



Supplemental Figure S3: Map quality and structural features of the PLRV xrRNA_{LT}. (A) Two xrRNAs form a dimer in the asymmetric unit. Blue, iridium(III) hexammine molecules used for experimental phasing. (B) Structural alignment of molecules 1 and 2 in the asymmetric unit (RMSD ~ 0.4 Å). (C) Schematic representation of xrRNA conformations. Left: Open and closed (modeled) conformations in solution. The 5' end of the RNA structure is in blue and the pseudoknot in orange. Note that in the closed conformation the PK forms a protective ring around the 5' end. Right: Dimer conformation solved by x-ray crystallography. (D) Overall quality of the map used for model building. The final structure is shown with carbon atoms in green. A symmetry-related molecule is shown in grey to help locate the L2A_{CN} – J1/2 – J1/3_{PK} interface further detailed in panel (E). (E) Stacking, base-pairing and other structural features at the L2A_{CN} – J1/2 – J1/3_{PK} interface. Nucleotides belonging to the second molecule in the asymmetric unit or to symmetry-related molecules in the crystals are denoted by asym and sym, respectively. The composite 2F_o–|F_c| map was calculated in Phenix using default parameters. Inset: lower contour level at 1.0 σ for U16.