Supplementary Table S1.
Comparison of pseudo-rotation angles of Z-RNA, Z-DNA (bound by Zα) and Z-RNA in high salt.

Table S1. Comparison of sugar packer parameters of Z-RNA and Z-DNA

	Z-RNA (this work)		Z-DNA [1] 1QBJ		High Salt Z-RNA [2] 1T4X model 1	
Strand I	Pseudo-rotation angle	Puckering	Pseudo-rotation angle	Puckering	Pseudo-rotation angle	Puckering
1 C	147.2	C2'-endo	160.8	C2'-endo	200.1	C3'-exo
2 G	28.7	C3'-endo	25.8	C3'-endo	50.8	C4'-exo
3 C	162.2	C2'-endo	160.4	C2'-endo	138.0	C1'-exo
4 G	17.2	C3'-endo	20.9	C3'-endo	44.0	C4'-exo
5 C	155.1	C2'-endo	157.3	C2'-endo	160.8	C2'-endo
6 G	19.6	C3'-endo	164.1	C2'-endo	23.5	C3'-endo
Strand II						
1 G	177.9	C2'-endo	170.4	C2'-endo	27.1	C3'-endo
2 C	157.4	C2'-endo	159.0	C2'-endo	163.9	C2'-endo
3 G	25.8	C3'-endo	27.0	C3'-endo	47.5	C4'-exo
4 C	161.0	C2'-endo	159.2	C2'-endo	131.2	C1'-exo
5 G	36.6	C3'-endo	25.5	C3'-endo	46.8	C4'-exo
6 C	157.2	C2'-endo	154.3	C2'-endo	197.9	C3'-exo

References

1. Schwartz, T., Rould, M.A., Lowenhaupt, K., Herbert, A., and Rich, A. (1999). Crystal structure of the Zalpha domain of the human editing enzyme ADAR1 bound to left-handed Z-DNA. Science *284*, 1841-1845.
2. Popenda, M., Milecki, J., and Adamiak, R.W. (2004). High salt solution structure of a left-handed RNA double helix. Nucleic Acids Res *32*, 4044-4054.

Supplementary Table S2.

Detailed parameters defining sugar conformation in the Zα/RNA complex.

Source 3DNA[1]

Note:

v0: C4'-O4'-C1'-C2'
v1: O4'-C1'-C2'-C3'
v2: C1'-C2'-C3'-C4'
v3: C2'-C3'-C4'-O4'
v4: C3'-C4'-O4'-C1'

tm: amplitude of pseudorotation of the sugar ring
P: phase angle of pseudorotation of the sugar ring

alpha: O3'(i-1)-P-O5'-C5'
beta: P-O5'-C5'-C4'
gamma: O5'-C5'-C4'-C3'
delta: C5'-C4'-C3'-O3'
epsilon: C4'-C3'-O3'-P(i+1)
zeta: C3'-O3'-P(i+1)-O5'(i+1)
chi for pyrimidines(Y):
O4'-C1'-N1-C2
chi for purines(R):
O4'-C1'-N9-C4

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-30.6	38.6	-32.1	15.2	9.6	38.2	147.2	C2'-endo
2 G	-5.9	-15.4	29.2	-33.5	25.1	33.3	28.7	C3'-endo
3 C	-26.6	41.9	-41.8	26.9	-0.3	43.9	162.2	C2'-endo
4 G	0.6	-15.8	23.9	-24.1	14.9	25.0	17.2	C3'-endo
5 C	-28.1	40.0	-36.2	20.8	4.5	39.9	155.1	C2'-endo
6 G	-0.4	-11.5	18.3	-18.9	12.3	19.4	19.6	C3'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-16.1	37.8	-43.8	36.3	-12.6	43.8	177.9	C2'-endo
2 C	-31.5	46.3	-43.0	26.1	3.4	46.6	157.4	C2'-endo
3 G	-3.6	-14.4	25.6	-28.4	20.4	28.4	25.8	C3'-endo
4 C	-27.4	42.8	-41.2	26.7	0.2	43.6	161.0	C2'-endo
5 G	-10.7	-11.2	26.9	-33.8	28.3	33.6	36.6	C4'-exo
6 C	-28.2	41.5	-38.1	23.3	2.8	41.3	157.2	C2'-endo

Strand I

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 C	---	148.5	47.6	137.0	-100.0	74.9	-136.8
2 G	70.3	-167.9	169.4	86.9	-110.0	-70.9	59.4
3 C	-146.7	-125.0	53.8	147.9	-98.9	77.8	-142.1
4 G	63.4	-170.0	-179.3	99.9	-125.7	-47.3	61.4
5 C	-164.9	-133.9	59.9	143.3	-102.2	79.2	-145.7
6 G	58.2	-174.1	-174.9	97.1	---	---	65.9

Strand II

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 G	93.8	179.0	-172.3	159.1	---	---	77.6
2 C	-158.7	-130.3	69.2	145.7	-94.6	49.7	-149.3
3 G	56.0	-164.6	-178.5	92.0	-115.0	-66.9	59.3
4 C	-149.2	-125.7	56.2	148.3	-97.7	79.2	-141.0
5 G	72.8	-170.9	171.3	86.4	-110.1	-70.9	56.0
6 C	---	-171.8	61.1	144.0	-91.6	72.3	-138.1

References

1. Lu, X.J., and Olson, W.K. (2003). 3DNA: a software package for the analysis, rebuilding and visualization of three-dimensional nucleic acid structures. Nucleic Acids Res *31*, 5108-5121.