Supplementary Data

Supplementary Table 1. X-ray data statistics.

Crystal	$(GCUGCUGC)_2$	$[(CUG)_6]_2$ by Mooers *et al.* (2005)
Beamline	EMBL-X13	ALS BL 8.2.2.
Temperature (K)	100	100
Wavelength (Å)	0.808	0.8860
Space group	C2	R3:H
Unit-cell parameters (Å)	a = 37.0 b = 38.9 c = 77.7 β = 90.0º	$a = b$ =39.1 c = 141.3
Resolution range (Å)	20.0 -1.23 (1.25-1.23) *	19.55-1.58 (1.62-1.58)
R_{merge} †	0.058 (0.30)	0.051 (0.365)
No. unique reflections	32055	11503
Completeness (%)	99.1 (98.1)	99.9 (99.9)
Mosaicity (º)	1.0	-
Data redundancy	7.1(6.2)	6.2 (5.1)
$\langle I/\sigma(I)\rangle$	21.3 (5.7)	40.5 (4.1)
Reflections > 2σ (%)	86 (72)	-
B-factor from Wilson plot (Å^2)	14.2	23.50

* Values in parenthesis are for the last resolution shell.

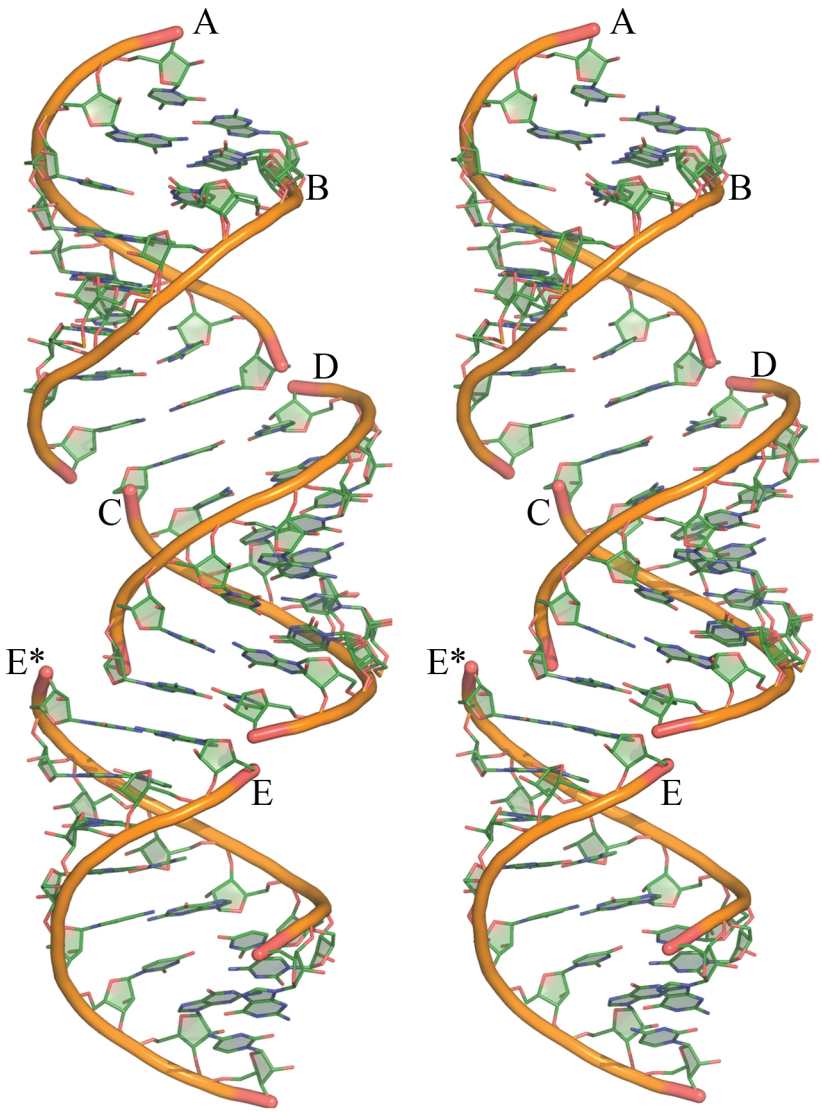
† $R_{\text{merge}} = \sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl)\rangle| / \sum_{hkl} \sum_i I_i(hkl)$, where $I_i(hkl)$ and $\langle I(hkl)\rangle$ are the observed individual and mean intensities of a reflection with the indices hkl, respectively, $\sum_i$ is the sum over i measurements of a reflection with the indices hkl, and $\sum_{hkl}$ is the sum over all reflections.

