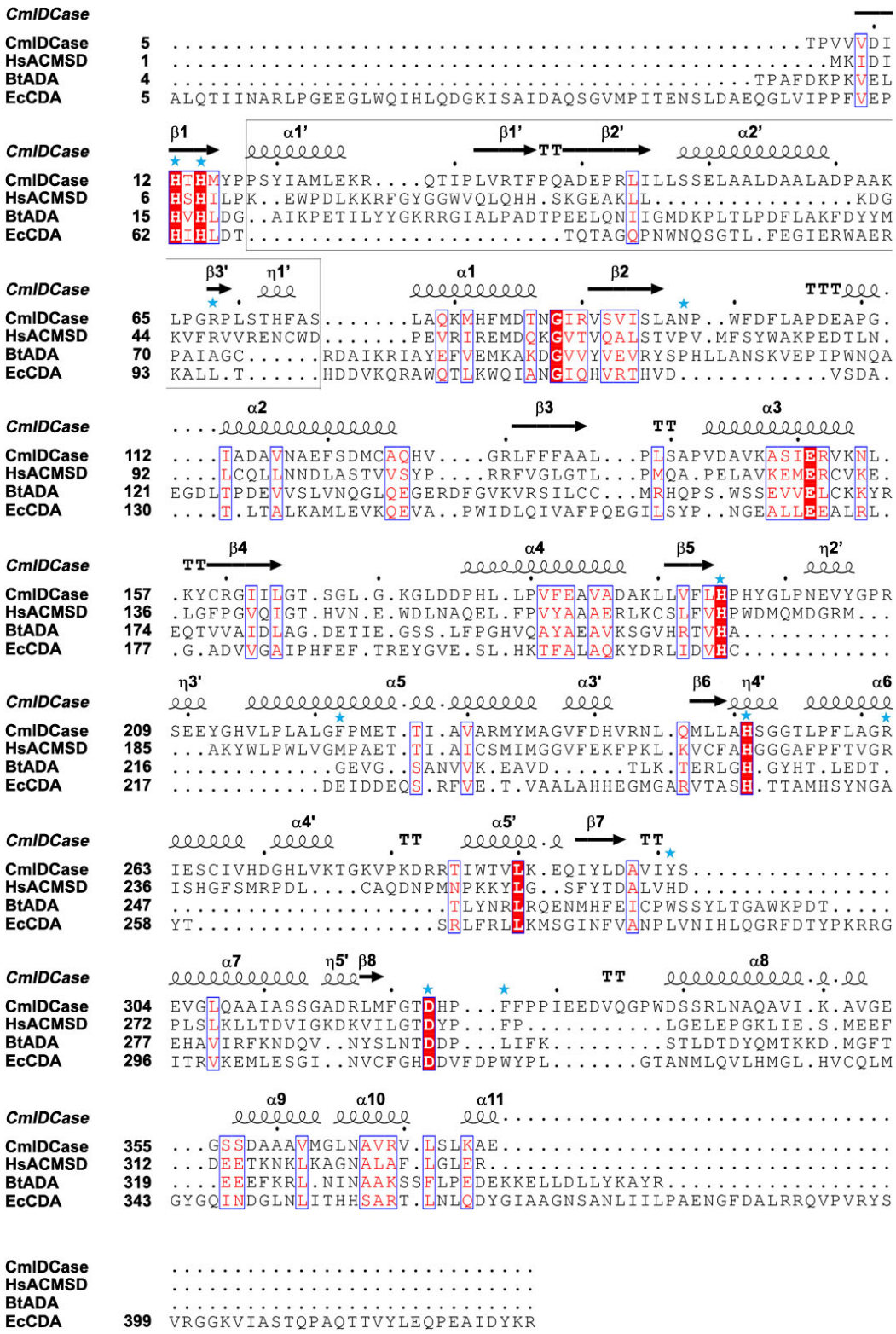
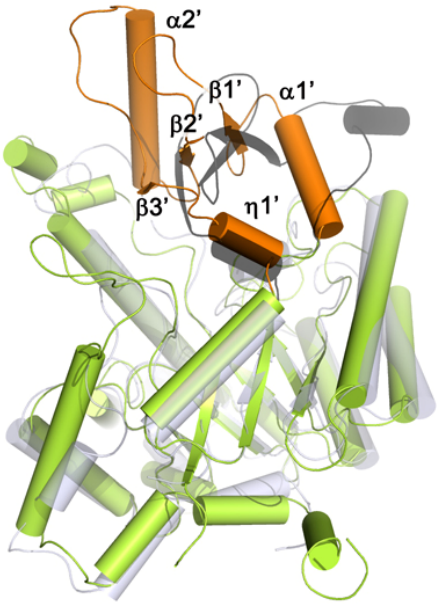
Supplementary information, Figure S8

