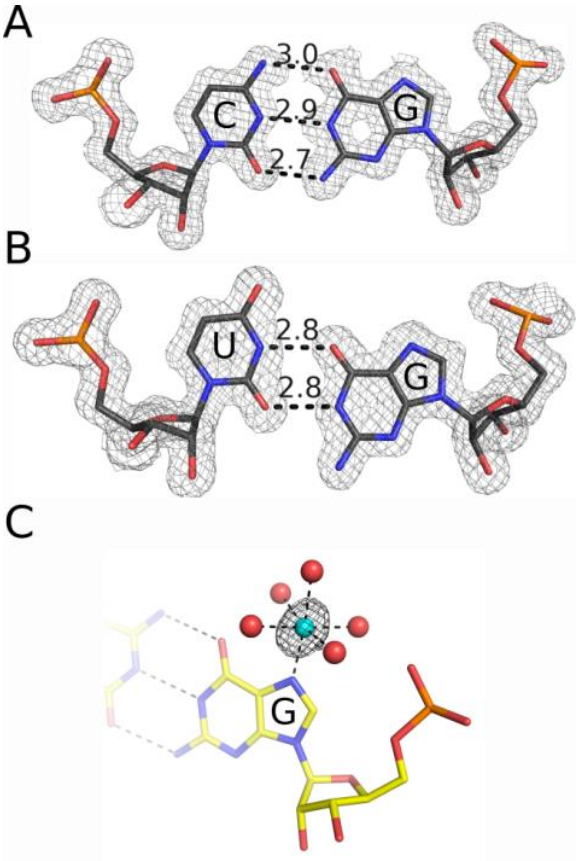
SUPPLEMENTARY DATA

to

Broken symmetry between RNA enantiomers in a crystal lattice

Agnieszka Kiliszek, Leszek Błaszczyk, Magdalena Bejger, Wojciech Rypniewski*

Institute of Bioorganic Chemistry, Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań, Poland.



Supplementary Figure S1. Base pairing and interactions with Zn^{2+} (**A**, **B**) C-G and U-G base pairs with the $2F_o$-F_c electron density map contoured at the 1σ level (gray contours). Distances of hydrogen bonds are marked in angstroms. (**C**) A hydrated Zn^{2+} ion (blue sphere) forming an inner complex with the N7 atom of residues G82 of chain K, with its anomalous electron density contoured at the 4 σ level (gray contours). The water molecules are shown as red spheres.

Supplementary Table S1. Summary of X-ray diffraction data.

