

Table S3: Reproduction of the crystal water molecules in simulations of the free A-site.

water molecule ↓	G1491U	G1491A	U1406C/U1495A	U1495C	NON_MUT
W1	—	—	+	+	+
W4	—	—	+	+	+
(W7)	(—)	(—)	(—)	(—)	(—)
W8 (W54)	—(—)	—(—)	—(—)	—(—)	—(—)
W9 (W2)	—(—)	—(+)	—(—)	—(+)	—(—)
W12	—	—	—	—	—
W13	—	—	—	—	—
W14	—	—	—	—	—
W15	—	—	—	—	—
W19	—	—	—	—	—
W20	—	—	—	—	—
W25	+	+	+	—	+
W27	—	—	—	—	—
W28	—	—	—	—	—
W32	—	—	—	—	—
W44	—	—	—	—	—
(W45)	(—)	(—)	(—)	(—)	(+)
W49	+ <i>(near)</i>	+	—	—	+
W51	+	+	+	+	—

Selected water molecules of the 1J7T crystal structure and the corresponding water density areas in MD simulations without the antibiotic. “+” denotes water density areas higher than 0.22 water molecules per  $\text{\AA}^3$  observed in the position of the corresponding crystallographic water molecule; “—” denotes lack of high water density in this position. Brackets denote analogous water molecules located in the other symmetric part of the RNA fragment.