Supplementary Figure S2. The dihydrolipoamide binding sites of the E2oCD and E2pCD

(A) Surface model of the dihydrolipoamide entrance in the active-site channel of the apo E. coli E2oCD structure (PDB code: 1C4T). (B) The apo A. vinelandii E2pCD structure
(PDB code: 1EAA). (C) The structure of E2pCD in complex with CoA in the “in” conformation (PDB code: 1EAD). The oxidized thiol group of the bound CoA is shown as a stick model. (D) The structure of E2pCD in complex with CoA in the “out” conformation (invisible) and dihydrolipoamide (as a stick model) (PDB code: 1EAB). The residues corresponding to the three gatekeeper residues in the E2bCD structures are colored in magenta. The region corresponding to the gating turn in the E2bCD structure is in red. (E) The model structure of dihydrolipoamide-bound bovine E2bCD in the open-gate conformation. The structure of *A. vinelandii* E2pCD-dihydrolipoamide complex was superimposed on the E2bCD-CoA (short soak) structure, and the position of the dihydrolipoamide was subsequently adjusted to fit the open gate of E2bCD.