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Supporting information for article:

Structure of glyoxysomal malate dehydrogenase (MDH3) from *Saccharomyces cerevisiae*

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Table S1 MDH sequences from UniProtKB (<http://www.uniprot.org/uniprot/>)

No .	Abbreviation	Organism	ID	Protein	Gene	Length
1	MDH3	<i>Saccharomyces cerevisiae</i>	P32419	Malate dehydrogenase , peroxisomal	MDH3	343
2	MDH1	<i>Saccharomyces cerevisiae</i>	P17505	Malate dehydrogenase , mitochondrial	MDH1	334
3	MDH2	<i>Saccharomyces cerevisiae</i>	P22133	Malate dehydrogenase , cytoplasmic	MDH2	377
4	Ca_cMDH	<i>Candida albicans</i>	P83778	Malate dehydrogenase , cytoplasmic	MDH1	337
5	Sp_mMDH	<i>Schizosaccharomyces pombe</i>	Q9Y7R8	Malate dehydrogenase , mitochondrial	MDH1	341
6	Zm_cMDH	<i>Zea mays (Maize)</i>	Q08062	Malate dehydrogenase , cytoplasmic	N/A	332
7	At_mMDH1	<i>Arabidopsis thaliana</i>	Q9ZP06	Malate dehydrogenase 1, mitochondrial	At1g53240	341
8	At_mMDH2	<i>Arabidopsis thaliana</i>	Q9LKA3	Malate dehydrogenase 2, mitochondrial	At3g15020	341
9	At_cMDH1	<i>Arabidopsis thaliana</i>	P93819	Malate dehydrogenase 1, cytoplasmic	MDH1	332
10	At_cMDH2	<i>Arabidopsis thaliana</i>	P57106	Malate dehydrogenase 2, cytoplasmic	MDH2	332
11	At_cMDH3	<i>Arabidopsis thaliana</i>	Q9FJU0	Malate dehydrogenase 3, cytoplasmic	MDH3	339
12	At_pMDH1	<i>Arabidopsis thaliana</i>	O82399	Malate dehydrogenase 1, peroxisomal	PMDH1	354
13	At_pMDH2	<i>Arabidopsis thaliana</i>	Q9ZP05	Malate dehydrogenase 2, peroxisomal	PMDH2	354
14	Cl_mMDH	<i>Citrullus lanatus (Watermelon)</i>	P17783	Malate dehydrogenase , mitochondrial	MMDH	347
15	Cl_gMDH	<i>Citrullus lanatus (Watermelon)</i>	P19446	Malate dehydrogenase , glyoxysomal	N/A	356

16	Os_cMDH	<i>Oryza sativa</i> (<i>Rice</i>)	Q7XDC8	Malate dehydrogenase , cytoplasmic	Os10g0478200	332
17	Os_gMDH	<i>Oryza sativa</i> (<i>Rice</i>)	Q42972	Malate dehydrogenase , glyoxysomal	Os12g0632700	356
18	Gm_gMDH	<i>Glycine max</i> (<i>Soybean</i>)	P37228	Malate dehydrogenase , glyoxysomal	N/A	353
19	Fa_mMDH	<i>Fragaria ananassa</i> (<i>Strawberry</i>)	P83373	Malate dehydrogenase , mitochondrial	MMDHI	339
20	Bn_mMDH	<i>Brassica napus</i> (<i>Rape</i>)	Q43744	Malate dehydrogenase , mitochondrial	MDH	341
21	Bn_gMDH	<i>Brassica napus</i> (<i>Rape</i>)	Q43743	Malate dehydrogenase 1, glyoxysomal	MDH1	358
22	Cs_gMDH	<i>Cucumis sativus</i> (<i>Cucumber</i>)	P46488	Malate dehydrogenase , glyoxysomal	MDHG	356
23	Eg_mMDH	<i>Eucalyptus gunnii</i> (<i>Cider gum</i>)	P46487	Malate dehydrogenase , mitochondrial	MDH	347
24	Mc_cMDH	<i>Mesembryanthemum crystallinum</i> (<i>Common ice plant</i>)	O24047	Malate dehydrogenase , cytoplasmic	MDH	332
25	Bv_cMDH	<i>Beta vulgaris</i> (<i>Sugar beet</i>)	Q9SML8	Malate dehydrogenase , cytoplasmic	NR1	332
26	Ms_cMDH	<i>Medicago sativa</i> (<i>Alfalfa</i>)	O48905	Malate dehydrogenase , cytoplasmic	CMDH	332
27	Hs_mMDH	<i>Homo sapiens</i> (<i>Human</i>)	P40926	Malate dehydrogenase , mitochondrial	MDH2	338
28	Hs_cMDH	<i>Homo sapiens</i> (<i>Human</i>)	P40925	Malate dehydrogenase , cytoplasmic	MDH1	334
29	Pa_mMDH	<i>Pongo abelii</i> (<i>Sumatran orangutan</i>)	Q5NVR2	Malate dehydrogenase , mitochondrial	MDH2	338
30	Mf_mMDH	<i>Macaca fascicularis</i> (<i>Crab-eating macaque</i>)	Q4R568	Malate dehydrogenase , mitochondrial	MDH2	338
31	Ss_mMDH	<i>Sus scrofa</i> (<i>Pig</i>)	P00346	Malate dehydrogenase , mitochondrial	MDH2	338
32	Ss_cMDH	<i>Sus scrofa</i> (<i>Pig</i>)	P11708	Malate dehydrogenase , cytoplasmic	MDH1	334

