



BIOLOGICAL
CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

Structural and functional analysis of betaine aldehyde dehydrogenase from *Staphylococcus aureus*

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Table S1. Changes in pKa values of some residues of the NAD- and substrate-binding sites.

Residue ^a	Wild-type				G234S mutant				model pKa
	4mpb	4mpy	4nu9	4nea	4qto	4qje	4q92	4qn2	
		NAD ⁺		NAD ⁺				NAD ⁺	
Asp111	7.44	6.83	7.02	8.49	6.76	6.46	6.72	6.59	3.80
Tyr158	16.85	16.22	14.42	15.86	15.70	15.76	17.09	16.61	10.00
Lys166	10.16	9.84	10.00	10.32	9.99	10.03	10.05		
Lys180	8.71	8.48	8.88	8.92	8.60	8.42	8.49	8.75	10.50
Asp218	3.00	3.30	2.98	3.26	2.71	2.93	3.16	3.18	3.80
Glu255	7.34	4.01	6.09	3.87	7.69	8.48	8.03	8.95	4.50
Cys289	N/A	N/A	13.43	14.70	N/A	N/A	N/A	14.14	9.00
Lys339	10.45	8.73	10.91	10.84	10.03	10.19	9.92	10.44	10.50
Glu390	7.01	6.77	4.81	7.92	7.77	7.26	5.58	4.97	4.50
His448	4.37	4.43	4.44	3.66	4.14	4.50	4.23	4.38	6.50
Tyr450	15.17	14.74	15.90	17.34	10.09	15.16	14.94	15.41	10.00
Glu467	4.77	4.97	4.72	4.86	4.82	4.82	4.41	5.26	4.50
NAD									
N7A	N/A	3.73	N/A	3.87	N/A	N/A	N/A	3.72	5.00
O1A	N/A	6.56	N/A	7.57	N/A	N/A	N/A	7.25	6.00
O2N	N/A	7.90	N/A	7.69	N/A	N/A	N/A	8.61	6.00
pH of a protein sample				8.3					
pH of crystallization	8.5	8.5	8.5	N/A	3.5	8.0	8.0	8.5	

^aChain A of each PDB entry was used only.

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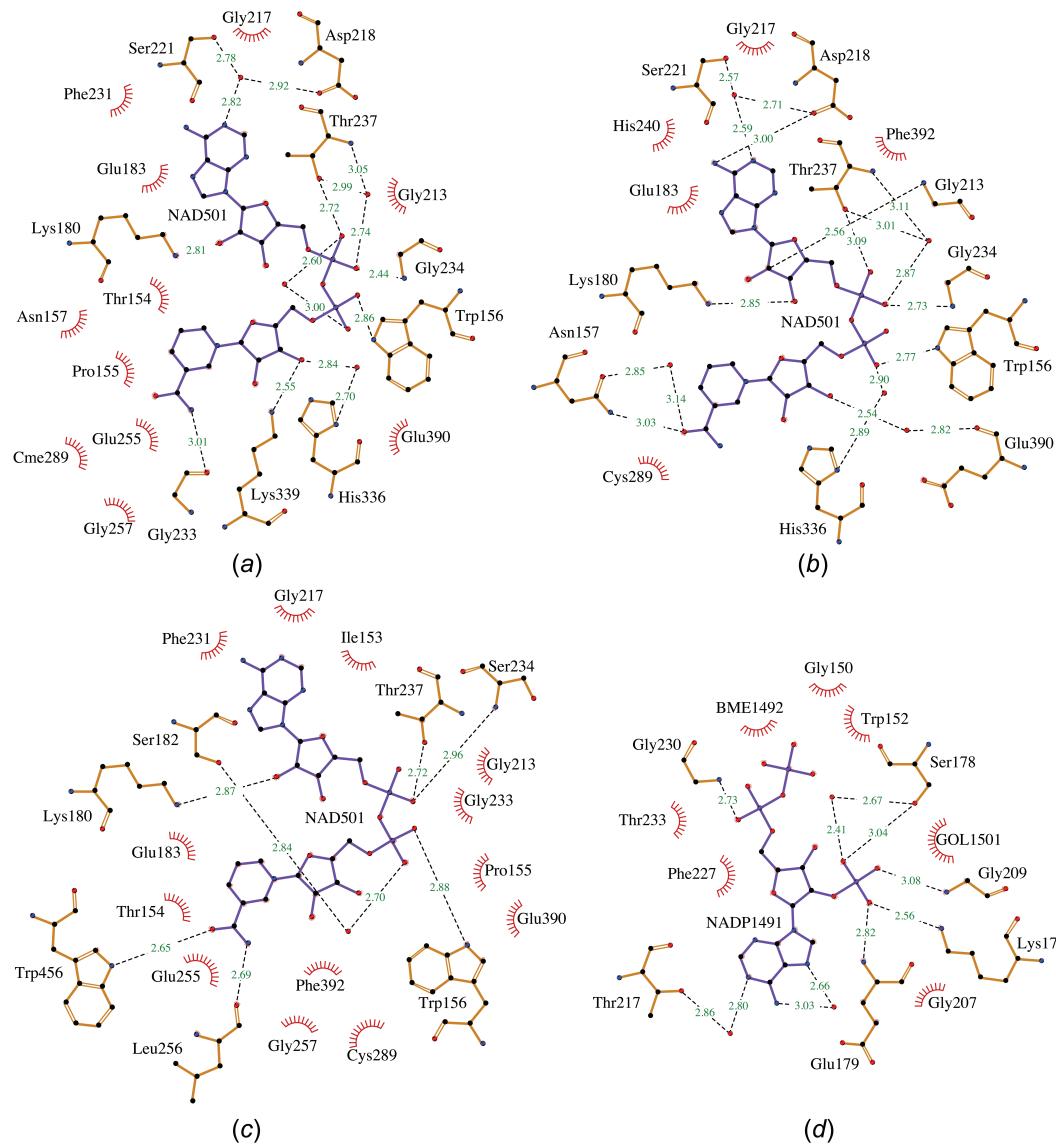


Figure S1. Details of the NAD–SaBADH interactions in NAD–SaBADH^{BME(-)} (a), NAD–SaBADH^{BME(+)} (b) and NAD–G234S–SaBADH^{BME(+)} (c). (d) Coordination of NADP⁺ in the PaBADH structure (PDB entry 2wme). The NMN moiety was not modelled

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in the 2wme structure and, thus, is not displayed. BME – β -mercaptoethanol; GOL – glycerol. Cme289 is BME-modified Cys289. Water molecules are red spheres.