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Supporting information for article:

Structure and functional properties of the cold-adapted catalase from *Acinetobacter* sp. Ver3 native to the Atacama plateau in northern Argentina

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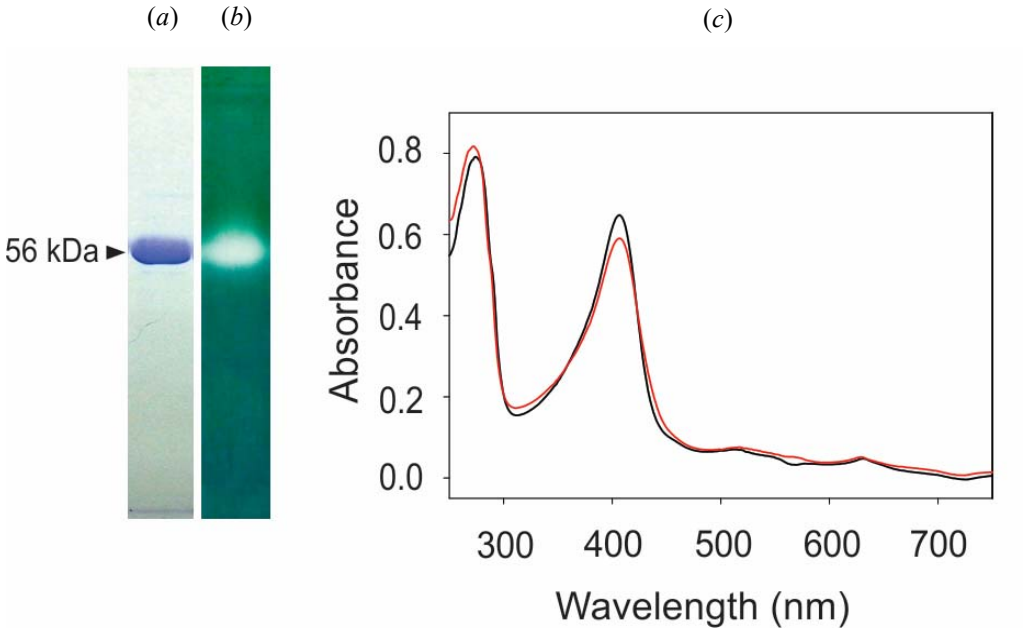

Figure S1 Purification of KatE1. (*a*) SDS-PAGE of purified KatE1. (*b*) Catalase activity staining of KatE1 after non-denaturing PAGE. (*c*) Absorption spectrum of purified KatE1 in the absence (black) or presence (red) of 10 mM sodium dithionite.

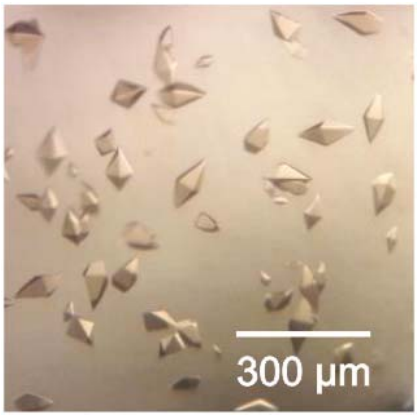

Figure S2 KatE1 crystals.

