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Supporting information for article:

Crystal structures of an archaeal RNase P protein Rpp38 in complex with RNA fragments containing a K-turn motif

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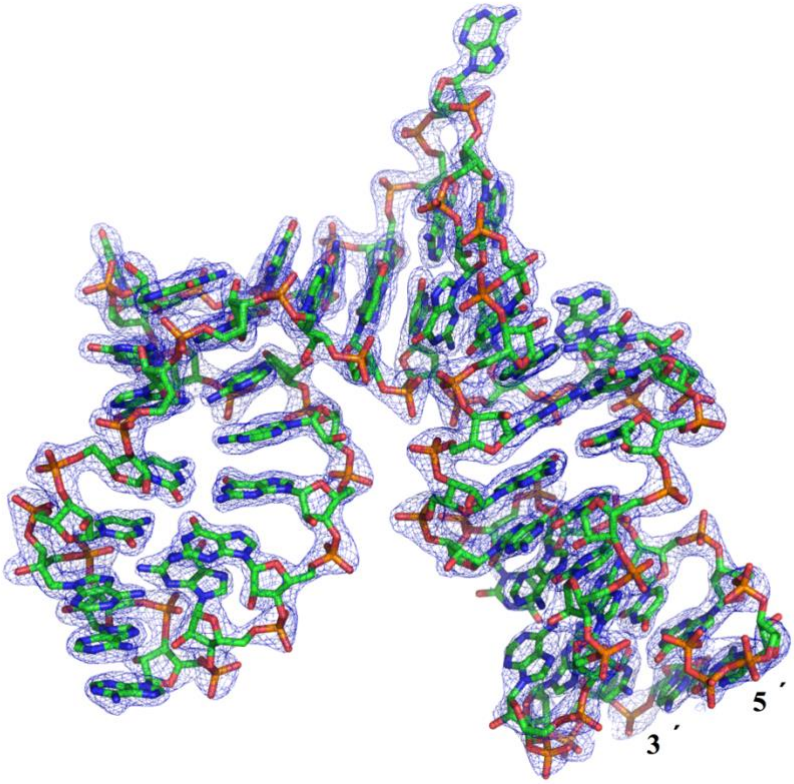

Figure S1. The (2*Fo*-*Fc*) electron density map of P12.2M (MolB)

The(2*Fo*-*Fc*) electron density map was made using Phenix.refine (Afonine *et al.*, 2012). The contour level is at the 1.5σ level. The figure was drawn with PyMol (http://pymol.sourceforge.net).