Crystal name	PDB code	Resoln. [Å]	Wave-length [Å]	R_{merge} [#]	$R^{\S}/R_{free}$ [$]	'hand' [£]	Anomal Corr	SigAno	Anomalous peak height [σ] [¥]							X-ray facility/date	DOI address of diffraction images [*]
									ZN1	ZN2	ZN3	ZN4	ZN7	ZN8	ZN10		
136-E1a	6ZQ9	1.50	1.283	0.079 (0.967)	0.201/0.250	+	0.20	0.75	16.5	16.1	7.0	12.1	15.6	9.4	8.7	EMBL/01-12-2018	10.18150/9ACEMY
140-F2a	6ZR1	1.53	1.283	0.086 (0.557)	0.203/0.253	+	0.21	0.80	18.3	15.3	9.1	9.8	12.1	10.8	7.5	EMBL/01-12-2018	10.18150/C7CNYT
140-F4a	6ZPF	1.44	1.283	0.052 (0.469)	0.201/0.251	+	0.35	0.88	24.1	21.0	9.5	6.4	19.8	13.9	6.3	EMBL/01-12-2018	10.18150/JV8T9Y
140-F6b	6ZRL	1.53	1.283	0.107 (0.731)	0.213/0.275	-	0.25	0.84	15.8	18.8	9.4	9.4	13.0	11.5	8.1	EMBL/01-12-2018	10.18150/SMC7KS
140-F6c	6ZRS	1.52	1.283	0.069 (0.566)	0.187/0.235	+	0.24	0.82	18.2	17.3	9.5	11.8	15.0	10.5	7.4	EMBL/01-12-2018	10.18150/BELVHE
143-A7d	6ZX8	1.98	1.283	0.099 (0.479)	0.173/0.259	+	0.12	0.62	6.8	7.6	4.9	5.5	9.5	4.8	2.2	BESSY/02-02-2019	10.18150/P4L74Z
143-A2c	7A9L	1.98	1.283	0.103 (0.407)	0.174/0.250	-	0.17	0.65	7.1	6.7	3.9	3.5	6.2	4.1	3.1	BESSY/02-02-2019	10.18150/Q4UKIN
136-E1b	7A9N	1.60	1.283	0.072 (0.472)	0.180/0.224	+	0.45	1.00	27.5	22.4	12.8	6.6	5.9	4.9	-	EMBL/01-05-2019	10.18150/IEYXA5
143-A11b	7A9O	1.60	1.283	0.089 (0.510)	0.191/0.228	+	0.47	0.96	19.3	16.4	9.0	11.2	10.5	9.2	7.5	EMBL/01-05-2019	10.18150/QFD8JM
140-F4b	6ZW3	1.50	1.283	0.168 (1.061)	0.213/0.272	-	-0.02	0.57	16.5	15.8	8.0	4.2	13.1	9.0	4.1	EMBL/01-12-2018	10.18150/KWD3XQ
140-F4c	6ZWU	1.53	1.283	0.135 (1.187)	0.198/0.252	-	-0.05	0.62	13.5	13.2	5.7	6.9	12.8	9.2	5.1	EMBL/01-12-2018	10.18150/GHURCS
141-A6	6ZX5	1.52	1.283	0.164 (1.526)	0.211/0.281	+	-0.11	0.53	10.3	9.2	5.2	8.1	9.8	5.3	4.1	EMBL/01-12-2018	10.18150/FVWGG8
143-D7b	7A9P	1.99	1.277	0.100 (0.256)	0.235/0.326	-	-0.17	0.61	4.7	7.0	2.7	2.8	5.4	5.8	-	BESSY/02-02-2019	10.18150/HLJBOJ
142-C1b	7A9Q	2.19	1.283	0.131 (0.452)	0.164/0.232	+	0.03	0.56	7.4	7.3	3.1	5.2	7.0	3.8	2.8	BESSY/02-02-2019	10.18150/4ZIRX1
142-C1c	7A9R	2.46	1.283	0.121 (0.352)	0.178/0.284	-	-0.10	0.54	5.3	4.8	2.6	3.1	4.1	3.8	-	BESSY/02-02-2019	10.18150/EBSJ8O
142-C1d	7A9S	2.30	1.283	0.133 (0.474)	0.169/0.274	+	-0.13	0.51	7.4	8.7	4.2	5.9	5.2	4.4	2.8	BESSY/02-02-2019	10.18150/DK6OUQ
141-A6b	7A9T	1.70	1.283	0.100 (0.350)	0.188/0.248	+	-0.02	0.63	11.8	9.9	4.8	5.7	5.3	5.1	3.8	EMBL/01-05-2019	10.18150/W45YHJ

[#] $R_{merge} = \Sigma_{hkl}\Sigma_i|I_i(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl}\Sigma_i I_i(hkl)$, where $I_i(hkl)$ is the integrated intensity of a given reflection and $\langle I(hkl)\rangle$ is the mean intensity of multiple corresponding symmetry-related reflections. The values in parentheses are for the highest resolution shell.

[§] $R = \Sigma_{hkl}||F_{obs}|-|F_{calc}|| / \Sigma_{hkl}|F_{obs}|$, where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively.

[$] R_{free} is R calculated using a randomly chosen subset of reflections excluded from the refinement.

[£] '+' indicates enantiomers D-(K:L)/L-(M:N) and '-' indicates L-(K:L)/D-(M:N)

[¥] The height of peaks on the anomalous map, in terms of r.m.s.d, corresponding to the Zn^{+2} sites, used to determine the 'hand' of the X-ray structures. The anomalous maps calculated for the opposite 'handedness' showed no significant peaks.

[*] The diffraction images are available at Macromolecular Xtallography Raw Data Repository (MX-RDR): mxrdr.icm.edu.pl

Supplementary Table S2. Helical parameters (based on crystal 140-F4a, PDB code 6ZPF) calculated using 3DNA {Olson, 2001 #76}.

