# Supplemental Data

# Structural Investigation of the GlmS Ribozyme Bound to Its Catalytic Cofactor

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Table S1. Data Collection, Phase Determination, and Refinement Statistics

| | Native | 2mM $Co(NH_3)^{6+}$ | 1mM $Co(NH_3)^{6+}$/IodoU | 5mM $Ir(NH_3)^{6+}$/IodoU |
|---|---|---|---|---|
| **Data Collection** | | | | |
| Space group | $P2_1$ | $P2_1$ | $P2_1$ | $P2_1$ |
| Cell dimensions | | | | |
| a, b, c (Å) | 48.13, 234.2, 105.0 | 48.44, 231.3, 106.2 | 48.99, 232.5, 106.5 | 48.60, 230.6, 106.2 |
| $\alpha, \beta, \gamma$ ($^o$) | 90.00, 90.65, 90.00 | 90.00, 92.59, 90.00 | 90.00, 92.20, 90.00 | 90.00, 92.84, 90.00 |
| Resolution (Å) | 39-2.50 (2.59-2.50) | 50-2.75 (2.85-2.75) | 50-2.75 (2.85-2.75) | 50-2.80 (2.90-2.80) |
| $R_{sym}$ (%)[a] | 6.2 (>100) | 13.8 (>100) | 13.8 (>100) | 13.9 (>100) |
| $\langle I \rangle / \langle \sigma I \rangle$[a] | 23.2 (1.1) | 12.2 (1.1) | 12.2 (1.1) | 10.2 (1.0) |
| Completeness (%)[a] | 99.8 (100) | 98.4 (95.9) | 98.4 (95.9) | 99.8 (98.6) |
| Redundancy[a] | 6.1 (5.9) | 7.5 (7.1) | 5.1 (4.5) | 7.3 (6.9) |
| **MIR(AS) Phasing** | | | | |
| No. $Co(NH_3)^{6+}$ | | 14 | 14 | |
| No. I | | | 4 | 4 |
| No. $Ir(NH_3)^{6+}$ | | | | 36 |
| Phasing power | | | | |
| Acentric[a] | | | 0.436 (0.288) | 0.947 (0.359) |
| Centric[a] | | | 0.336 (0.161) | 0.729 (0.226) |
| Rcullis[a] | | | 0.958 (1.386) | 0.835 (1.231) |
| Figure of merit[a] | | | 0.333 (0.100) | |
| **Refinement** | | | | |
| Resolution (Å) | 35.0-2.50 | | | |
| No. reflections[b] | 80129 (3987) | | | |
| $R_{work}/R_{free}$ (%) | 22.2 / 26.9 | | | |
| No. atoms | | | | |
| Protein | 2908 | | | |
| RNA | 13080 | | | |
| Ligand/Ion | 80 | | | |
| Water | 207 | | | |
| Mean B-factors | | | | |
| Protein | 55.2 | | | |
| RNA | 57.7 | | | |
| Ligand/Ion | 51.9 | | | |
| Water | 59.7 | | | |
| R.m.s. deviations | | | | |
| Bond lengths (Å) | 0.008 | | | |
| Bond angles ($^o$) | 1.562 | | | |

[a]Values in parentheses are for the highest resolution shell. [b]Values in parentheses are for the cross-validation test set.