

Supplementary figure 3. Difference in conformation of AMPPCP between the wild type and the His462Gln mutant. Atomic models are: molB in the wild type (atom color); AMPPCP in the mutant (pink) and its derivative (green) generated by adjusting the torsion angles in the triphosphate group so that the conformation becomes similar to the wild type as much as possible. It is impossible to bring the α -phosphate to the same position as that of the wild type, because the angles subtended by ribose and the C4*-C5* bond and that by C4*-C5*-O5* are different (in orange dotted circle). These differences show that the His462 side chain pushes the α -phosphate. Distances between the atoms in the His/Gln462 side chain and the α -phosphate are listed in Supplementary Table II.