Supplemental Data

Crystal structure of the lysine riboswitch regulatory mRNA element

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Supplemental Table 1: Data collection, phasing and refinement statistics

	Lysine-RNA complex Ir-hexammine derivative	Free RNA
Data collection		
Space group	$P3_2$	$P3_2$
Cell dimensions		
a, b, c (Å)	119.82, 119.82, 58.74	120.19, 120.19, 58.25
α, β, γ (°)	90, 90, 120	90, 90, 120
Wavelength (Å)	1.1050	1.5418
Resolution (Å)	40.0–2.8 (2.91 - 2.8)*	19.70–2.95 (3.06-2.95)
R_{sym} or R_{merge} (%)	8.4 (34.8)	9.0 (35.5)
I/σI	17.9 (4.4)	10.2 (3.4)
Completeness (%)	99.5 (96.6)	99.5 (100)
Redundancy	5.2 (3.7)	3.62 (3.63)
Refinement		
Resolution (Å)	32.6–2.8 (2.87-2.8)	17.11-2.95 (3.02-2.95)
No. reflections	23986 (97.7%)	19610 (99.4%)
R_{work}/ R_{free}	18.20/20.86	18.61/22.04
No. atoms	3631	3547
RNA	3491	3491
Ligand	10	N/A
Water	55	56
Atomic Displacement	54.61	54.92
Parameters (B-factors), all		
RNA	47.22	55.12
Ligand/ion	35.76	N/A
Water	39.14	42.87
r.m.s. deviations		
Bond lengths (Å)	0.005	0.004
Bond angles (°)	1.251	1.239
Maximum likelihood coordinate error (Å)	0.32	0.43

Data was collected from a single crystal.
*Highest resolution shell is shown in parenthesis.

Supplemental Table 2: SAXS Parameters

	Unfolded	Native	Native-Bound
parameters			
Guinier R_g, Å	41.8(±0.5)	29.7(±0.3)	31.1(±0.4)
Real space R_g, Å	47.3(±0.2)	32.0(±0.1)	31.5(±0.1)
D_{max} estimate, Å	172	108	108

Guinier R_g refers to radius of gyration determinations within the linear range of the scattering data when plotted as ln[I(q)] vs q^2. Real Space R_g refers to radius of gyration determinations based on the integration of the pair distribution function for each data set.

