

SUPPLEMENTARY MATERIAL

Table S1. Backbone torsion angles (deg) of d(ACCGGCCGGT)[a]

Base	α	β	γ	δ	ε	ζ	χ	*P*
A1	-67	164	68	80	-138	-65	-162	7
C2	-77	171	58	89	-155	-74	-159	8
C3	-45	164	59	73	-147	-79	-157	13
G4	-57	167	39	86	-160	-80	-156	5
G5	-57	159	42	88	-147	-75	-162	4
C6	-52	174	49	81	-153	-77	-160	16
C7	154	-164	47	86	-163	-70	-156	16
G8	-66	172	173	78	-145	-73	-169	12
G9	-82	-167	57	86	-170	-65	-158	26
T10			56	81			-138	20

[a]Torsion angles along the backbone of the oligonucleotide are defined as:

$$P\overset{\alpha}{-}O5'\overset{\beta}{-}C5'\overset{\gamma}{-}C4'\overset{\delta}{-}C3'\overset{\varepsilon}{-}O3'\overset{\zeta}{-}P$$

χ is the glycosyl angle, P is the pseudorotation angle. The nucleotides are numbered from C1 to G10 in one strand and from G20 to C11 in the other strand. Torsion angles are calculated using the program CURVES v.5.3 [R.Lavery and H.Sklenar (1989) *J. Biomol. Struct. Dyn.*, **6**, 655–667].

Table S2. Backbone torsion angles (deg) of r(GCG)d(TATACGC)[a]

Base	α	β	γ	δ	ε	ζ	χ	*P*
G1	-63	175	40	86	-143	-74	-180	8
C20			51	87			-160	19
C2	-70	-178	49	82	-159	-66	-156	10
G19	-68	-177	179	90	-152	-73	-173	17
G3	-70	175	51	82	-153	-76	-163	13
C18	139	-166	64	84	-162	-68	-153	19
T4	-70	167	50	84	-149	-75	-159	20
A17	-67	159	47	81	-159	-72	-159	20
A5	-53	171	63	80	-151	-73	-160	20
T16	-67	176	54	77	-154	-70	-153	17
T6	-61	162	44	87	-145	-86	-152	14
A15	-74	179	58	82	-169	-73	-168	18
A7	-67	163	51	83	-148	-80	-157	17
T14	-74	166	53	77	-148	-66	-160	6
C8	-83	175	57	83	-155	-63	-156	17
G13	-62	170	67	71	-148	-67	161	11
G9	-72	-172	57	81	-160	-61	-170	20
C12	-73	171	50	80	-156	-67	-159	18
C10			47	83			-156	24
G11	-68	180	57	80	-148	-72	-179	10

[a]See footnote for Table S1.

Table S3. Backbone torsion angles (deg) of r(GC)d(GTATAGCG)[a]

Base	α	β	γ	δ	ε	ζ	χ	*P*
G1	-69	173	-30	113	-135	-71	179	330
C20			63	83			-156	42
C2	-82	-178	44	80	-170	-62	-160	13
G19	-99	-172	68	96	-168	-65	-176	55
G3	-81	-171	70	90	-168	-73	-167	21
C18	-78	-166	41	135	-179	-109	-122	142
T4	137	164	55	84	-143	-70	-146	16
A17	-36	165	47	86	-149	-85	-155	25
A5	-73	175	-169	84	-154	-69	-163	20
T16	-62	170	54	84	-151	-79	-153	18
T6	-69	172	53	88	-161	-77	-159	22
A15	-81	-176	56	86	-169	-67	-156	6
A7	-62	170	47	83	-156	-73	-149	14
T14	-73	177	47	85	-162	-66	-159	17
C8	-69	175	53	83	-160	-68	-155	19
G13	-68	-179	54	87	-155	-72	167	12
G9	-67	-178	51	76	-161	-66	-167	21
C12	-50	168	37	85	-158	-83	-162	19
C10			50	89			-158	20
G11	-53	179	67	81	-147	-73	-171	11

[a]See footnote for Table S1.

Table S4. Backbone torsion angles (deg) of r(G)d(CGTATACGC)[a]

Base	α	β	γ	δ	ε	ζ	χ	*P*
G1	-71	167	49	85	-142	-73	-180	14
C20			56	82			-154	36
C2	138	-176	63	92	-176	-66	-167	31
G19	-80	179	-178	98	-135	-65	-178	346
G3	-65	-171	-170	95	-153	-74	176	14
C18	154	-166	66	86	178	-78	-152	24
T4	120	-162	38	96	-141	-75	-146	16
A17	-73	166	41	87	-156	-71	-148	17
A5	-75	172	-163	89	-159	-74	-159	15
T16	-66	178	54	82	-159	-81	-151	17
T6	-68	169	58	74	-151	-62	-154	9
A15	-72	177	48	88	-158	-75	-164	18
A7	127	-168	58	78	-162	-70	-158	16
T14	-73	-179	49	81	-156	-69	-158	16
C8	-59	173	-161	88	-152	-68	-164	0
G13	-79	-173	-176	89	-156	-69	-167	6
G9	-64	174	51	83	-161	-77	-156	17
C12	138	-157	51	84	-163	-76	-155	25
C10			56	82			-150	12
G11	-62	166	172	87	-146	-75	-172	358

[a]See footnote for Table S1.

