

Table S2. Sharp Backbone Kinks in RNA Structures

PDB ID	Chain	Nucleotide Number	Nucleotide Name	Angle ^a	Molecule
1ET4	A	214	A	47.77	vitamin B(12) RNA aptamer
1SDS	D	210	U	50.44	protein L7Ae bound to a K-turn derived from an archaeal box H/ACA sRNA
1MMS	C	1071	G	42.36	ribosomal protein L11-RNA complex
1S72	0	1105	C	46.29	<i>H. marismortui</i> large ribosomal subunit
1S72	0	1369	A	46.57	<i>H. marismortui</i> large ribosomal subunit
1S72	0	1533	A	49.82	<i>H. marismortui</i> large ribosomal subunit
1S72	0	174	A	50.64	<i>H. marismortui</i> large ribosomal subunit
1S72	0	1776	A	48.93	<i>H. marismortui</i> large ribosomal subunit
1S72	0	2007	A	47.82	<i>H. marismortui</i> large ribosomal subunit
1S72	0	212	A	50.76	<i>H. marismortui</i> large ribosomal subunit
1S72	0	357	A	49.23	<i>H. marismortui</i> large ribosomal subunit
1S72	0	893	C	49.73	<i>H. marismortui</i> large ribosomal subunit
1XMQ	A	508	C	49.27	t6A37-ASLLysUUU AAA-mRNA bound to the decoding center
1MSY	A	2654	A	50.58	GUAA tetraloop mutant of Sarcin/Ricin domain from <i>E. coli</i> 23 S rRNA
4FAQ	A	1	G	50.12	<i>O. iheyensis</i> group II intron before 5' exon hydrolysis
4E8K	B	6	U	137.6	<i>O. iheyensis</i> group II intron before SER

^a: defined as the angle formed by three consecutive phosphorus atoms.

Table S3. Properties of the Different Metal Ions Used in This Work

metal class	ion	cationic radius (Å) ^a	hydration energy (kJ/mol) ^{b, d}	Lewis acid strength ^a	absolute hardness (η) ^{b, c, e}	absolute electronegativity (χ) ^{b, e}
alkaline metal ions	Li ⁺	0.60	-514.10	0.188	35.12	40.52
	Na ⁺	0.95	-405.40	0.148	26.21	21.08
	K ⁺	1.33	-334.72	0.112	17.99	13.64
	Rb ⁺	1.48	-310.50	0.102	11.70	15.77
	Cs ⁺	1.69	-278.00	0.094	10.60	14.50
other monovalent metal ions	Tl ⁺	1.49	-325.90	0.120	7.16	13.27
alkali earth metal ions	Mg ²⁺	0.65	-1922.10	0.334	47.59	32.55
	Ca ²⁺	0.99	-1592.40	0.274	19.52	31.39
	Ba ²⁺	1.35	-1303.70	0.195	12.80	na

a: (Brown, 1988); b: (Feig and Uhlenbeck, 1999); c: (Essington, 2005); d: (Payzant et al., 1973); e: absolute hardness (η) and absolute electronegativity (χ) are defined according to Pearson (Pearson, 1988); na = not available ; dark green indicates strong and light green weak X-ray anomalous scattering properties.

References

- Brown, I.D. (1988). What factors determine cation coordination numbers? *Acta Crystallogr. B* *44*, 545–553.
- Essington, M.E. (2005). *Soil and water chemistry: an integrative approach* (Boca Raton: CRC Press).
- Feig, A.L., and Uhlenbeck, O.C. (1999). The role of metal ions in RNA biochemistry. In *The RNA world*, R.F. Gesteland, T.R. Cech, and J.F. Atkins, eds. (New York: Cold Spring Harbor Laboratory Press), pp. 287–320.
- Payzant, J.D., Cunningh, A.J., and Kebarle, P. (1973). Gas-phase solvation of ammonium ion by NH₃ and H₂O and stabilities of mixed clusters NH₄⁺(NH₃)_n(H₂O)_w. *Can. J. Chem.* *51*, 3242–3249.
- Pearson, R.G. (1988). Absolute Electronegativity and Hardness - Application to Inorganic-Chemistry. *Inorg. Chem.* *27*, 734–740.

Table S4. Kinetic Parameters of the Wild-Type Intron and Mutants

Construct	k_1^a	k_2^a
wt	100	100
G288A	0.79 ± 0.08	1.49 ± 0.29
G288C	1.87 ± 1.08	1.22 ± 0.42
G288U	10.1 ± 1.75	4.96 ± 1.33
C377A	69.4 ± 7.14	38.4 ± 16.6
C377G	9.53 ± 1.28	2.66 ± 0.01
C377U	214 ± 35.4	105 ± 15.8

^a: first (k_1) and second (k_2) splicing step rates for the indicated mutants relative to wild type (wt, $k_1 = 0.011 \pm 0.003 \text{ min}^{-1}$, $k_2 = 0.094 \pm 0.012 \text{ min}^{-1}$, set to 100 %). The standard deviation was calculated from three independent experiments.