33	Mm_mMDH	<i>Mus musculus</i> (Mouse)	P08249	Malate dehydrogenase, mitochondrial	Mdh2	338
34	Mm_cMDH	<i>Mus musculus</i> (Mouse)	P14152	Malate dehydrogenase, cytoplasmic	Mdh1	334
35	Bt_mMDH	<i>Bos Taurus</i> (Bovine)	Q32LG3	Malate dehydrogenase, mitochondrial	MDH2	338
36	Bt_cMDH	<i>Bos Taurus</i> (Bovine)	Q3T145	Malate dehydrogenase, cytoplasmic	MDH1	334
37	Rn_mMDH	<i>Rattus norvegicus</i> (Rat)	P04636	Malate dehydrogenase, mitochondrial	Mdh2	338
38	Rn_cMDH	<i>Rattus norvegicus</i> (Rat)	O88989	Malate dehydrogenase, cytoplasmic	Mdh1	334
39	Fc_mMDH	<i>Felis catus</i> (Cat)	K0J107	Malate dehydrogenase, mitochondrial	MDH2	338
40	Fc_cMDH	<i>Felis catus</i> (Cat)	Q7YRU4	Malate dehydrogenase, cytoplasmic	MDH1	334
41	Gg_cMDH	<i>Gallus gallus</i> (Chicken)	Q5ZME2	Malate dehydrogenase, cytoplasmic	MDH1	334
42	Xt_cMDH	<i>Xenopus tropicalis</i> (Western clawed frog)	Q6DIY9	Malate dehydrogenase, cytoplasmic	mdh1	334
43	XI_cMDH	<i>Xenopus laevis</i> (African clawed frog)	Q6PAB3	Malate dehydrogenase, cytoplasmic	mdh1	334
44	Eg_cMDH	<i>Echinococcus granulosus</i> (Hydatid tapeworm)	Q04820	Malate dehydrogenase, cytoplasmic	MDH	332

