301(19)	1.305(6)
C8-N9	1.378(4)	1.340(7)	1.348(17)	1.365(13)	1.390(19)	1.378(7)	1.374(7)
rmsd (78 bonds)	0.0038	0.0096	0.0163	0.0193	0.0139	0.0119	
2’-Deoxyribose (average of 12 bonds)							
C1'-C2'	1.527(3)	1.557(32)	1.553(45)	1.564(43)	1.532(7)	1.519(25)	1.521(14)
C1'-O4'	1.421(8)	1.435(25)	1.434(32)	1.440(37)	1.425(13)	1.445(31)	1.420(13)
C2'-C3'	1.521(4)	1.507(26)	1.519(47)	1.520(39)	1.494(13)	1.506(15)	1.518(10)
C3'-C4'	1.533(5)	1.554(25)	1.525(26)	1.568(26)	1.520(13)	1.538(7)	1.528(10)
C3'-O3'	1.436(7)	1.409(18)	1.443(28)	1.442(29)	1.423(11)	1.422(10)	1.431(13)
C4'-C5'	1.510(6)	1.533(15)	1.533(28)	1.528(22)	1.505(16)	1.518(12)	1.511(8)
C4'-O4'	1.439(7)	1.429(26)	1.433(38)	1.446(23)	1.434(12)	1.439(14)	1.446(11)
C5'-O5'	1.434(9)	1.416(20)	1.439(33)	1.424(32)	1.438(10)	1.436(14)	1.440(16)
rmsd (96 bonds)	0.0064	0.0240	0.0353	0.0321	0.0122	0.0175	
Phosphodiester (average of 10 bonds)							
P^{+}-O3'	1.593(7)	1.586(17)	1.610(32)	1.601(13)	1.588(24)	1.603(9)	1.607(12)
P-O5'	1.595(9)	1.623(15)	1.620(40)	1.602(23)	1.591(16)	1.599(10)	1.593(10)
P-OP1	1.491(5)	1.430(33)	1.441(48)	1.461(36)	1.489(20)	1.493(14)	1.485(17)
P-OP2	1.494(7)	1.449(46)	1.477(62)	1.465(27)	1.503(19)	1.495(10)	1.485(17)
rmsd (40 bonds)	0.0064	0.0306	0.0469	0.0262	0.0200	0.0108	

Angles

	curr	1D48	1DCG	2DCG	1I0T	1ICK	Parkinson
Cytosine (average of 6 angles)							
C2-N1-C6	120.9(3)	121.3(6)	121.8(12)	120.6(14)	120.7(12)	120.4(8)	120.3(4)
C2-N1-C1'	118.8(7)	116.0(9)	115.6(16)	116.9(10)	118.5(15)	118.8(8)	118.8(11)
C6-N1-C1'	120.3(8)	122.6(6)	122.6(11)	122.5(15)	120.6(10)	120.8(10)	120.8(12)
N1-C2-N3	119.3(3)	116.3(9)	116.7(15)	118.3(13)	118.8(15)	119.1(13)	119.2(7)
N1-C2-O2	119.0(4)	123.7(10)	121.8(12)	120.8(18)	118.7(9)	119.5(9)	118.9(6)
N3-C2-O2	121.7(4)	119.9(10)	121.4(16)	120.9(15)	122.6(8)	121.5(11)	121.9(7)
C2-N3-C4	120.1(2)	123.8(13)	122.2(19)	121.3(11)	120.4(11)	119.6(7)	119.9(5)