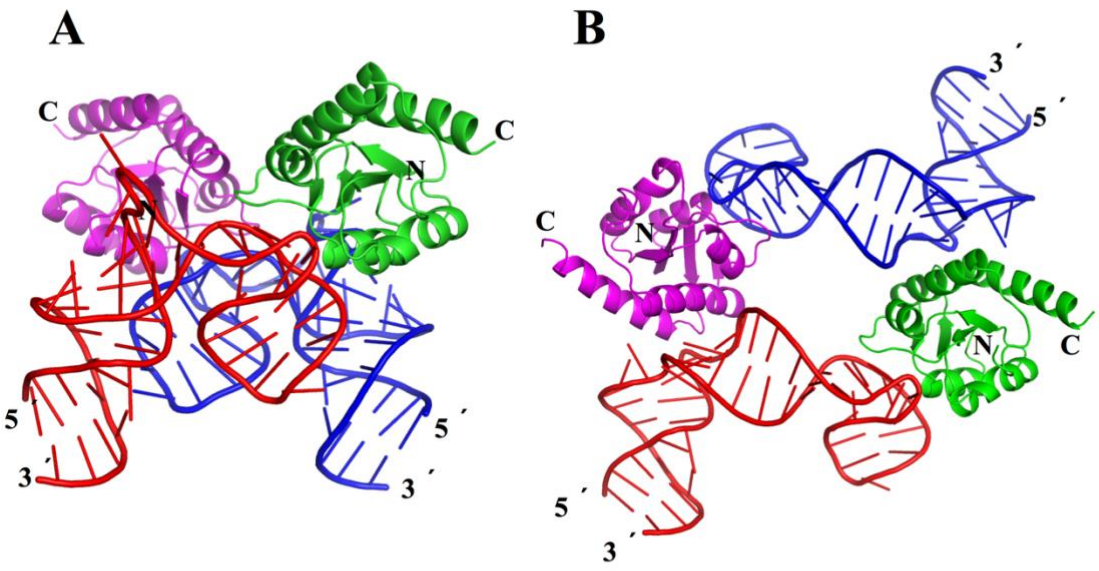

Figure S2. Structure of *Pho*Rpp38 in complex with P12.2M or P12.1M

The crystal structures of *Pho*Rpp38 in complex with P12.2M (A) or P12.1M (B) observed in the asymmetric units are presented. *Pho*Rpp38 is represented by its cartoon diagram with MolA and MolC colored green and magenta, while P12.2M and P12.1M are drawn in cartoon form with MolB and MolD colored red and blue, respectively.

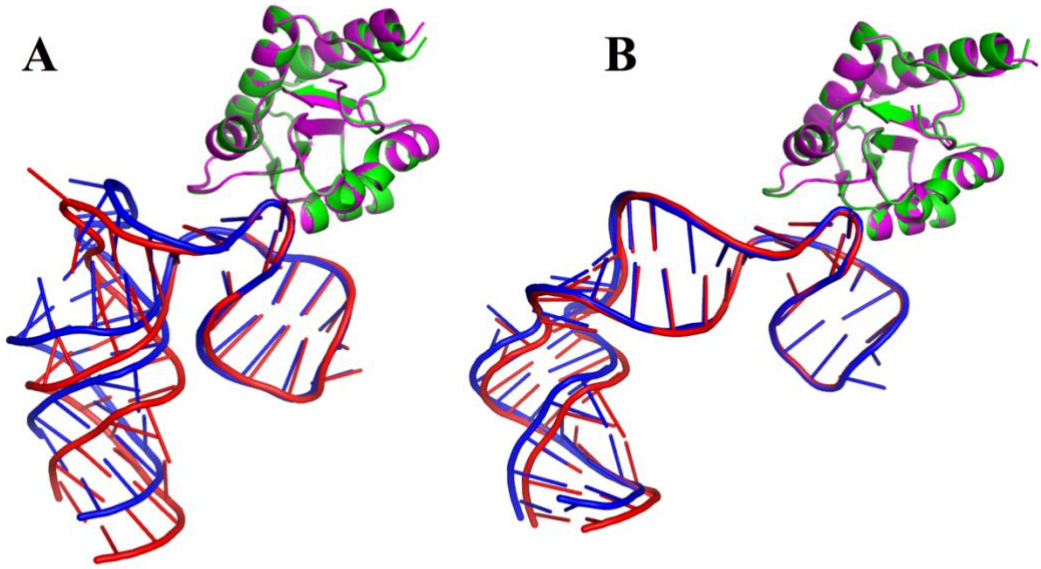

Figure S3 Structural comparison of the *Pho*Rpp38-P12.2M and P12.1M complexes

Superposition of the backbone atoms of the two independent copies in the asymmetric units of the *Pho*Rpp38-P12.2M (A) or P12.1M (B) complexes. MolA (green), MolB (red), MolC (magenta), MolD (blue).