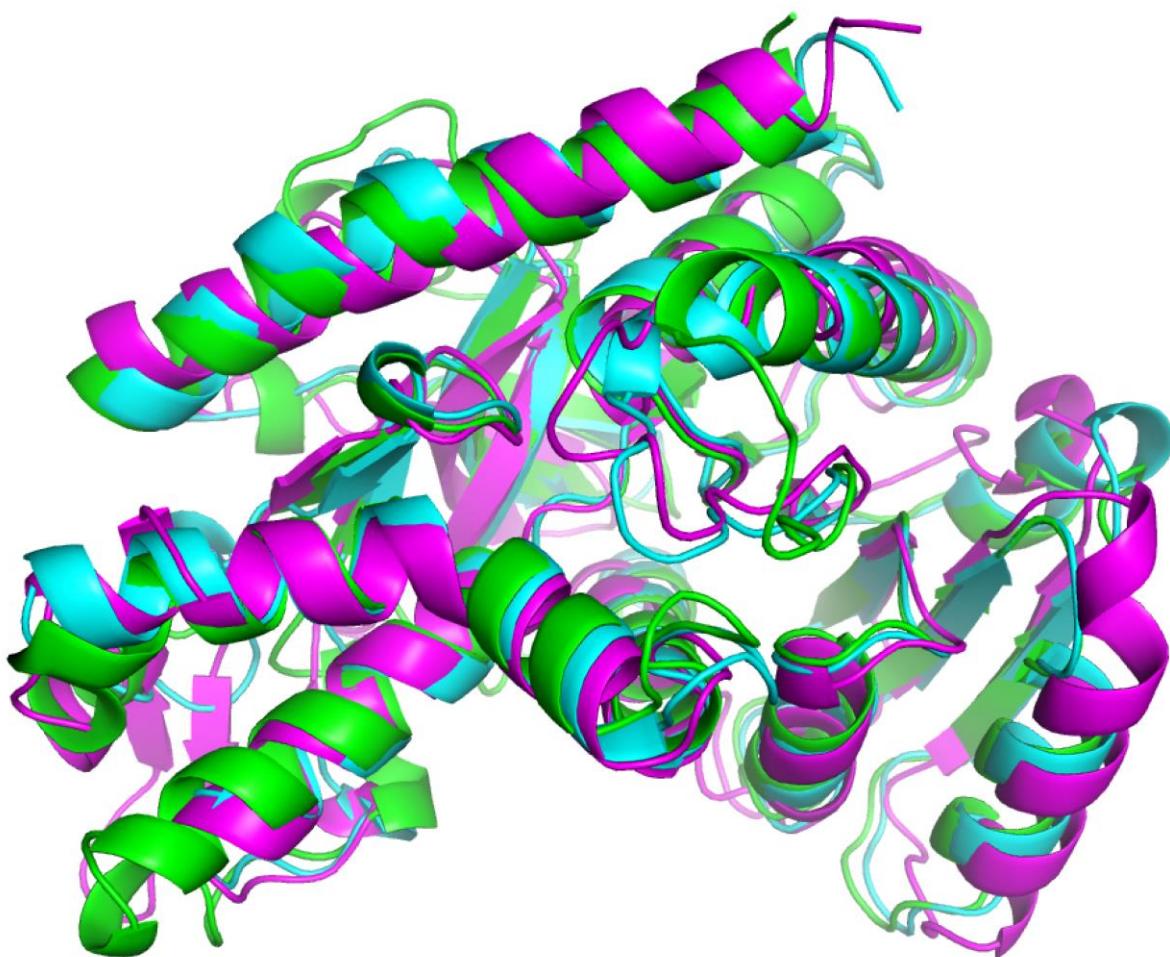


Figure S1 Comparison of yeast MDH3 (green) with porcine mitochondrial (PDB entry 1mld, cyan) and cytosolic (PDB entry 4mdh, magenta) MDHs. Structure overlay and calculation of RMSD, based on secondary structure matching, were performed using *Superpose* (Krissinel & Henrick, 2004) from the CCP4 suite.

