



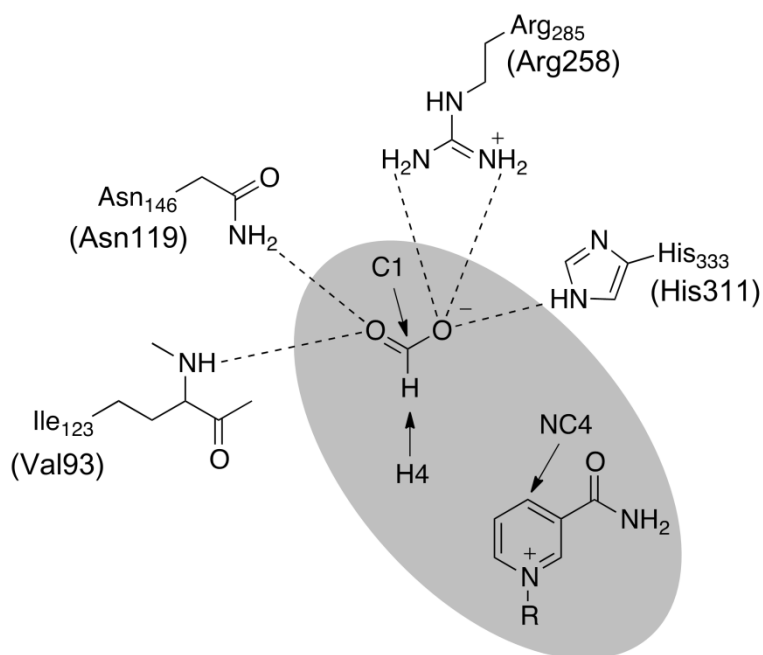
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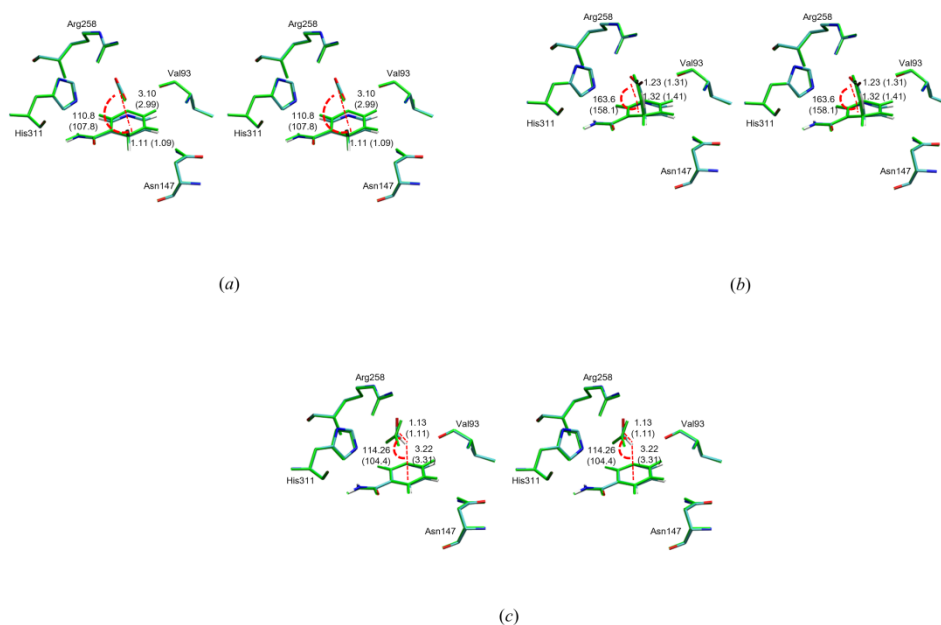
**Supporting information for article:**

**Structural insights into the efficient CO<sub>2</sub>-reducing activity of an NAD-dependent formate dehydrogenase from *Thiobacillus* sp. KNK65MA**

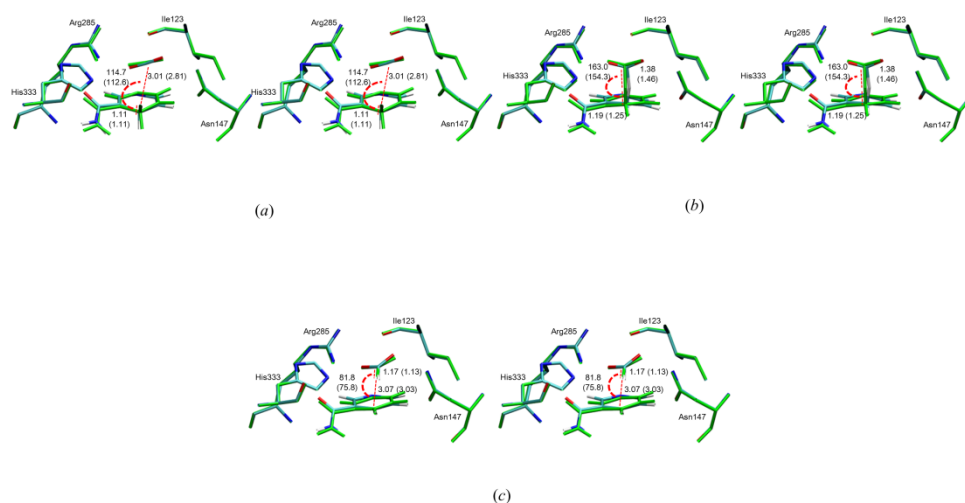
**Hyunjun Choe, Jung Min Ha, Jeong Chan Joo, Hyunook Kim, Hye-Jin Yoon, Seonghoon Kim, Sang Hyeon Son, Robert M. Gengan, Seung Taeg Jeon, Rakwoo Chang, Kwang Deog Jung, Yong Hwan Kim and Hyung Ho Lee**



