

Supplementary table SI Interactions between phosphate groups of the bound nucleotides and the ATP lid of PDK3

ADP			ATP		
ADP	PDK3	Distance (Å)	ATP	PDK3	Distance (Å)
O1 α	L328 N	3.09	O1 α	N251 ND2	3.16
O2 α	N251 OD1	3.26		N251 OD1	2.70
O1 β	F324 O	2.84	O2 α	L328 N	2.91
O3 β	N251 OD1	3.19	O1 β	S306 OG	2.74
	R254 NH2	2.70	O2 β	N251 OD1	3.02
			O3 β	G323 N	3.27
			O1 γ	G325 N	2.85
				Y326 N	2.80
			O2 γ	G327 N	3.28
				E247 OE1	3.27

Distances were calculated using the program CONTACT in the CCP4 package (Collaborative Computational Project, 1994).