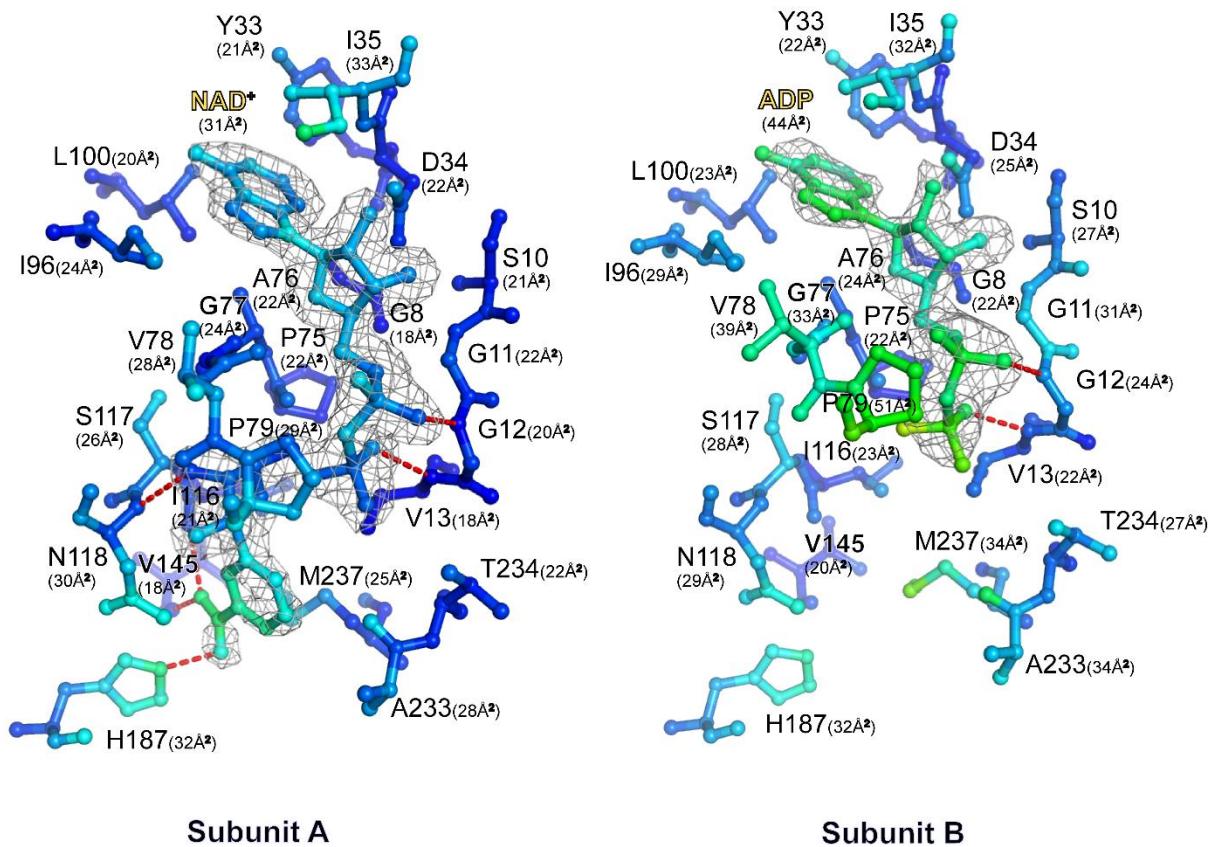
**Subunit A****Subunit B**

Figure S2 NAD⁺ and ADP were modeled with the electron density map ($F_0 - F_c$ omit map contoured at 3σ). The stick model was colored according to its temperature factor using dark blue (low B -factor) to yellow green (high B -factor). Stick model was labeled for its residue numbers and average B -factor values in parentheses.

