Structural analysis of multi-functional enzyme FadB from *Cupriavidus necator* H16: Non-formation of FadAB complex

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*Cupriavidus necator* H16 is a gram-negative chemolithoautotrophic bacterium and has been extensively studied for biosynthesis and biodegradation of polyhydroxyalkanoate (PHA) plastics [1-2]. To increase understanding of fatty acid metabolism for PHA production, we determined the crystal structure of FadB from *Cupriavidus necator* H16 (*CnFadB*). The predicted model of *CnFadB* by AlphaFold was used to solve the phase problem of the crystals of the protein. The *CnFadB* structure consists of two distinctive domains, an N-terminal ECH domain and a C-terminal HAD domain, and the substrate- and cofactor-binding modes of the two functional domains were identified. Importantly, unlike other known FadB enzymes that exist as a dimer in a form complexed with FadA [3], *CnFadB* functions as a monomer without forming a complex with *CnFadA*. SAXS measurement further proves that *CnFadB* exists as a monomer in solution. Non-sequencing action of FadA and FadB in *C. necator* seems to be beneficial for minimizing the metabolic interference between β-oxidation and PHA synthesis/degradation.

Figure 1. Structural superposition of the *CnFadB* onto the molecular envelope calculated from the SAXS data.


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