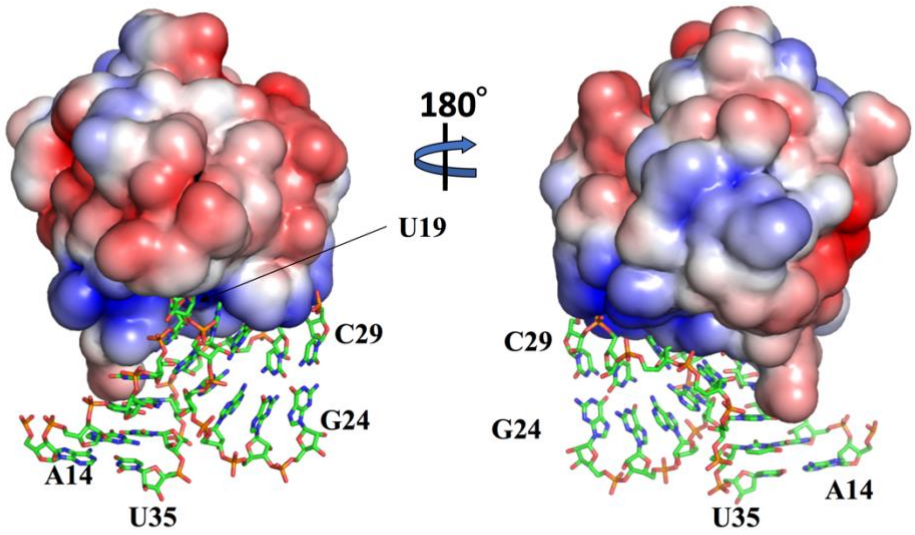

Figure S4. The electrostatic potential of the *Pho*Rpp38 surface

Surfaces are colored according to their electrostatic potential as calculated by the program APBS (Baker *et al*., 2001). The surface potential is displayed as a color gradient from red (negative) to blue (positive), showing a positive charge cluster in *Pho*Rpp38. The positive charges are located predominantly in the P12.2M binding region. Nucleotides located at the interface are shown.

Figure S5. Structural comparison of the K-turns

Superposition of the backbone atoms of the K-turn motifs in the two independent copies in the asymmetric units of the *Pho*Rpp38-P12.2M complexes (MolB, red and MolD, blue), the structure (MolB, magenta) in the*Pho*Rpp38-P12.1M complex, and that of the *Pho*Rpp38-SL12M (MolB, cyan). The bending angles for the K-turns in P12.2M (MolB), P12.2M (MolD), P12.1M (MolB), and SL12M (MolB) are 49.1°, 52.6°, 53.9°, and 40.9°, respectively

