

Supplementary figure 5. Structure of ADP-Mg²⁺ bound to CopA-PN. The small spheres represent Mg²⁺ (green) and coordinating water molecules (red) in MolA (**A**, **B**) and in MolB (**C**). The blue broken lines show likely hydrogen bonds. The cyan net in **A** represents a simulated annealed omit map for ADP and Mg²⁺ contoured at 4.5 σ . Both MolA and MolB contain a Mg²⁺. Two oxygen atoms in α - and β -phosphates and four water molecules complete the octahedral coordination sphere of Mg²⁺ (**B**).