N3-C4-C5	121.6(2)	117.9(11)	120.2(14)	120.2(13)	122.3(12)	122.3(5)	121.9(4)
N3-C4-N4	118.3(2)	118.8(15)	117.8(21)	118.9(17)	119.0(7)	117.8(10)	118.0(7)
C5-C4-N4	120.2(2)	123.4(14)	122.0(20)	120.8(23)	118.7(11)	119.8(14)	120.2(7)
C4-C5-C6	117.4(3)	117.9(4)	117.8(14)	117.4(21)	116.8(17)	116.7(4)	117.4(5)
C5-C6-N1	120.8(2)	122.6(6)	121.2(11)	122.1(7)	121.0(9)	121.8(4)	121.0(5)
rmsd (72 angles)	0.41	1.01	1.55	1.54	1.17	0.90	
Cytidine sugars (average of 6 angles)							
N1-C1'-C2'	115.3(4)	115.8(7)	114.8(22)	116.5(7)	115.5(9)	117.4(13)	114.2(16)
N1-C1'-O4'	108.1(6)	107.6(12)	108.0(17)	106.7(10)	107.9(10)	105.2(12)	107.8(8)
C2'-C1'-O4'	106.8(6)	106.5(14)	105.1(20)	105.5(27)	106.3(12)	106.6(10)	106.1(11)
C1'-C2'-C3'	103.8(18)	103.5(21)	102.6(20)	104.1(27)	103.6(29)	104.7(23)	102.7(14)
C2'-C3'-C4'	103.0(3)	105.1(13)	106.3(26)	104.2(21)	104.4(5)	103.7(8)	103.2(10)
C2'-C3'-O3'	110.7(23)	114.0(15)	112.0(41)	111.2(19)	110.9(16)	112.4(22)	110.6(27)
C4'-C3'-O3'	109.5(16)	105.9(6)	107.1(30)	106.8(20)	110.3(14)	110.7(22)	110.3(22)
C3'-C4'-C5'	112.9(8)	112.4(11)	112.1(24)	111.5(16)	113.2(8)	114.9(14)	114.7(15)
C3'-C4'-O4'	106.1(5)	105.0(7)	104.9(22)	103.6(15)	105.9(9)	106.2(8)	105.6(10)
C5'-C4'-O4'	109.1(4)	109.4(8)	108.6(21)	108.1(15)	109.3(7)	109.2(6)	109.4(16)
C1'-O4'-C4'	110.4(6)	111.4(18)	112.2(11)	111.0(19)	110.2(7)	109.2(6)	109.7(14)
C4'-C5'-O5'	107.8(8)	105.3(19)	104.5(35)	105.7(12)	109.4(7)	109.4(7)	110.2(14)
C3'-O3'-P^{+}	121.6(5)	124.4(5)	123.7(50)	121.6(9)	123.9(23)	122.0(10)	119.7(12)
C5'-O5'-P	119.2(11)	116.2(18)	118.1(28)	119.6(19)	119.7(11)	120.8(11)	120.9(16)
rmsd (82 angles)	0.73	1.59	1.98	1.89	1.21	1.11	
Guanine (average of 6 angles)							
C6-N1-C2	124.3(3)	120.5(7)	122.5(6)	123.5(14)	124.7(9)	125.0(5)	125.1(6)
N1-C2-N3	124.2(3)	128.0(8)	125.0(10)	124.1(15)	124.3(7)	123.9(4)	123.9(6)
N1-C2-N2	116.5(2)	119.6(13)	18.3(17)	117.6(17)	116.9(11)	116.8(9)	116.2(9)
N3-C2-N2	119.4(3)	112.4(10)	16.6(11)	118.2(11)	118.8(14)	119.4(12)	119.9(7)
C2-N3-C4	112.0(2)	109.5(8)	111.9(14)	111.9(9)	111.7(8)	112.1(7)	111.9(5)
N3-C4-C5	128.3(4)	128.7(5)	127.8(12)	128.7(13)	128.2(4)	128.2(7)	128.6(5)
N3-C4-N9	126.5(6)	127.6(7)	127.2(17)	126.2(15)	126.2(7)	126.3(7)	126.0(6)
C5-C4-N9	105.2(3)	103.7(3)	105.1(12)	105.1(17)	105.6(7)	105.5(10)	105.4(4)

