The high-resolution structure of dihydrodipicolinate synthase from *Escherichia coli* bound to its first substrate, pyruvate

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Supporting Information

Figure S1 Possible hydrogen bonding networks in the vicinity of the lysine-bound pyruvate moiety. A. If the pyruvate carboxylate is either deprotonated or protonated cis to the imine group, asparagine 248 must be oriented such that the –NH2 group hydrogen bonds to the threonine 45 –OH. This is the orientation that has been modelled in 3DUO. B. If the pyruvate carboxylic acid group is protonated trans to the imine group, then the side chain of asparagine 248 can be oriented either way around.

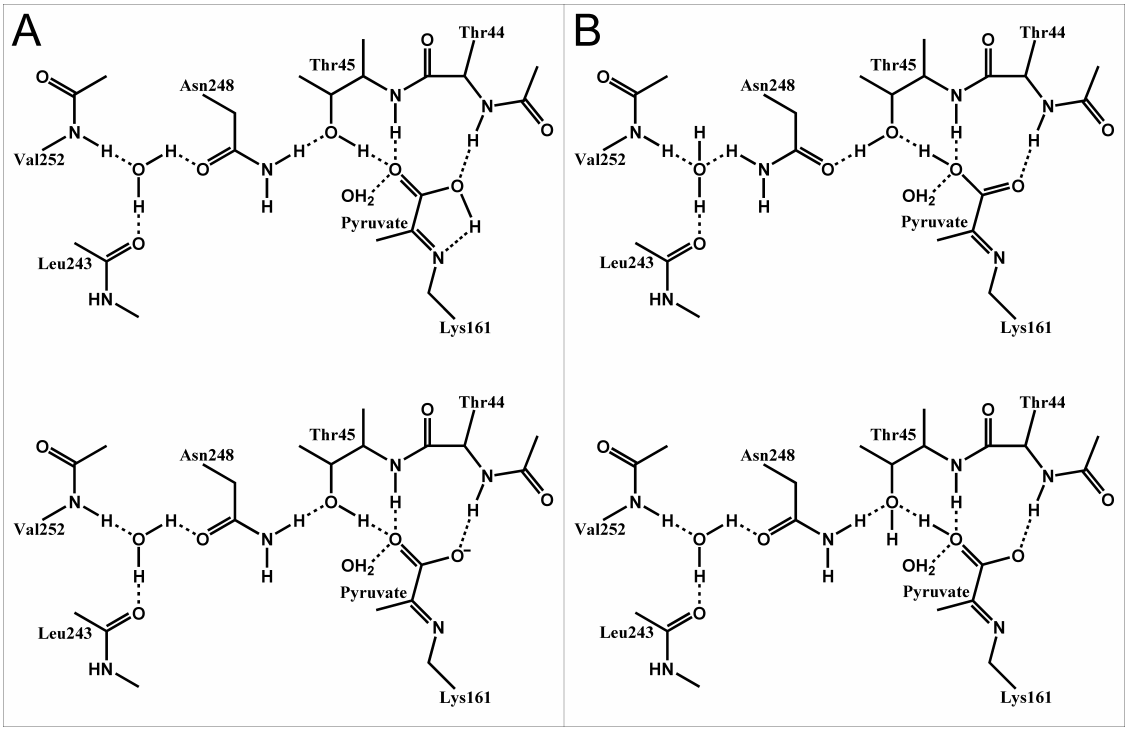

Figure S2 Active site of partially refined structure, prior to modelling of pyruvate moiety, showing excess electron density near the NZ of lysine 161 in chains A and B as indicated. $2F_o$-F_c density, coloured grey, is contoured at 1.0 σ, F_o-F_c density is contoured at 3.0 σ (green) and -3.0 σ (red). Images generated using PYMOL [Delano, W.L. (2002). *The PyMOL Molecular Graphics System*].