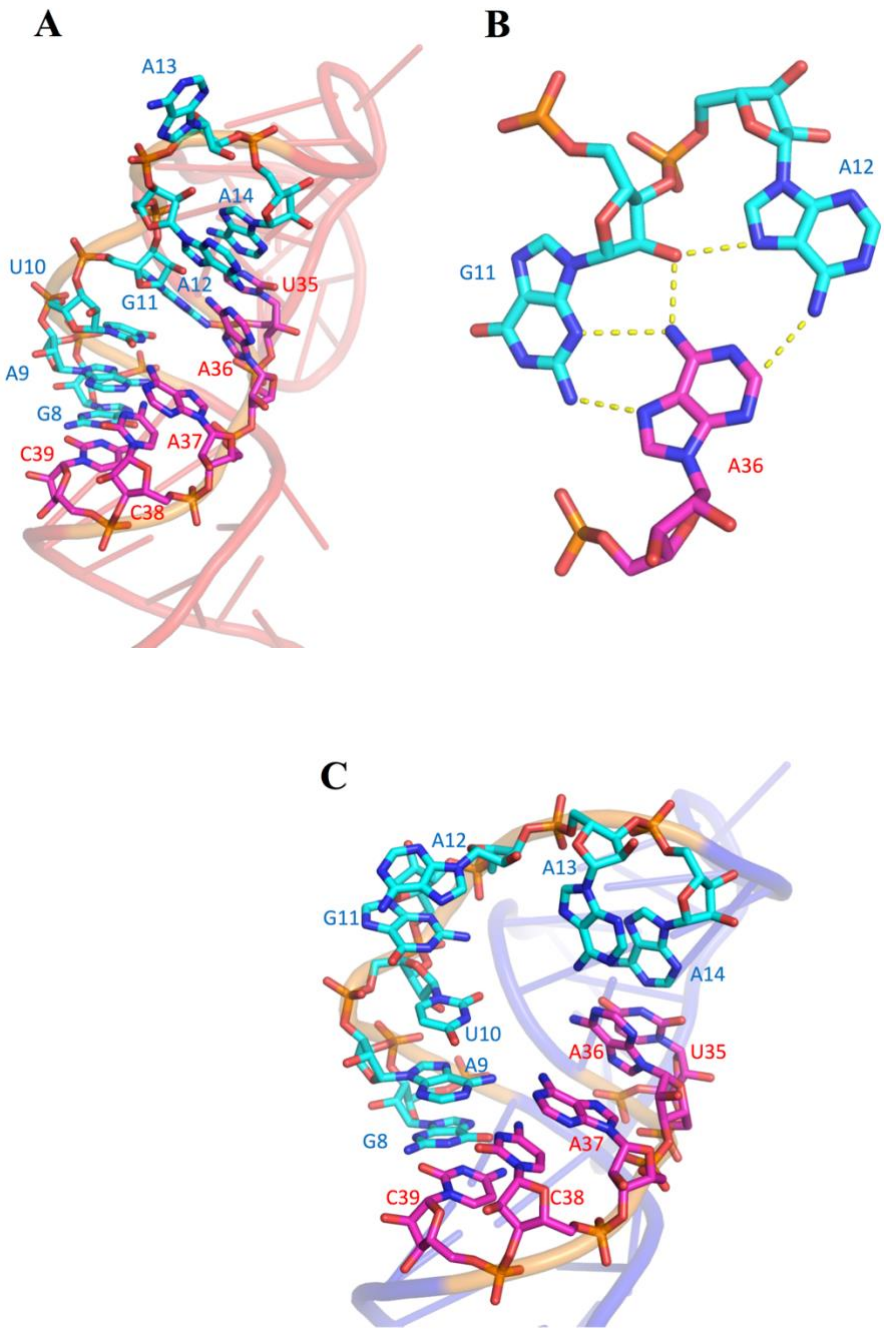

Figure S6. Structure of the single-stranded loops connecting P12.1 and P12.2

The structure of the single-stranded loops connecting P12.1 and P12.2 observed in MolB (A and B) and MolD (C) in the *Pho*Rpp38-P12.2M complex are presented. In the MolB structure, G11, A12, and A36 interact with each other by base triple (B)

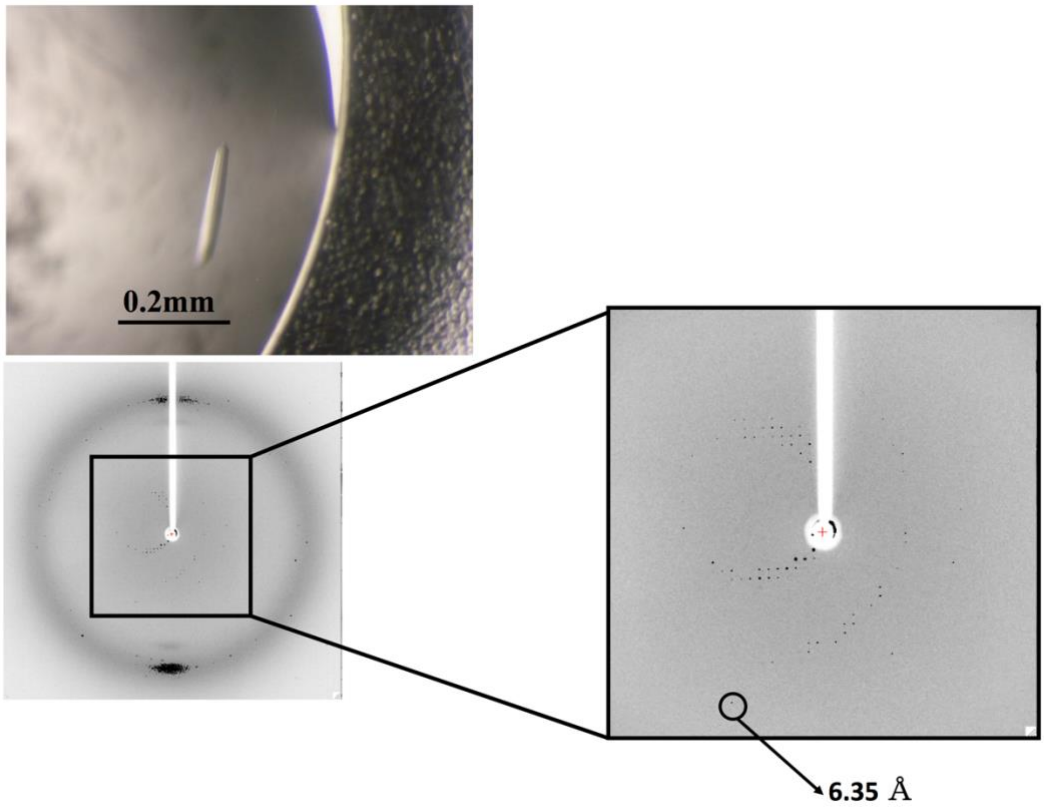

Figure S7. Crystallization of the P10/12 in complex with *Pho*Rpp21, *Pho*Rpp29, and *Pho*Rpp38

The P10/12 RNA fragment in complex with *Pho*Rpp21, *Pho*Rpp29, and *Pho*Rpp38 was purified by a Ni-NTA column and crystallized. The conditions produced crystals that diffracted to a resolution of up to 6.35 Å