High salt solution structure of a left-handed RNA double helix

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SUPPLEMENTARY MATERIAL

Table S1. ^{1}H NMR chemical shifts δ_H (p.p.m.) of $(CGCGCG)_2$ in the Z-RNA form at 303 K in D_2O.

Residue	H8/H6	H5	H1′	H2′	H3′	H4′	H5′	H5″	imino	amino	
C1	7.33	5.88	5.83	3.88	4.45	3.76	3.01	2.57	-	8.28	6.29
G2	7.84	-	5.95	4.45	5.26	4.35	4.24	4.24	13.14	-	-
C3	7.25	5.27	5.85	4.00	4.61	3.93	3.88	2.51	-	8.54	5.84
G4	7.91	-	5.96	4.49	5.20	4.35	4.29	4.20	13.01	-	-
C5	7.34	5.37	5.92	4.06	4.65	3.99	3.89	2.65	-	8.51	5.86
G6	7.86	-	5.90	5.11	4.79	4.32	4.24	4.22	13.04	-	-

Table S2. Experimental $J_{1',2'}$, $J_{2',3'}$ and $J_{3',4'}$ coupling constants, sugar pucker parameters [a)] and percentage of N conformers for $(CGCGCG)_2$ in the Z-RNA form.

Residue	coupling constants [Hz] [b)]			PSEUROT[c)]					12 final structures [d)]	
	$J_{1',2'}$	$J_{2',3'}$	$J_{3',4'}$	P_N	Φ_N	P_s	Φ_s	$\%_N$	P	Φ
C1	8.0	4.7	≤1.0	17 (16)	31 (6)	177 (17)	39 (6)	2	198 (1)	35 (1)
G2	≤1.0	5.5	9.8	35 (2)	40 (2)	-	-	100	48 (2)	41 (1)
C3	7.8	4.4	0.9	-28 (14)	36 (4)	185 (17)	41 (6)	2	135 (3)	40 (2)
G4	≤1.0	5.9	9.2	32 (1)	35 (1)	-	-	100	44 (2)	36 (2)
C5	7.8	3.9	1.4	-21 (15)	29 (7)	184 (22)	48 (8)	6	162 (3)	41 (1)
G6	3.8	6.2	5.2	48 (16)	27 (9)	190 (59)	25 (8)	68	24 (4)	36 (1)

[a)] average values are given with standard deviations in parentheses.
[b)] ± 1Hz
[c)] all five values P_N, P_S, Φ_N, Φ_S, $\%_N$ were fitted to experimental data. Initial values of Φ_N, Φ_S were of 30° and initial $\%_N$ was 50%. Initial values of P_N and P_S changed independently from 0° to 360° every 10°. For statistics, only results giving r.m.s.d. values less than 0.5 [Hz] were employed.
[d)] ref (37)

Table S3. Backbone and glycosidic torsion angles[a)] for 12 conformers representing the refined structure of $(CGCGCG)_2$ in the Z-RNA form (*left column*) and 11 reference X-ray Z-DNA structures [b)] of d$(CGCGCG)_2$ (*right column*).

Res.	α		β		γ		δ		ε		ζ		χ	
C1	-	-	-	-	46(2)	39(38)	153(1)	143(6)	-68(1)	-93(4)	76(2)	75(5)	-151(2)	-150(5)
G2	49(4)	65(5)	-163(2)	-172(3)	-175(3)	177(3)	81(1)	95(7)	-104(1)	-117(7)[c] -161(5)[d]	-55(2)	-64(17)[c] 59(8)[d]	60(2)	62(5)
C3	-145(2)	-150(9)[c] 165(5)[d]	175(4)	-132(15)[c] 155(6)[d]	71(1)	54(4)	127(2)	147(4)	-72(1)	-95(5)	76(2)	75(4)	-159(2)	-156(4)
G4	69(3)	66(5)	-159(1)	-174(6)	172(1)	179(3)	86(2)	95(5)	-105(1)	-123(9)[c] -176(4)[d]	-65(3)	-55(16)[c] 67(5)[d]	61(1)	60(6)
C5	-134(4)	-155(8)[c] 169(3)[d]	-158(3)	-133(12)[c] 163(5)[d]	54(4)	49(7)	146(1)	141(5)	-83(4)	-95(4)	71(1)	70(7)	-141(2)	-155(6)
G6	62(2)	79(7)	-165(1)	-179(5)	-173(1)	176(3)	84(1)	148(5)	-	-	-	-	47(2)	76(3)

[a)] P $^{\alpha}$ O5′ $^{\beta}$ C5′ $^{\gamma}$ C4′ $^{\delta}$ C3′ $^{\varepsilon}$ O3′ $^{\zeta}$ P ; average values with standard deviations in parentheses are given
[b)] PDB ID: 131D, 1D39, 1D48, 1DCG, 1DJ6, 1I0T, 1ICK, 292D, 293D, 2DCG, 336D.
[c)] GpC step typical of the Z_I-DNA form
[d)] GpC step typical of the Z_{II}-DNA form