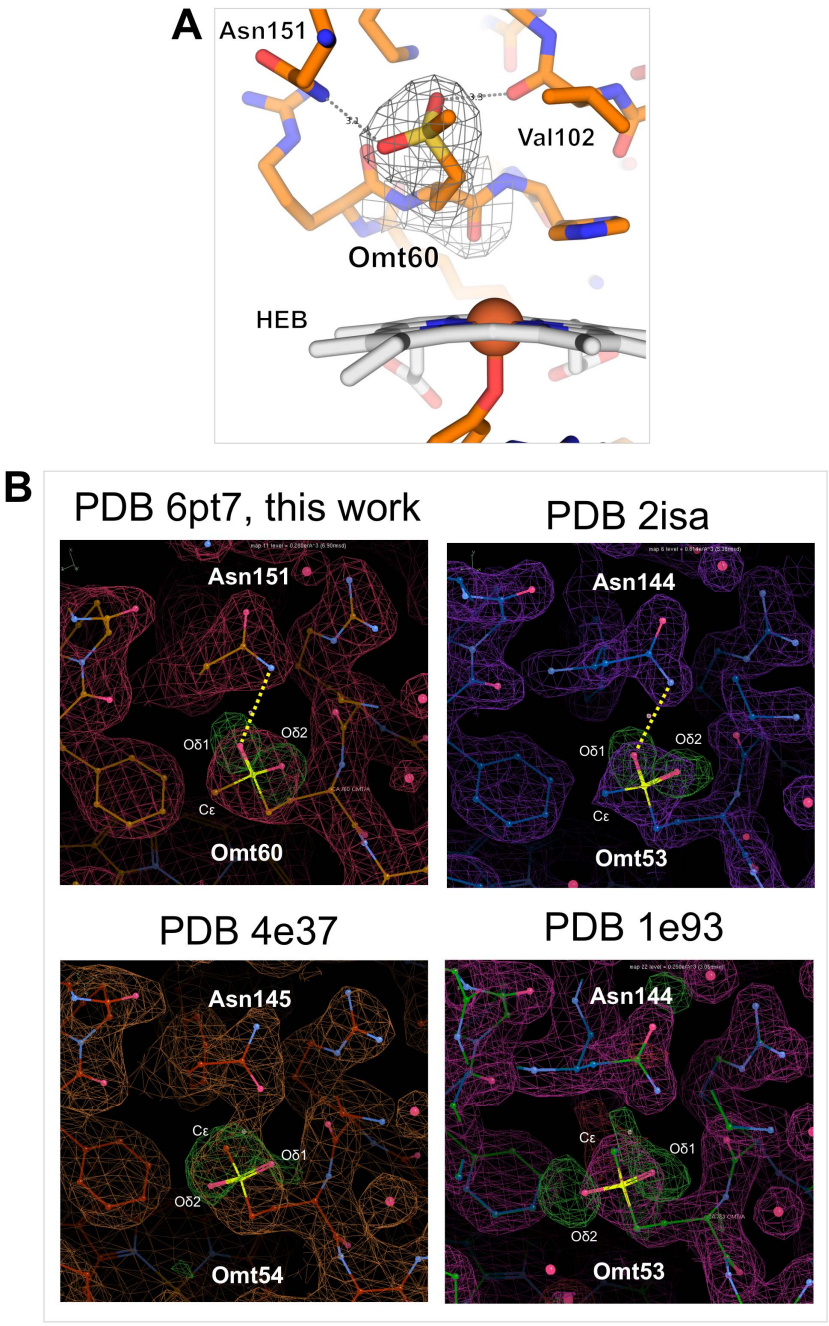

Figure S3 (A) Electron density around residue Met60 of KatE1 structure, PDB 6pt7 (Fourier $2F_O - F_C$ map, contoured at 1.0 σ). (B) Simple difference Omit maps (obtained after one refinement cycle using Met instead of Omt) for catalases from *Acinetobacter* Ver3 (PDB 6pt7, this work), *Vibrio salmonicida* (PDB 2isa), *Pseudomonas aeruginosa* (PDB 4e37), and *Proteus mirabilis* (PDB 1e93). Note that the conformation of Omt for optimal H-bonding (dotted yellow lines) with the indicated Asn residue has been refined in structures PDB 6pt7 (this work) and PDB 2isa. Experimental data for structures 1e93, 4e37 and 2isa were obtained from PDB REDO (https://pdb-redo.eu/).