C4-C5-C6	118.6(2)	116.5(5)	117.2(12)	118.1(10)	119.0(9)	119.1(9)	118.8(6)
C4-C5-N7	111.1(4)	113.0(6)	111.8(10)	112.1(11)	110.6(12)	110.8(6)	110.7(5)
C6-C5-N7	130.4(4)	130.5(8)	130.9(10)	129.8(12)	130.4(16)	130.2(6)	130.4(6)
C5-C6-N1	112.5(3)	116.8(9)	115.6(11)	113.5(13)	112.0(15)	111.8(9)	111.5(5)
C5-C6-O6	126.9(3)	123.1(9)	125.0(13)	126.6(9)	126.8(12)	127.8(12)	128.6(6)
N1-C6-O6	120.6(2)	120.2(5)	119.4(9)	119.9(15)	121.2(7)	120.4(7)	119.9(6)
C5-N7-C8	104.2(3)	102.7(4)	103.5(11)	103.6(13)	104.7(14)	103.9(4)	104.3(5)
N7-C8-N9	113.4(2)	113.8(5)	113.4(13)	113.4(14)	113.2(5)	114.1(6)	113.1(5)
C8-N9-C4	106.3(2)	106.8(6)	106.1(11)	105.7(19)	105.9(8)	105.7(6)	106.4(4)
C4-N9-C1'	129.0(7)	128.9(6)	130.0(13)	129.8(15)	129.0(13)	129.0(9)	**126.5(13)**
C8-N9-C1'	124.5(7)	124.2(8)	123.8(9)	124.4(15)	124.7(14)	125.3(9)	**127.0(13)**
rmsd (114 angles)	0.38	0.74	1.20	1.38	1.07	0.79	
Guanosine sugars (average of 6)							
N9-C1'-C2'	115.3(4)	115.8(7)	114.8(22)	116.5(7)	115.5(9)	117.4(13)	114.2(16)
N9-C1'-O4'	108.1(6)	107.6(12)	108.0(17)	106.7(10)	107.9(10)	105.2(12)	107.8(8)
C2'-C1'-O4'	106.8(6)	106.5(14)	105.1(20)	105.5(27)	106.3(12)	106.6(10)	106.1(11)
C1'-C2'-C3'	103.8(18)	103.5(21)	102.6(20)	104.1(27)	103.6(29)	104.7(23)	102.7(14)
C2'-C3'-C4'	103.0(3)	105.1(13)	106.3(26)	104.2(21)	104.4(5)	103.7(8)	103.2(10)
C2'-C3'-O3'	110.7(23)	114.0(15)	112.0(41)	111.2(19)	110.9(16)	112.4(22)	110.6(27)
C4'-C3'-O3'	109.5(16)	105.9(6)	107.1(30)	106.8(20)	110.3(14)	110.7(22)	110.3(22)
C3'-C4'-C5'	112.9(8)	112.4(11)	112.1(24)	111.5(16)	113.2(8)	114.9(14)	114.7(15)
C3'-C4'-O4'	106.1(5)	105.0(7)	104.9(22)	103.6(15)	105.9(9)	106.2(8)	105.6(10)
C5'-C4'-O4'	109.1(4)	109.4(8)	108.6(21)	108.1(15)	109.3(7)	109.2(6)	109.4(16)
C1'-O4'-C4'	110.4(6)	111.4(18)	112.2(11)	111.0(19)	110.2(7)	109.2(6)	109.7(14)
C4'-C5'-O5'	107.8(8)	105.3(19)	104.5(35)	105.7(12)	109.4(7)	109.4(7)	110.2(14)
C3'-O3'-P^{+}	121.6(5)	124.4(5)	123.7(50)	121.6(9)	123.9(23)	122.0(10)	119.7(12)
C5'-O5'-P	119.2(11)	116.2(18)	118.1(28)	119.6(19)	119.7(11)	120.8(11)	120.9(16)
rmsd (82 angles)	1.05	1.35	2.73	1.81	1.32	1.36	
Phosphodiester (average of 10)							
O3'-P-O5'	103.6(26)	107.3(23)	104.0(36)	103.1(25)	103.4(19)	103.4(24)	104.0(19)
O3'-P-OP1	109.8(23)	107.7(16)	108.4(46)	109.1(29)	108.9(19)	109.2(27)	107.4(32)

O3’-P-OP2	106.3(29)	103.8(18)	104.0(58)	106.4(30)	106.4(27)	106.5(26)	108.3(32)
O5’-P-OP1	107.2(26)	105.9(38)	107.1(44)	107.7(17)	108.2(30)	109.1(26)	108.1(29)
O5’-P-OP2	110.3(5)	108.7(39)	108.3(44)	108.9(17)	109.2(25)	108.9(15)	108.3(27)
OP1-P-OP2	118.6(9)	122.7(23)	122.8(66)	120.0(23)	119.6(12)	118.7(14)	119.6(15)
rmsd (60 angles)	2.18	2.79	4.99	2.46	2.28	2.25	