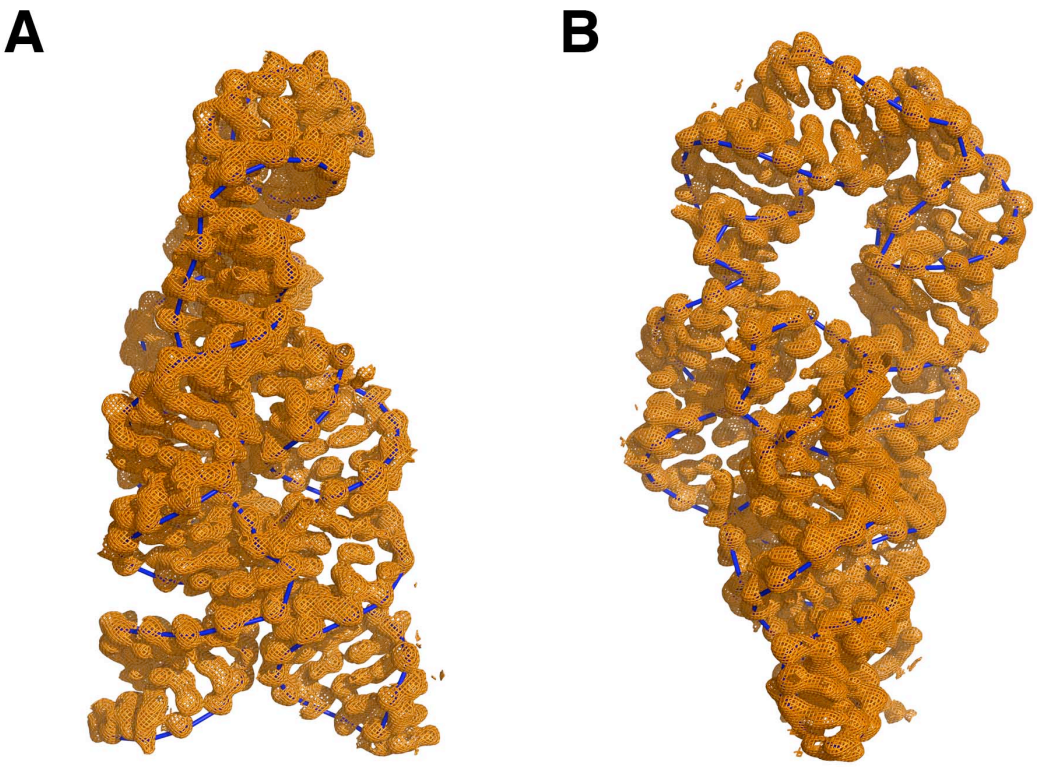

Figure S1. Experimental electron density map. The experimental electron density map (orange mesh) for a single asymmetric unit, unbiased by model phases and contoured at 1.0σ. The final model (blue ribbon) is overlaid on the map to provide perspective. (A) and (B) correspond to the same views depicted in Figure 1C.

