

Supplemental Figure S4: Structural details of guanidinium binding to the PLRV xrRNA_{LT}. (A) Guanidinium molecules (carbon atom in magenta) bind near the J1/2 region of PLRV (left), where iridium(III) hexammine ligands (blue) bind in the SCNMV structure (right). The composite 2IF_oI-IF_cI map was calculated in Phenix using default parameters. (B) Stacked guanidiniums form a 'spine' in the deep groove of G34–G36. (C) A guanidinium similarly bridges a phosphate oxygen and the Hoogsteen side of a downstream guanine in PLRV and in a guanidinium-II riboswitch (Reiss and Strobel 2017).