Supplementary Table 2. Helical parameters calculated using 3DNA, based on C1'-C1' distances.

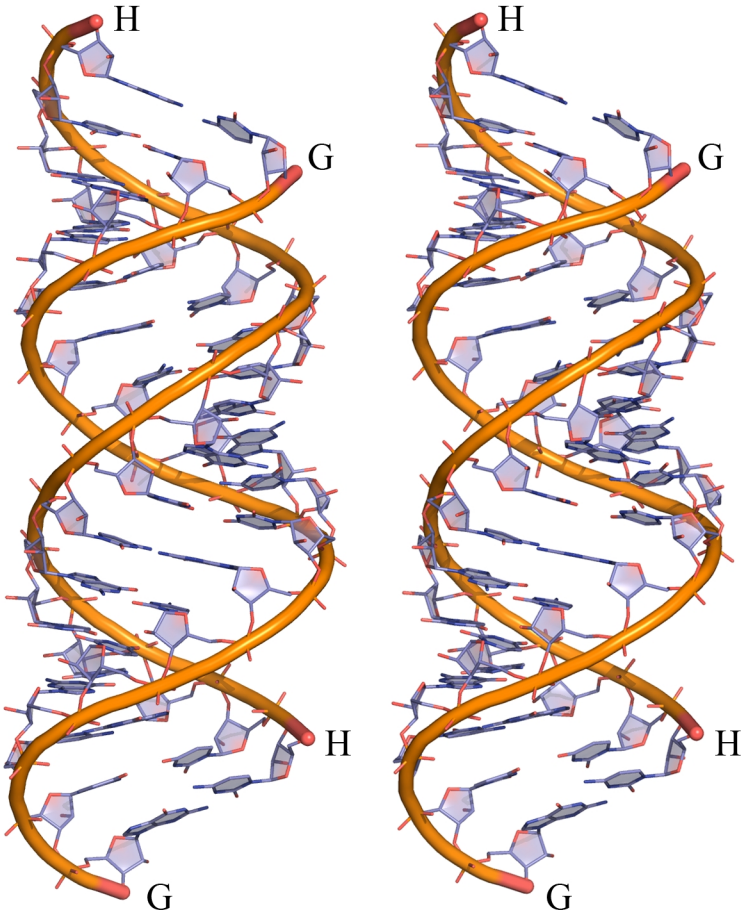
Bp	*Displacement (Å)*				*Angle (°)*				*Twist (°)*				*Rise (Å)*				*Opening (°)*			
	AB	CD	EE'	$(CUG)_6$	AB	CD	EE'	$(CUG)_6$	AB	CD	EE'	$(CUG)_6$	AB	CD	EE'	$(CUG)_6$	AB	CD	EF	$(CUG)_6$
G-C	6.8	5.9	6.8		14.4	15.7	12.5		27.1	33.5	34.4		3.3	2.5	2.7		-1.1	2.1	-2.3	
C-G	6.3	6.5	7.2	6.8	14.6	14.2	10.2	20.5	44.8	34.9	33.7	39.0	2.8	2.3	2.4	2.0	0.1	-1.2	-1.0	-13.2
U-U	6.5	6.6	7.1	6.8	14.0	15.3	11.3	18.2	33.8	34.6	35.0	31.9	2.2	2.9	2.7	2.4	-31.5	-34.4	-30.6	-21.2
G-C	5.2	6.2	6.4	6.9	15.0	15.7	14.1	13.8	22.3	33.2	27.7	33.3	2.7	2.9	2.9	2.7	-2.1	-0.5	0.5	-6.8
C-G	5.8	6.4	6.4	6.8	11.4	15.0	14.1	13.1	40.9	30.2	35.0	31.7	3.2	2.4	2.7	2.8	0.1	-4.4	0.5	0.8
U-U	7.1	6.4	7.1	6.4	7.4	15.3	11.3	12.5	26.5	41.4	33.7	35.0	2.9	2.3	2.4	2.6	-16.4	-21.2	-30.6	-22.1
G-C	7.1	6.3	7.2	5.7	9.9	14.7	10.2	14.9	31.5	31.8	34.4	35.1	2.4	2.8	2.7	2.4	1.3	1.9	-1.0	-3.5
C-G	6.4	7.0	6.8	5.6	14.1	12.1	12.5	17.8				36.3				2.4	0.6	-1.5	-2.3	-1.5
U-U				6.1				14.2				34.9				2.7				-21.0
G-C				6.8				12.5				31.1				2.7				-0.7
C-G				7.5				7.7				32.9				3.3				1.7
U-U				7.8				8.0				33.6				2.8				-11.9
G-C				6.6				13.3				27.7				2.4				-5.1
C-G				5.9				18.3				29.3				2.3				1.9
U-U				7.0				14.9				34.5				2.7				-28.0
G-C				7.9				13.0				32.4				2.7				-2.2
C-G				8.1				12.9				32.3				2.6				2.0
U-U				7.7				16.1				40.5				2.3				-14.8
G-C				7.2				18.1												1.3
Average	6.4	6.4	6.9	6.9	12.6	14.7	12.0	14.4	32.4	34.2	33.4	33.6	2.8	2.6	2.7	2.6	-6.1	-7.4	-8.4	-8.0
s.d.	0.6	0.3	0.4	0.8	2.8	1.2	1.6	3.4	8.1	3.6	2.6	3.2	0.4	0.3	0.2	0.3	11.8	13.2	13.7	9.8