Table S4. Lower (*left column*) and upper (*right column*) limits [°] for the initial torsion angle restraints used in the structure determination (CYANA) of $(CGCGCG)_2$ in the Z-RNA form

Residue	β		γ		χ		ν_1		ν_2		δ		ε	
C1 (C7	132	228	40	70	-200	-120	17	50	-50	-23	127	168	188	292
G2 (G8	165	195	na	na	26	106	-18	-8	27	39	75	85	188	292
C3 (C9	132	228	40	70	-200	-120	17	50	-50	-23	127	168	188	292
G4 (G10)	165	195	na	na	26	106	-16	-7	23	35	80	90	188	292
C5 (C11)	132	228	40	70	-200	-120	16	50	-50	-26	127	170	188	292
G6 (G12)	165	195	na	na	26	106	-18	44	-29	39	75	123	-	-

Fig. S1. ^{1}H NMR spectra of $(CGCGCG)_2$ at 0M (right-handed form) (*bottom*) and 6M $NaClO_4$ (left-handed form) (*top*).

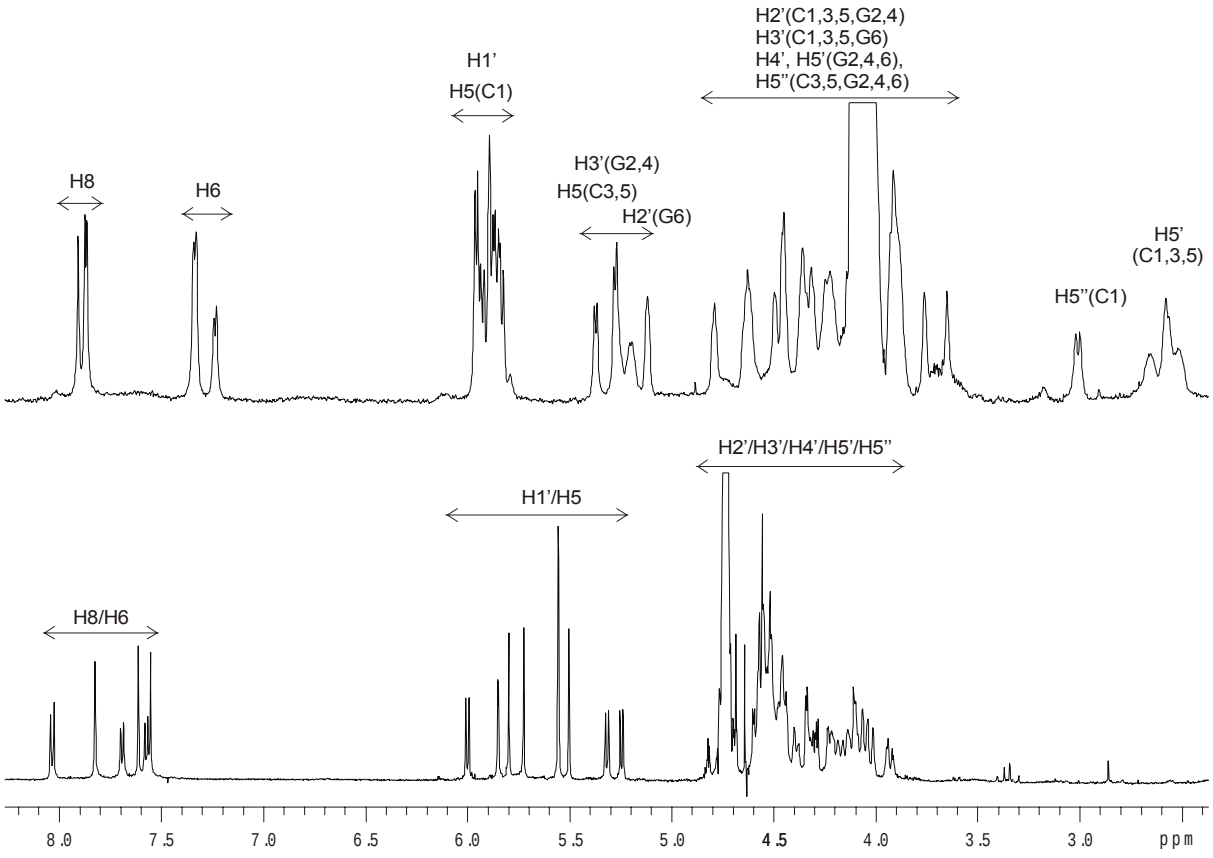

Fig. S2. Applied protocol for the structure determination (CYANA) of the $(CGCGCG)_2$ in Z-RNA form. At the structure calculation stage, the TAD algorithm was implemented to a new subroutine *ndrs.cya* which allows for automatic NOE distance restraints selection.