SUPPORTING MATERIAL FOR:

Effect of loop residues in four-stranded dimeric structures stabilized by minor groove tetrads.

Núria Escaja[a], Irene Gómez-Pinto[b], Júlia Viladoms[a], Enrique Pedroso[a] and Carlos González[b]

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Figure S1: CD spectral data. **A**: CD spectra of d<pGCTGCT> and d<pCGTCGT> in low salt conditions. **B**: CD melting curve at high salt concentration buffer. **C** and **D**: CD spectra at low salt conditions and in high salt concentration buffer. **E** to **H**: Series of CD spectra of the octameric sequences at different temperature and salt conditions.
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Table S1. Assignment list of d<pGCTCGCTC> at T=5ºC, 1.2 mM oligonucleotide concentration
Buffer conditions: 25 mM phosphate buffer pH 7, 10 mM $MgCl_2$, 100 mM NaCl

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	13.39	n.o.	n.o.	7.99	-	6.07	2.72	2.90	4.39		3.87	3.98
C2	-	8.50	6.68	7.55	5.45	6.48	2.08	2.19	4.57	4.27	3.88	4.19
T3	n.o.	-	-	7.47	1.56	5.73	2.23	1.89	4.46	3.97	3.45	3.13

*Chemical shifts of exchangeable protons are given at T=5ºC

Table S2. Assignment list of d<pGCATGCAT> at T=25ºC, 0.5 mM oligonucleotide concentration
Buffer conditions: 25 mM phosphate buffer pH 7

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	n.o.	n.o.	n.o.	7.99	-	6.15	2.76	2.98	4.83	4.42	3.84	4.09
C2	-	n.o.	n.o.	7.46	5.43	6.09	1.96	2.33	4.56	4.12	3.96	
A3	-	n.o.	n.o.	8.47	7.99	6.42	2.97	2.88	4.87	4.48	3.88	4.09
T4	n.o.	-	-	7.68	1.50	5.55	1.90	2.20	4.76	4.30	4.14	

*At T=5ºC the monomeric form coexits with an important population of the dimeric form. Exchangeable protons of the monomeric form are overlapped with those corresponding to the dimer, that are sharper and more intense.

Table S3. Assignment list of d<pGCATGCAT> at T=25ºC, 5 mM oligonucleotide concentration
Buffer conditions: 25 mM phosphate buffer pH 7

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	12.85	8.84	6.08	8.13	-	6.22	2.75	3.01	5.02	4.55	4.01	4.27
C2	-	8.23	6.32	7.50	5.26	6.62	2.56	2.73	5.06	4.59	4.33	4.44
A3	-	n.o.	n.o.	8.09	7.97	6.09	1.97	2.55	4.74	3.47	3.69	3.81
T4	n.o.	-	-	7.84	1.92	6.49	2.34	2.57	4.55	4.68	4.09	4.23

*Chemical shifts of exchangeable protons are given at T=5ºC

Table S4. Assignment list of d<pGCTAGCTA> at T=25ºC, 0.5 mM oligonucleotide concentration
Buffer conditions: 25 mM phosphate buffer pH 7

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	n.o.	n.o.	n.o.	7.94	-	6.01	2.75		4.91	4.41	4.05	4.18
C2	-	n.o.	n.o.	7.62	5.66	6.12	2.09	2.48	4.72	4.23	4.02	
T3	n.o.	-	-	7.51	1.87	6.05	1.87	2.27	4.70	4.21	3.91	3.98
A4	-	n.o.	n.o.	8.17	8.06	6.07	2.49	2.61	4.86	4.24	3.90	4.03

*At T=5ºC the monomeric form coexits with an important population of the dimeric form. Exchangeable protons of the monomeric form are overlapped with those corresponding to the dimer, that are sharper and more intense.