Definitions of displacement, angle, twist, rise and opening according to Dickerson *et al*., J. Mol. Biol. (1989) 205, 787-791.

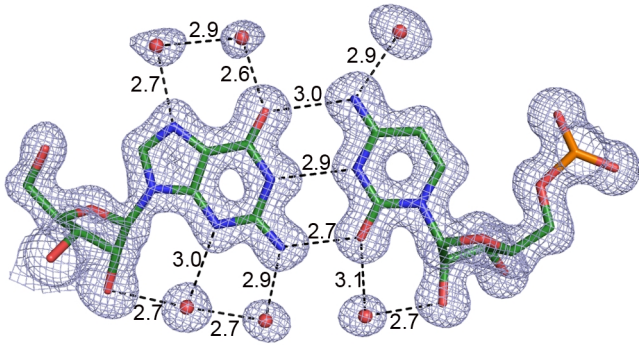
A



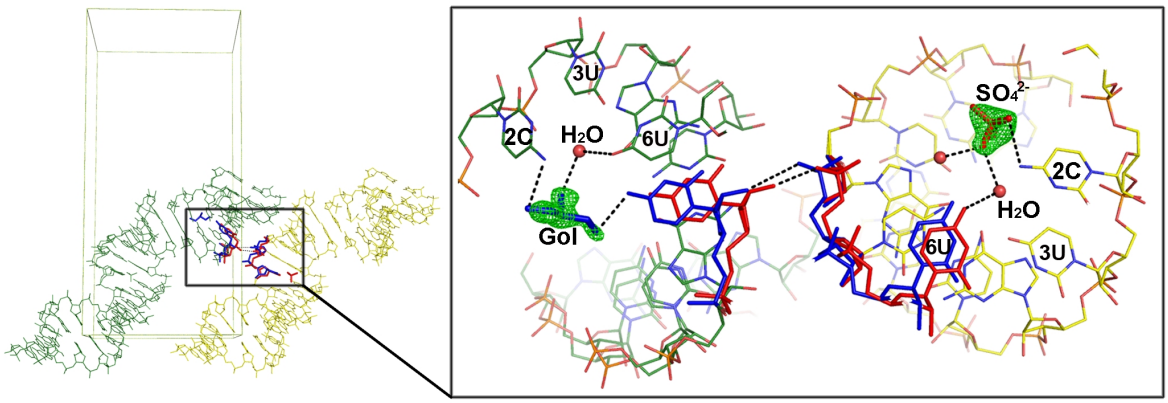
B



Supplementary Figure 1. Stereo pairs of (A) the $(GCUGCUGC)_2$ crystal structure showing duplexes A+B, C+D and E+E* (* indicates a symmetry-related strand) as they stack in the crystal lattice. (B) shows $[(CUG)_6]_2$ detwinned model.



Supplementary Figure 2. A representative GC pair from the monoclinic $(GCUGCUGC)_2$ structure showing the regular hydration pattern. The $2F_o$-F_c map is contoured at the 1σ level.



Supplementary Figure 3. Ligand interactions in the monoclinic structure. Two strands are in contact in the crystal lattice. The binding of glycerol and sulphate molecules is associated with local disorder of two neighbouring RNA strands. The sites of both ligands are half occupied thus either the glycerol or the sulphate is bound. The omit electron density map (green contours) is shown at the 3 σ level.