



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 75 (2019)

Supporting information for article:

Changes in the allosteric site of human liver pyruvate kinase upon activator binding include the breakage of an intersubunit cation– π bond

Jeffrey S. McFarlane, Trey A. Ronnebaum, Kathleen M. Meneely, Annemarie Chilton, Aron W. Fenton and Audrey L. Lamb

Table S1 Structural Alignments of Monomers

Variant	C436M	D499N	W527H	GGG	S531E
C436M	X	0.27-0.48	0.37-0.6	0.47-2.23	0.44-1.92
D499N	0.27-0.48	X	0.27-0.48	0.37-0.60	0.41-0.69
W527H	0.37-0.6	0.27-0.48	X	0.42-0.61	0.42-0.65
GGG	0.47-2.23	0.37-0.60	0.42-0.61	X	0.4-1.82
S531E	0.44-1.92	0.41-0.69	0.42-0.65	0.4-1.82	X

Rmsd values are reported in Å for alignments over the full length of each monomer. Ranges demonstrate the variation in rmsd values for the alignment of different monomers. Alignments performed by PDBeFold.

Table S2 Structural Alignments of Tetramers

Variant	D499N	W527H	GGG	S531E
D499N	X	0.47	1.44	1.45
W527H	0.47	X	1.35	1.69
GGG	1.44	1.35	X	1.73
S531E	1.45	1.69	1.73	X

Rmsd values are reported in Å for alignments over the full length of the A and C domains for each tetramer (excluding the B domain, residues 130-230). Alignments performed using the combinatorial extension (CE) algorithm in PyMOL.

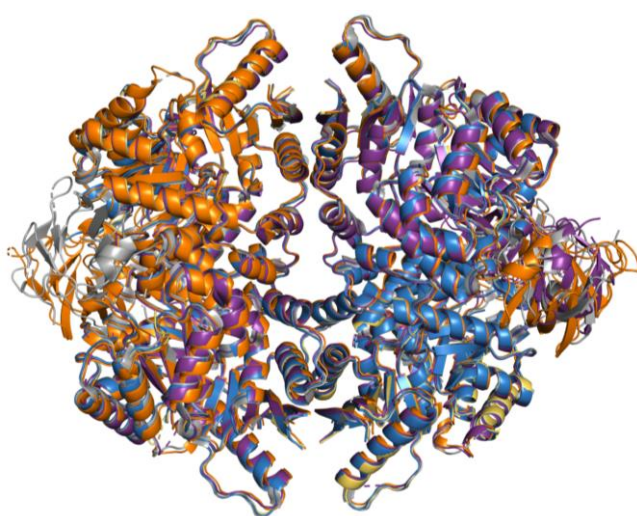


Figure S1 Tetramer Overlays. Overlay of D499N (blue), W527H (yellow), GGG (orange), S531E (purple) and C436M (gray) demonstrating high structural homology for the A and C domains.

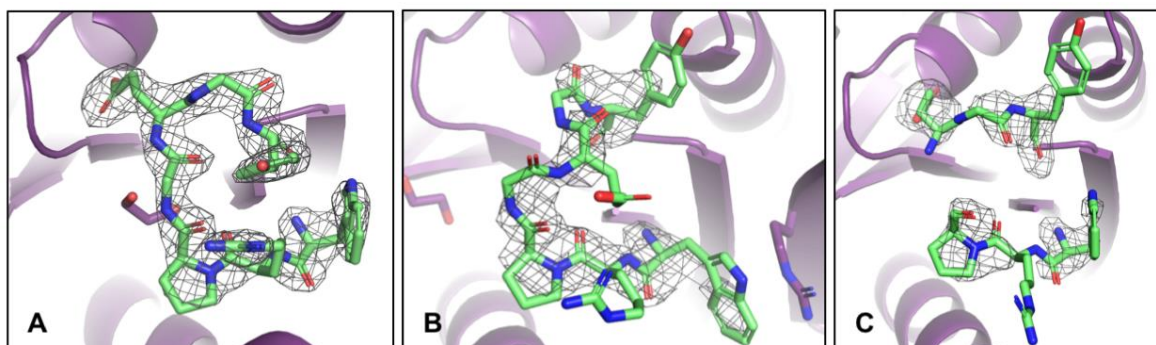


Figure S2 Conformational variation of the S531E allosteric loop. A. Chain C showing S531E bound in the 6' phosphate binding site. Wireframe is a mF_o-DF_c omit map contoured 4.0σ . B. Chain B showing the allosteric loop sampling an open conformation with partial occupancy. Wireframe is a mF_o-DF_c omit map contoured 3.0σ . C. Chain F showing incomplete density for the allosteric loop in a closed conformation. Wireframe is a mF_o-DF_c omit map contoured 3.0σ .

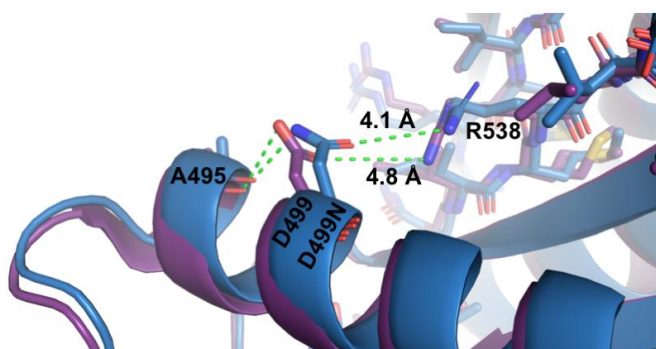


Figure S3 Comparison of D499N and C436M C-C interface. Overlay of C436M (purple) and D499N (blue) showing the position of residue 499. Alignment is of the AC domains and was performed by PDBeFold.