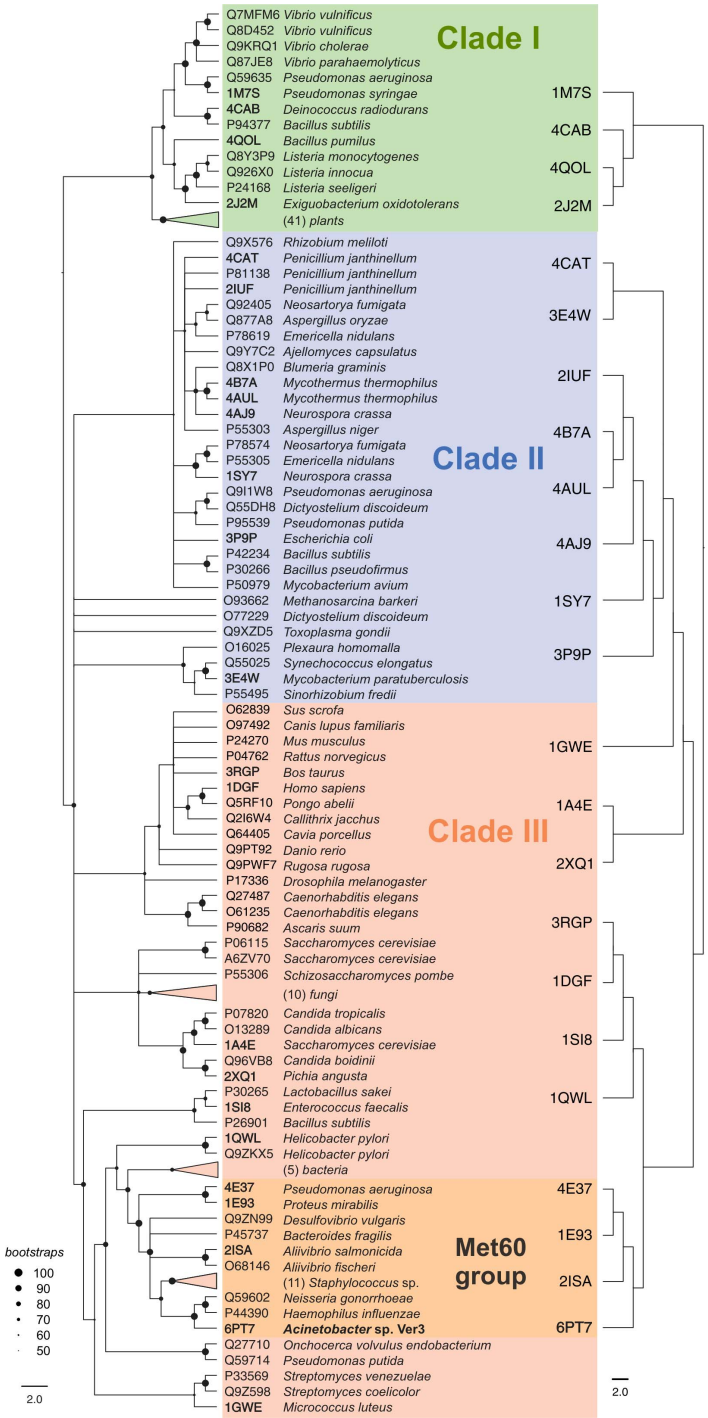

Figure S4 Cladistic and structural comparison of 152 heme catalases. Both the maximum-likelihood bootstrapped cladogram (*left*) and structural DALI *Z*-score distance phenogram (*right*) were reordered by tanglegram calculation of midpoint-rooted trees in order to match equivalent clades. Taxa are identified by their corresponding UniProt or PDB database entries, when available. Clades I, II and III in the tanglegram were defined according to literature assignments of PDB entries, and by extrapolating the structural phenogram topology onto the cladogram.