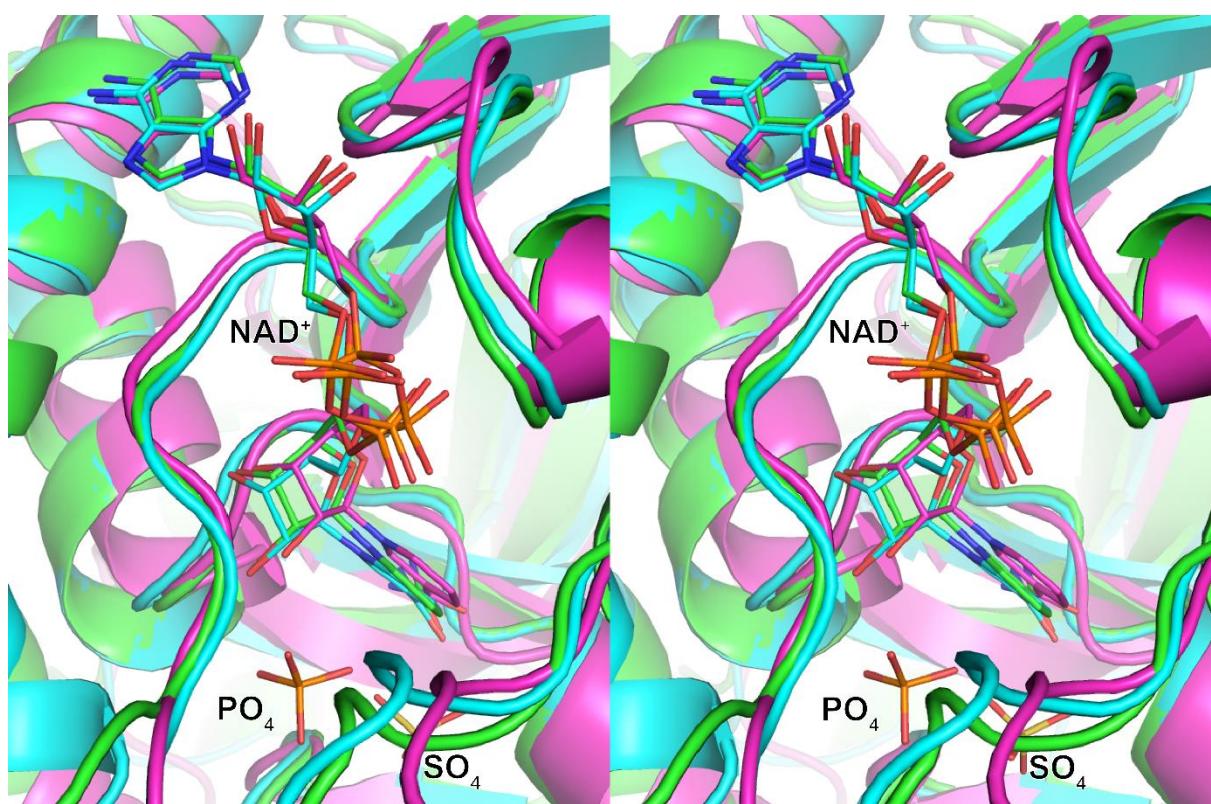


Figure S3 Comparison of NAD⁺-binding sites of the yeast MDH3 (green), human mitochondrial MDH (PDB entry 4wlv, cyan) and porcine cytosolic MDH (PDB entry 4mdh, magenta).

