

Supplementary Table 2. Metal ions in cryo-EM structures of the *Tetrahymena* ribozyme including bond lengths, bond angles and comparison with other group I introns

Metal	Region	The holo L-16 Scal <i>Tetrahymena</i> ribozyme		The apo L-21 Scal <i>Tetrahymena</i> ribozyme		Other models that have this metal
		Bond length	Bond angle	Bond length	Bond angle	
P4-J4/5-P5-P5a						
M ₁	P4 major	G111 N7, 3.75 Å	n.a.	G111 O6, 4.19 Å	n.a.	
M ₂	Bridging J4/5 and J6/7	A207 OP1*, 2.07 Å C262 OP1, 2.03 Å	A207-M-C262, 145°	A207 OP1, 2.05 Å C262 OP1, 2.49 Å	A207-M-C262, 142°	
M ₃	P5 major groove	G116 O6, 3.61 Å	n.a.	A114 OP2, 3.05 Å	n.a.	1GID, 1HR2, 1U6B
Metal core						
M ₄	P5a A-rich bulge	A184 OP1, 1.86 Å A186 OP1, 2.21 Å A187 OP2, 1.81 Å G188 OP2, 2.29 Å	A184-M-G188, 106° A184-M-A186, 80.1° A184-M-A187, 149° A186-M-A187, 80.3° A186-M-G188, 152° A187-M-G188, 81.9°	A184 OP1, 1.80 Å A186 OP1, 1.83 Å A187 OP2, 1.92 Å G188 OP2, 3.45 Å	A184-M-G188, 82.4° A184-M-A186, 91.5° A184-M-A187, 171° A186-M-A187, 88.5° A186-M-G188, 159° A187-M-G188, 101°	1GID, 1HR2, 1X8W
M ₅	P5a A-rich bulge	A183 OP1, 2.30 Å A184 OP2, 2.11 Å A186 OP2, 2.50 Å	A183-M-A184, 76.3° A183-M-A186, 98.0° A184-M-A186, 72.9°	A183 OP1, 2.22 Å A184 OP2, 2.22 Å A186 OP2, 2.24 Å	A183-M-A184, 84.1° A183-M-A186, 95.2° A184-M-A186, 76.6°	1GID, 1HR2
M ₆	P5a A-rich bulge	G188 O6, 1.96 Å	n.a.	G188 N7, 3.03 Å	n.a.	1GID, 1HR2
P5b and tetraloop						
M ₇	P5b major groove	G163 N7, 3.07 Å G164 O6, 2.50 Å	G163-M-G164, 83.9°	G163 N7, 2.79 Å G164 O6, 1.85 Å	G163-M-G164, 107°	1HR2
M ₈	P5b major groove	G160 O6, 4.16 Å	n.a.	A139 OP1, 3.77 Å	n.a.	
M ₉	P5b major groove	G148 N7, 3.02 Å	n.a.	G148 O6, 3.67 Å	n.a.	1GID, 1HR2,
M ₁₀	L5b GAAA	G150 OP2, 2.33 Å	n.a.	G149 OP2, 2.46 Å	n.a.	
P3-P6						
M ₁₁	Between P3 and P6	A256 OP1, 2.51 Å U273 OP1, 2.54 Å	A256-M-U273, 89.6°	A256 OP1, 2.00 Å U273 OP1, 2.53 Å	A256-M-U273, 88.5°	1X8W
M ₁₂	P3 major groove	U300 O4, 4.57 Å	n.a.	G276 N7, 4.01 Å	n.a.	
M ₁₃	P6 major groove	C217 OP2, 4.05 Å	n.a.	C217 OP2, 3.41 Å	n.a.	
P6-J6a/6-J6/7-J8/7 cluster close to catalytic site						
M ₁₄	P6 major groove	U259 N3, 3.31 Å	n.a.	A214 OP2, 2.12 Å	n.a.	1HR2
M ₁₅	Bridging J6a/6 and J8/7	G257 OP1, 2.34 Å U258 OP2, 2.28 Å C260 O2, 3.28 Å U305 OP2, 2.47 Å	G257-M-U305, 94.8° G257-M-U258, 81.1° G257-M-C260, 143° U258-M-U305, 114° U258-M-C260, 119° C260-M-U305, 103°	G257 OP1, 2.65 Å U258 OP2, 2.28 Å C260 O2, 2.67 Å U305 OP2, 2.14 Å	G257-M-U305, 90.7° G257-M-U258, 73.0° G257-M-C260, 126° U258-M-U305, 105° U258-M-C260, 122° C260-M-U305, 126°	1U6B, 1Y0Q
M ₁₆	Between P6 and J6a/6	U258 OP1, 2.57 Å	n.a.	U258 OP1, 2.49 Å	n.a.	1U6B
M ₁₇	Between J6/7 and P7	U259 OP2, 2.68 Å	n.a.	U259 OP2, 2.17 Å	n.a.	1U6B, 1Y0Q