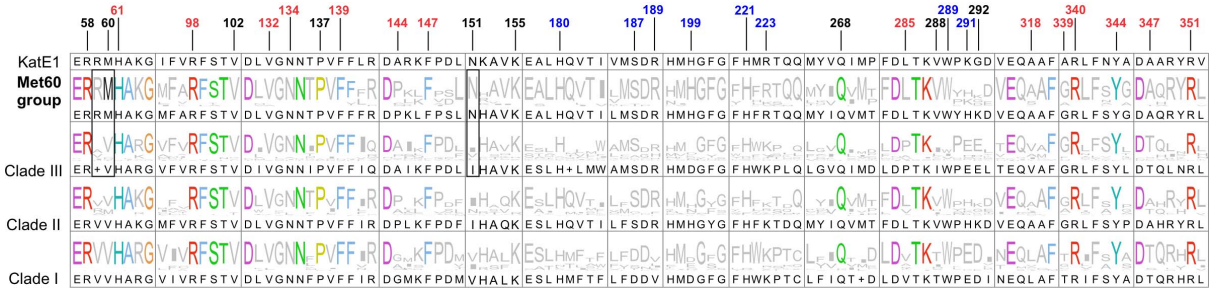

Figure S5 Multiple sequence alignment of the 152 heme catalases used for cladogram calculation, expressed as consensus sequences, highlighting clades I, II, III, and the Met60 group (also part of clade III), according to the tanglegram. Amino acid numbering corresponds to the sequence of KatE1, indicated on top. Residues involved in HEB and NADP binding are indicated by *red* and *blue* numbers, respectively. Black boxes highlight conserved residues in the Met60 group.

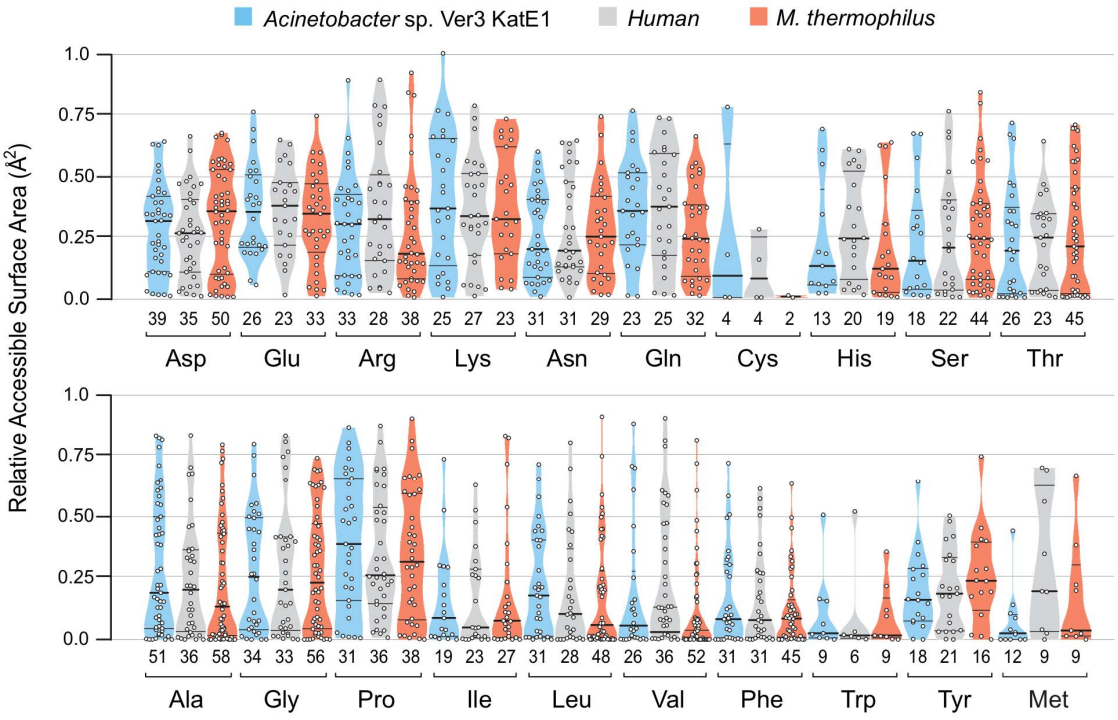

Figure S6 Dot density plots of relative accessible solvent area (RASA) of all amino acid residues in crystallographic structures of cold-adapted *Acinetobacter* sp. Ver3 KatE1 (PDB 6pt7, 53.0 kDa, *blue*), mesophilic human erythrocyte catalase (PDB 1dgf, 56.5 kDa, *green*), and *Mycothermus thermophilus* catalase phenol oxidase (PDB 4aum, 79.2 kDa, *red*), the only thermophilic catalase with available experimentally determined structure.