

Supporting Information

QM/MM studies on the mechanism of unusual bifunctional fructose-1,6-bisphosphate aldolase/phosphatase

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Figure S1

The crystal structures of FBPA/P (a) in FBPA form (PDB ID: 3R1M) and (b) in FBPP form (PDB ID: 1UMG).

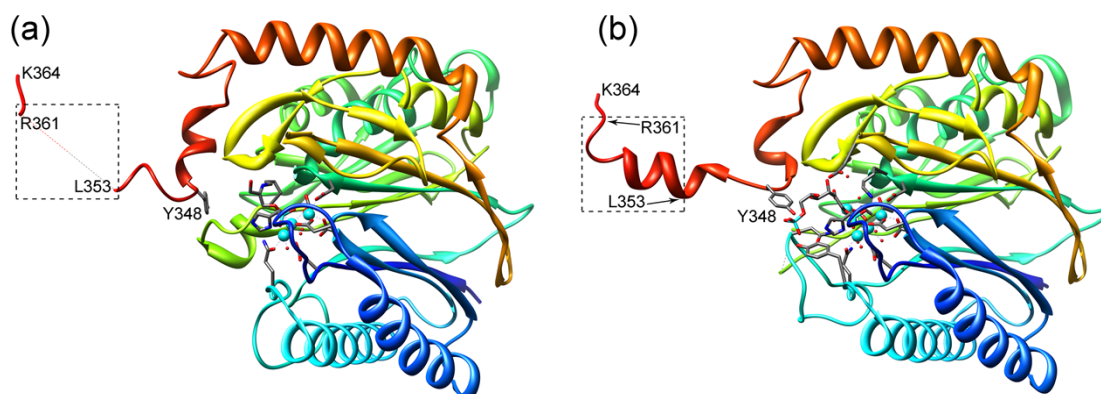


Figure S2

Time dependences of RMSDs (ps) from MD simulations. The RMSDs of two models to itself are present, and black line for DHAP-protein complex, red one for GA3P-protein complex.

