

Supporting Information

Role of Hydrophilic Residues in Proton Transfer

During Catalysis by Human Carbonic Anhydrase II

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Contents: Two pages total containing two tables. Table SI1 contains the dihedral angles of three residues in the active-site cavity of wild-type HCA II and the variants N62A,V,D,T. Table SI2 contains the B factors for the ordered water molecules in the active-site cavity of the same variants.

Table SI1. Dihedral angles (°) for the side chains of three residues in the active-site cavity of five variants of HCA II.

	N62A	N62V	N62D	N62T	Wild type ^a
His 64 χ_1	49 ^b	51 ^b	-56 ^c	50/-45 ^d	44/-39 ^d
His 64 χ_2	89 ^b	91 ^b	111 ^c	82/99 ^d	95/98 ^d
Asn 67 χ_1	-54	-67	-55	-69	-79
Asn 67 χ_2	151	173	145	177	-178
Gln 92 χ_1	63	56	63	55	53
Gln 92 χ_2	108	103	108	104	106
Gln 92 χ_3	-51	-32	-64	-31	-31

^a Data from the Protein Data Bank, accession code 2CBA. ^bInward conformation. ^cOutward conformation. ^d Inward and outward orientations.

Table SI2. B-factors (\AA^2) for the ordered water molecules in the active-site cavity of HCA II and variants.

	Wild type ^a	N62A	N62V	N62T	N62D	Mean / Std.Dev
Zn	7.8	11.9	9.5	6.8	9.3	9.06 / 1.9
Zn-OH	8.3	17.2	12.4	8.0	10.0	11.18 / 3.7
W1	17.7	21.1	18.4	14.0	15.2	17.28 / 2.7
W2	19.1	26.0	21.1	20.2	20.2	21.32 / 2.7
W3a	15.5	26.4	18.7	16.5	16.0	18.62 / 4.5
W3b	17.5	30.2	24.4	26.8	22.6	24.3 / 4.7

^aData from the Protein Data Bank, accession code 2CBA.