Table S5. Assignment list of d<pGCTAGCTA> at T=25ºC, 5 mM oligonucleotide concentration
Buffer conditions: 25 mM phosphate buffer pH 7

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	13.47	9.28	6.31	8.17	-	6.35	2.77	3.11	5.06	4.65	4.06	4.31
C2	-	8.79	6.52	7.48	5.41	6.59	2.37		5.06	4.53	4.20	4.35
T3	n.o.	-	-	7.39	1.84	5.94	1.92	2.41	4.70	3.48	3.32	3.67
A4	-	n.o.	n.o.	8.52	8.29	6.65	2.79		4.68	4.73	4.13	4.28

*Chemical shifts of exchangeable protons are given at T=5ºC

Table S6. Assignment list of d<pGCTTTGCTTT> at T=5ºC, 1mM oligonucleotide concentration Buffer conditions: 25 mM phosphate buffer pH 7

	H1/H3*	H42/H22*	H41/H21*	H6/H8	H5/Me	H1'	H2'	H2"	H3'	H4'	H5'	H5"
G1	13.37	8.83	6.54	8.08	-	6.01	2.72	2.80	4.85	4.41	4.03	4.13
C2	-	8.59	6.81	7.52	5.36	6.27	2.06	2.29	4.57	4.42	4.24	4.28
T3	n.o.	-	-	7.85	1.96	6.37	2.06	2.53	4.81	4.27	-	-
T4	n.o.	-	-	7.58	1.68	5.89	1.97	2.29	4.69	3.90	4.1	
T5	n.o.	-	-	7.54	1.79	6.11	2.15	2.38	4.76	4.06	3.45	3.67

*Chemical shifts of exchangeable protons are given at T=5ºC

Table S7. Mass spectrometry characterization of the studied oligonucleotides

Sequence	Calculated Mass	MALDI-TOF[a]
d<pGCTGCT>	1845.16	1842.01
d<pCGTCGT>	1845.16	1842.22
d<pGCATGCAT>	2471.58	2470.39
d<pGCTAGCTA>	2471.58	2470.80
d<pGCTTTGCTTT>	3061.94	3058.62
d<pCGTTTCGTTT>	3061.94	3057.94

[a] Sample preparation: 1μL of 0.1 M ammonium citrate solution is added to 1μL of oligonucleotide solution (25-50 μM in H_2O). After few seconds, 1μL of the mixture is added to 1μL of matrix solution, deposited onto the plate and allowed to dry.
Matrix solution: 0.5 M 2,4,6-trihydroxyacetophenone 82,4,6-THAP) in EtOH.