M18	J8/7	U305 OP1, 2.65 Å	n.a.	U305 OP1, 2.58 Å	n.a.	
M19	J8/7	A301 OP2, 2.32 Å A302 OP1, 2.45 Å	A301-M-A302, 79.7°	A301 OP2, 2.22 Å A302 OP1, 1.81 Å	A301-M-A302, 89.1°	
M20	Between P8 and P2	G32 OP1, 4.38 Å	n.a.	A299 O2', 3.88 Å	n.a.	
M21	P8 major	G280 O6, 2.96 Å	n.a.	G281 N7, 4.73 Å	n.a.	
P14						
M22	P14 major groove	A171 OP2, 2.75 Å	n.a.	A171 OP2, 2.05 Å	n.a.	1GID, 1HR2
M23	P14 major groove	A172 OP2, 2.49 Å A173 OP2, 3.20 Å	A172-M-A173, 73.3°	A172 OP2, 2.04 Å A173 OP2, 2.60 Å	A172-M-A173, 72.5°	1GID, 1HR2, 1X8W
M24	P14 major groove	A42 O2', 4.01 Å	n.a.	A42 O2', 3.63 Å	n.a.	
Catalytic site						
M25	P7 major groove	G312 N7, 3.80 Å	n.a.	G312 O6, 4.21 Å	n.a.	
M26	Between P4 and J8/7	U(-1) O3', 2.41 Å A304 OP1, 2.65 Å A306 OP2, 2.18 Å C208 OP1, 2.54 Å	C208-M-A304, 64.1° C208-M-A306, 88.8° U(-1)-M-C208, 76.6° U(-1)-M-A306, 155° U(-1)-M-A304, 94.9° A304-M-A306, 96.4°	A304 OP1, 2.78 Å A306 OP2, 2.26 Å	A304-M-A306, 64.5°	1U6B, 1X8W, 1Y0Q
M27	P7 major groove	G414 O2', 1.50 Å C262 OP2, 2.53 Å A306 OP1, 2.44 Å	G414-M-C262, 80.7° C262-M-A306, 95.4° G414-M-A306, 95.5°	n.a.	n.a.	1U6B
M28	P7 major groove	U307 OP2, 2.26 Å A308 OP2, 2.28 Å	U307-M-A308, 94.3°	U307 OP2, 2.20 Å A308 OP2, 2.21 Å	U307-M-A308, 91.2	1U6B, 1Y0Q
P1-P2-P2.1						
M29	Between P1 and P2.1	A94 OP1, 2.76 Å	n.a.	n.a.	n.a.	
M30	Between P1 and P2	A28 OP2, 2.25 Å	n.a.	n.a.	n.a.	
M31	P2.1 major groove	G91 O6, 3.26 Å	n.a.	n.a.	n.a.	

*OP1 normally indicates *pro-S* oxygen, whereas OP2 normally indicates *pro-R* oxygen in nucleic acids.