

Supplementary Table II

Distance between His/Gln462 and the α -phosphate

Protein atom		AMPPCP (WT)		AMPPCP (mutant)	
		O2 α	O5*	O2 α	O5*
His462 WT	N ϵ 2	3.14	4.00	2.40	3.73
	C ϵ 1	4.32	4.70	3.61	4.42
	C ϵ 2	3.66	4.94	2.96	4.64
Gln462 mutant	N ϵ 2	3.70	4.00	2.99	3.70

The atomic models for MolB of the wild type and the His462Gln mutant are superimposed (Fig. 4) and the distances (\AA) between the atoms of His/Gln462 and the closest two oxygen atoms in AMPCP (O2 α and O5*) are measured.