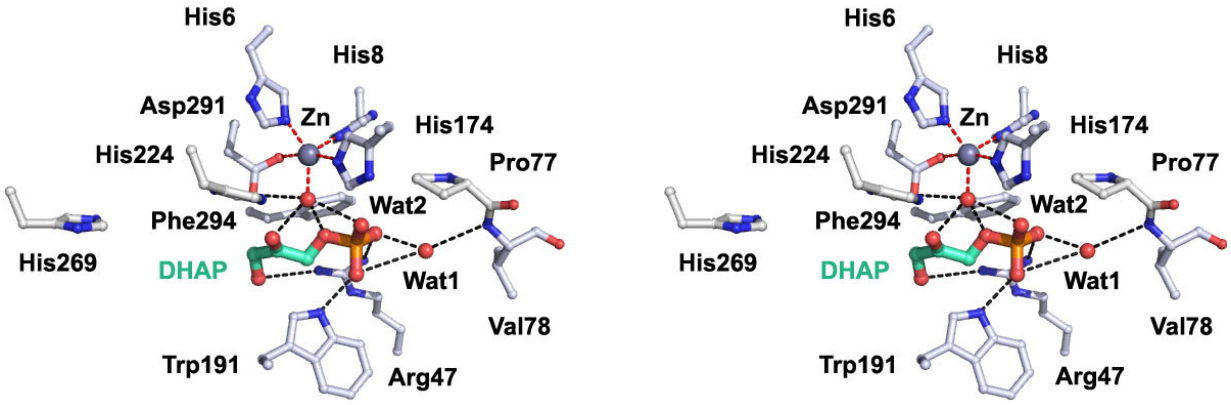
A



B



C



D

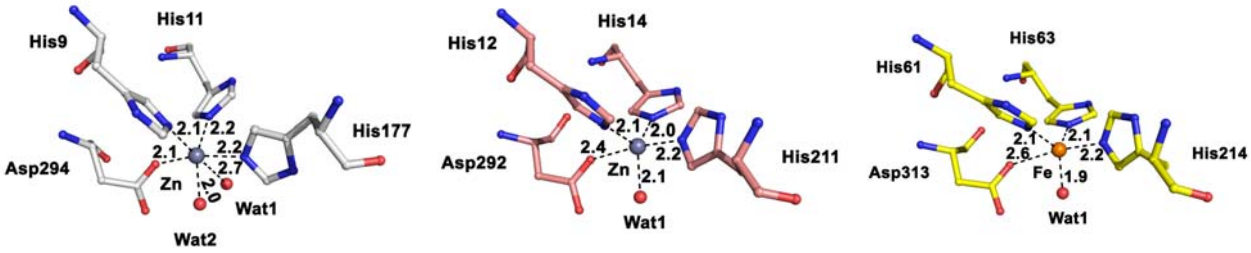


Figure S8 Comparison of CmIDCase with members of the $(\beta/\alpha)_8$ barrel-containing amidohydrolase

superfamily. **(A)** Structure-based sequence alignment of CmIDCase and several representative members of the $(\beta/\alpha)_8$ barrel-containing amidohydrolase superfamily. The abbreviations used are as follows: CmIDCase, *C. militaris* IDCase; HsACMSD, *H. sapiens* ACMSD; BtADA, *B. taurus* adenosine deaminase; and EcCDA, *E. coli* cytosine deaminase. The structure alignment of the apo CmIDCase, the HsACMSD-DHAP complex (PDB code 2WM1), the apo BtADA (PDB code 1VFL), and the apo EcCDA (PDB code 1K6W) was performed using the Dali server (http://ekhidna.biocenter.helsinki.fi/dali_server). The secondary structures of CmIDCase are placed on the top of the alignment. The key residues of CmIDCase involved in the catalysis, the metal binding, and the substrate binding are marked with blue asterisks. The insertion domains (boxed) in these proteins show notable differences in both sequence and structure. **(B)** Structural comparison of the apo CmIDCase and the HsACMSD-DHAP complex. Superposition was based on the $(\beta/\alpha)_8$ barrel domain. The insertion domain of CmIDCase is colored in orange and the other regions in green. The insertion domain of HsACMSD is colored in dark gray and the other regions in light gray. For clarity, only the secondary structures of the insertion domain in CmIDCase are labeled. **(C)** A stereoview of the **s**tructure of the active site in the HsACMSD-DHAP complex showing the interactions of the Zn^{2+} and the ligand with the surrounding residues. **(D)** Structure of the metal-binding site in the structures of the apo *Pseudomonas fluorescens* ACMSD (PDB code 2HBV) (top panel), the apo BtADA (middle panel), and the apo EcCDA (bottom panel). The coordinating residues are shown in ball-and-stick models. The coordination bonds between the metal ion and the ligands are indicated with dashed lines and bond lengths (Å). Zn^{2+}, Fe^{2+}, and the water molecules are shown with gray, orange, and red spheres, respectively.