Table S5. Helical parameters for d(ACCGGCCGGT)[a]

Base	x-disp	Roll	Tilt	Incl	ω	κ	Ω	Rise (Å)
A1 . G20	-4.33	-0.2	-2.7	12.7	-15.7	-4.5	37.4	2.68
C2 . G19	-3.85	-1.4	-0.7	10.2	-15.6	8.3	34.4	2.99
C3 . A18	-4.13	5.2	-4.5	10.9	-15.5	7.8	28.3	2.61
G4 . G17	-4.05	1.9	-0.7	9.6	-12.4	10.4	35.5	2.80
G5 . T16	-4.23	-1.5	0.0	11.0	-20.2	1.8	34.8	2.98
C6 . A15	-4.23	1.9	0.7	11.0	-20.2	-1.8	35.5	2.80
C7 . A14	-4.05	5.2	4.5	9.6	-12.4	-10.4	28.3	2.61
G8 . G13	-4.13	-1.4	0.7	10.9	-15.5	-7.8	34.4	2.99
G9 . C12	-3.85	-0.2	2.7	10.2	-15.6	-8.3	37.4	2.68
T10 . C11	-4.33			12.7	-15.7	4.4		

[a]These parameters are calculated using the program CURVES v.5.3 [R.Lavery and H.Sklenar (1989) *J. Biomol. Struct. Dyn.*, **6**, 655–667].

Table S6. Helical parameters for r(GCG)d(TATACGC)[a]

Base	x-disp	Roll	Tilt	Incl	ω	κ	Ω	Rise (Å)
G1 . C20	-4.74	-7.6	1.4	11.6	-7.3	4.1	37.5	2.76
C2 . G19	-4.26	9.2	-1.2	12.5	-15.1	3.8	30.7	2.93
G3 . C18	-4.53	-2.9	-2.0	13.5	-17.4	-12.8	33.1	2.40
T4 . A17	-4.50	6.2	1.4	14.5	-10.9	-4.6	31.0	2.52
A5 . T16	-4.47	-2.5	-0.2	15.4	-16.8	1.7	34.7	2.48
T6 . A15	-3.99	8.1	0.6	14.6	-18.2	7.5	31.1	2.64
A7 . T14	-4.43	-3.1	2.9	14.1	-15.8	9.4	32.9	2.59
C8 . G13	-4.32	5.5	-2.4	15.3	-21.3	10.6	34.1	3.13
G9 . C12	-4.53	-6.5	2.2	12.1	-12.5	-3.5	34.5	2.71
C10 . G11	-4.20			13.8	-0.3	-0.6		

[a]See footnote for Table S5.

Table S7. Helical parameters for r(GC)d(GTATACGC)[a]

Base	x-disp	Roll	Tilt	Incl	ω	κ	Ω	Rise (Å)
G1 . C20	-4.42	-9.4	-1.9	11.2	-5.4	3.7	38.3	3.23
C2 . G19	-4.13	1.4	2.5	8.4	-16.4	3.7	33.3	3.67
G3 . C18	-4.07	4.7	-7.6	12.9	-1.4	-20.4	31.1	2.13
T4 . A17	-4.52	16.1	-2.6	10.9	-12.9	-6.7	26.8	2.22
A5 . T16	-4.17	-2.7	-2.5	11.2	-11.0	-0.1	34.0	2.80
T6 . A15	-3.95	8.1	-1.7	9.3	-15.0	6.1	33.1	2.62
A7 . T14	-4.24	2.2	-2.0	8.2	-16.0	8.8	31.6	2.96
C8 . G13	-4.25	3.7	-6.3	6.2	-12.0	7.1	27.8	3.37
G9 . C12	-4.24	0.4	-1.1	2.4	1.0	-0.3	28.8	3.02
C10 . G11	-4.37			2.9	4.5	6.3		

[a]See footnote for Table S5.

Table S8. Helical parameters for r(G)d(CGTATACGC)[a]

Base	x-disp	Roll	Tilt	Incl	ω	κ	Ω	Rise (Å)
G1 . C20	-4.45	-3.6	-1.7	9.9	-8.0	0.2	38.0	2.91
C2 . G19	-4.67	0.1	4.1	6.9	-9.5	0.1	26.6	3.43
G3 . C18	-4.16	-2.3	-4.5	12.0	-13.7	-13.8	37.3	2.58
T4 . A17	-5.00	15.1	0.4	12.2	-16.0	-11.1	29.3	2.18
A5 . T16	-4.09	-1.7	-0.9	14.0	-8.9	-3.5	33.6	2.56
T6 . A15	-4.63	10.3	2.4	12.4	-14.1	3.2	34.4	2.49
A7 . T14	-4.53	-1.7	3.5	11.3	-22.6	-1.5	33.2	2.62
C8 . G13	-4.24	3.0	-1.9	9.4	-13.8	-1.6	26.4	3.14
G9 . C12	-4.54	-6.1	-2.1	8.5	-13.1	-2.4	34.6	2.91
C10 . G11	-4.55			8.4	0.4	6.6		

[a]See footnote for Table S5.