K+L duplex

Local base-pair parameters

B.p.	Shear [Å]	Stretch [Å]	Stagger [Å]	Buckle [°]	Propllr. [°]	Openg. [°]	Displ. [Å]	Angle [°]	Twist [°]	Rise [Å]
1 c-g	-0.0	-0.1	0.2	4.5	-7.0	-2.0	5.9	13.2	28.0	3.0
2 u-g	2.4	-0.6	-0.1	9.6	-19.7	-0.9	5.3	9.7	44.4	2.6
3 g-u	-2.3	-0.7	0.2	-1.0	-9.3	-3.1	5.8	11.1	27.2	2.9
4 g-c	-0.3	-0.2	0.4	4.7	-15.3	0.4	5.7	12.3	38.1	2.4
5 g-c	-0.1	-0.3	0.1	-2.7	-14.8	-3.9	5.8	11.6	32.4	2.6
6 c-g	0.2	-0.2	0.1	-1.1	-15.8	1.0	5.8	10.4	36.3	2.7
7 g-c	-0.3	-0.3	-0.1	-10.4	-16.8	-3.0	5.9	10.5	32.2	2.9
8 g-c	-0.2	-0.1	0.1	-7.8	-8.0	-3.3	5.9	15.0		
ave.	-0.1	-0.3	0.1	-0.5	-13.3	-1.9	5.8	11.7	34.1	2.7
s.d.	1.3	0.2	0.1	6.7	4.6	1.8	0.2	1.6	5.6	0.2

Local base-pair step parameters

Step	Shift [Å]	Slide [Å]	Rise [Å]	Tilt [°]	Roll [°]	Twist [°]
1 cu/gg	0.0	-1.1	3.2	0.9	7.2	39.8
2 ug/ug	-0.9	-2.3	3.1	-5.0	15.1	18.0
3 gg/cu	0.1	-1.0	3.2	0.2	2.3	37.4
4 gg/cc	-0.3	-1.2	3.3	0.1	7.3	38.3
5 gc/gc	0.4	-1.3	3.2	0.1	2.0	33.3
6 cg/cg	0.1	-1.7	3.3	3.6	14.8	32.3
7 gg/cc	0.3	-1.5	3.2	2.0	7.7	31.4
ave.	-0.0	-1.4	3.2	0.3	8.1	32.9
s.d.	0.4	0.4	0.1	2.6	5.3	7.3

M+N duplex

Local base-pair parameters

B.p.	Shear [Å]	Stretch [Å]	Stagger [Å]	Buckle [°]	Propllr. [°]	Openg. [°]	Displ. [Å]	Angle [°]	Twist [°]	Rise [Å]
1 c-g	0.0	-0.1	0.2	5.0	8.0	2.6	6.0	13.8	-25.3	3.0
2 u-g	-2.5	-0.6	0.0	8.7	18.0	-2.1	5.6	9.8	-45.4	2.6
3 g-u	2.1	-0.6	0.1	-2.5	12.6	2.2	5.6	10.8	-27.6	2.8
4 g-c	0.1	-0.1	0.3	2.5	17.4	0.5	5.7	12.1	-37.0	2.5
5 g-c	0.3	-0.2	0.0	-5.6	16.1	1.8	5.9	11.7	-31.2	2.9
6 c-g	-0.5	-0.2	0.1	0.0	13.2	-1.6	5.6	11.9	-37.9	2.6
7 g-c	0.3	-0.3	-0.1	-9.4	19.8	3.3	5.5	11.0	-33.0	2.9
8 g-c	0.2	-0.2	0.1	-7.0	9.4	3.1	5.7	14.5		
ave.	0.0	-0.3	0.1	-1.0	14.3	1.2	5.7	12.0	-33.9	2.8
s.d.	1.3	0.2	0.1	6.3	4.2	2.1	0.2	1.5	6.3	0.2

Local base-pair step parameters

Step	Shift [Å]	Slide [Å]	Rise [Å]	Tilt [°]	Roll [°]	Twist [°]
1 cu/gg	-0.0	-1.2	3.2	-0.6	-7.9	-38.3
2 ug/ug	0.6	-2.2	3.1	-2.7	-15.7	-19.6
3 gg/cu	0.1	-1.1	3.2	0.1	-2.5	-37.2
4 gg/cc	0.2	-1.2	3.3	0.7	-8.1	-35.3
5 gc/gc	-0.6	-1.0	3.1	-0.1	-4.3	-34.5
6 cg/cg	-0.0	-1.5	3.4	3.7	-13.0	-32.4
7 gg/cc	-0.3	-1.2	3.2	1.1	-7.7	-32.0
ave.	0.0	-1.3	3.2	0.5	-8.4	-32.7
s.d.	0.4	0.4	0.1	1.9	4.6	6.2

Supplementary Table S3. Intermolecular contacts in the crystal structure of D-(K:L)/L-(M:N) RNA duplexes (based on crystal 140-F4a, PDB code 6ZPF), other than base-pairing and base-stacking contacts. The distance range is 2.15-3.25 Å, W stands for water molecule, symmetry-related molecules are marked with *, direct contacts between neighboring RNA duplexes are underscored, lattice contacts with no symmetric counterparts are highlighted in color.

