

Structure and folding of a rare, natural kink turn in RNA with an A•A pair at the 2b•2n position.

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Supplementary Information

Figures.

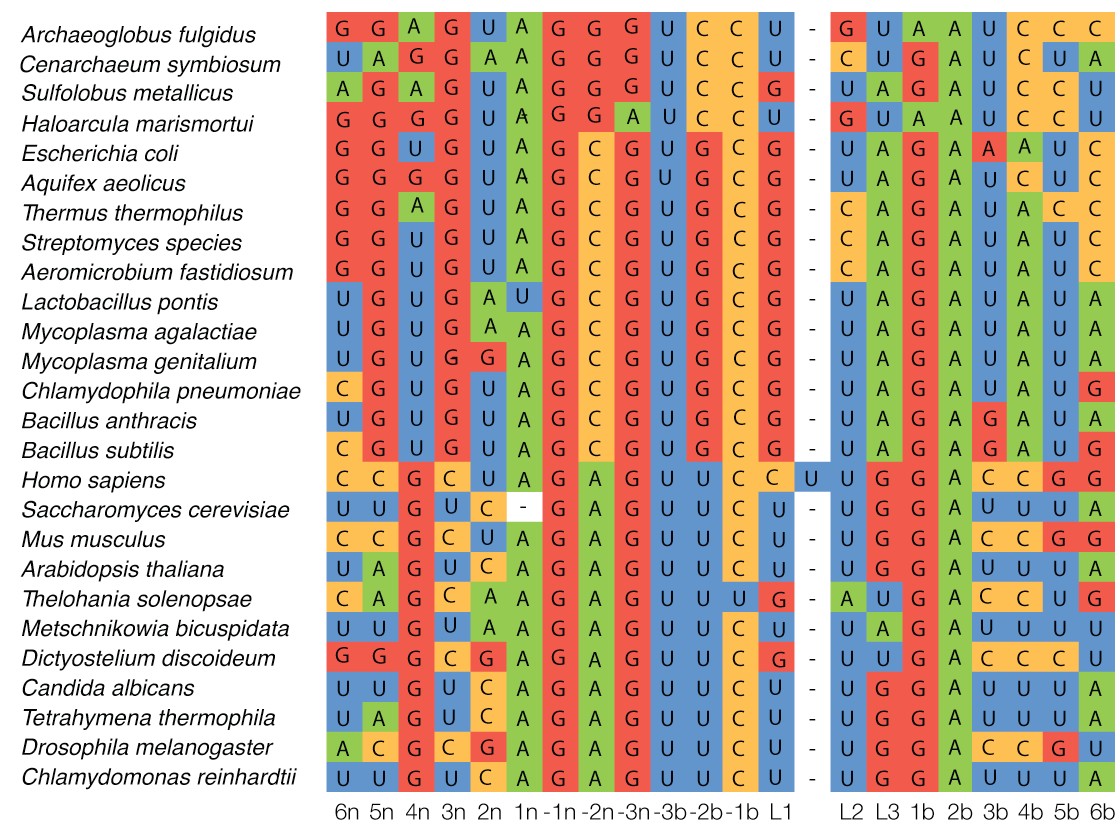


Figure S1. Alignment of the set of Kt-23 sequences from the selected model organisms taken from the complete small-subunit rRNA database (Cannone et al., 2002), visualized using Jalview 2.7 (Waterhouse et al., 2009).