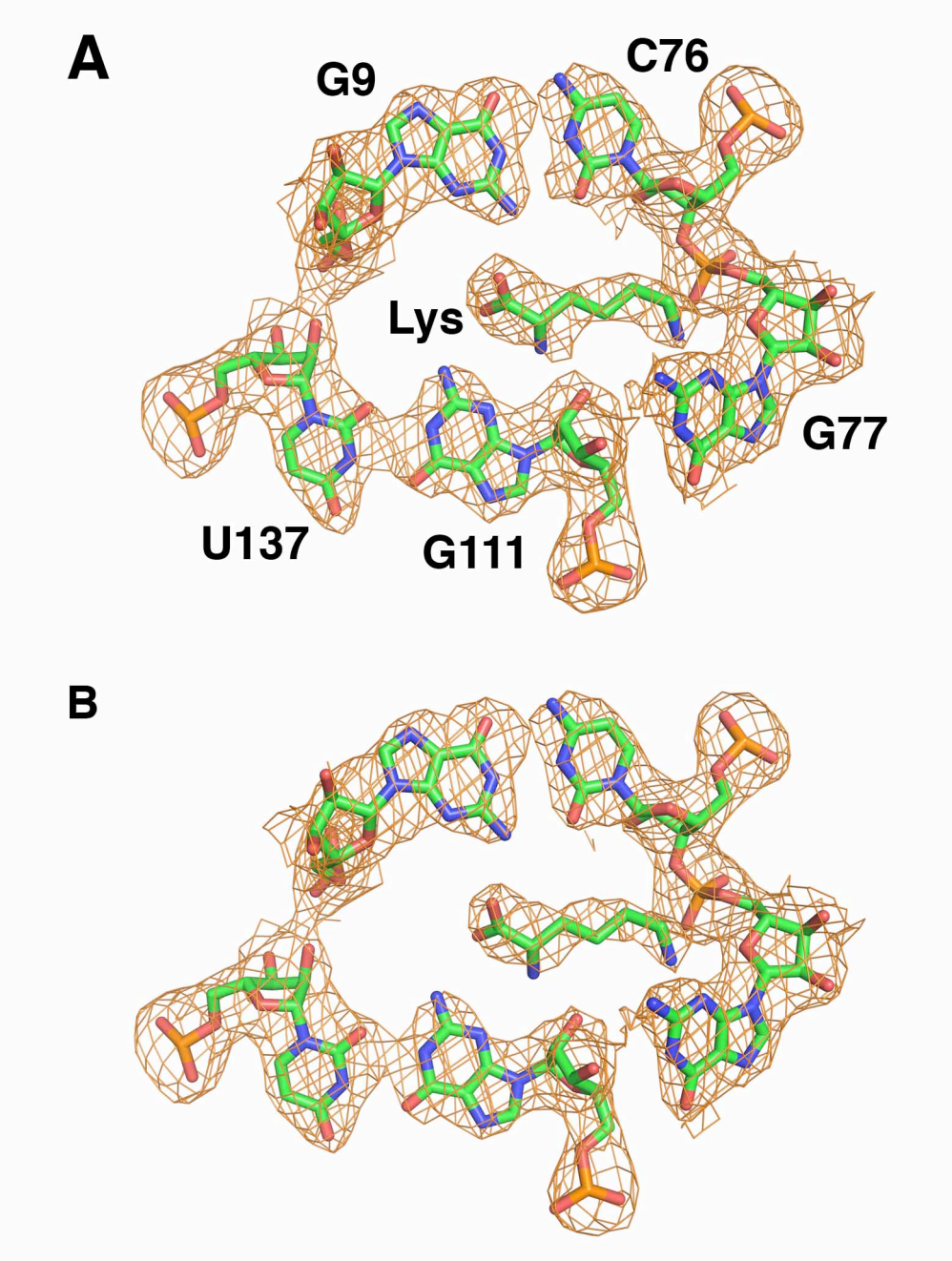

Figure S2. Maps of the ligand binding pocket. (A) Final 2Fo-Fc map contoured at 1.0σ around the nucleotide residues that define the binding pocket and lysine. (B) Simulated annealing omit map in which residues 76, 77, 111 were omitted along with lysine. Note that the density around the ligand remains defined for the entire amino acid and its positioning within the pocket is unambiguous.

