

Supplementary figure 2. Identification of AMPPCP and divalent cations associated with it. **(A)** A simulated annealed omit map (cyan net) contoured at 4.5σ of AMPPCP-Mg²⁺ and its coordinating water molecules. The orange net represents an anomalous Fourier difference map for I of 2'-I AMPPNP contoured at 6σ . **(B)** An anomalous Fourier difference map for Mn of AMPPCP-Mn²⁺ contoured at 6σ (red net), and an $|F_{\text{obs}}| - |F_{\text{obs}}|$ (native - Mg²⁺-removed) map contoured at 6σ representing Mg²⁺ (green net). Mg²⁺ was removed by soaking the crystals in the crystallization buffer without Mg²⁺. AMPPCP is shown in ball-and-stick.