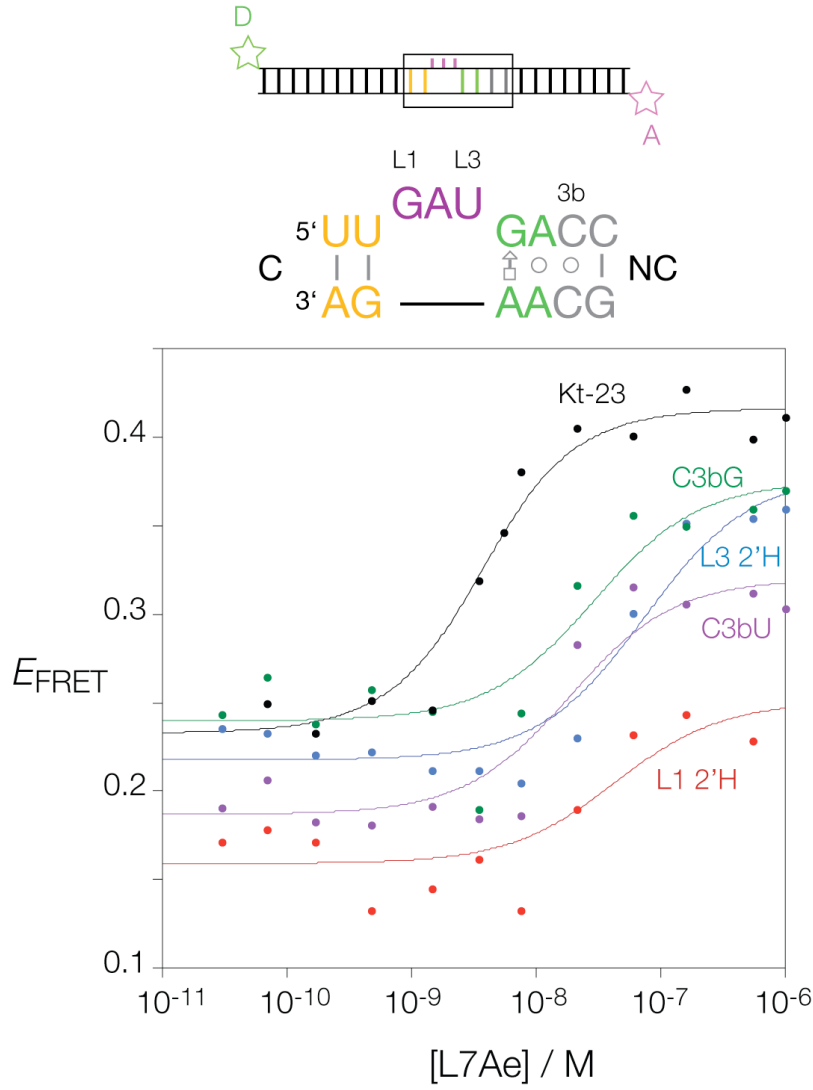


Figure S2. Steady-state FRET analysis of the folding of *T. solenopsae* Kt-23 and variant sequences induced by L7Ae binding. The k-turn sequence was centrally located within a 25 bp RNA duplex terminally labelled with fluorescein (donor, D) and Cy3 (acceptor, A) fluorophores. FRET efficiency was measured in the steady-state for each variant Kt-23 sequence. The change in E_{FRET} was fitted using a model of stoichiometric binding, ie

$$E_{\text{FRET}} = E_0 + \Delta E_{\text{FRET}} \cdot \frac{(1 + K_A P_T + K_A R_T) - \sqrt{(1 + K_A P_T + K_A R_T)^2 - 4 R_T K_A^2 P_T}}{2 R_T K_A}$$

The results are tabulated in Table 1 in the main text.

