Suppl. Table 1: **Number of the atomic contacts of various nucleotides bound to PGK (A), PK (B) and CK (C) as determined by docking**

A.)

Interacting side-chain of PGK	D-ADP crystal structure	D-2'-dADP	L-ADP	D-GDP	D-CDP	L-CDP	D-GDP	D-UDP	D-2'-dTDP
Gly 213	10	8	11	7	9	10	7	12	7
Ala 214	2 + 7[§]	0 + 9	2 + 8	1 + 6	1 + 7	2 + 6	1 + 6	1 + 9	2 + 7
Lys 215	0	2	0	1	0	0	1	0	2
Lys 219	4	4	4	4	4	4	4	4	5
Gly 237	6	4	5	4	5	6	4	4	5
Gly 238	2 + 3	0 + 2	2 + 2	1 + 2	1 + 2	0 + 2	1 + 2	1 + 2	1 + 3
Leu 256	4	4	4	1	1	0	1	0	0
Phe 291	1	1	1	1	0	0	1	0	0
Gly 312	1 + 1	0	1 + 0	0	0	0	0	0	1
Leu 313	4	3	1	1	2	0	1	0	4
Asn 336	2	2	2	2	2	2	2	2	1
Pro 338	11	10	14	1 + 10	6	13	1 + 10	10	1 + 7
Val 339	1	0	2	0	1	2	0	3	2
Gly 340	6	5	1 + 7	1 + 8	7	1 + 9	1 + 8	6	3 + 9
Val 341	11	14	10	8	13	9	8	9	14
Phe 342	1	3	1 + 1	2	2	2	2	2	0
Gly 343	3 + 2	0 + 2	4 + 2	3 + 2	4 + 2	4 + 2	3 + 2	4 + 2	1 + 2
Gly 373	1	1	1	1	1	0	1	1	1
Asp 374	1 + 6	1 + 6	1 +4	1 + 7	1 + 5	0 + 6	1 + 7	1 + 6	1 + 6
Thr 375	2	2	2	2	2	2	2	2	0

[§] Where two different values are given, the first one refers to the number of H-bonds plus ionic interactions, while the second one refers to the number of hydrophobic contacts

B.)

Interacting side-chain of PK	D-ATP	D-ADP	D-2'-dADP	L-ADP	D-CDP	L-CDP
Thr 49	1	2	2	4	2	4
Ile 50	0	0	0	3 + 2	0	1 + 4
Gly 51	2	3	0	4	1	2
Pro 52	5	7	0	1	3	0
Arg 72	8	2	0	4	5	5
Leu73	0	0	0	0	0	4
Asn 74	4	3 + 3	3 + 3	3 + 9	2 + 2	3 + 10
His 77	1 + 18	0 + 10	5 + 21	7	14	1 + 8
Gly 78	0	2	0	0	1	0
Tyr 82	2	2 + 22	0	4	1 + 3	1
His 83	1	2	0	1 + 3	2	1 + 3
Arg 119	6	3	5	2	3	3
Lys 206	2	0	0	0	0	0
Lys 269	1	0	1	0	0	0
Ser 361	0	0	4	3	4	3
Gly 362	1	0	1 + 2	3	2	1
Ala 365	1	5	5	7	3	6
Lys 366	3	0	0	4	0	3

C.)

Interacting side-chain of CK	D-ADP	D-2'-dADP	L-ADP	D-CDP	L-CDP
Ser 128	1 + 2	1	1 + 2	3 + 2	0
Arg 130	4 + 19	7 + 14	4 + 15	4 + 15	2 + 7
Arg 132	4	3	2	3	2
His 191	14	1 + 14	1 + 13	0 + 15	5
Leu 193	0	0	0	0	1
Asp 195	0	0	0	0	0
Trp 228	5	3	4	2	3
Arg 236	3	3	2	3	2
Arg 292	8 + 1	7	7 + 1	3 + 1	5 + 1
Val 295	2	0	2	0	0
His 296	16	10	1 + 16	13	2 + 4
Arg 320	6	3	5	4	3
Thr 322	1	0	0	0	1
Gly 323	4	1 + 5	2	1 + 1	1 + 6
Gly 324	3	5	4	1 + 3	1 + 4
Val 325	1	1	1	1	1
Asp 335	1 + 1	2 + 2	1 + 3	1	1 + 3