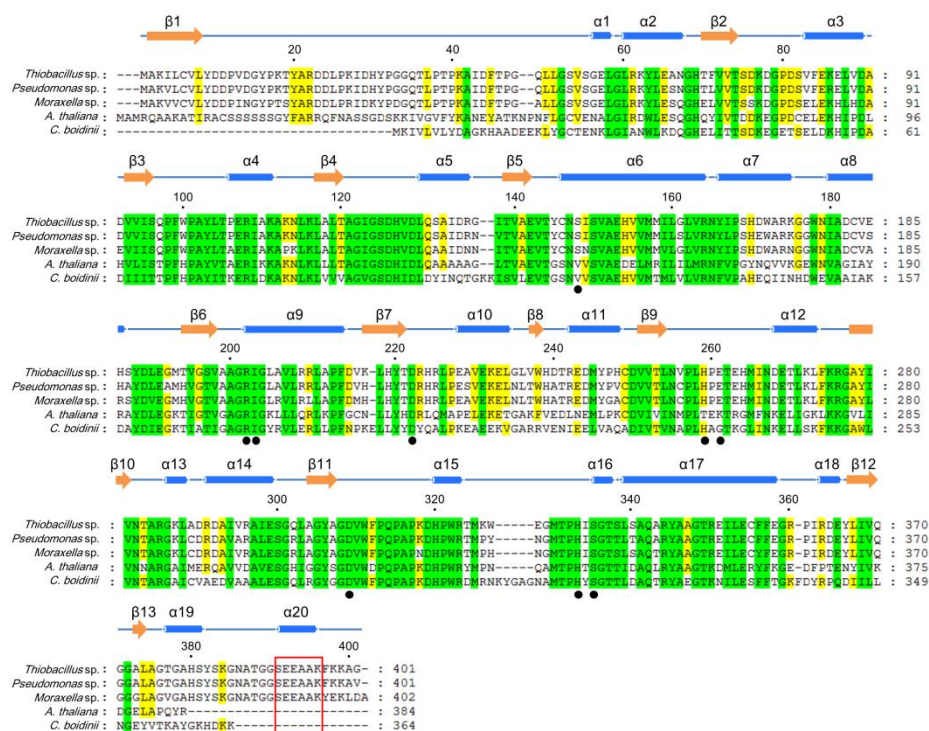
**Figure S1** QM region setup for the active site of TsFDH. The corresponding residues of CbFDH are given in parentheses.



**Figure S2** Optimized geometries (stereo) of the active site of CbFDH for the  $\text{CO}_2 \rightarrow$  formate conversion: (a) reactant, (b) transition, and (c) product states. Colored stick models represent the structures optimized with SCC-DFTB and geometries with green color correspond to those optimized with B3LYP/6-31+G(2d,2p). Some important bond lengths and angles are also shown for structures optimized by SCC-DFTB and B3LYP/6-31+G(2d,2p) (in parentheses).



**Figure S3** Optimized geometries (stereo) of the active site of TsFDH for the  $\text{CO}_2 \rightarrow$  formate conversion: (a) reactant, (b) transition, and (c) product states. Colored stick models represent the structures optimized with SCC-DFTB and geometries with green color correspond to those optimized with B3LYP/6-31+G(2d,2p). Some important bond lengths and angles are also shown for structures optimized by SCC-DFTB and B3LYP/6-31+G(2d,2p) (in parentheses). It is noted that Asn119 in these snapshots are hidden by NAD.



**Figure S4** Multiple sequence alignment of FDHs. TsFDH (UniProtKB/Swiss-Prot accession number Q76EB7) was aligned with PsFDH (UniProtKB/Swiss-Prot accession number P33160), MsFDH (UniProtKB/Swiss-Prot accession number O08375), AtFDH (UniProtKB/Swiss-Prot accession number Q9S7E4), and CbFDH (UniProtKB/Swiss-Prot accession number O13437). Residues that interact with NAD<sup>+</sup> are marked with black dots. Secondary structure elements of TsFDH assigned by PyMOL are indicated above the sequences. Residues that are strictly conserved and partially conserved among these species are shown in green and yellow, respectively. The figure was drawn with *ClustalX* (Larkin *et al.*, 2007) and *GeneDoc* (Nicholas *et al.*, 1997).