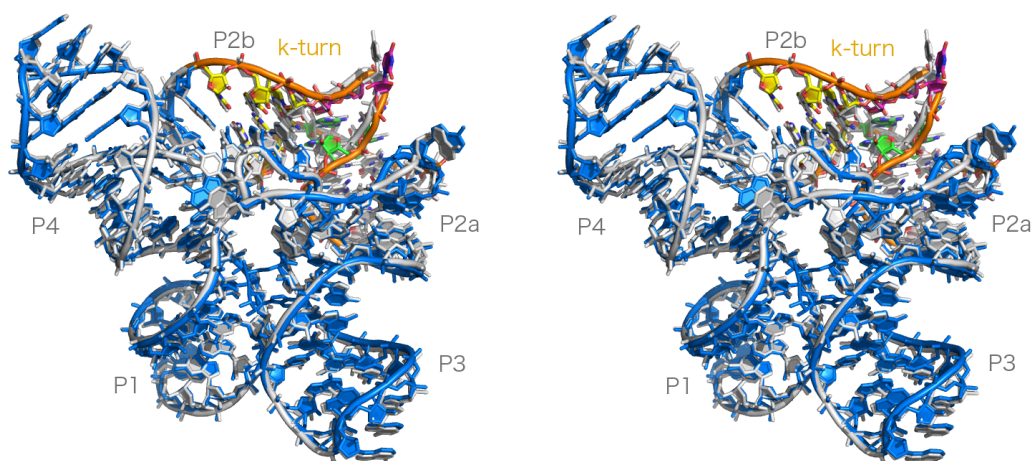


Figure S3. Parallel eye stereo view of an overlay of the crystal structures of the SAM-I riboswitch with the *T. solenopsae* k-turn (blue) and that with its natural k-turn (grey, PDB file 3GX5 (Montange et al., 2010)). The k-turn region is highlighted.

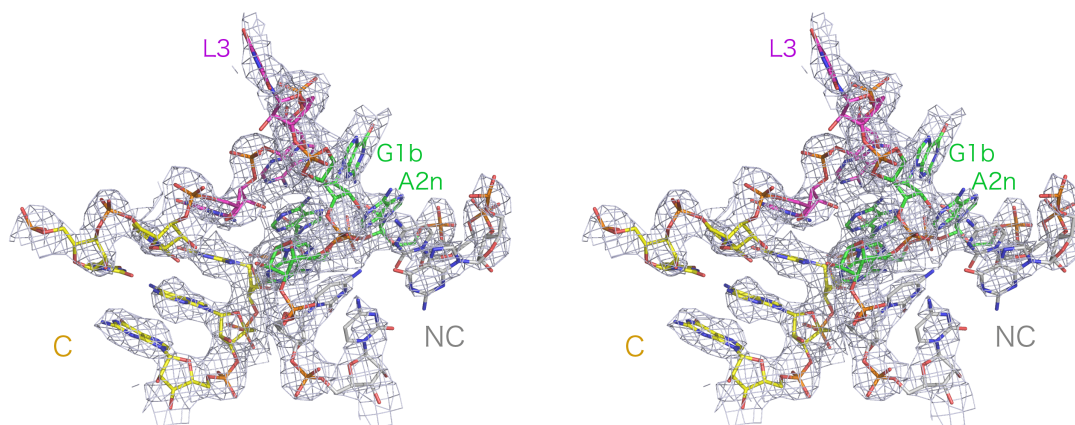


Figure S4. Composite omit map of the k-turn region of the modified SAM-I riboswitch. Parallel eye stereo view from the side of the bulge-containing strand.