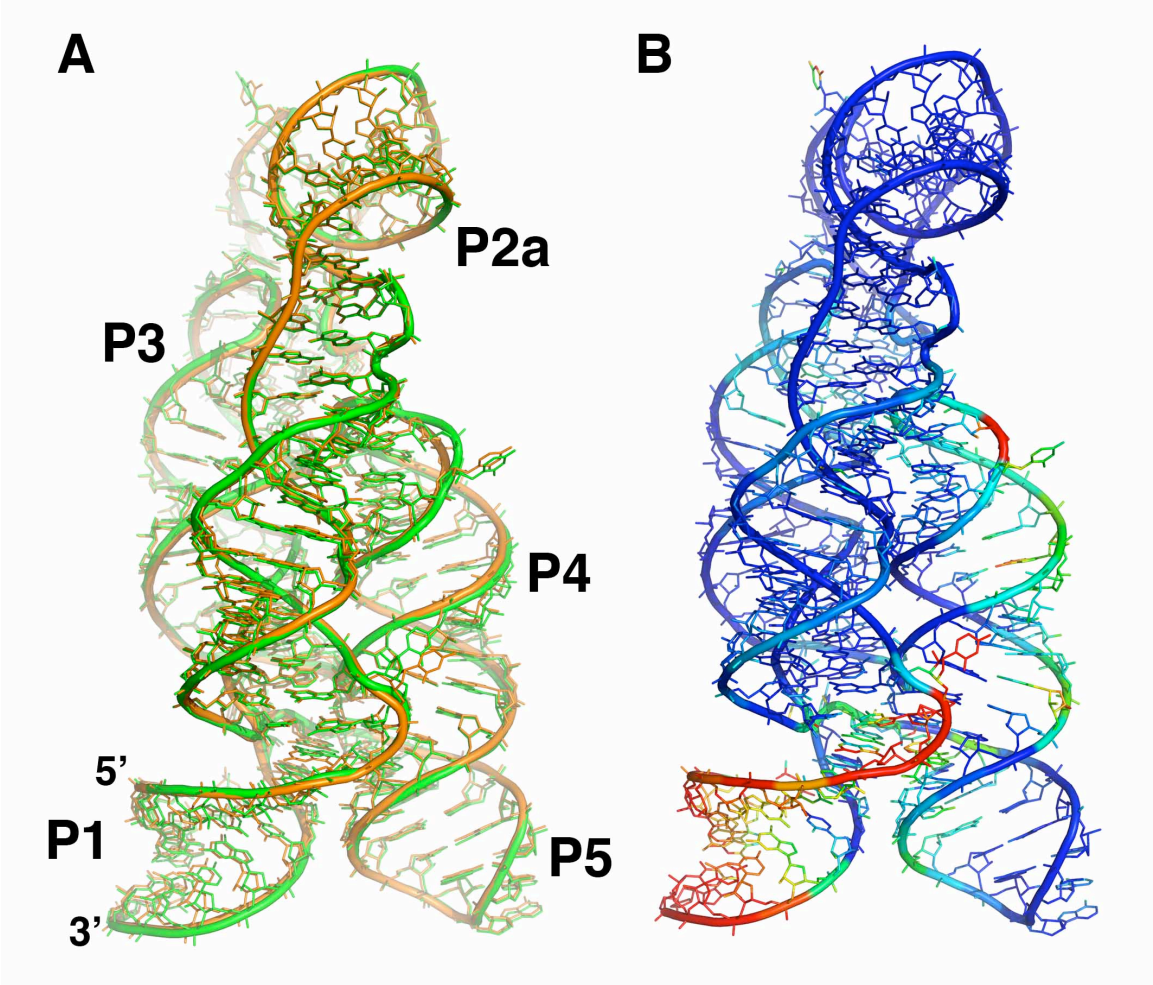

Figure S3. **Superposition of free and bound lysine riboswitch. (A)** Superpositioning of the free (orange) and bound (green) structures of the lysine riboswitch using the Theseus alignment program. The two structures superposition with a maximum liklihood r.m.s.d. of 0.08 Å (classical pairwise r.m.s.d. is 0.70 Å). **(B)** Map of the estimated variance between the two structures in atomic coordinates between the two structures; blue represents low variance (<1 $Å^2$) and red denotes high variance (>10 $Å^2$).

