

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

<b>ADP</b>			<b>ATP</b>		
ADP	PDK3	Distance (Å)	ATP	PDK3	Distance (Å)
O1 $\alpha$	L328 N	3.09	O1 $\alpha$	N251 ND2	3.16
O2 $\alpha$	N251 OD1	3.26		N251 OD1	2.70
O1 $\beta$	F324 O	2.84	O2 $\alpha$	L328 N	2.91
O3 $\beta$	N251 OD1	3.19	O1 $\beta$	S306 OG	2.74
	R254 NH2	2.70	O2 $\beta$	N251 OD1	3.02
			O3 $\beta$	G323 N	3.27
			O1 $\gamma$	G325 N	2.85
				Y326 N	2.80
			O2 $\gamma$	G327 N	3.28
				E247 OE1	3.27

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