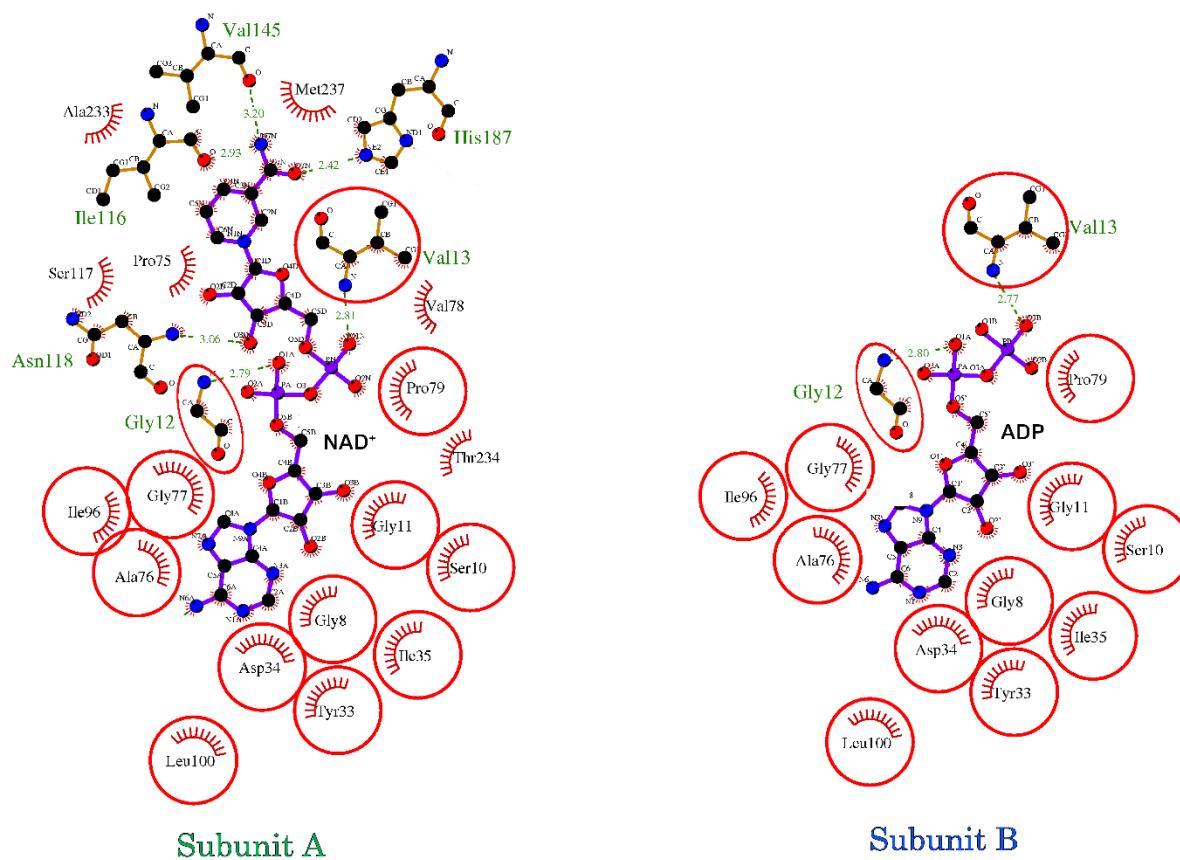


Figure S4 Schematic representation of interactions between MDH3 and cofactors. Interactions of MDH3 with NAD⁺ (left), and ADP (right) were investigated using *LIGPLOT* (Wallace *et al.*, 1995). Hydrogen bonds are indicated with dashed lines and distances, and hydrophobic interactions are represented using arcs with spokes radiating toward the ligand atoms they contact. Interacting residues conserved between subunits A (left) and B (right) are indicated in red circles.

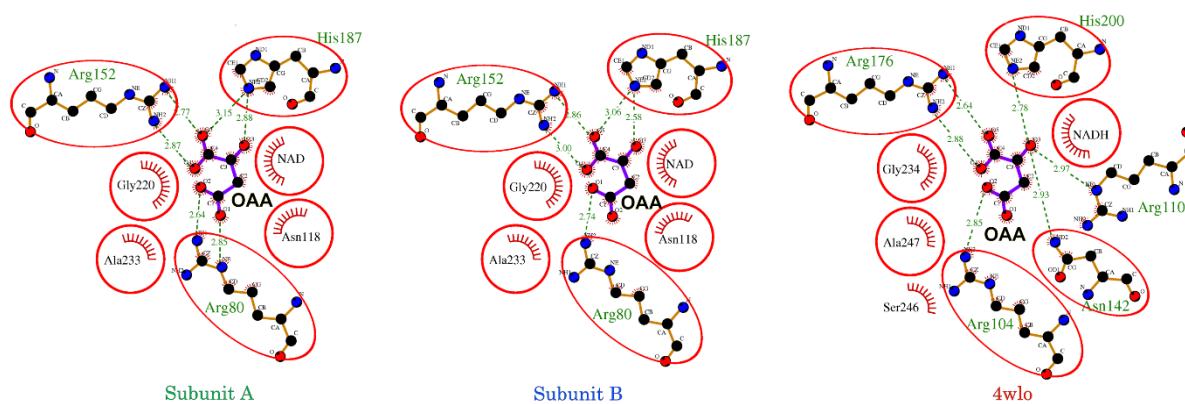


Figure S5 Comparison of the OAA binding site between subunits A and B of yeast MDH3 and human mitochondrial MDH. Hydrogen bonds are indicated with dashed lines, and hydrophobic interactions are represented using arcs with spokes radiating toward the ligand atoms they contact. Interacting residues conserved between subunits A and B of yeast MDH3 and human mitochondrial MDH are indicated in red circles.