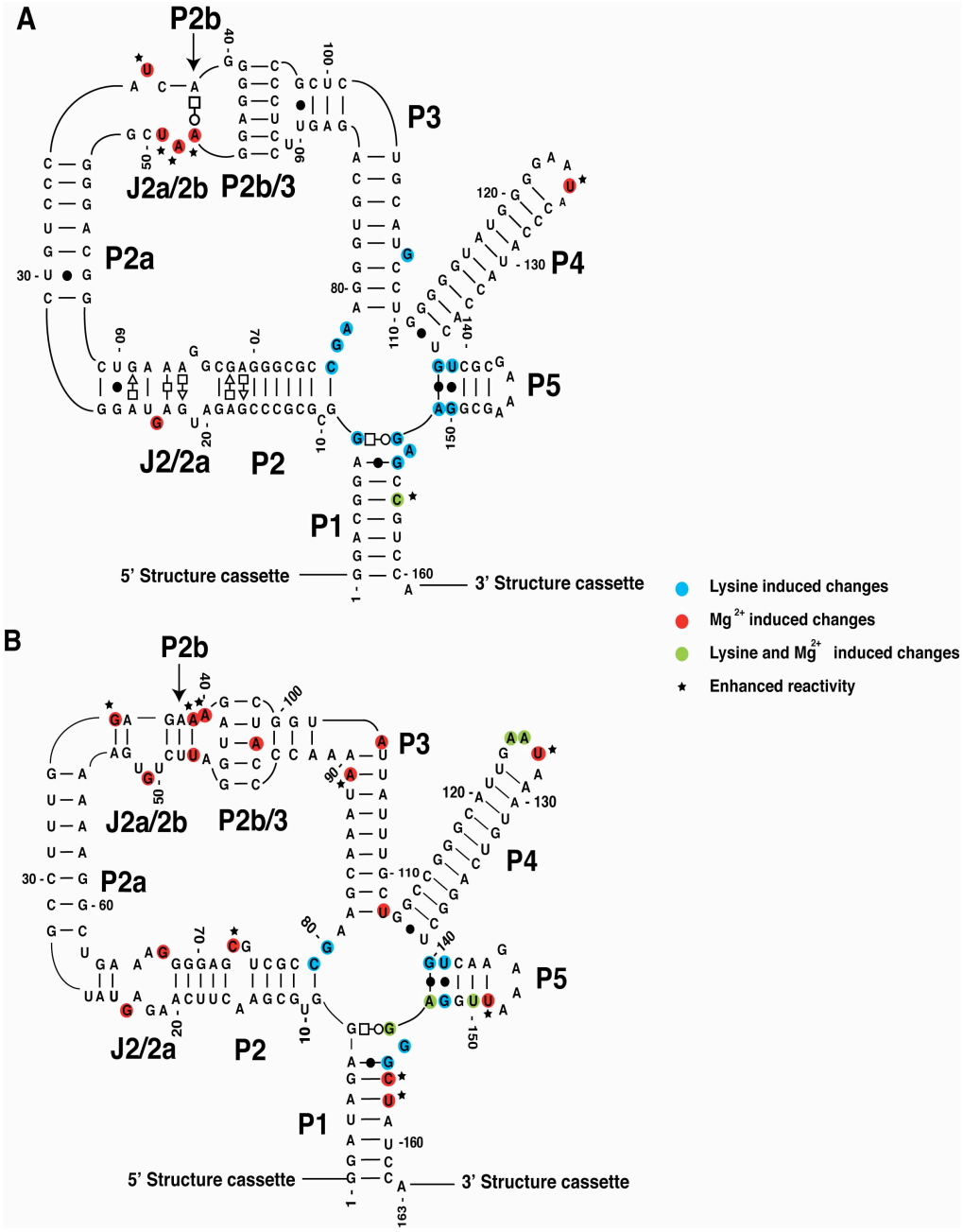

Figure S4. Sequence and structure of RNAs used in SHAPE experiments. The labeling of paired regions has been retained from Fig. 1B; non-canonical base pairing interactions shown in the secondary structure of the *B. subtilis* variant are inferred from the crystal structure of the *T. maritima* variant. (A) The *T. maritima* construct used in the crystallographic studies is shown with the structure cassettes on either end. (B) The riboswitch upstream of the *lysC* gene in *B. subtilis*. Note that the P5 region has been truncated to the same length as the *T. maritima* construct for consistency. The 5' and 3' structure cassettes are illustrated in the literature (*19*). Annotation of reactivity patterns from chemical probing (Figure S5) is denoted on each, per the legend to the right.

