

Fig. S1

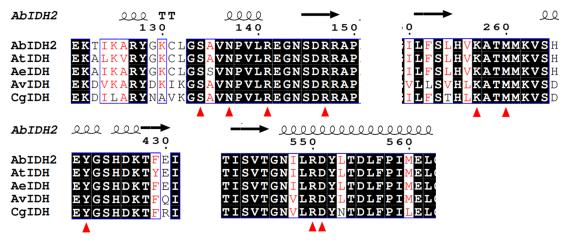
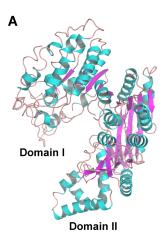
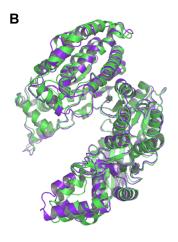
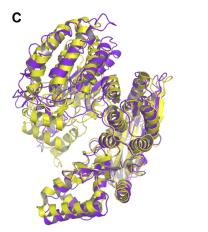


Fig. S2







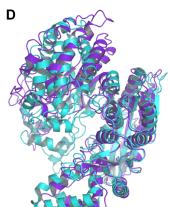


Fig. S3

Figure legends

Fig. S1. The sequence alignment of the dimeric AbIDH2 with its homologous IDHs from *Azoarcus tolulyticus* (AtIDH, GenBank Accession WP_076602605.1) and *Acidovorax ebreus* (AeIDH, GenBank Accession WP_015913126.1) and two typical monomeric NADP-IDHs from *Azotobacter vinelandii* (AvIDH, GenBank Accession No. BAA11169.1) and *Corynebacterium glutamicum* (CgIDH, GenBank Accession No. WP_011013800.1). The residue numbering in the figure is based on AbIDH2 sequence. The conserved residues are shaded by black. The residues that involved in NADP⁺ binding are marked by red pentagram \bigstar .

Fig. S2. The sequence alignment of the dimeric AbIDH2 with its homologous IDHs from *Azoarcus tolulyticus* (AtIDH, GenBank Accession WP_076602605.1) and *Acidovorax ebreus* (AeIDH, GenBank Accession WP_015913126.1) and two typical monomeric NADP-IDHs from *Azotobacter vinelandii* (AvIDH, GenBank Accession No. BAA11169.1) and *Corynebacterium glutamicum* (CgIDH, GenBank Accession No. WP_011013800.1). The residue numbering in the figure is based on AbIDH2 sequence. The conserved residues are shaded by black. The residues that involved in substrate binding are marked by red triangle \blacktriangle .

Fig. S3. (A), Overall AbIDH2 monomer structure is resolved into domain I and domain II. There are 12 α -helices and 7 β -strands in domain I, and 18 α -helices and 20 β -strands in domain II. (B), Superimposition of apo-AtIDH2 (purple) and apo-CgIDH (green, 2b0t) secondary structures. (C), Superimposition of apo-AtIDH2 (purple) and AvIDH-isocitrate (yellow, 1jtw) secondary structures. (D), Superimposition of apo-AtIDH2 (purple) and AvIDH-isocitrate (yellow, 1jtw) secondary structures. (D), Superimposition of apo-AtIDH2 (purple) and AvIDH-isocitrate (yellow, 1jtw) secondary structures. (D), Superimposition of apo-AtIDH2 (purple) and AvIDH2 (purple) and A