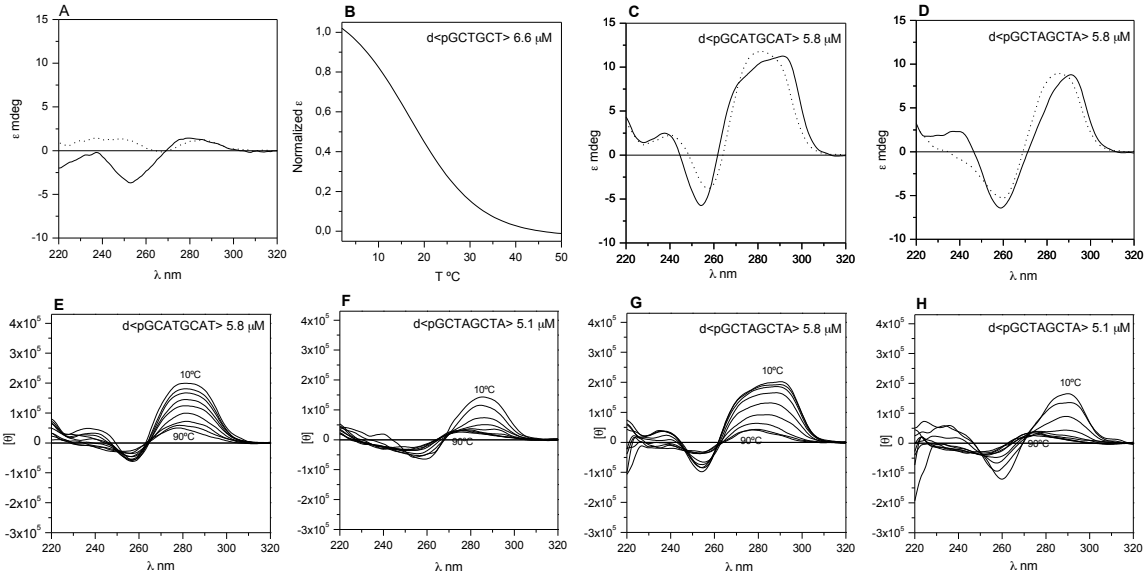

Figure S1. CD data. **A**: CD spectra of d<pGCTGCT> (solid line) and d<pCGTCGT> (dotted line) in low salt conditions. **B**: CD melting curve at high salt concentration buffer. **C** and **D**: CD spectra at low salt conditions (dotted line) and in high salt concentration buffer (solid line). **E**, **F**, **G** and **H**: Series of CD spectra at different temperature at low salt conditions (**E** and **F**) and in high salt concentration buffer (**G** and **H**). Experimental conditions: Low salt conditions: water solution. High salt concentration buffer: 10 mM Na_2PIPES buffer, pH 7, 10 mM $MgCl_2$, 100 mM NaCl.

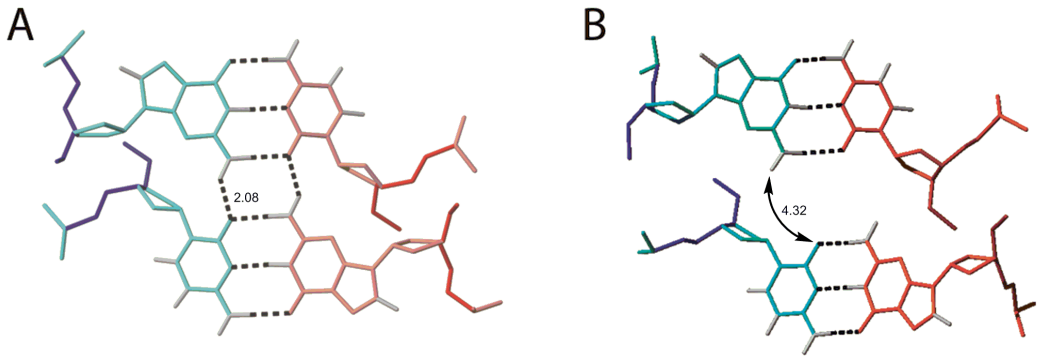

Figure S2. Details of the direct G:C:G:C minor groove tetrads in d<pGCTCGCTT> (A) and d<pGCTGCT> (B). Distances between O2(C)-H21(G) through minor groove are given in Å.

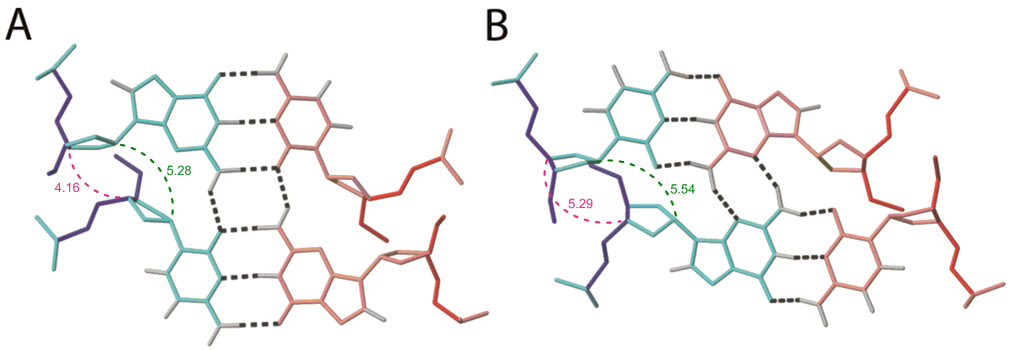

Figure S3. Details of the direct (A) and slipped (B) minor groove G:C:G:C tetrads. Distances C1'-C1' (green) and C4'-C4' (pink) are given in Å.