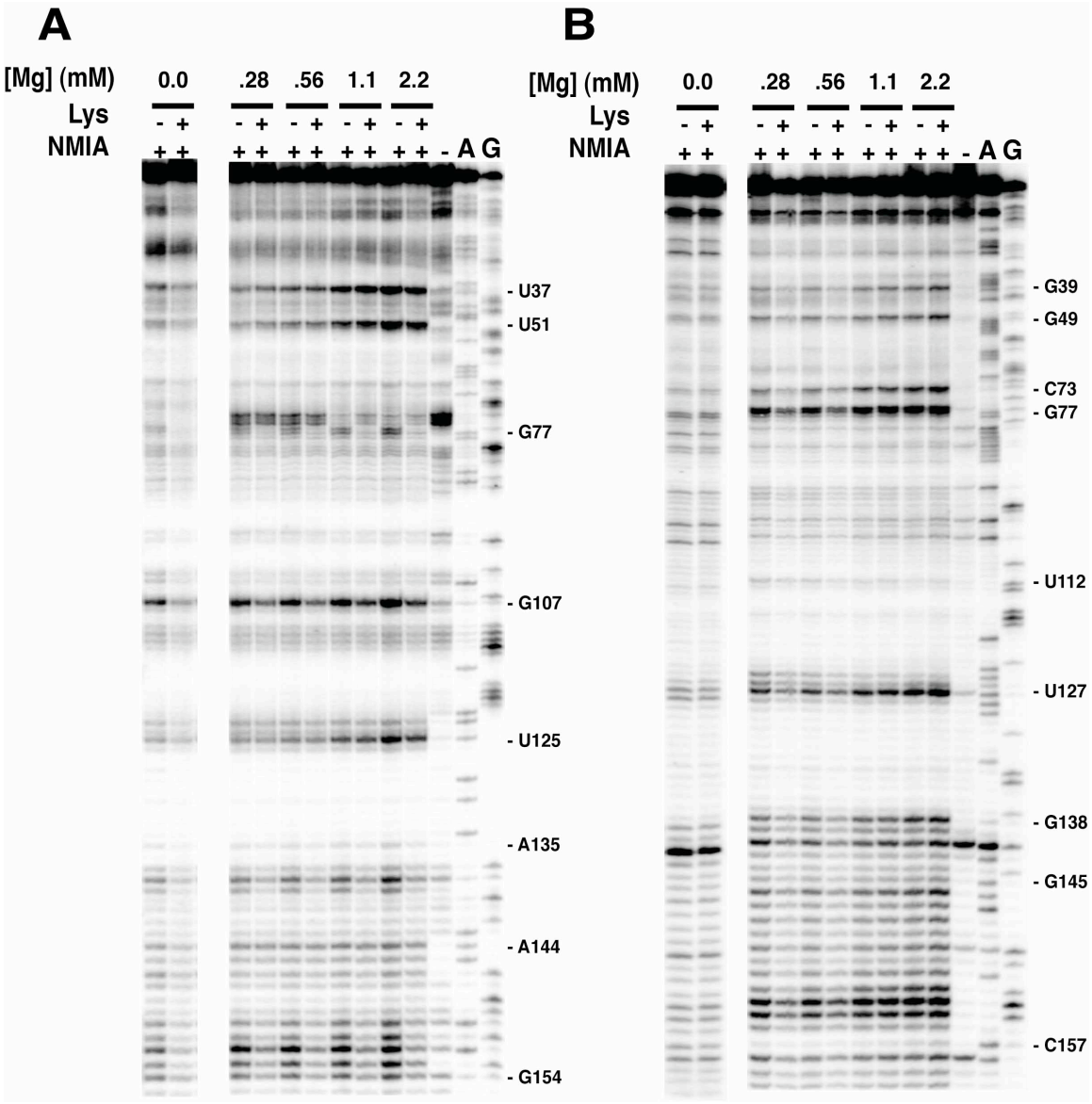

Figure S5. SHAPE probing of the *T. maritima asd* (left) and *B. subtilis lysC* (right) lysine riboswiches. The overall pattern of chemical reactivity demonstrates the overall similarity in the global structure of two lysine riboswitch variants in their response to both magnesium and lysine.

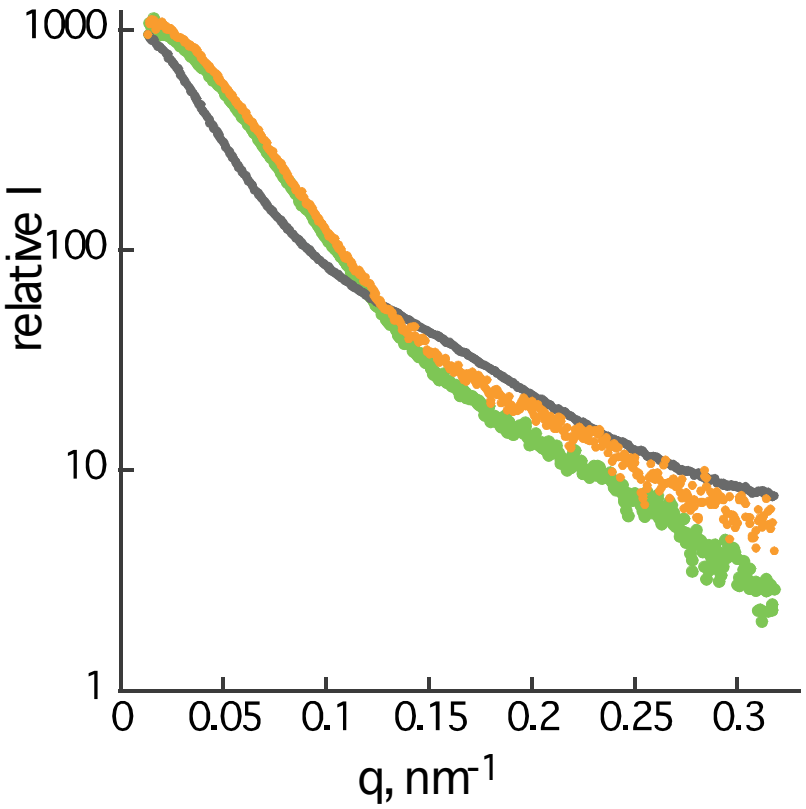

Figure S6. Experimental SAXS curves. Data corresponding to free (EDTA, grey; magnesium, orange) and lysine-bound (green) riboswitch RNA plotted on a relative intensity scale.