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Supporting information for article:

Structure of α-carbonic anhydrase from the human pathogen *Helicobacter pylori*

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Table S1 List of bacteria and archea whose CA crystal structure is known.

The third column refers to the number of files present in the PDB.

	Type	Number of structures	Ligands or variants
Bacteria			
Escherichia coli	β, γ	6	Bicarbonate, MSE
Chlostridium difficile	γ	1	
Halothiobcillus neapolitanus	β	1	
Haemophilus inlueanzae	β	14	Co substituted, bicarbonate,, Y181F, V47A, G41A, D44N, W39F
Micobacterium tubercolosis	β	2	Thiocyanate ion
Neisseria gonorreae	α	2	
Salmonella enterica	β	1	
Streptococcus mutans	?	1	
Sulfurihydrogenibium yellostonense	α	1	AZM
Thermosynecoccus elongatus	γ	3	
Thermovibrio ammonificans	α	3	Sulfanilamide, AZM, B3P
Archea			
Methanobacterium thermoautotrophicum	β	1	
Methanosarcina thermophila	γ	12	W19A, W19F, W19N, Y200A, Co substituted, bicarbonate

Table S2 Residues forming H-bonds at the interface between monomers A and B

Interactions mediated by water molecules are not taken into account.

Chain B	Chain A	Distance (Å)
Thr62 Oγ1	His61 O	2.67
Asn236 Nδ2	Tyr104 OH	2.92
Val238 N	Asn187 Oδ1	2.83
Arg183 NH1	Asp234 O	2.92
Asn187 Nδ2	Asn236 O	2.84
Arg100 NH2	Thr237 O	3.00
Asp64 Oδ1	His61 Nδ1	3.29
Asp64 Oδ2	His61 Nδ1	3.00
Asp64 Oδ2	His61 N	2.96
Asp67 Oδ2	His58 Nε2	2.79
Asp67 Oδ2	Tyr60 OH	2.58
Tyr104 OH	Asn236 Nδ2	2.95
Asn187 Oδ1	Val238 N	2.75
Asn236 O	Asn187 Nδ2	2.83
Thr237 O	Arg100 NH2	3.01
Asp64 Oδ1	His61 Nδ1	3.29
Asp64 Oδ2	His61 Nδ1	3.00
Asp67 Oδ2	His58 Nε2	2.79

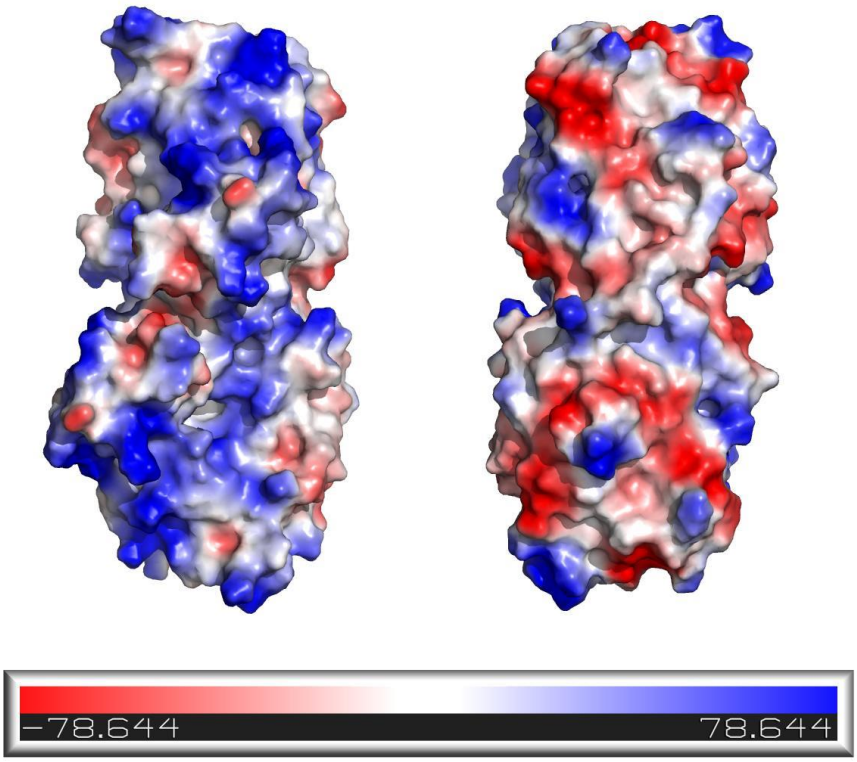

Figure S1 Qualitative electrostatic surface of HpαCA dimer. The face of the enzyme that presents the two openings of the active site cavity is on the left. The right pictures is rotated 180°. The image shows that also in the dimer, as happens in the monomer, one face is mostly positively charged, whilst in the opposite face negative charges are prevalent.