Residue	Atom	Chain K	Chain M	Residue	Atom	Chain L	Chain N
C79	O5’		W141	**C90**	O5’	O3’ G97N, W143	O3’ G97L*, W135, W89*, W91*
	O4’	W38			O2’	W93, W182	W151*
	O2’	W79, W98	W59		N4		W107
	O2	W194			O2	W160, W182	W147*, W151*
U80	OP1	W69		**C91**	OP1	W51, W143	W52, W135
	O4’	W73	W59		OP2	W175, W176	W99
	O3’	W56	W190		O2’	W56*	W32*
	O2’	W44, W56	W32, W50		N4	W110, W165	W144
	O2	W44	W50		O2	W20	W11
	O4	W75,W189					
G81	OP1	W22, W28	W5, W113	**G92**	OP1	W4	W7, W65
	OP2	W145	W80, W190		OP2	W103	
	O4’	O4’ G92L*	O4’ G92N*		O5’	W4	
	O3’	W20*	W11*		O4’	O4’ G81K*	O4’ G81M*
	O2’	N2 G85K*, W43*, W106*	N2 G85M* (3.5Å), W155		O2’	N2 G96L*, W139	N2 G96N*
	N7		W113		N7	W157	W65, W136
	N3	W139*			O6	W165	W84, W136
	O6	W75			N3	W106	W155*
	N2	W31, W170	W101, W102				
	N3	W139*					
G82	OP1	W22, W118	W5, W64, W80	**C93**	OP1	W4, W29	W1, W7
	OP2	O2’ G86K*, W140*	O2’ G86M*, W105		OP2	O2’ G97L*, W18	O2’ G97N*, W25
	O3’	W49*	W15*		O3’	W21*	W45*
	O2’	W39, W49*	W14*, W15*, W166*		O2’	W16, W21*	W58
	N7	ZN1, W2, W22, W117, W118	ZN2, W5, W27, W64, W112		N4	W72, W162	W163
	O6	W117	W112		O2	W96	W58
	N2	W67	W76				
G83	OP1	W37, W55, W187	W33, W63, W88	**C94**	OP1	W48, W74	W40, W61*
	OP2	W47, W66	W134, W9*		OP2	W14, W12*	W23, W94
	O5’	W187			O5’		W40
	O4’	W39			O3’		W57
	O2’		W12, W19, W46		O2’	W9*, W26*	W57
	N7	W37	W33		N4	W142	W127
	O6	W2	W27		O2	W41	W137
	N3	W41	W19				

C84			
	OP1	W149, W187	W63, W179
	OP2	W82	W26, W146, W16*
	O5’	W149	W179
	O2’		C5’ G96L* (3.0Å), W17
	O2	W96	W17
	N4	W10	

U95			
	OP1	W48, W83, W100	W40
	OP2	W14, W46*	
	O4’	W90*	
	O2’	C5’ G85M* (3.2Å), W31, W90*	W102
	O4	W77, W129, W189	W30

G85			
	OP1	W121, W149	W70, W179
	OP2		W8, W111, W31*
	C5’		O2’ U95L* (3.2Å)
	O4’		W17
	O3’		W90
	O2’	W43, W49, W171*	W3, W15, W166
	N7	W120, W159	W183
	O6	W122	W156
	N3	W43	W3
	N2	O2’ G81K*	O2’ G81M* (3.5Å)

G96			
	OP1	W79, W186	W85, W133
	OP2	W13, W192, W17*	
	O5’	W79	
	C5’	O2’ C84M* (3.0Å)	
	O4’		W102
	O2’	W21, W8*	W45, W178
	N7	W129, W138	
	O6		W188
	N2	O2’ G92L*, W44	O2’ G92N*, W50

G86			
	OP1	W121	W196, W38*
	OP2	W42, W47*	W24, W90
	O4’	W154*	
	O3’	W141, W185, W55*	W184, W88*
	O2’	OP2 G82K*, W197, W55*,	OP2 G82M*, W88*, W105*
	N7	W120	W150
	O6	W122	W156
	N3	W140	W105*
	N2	W20, W140	W11*

G97			
	OP1	W79, W97	W85, W86
	OP2	W60, W71, W12*	W78, W87 W23*
	O3’	O5’ C90N*, W89, W91	O5’ C90L*, W61
	O2’	OP2 C93L*, W74*	OP2 C93N*, W61
	N7	W130	W132
	O6	W147	W160, W188
	N3		W25*
	N2	W18*	W25*