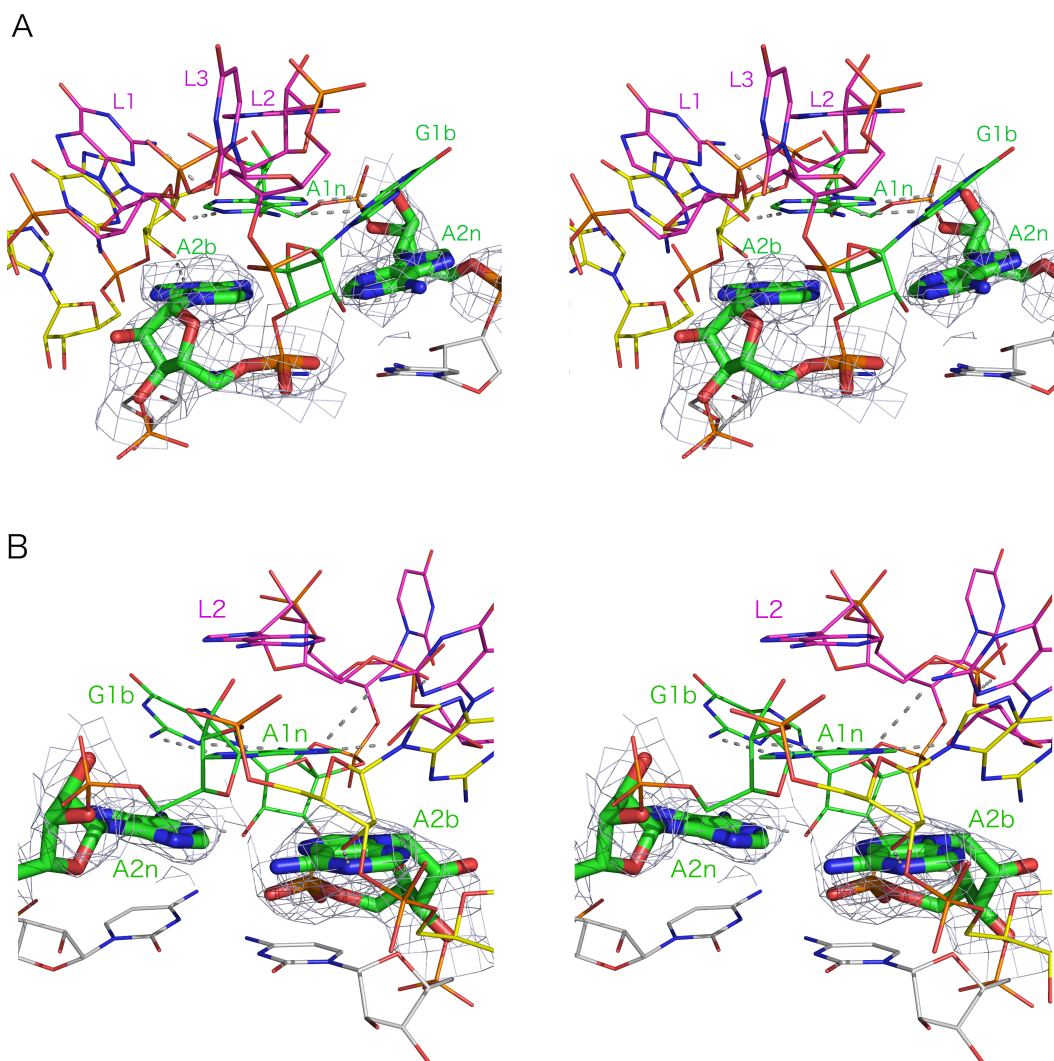


Figure S5. Two parallel eye stereo views of the composite omit map of the k-turn region of the modified SAM-I riboswitch, with the electron density drawn on nucleotides 2b and 2n.

A. View from the side of the bulge-containing strand.

B. View from the side of the non-bulge-containing strand.

References

- Cannone JJ, Subramanian S, Schnare MN, Collett JR, D'Souza LM, Du Y, Feng B, Lin N, Madabusi LV, Muller KM, Pande N, Shang Z, Yu N, Gutell RR. 2002. The comparative RNA web (CRW) site: an online database of comparative sequence and structure information for ribosomal, intron, and other RNAs. *BMC Bioinformatics* 3:2.
- Montange RK, Mondragon E, van Tyne D, Garst AD, Ceres P, Batey RT. 2010. Discrimination between closely related cellular metabolites by the SAM-I riboswitch. *J Molec Biol* 396:761-772.
- Waterhouse AM, Procter JB, Martin DMA, Clamp M, Barton GJ. 2009. Jalview Version 2 - a multiple sequence alignment editor and analysis workbench. *Bioinformatics* 25:1189-1191.