



**Supplementary figure S1** Sequence alignments of human PDK isoforms, BCK and lipoyl domains

(A) Sequence alignments of human PDK isoforms and the cognate BCK were carried out with ClustalW (Thompson et al., 1994) and drawn by ESPript (Gouet et al., 1999). Conserved residues are colored in *red* and similar residues in *yellow*. The secondary structures of PDK3 and rat BCK are shown above and below the alignments, respectively. Wavy lines indicate disordered regions in crystal structures. The ATP lid and C-terminal tail of PDK3 are indicated by *red* arrows. Conserved residues participating in the lipoyl-binding pocket are marked with a *red* asterisk \*. Residues that interact with the phosphate group of bound ATP are indicated with a *blue* asterisk \* (*cf.* supplementary table SI). (B) Sequence alignments of lipoyl-bearing domains in human PDC were performed as described above. Sequence designations are as follows: E2p-LBD1, the outer lipoyl (L1) domain of E2p; E2p-LBD2, the inner lipoyl (L2) domain of E2p; E3bp-LBD, the lipoyl domain of E3-binding protein. Negative numbers for E2p-LBD1 and E3bp-LBD denote residues in mitochondrial targeting sequences. Secondary structures from the present crystal structure and the published NMR structure (Howard et al., 1998) are shown above and below the aligned sequences, respectively. lip, the lipoyl-lysine residue.