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Supporting information for article:

Structure of *Streptococccus agalactiae* glyceraldehyde 3-phosphate dehydrogenase holoenzyme reveals a novel surface

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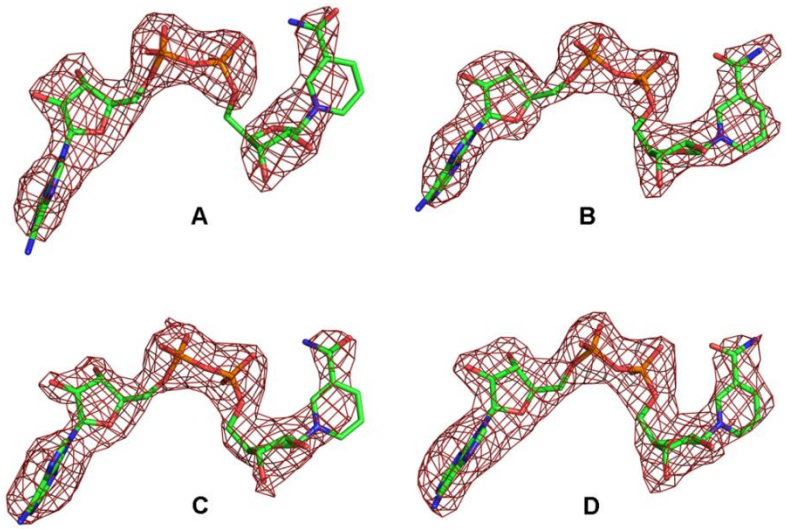

Figure S1 The figure shows the Fo-Fc omit map (3σ contour level) of NAD molecules in subunits A through D. The difference electron density is represented as a mesh in firebrick red. NAD molecules are shown as stick models (color code: C green; O red, N blue, P orange).

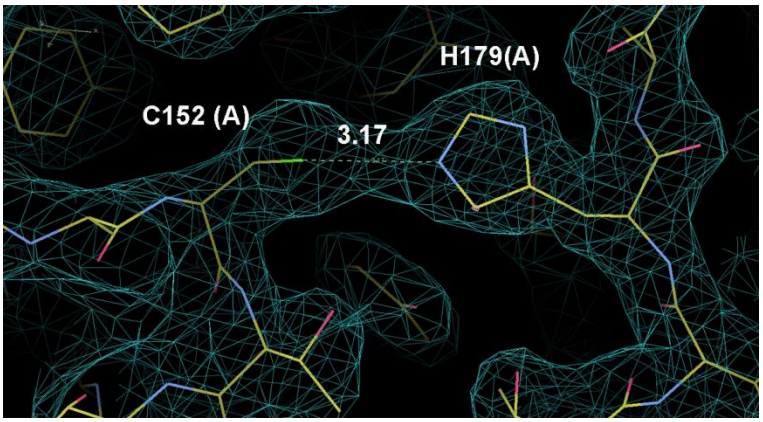

Figure S2 Hydrogen-bonding interactions between residues Cys152 and His179 in GBS GAPDH. The figure shows a screen snapshot taken in Coot displaying the GBS GAPDH coordinates and the 2Fo-Fc electron density map (1σ contour level). The electron density map is represented as a mesh in bluish green. Residues C152 and H179 are labeled and the hydrogen-bonding distance of 3.17 Å in subunit A is shown (green dashed line). Very similar distances are observed in the other subunits. Residue C152 shows only one conformation.

Table S1 Protein-NAD interactions.

NAD401: Chain A

Atom	Distance [Å]	Atom	Residue/Water	Chain
O2B	2.52	OD1	ASP34	A
O2N	2.58	O	HOH417	A
O2A	2.68	O	HOH407	A
O3D	2.71	O	HOH411	A
O2N	2.85*	N	ARG12	A
O3B	2.86	OD2	ASP34	A
O2A	2.88*	N	ARG12	A
N1A	2.89	O	HOH418	A
O2N	2.97*	N	ILE13	A
N6A	3.10*	O	ARG78	A
O4D	3.13	OG1	THR121	A
O4D	3.23	O	THR121	A
O7N	3.33*	ND2	ASN316	A
O5B	3.34	O	HOH417	A
C5A	3.44	CD1	LEU35	A
C4N	3.46	CB	CYS152	A
O3B	3.46	OD1	ASP34	A
C4A	3.49	CG2	THR97	A
C5N	3.50	CB	CYS152	A

NAD401: Chain B

Atom	Distance [Å]	Atom	Residue/Water	Chain
O2B	2.49	OD1	ASP34	B
O2N	2.73	O	HOH412	B
O3B	2.80	OD2	ASP34	B
N6A	2.82*	O	ARG78	B
O2A	2.85	O	HOH404	B
N1A	2.88	O	HOH425	B
O2A	2.93	O	HOH405	B
O2N	3.01*	N	ILE13	B
O2A	3.03*	N	ARG12	B
O2N	3.05*	N	ARG12	B
O4D	3.09*	OG1	THR121	B
O1N	3.27	O	HOH406	B
O4D	3.27	O	THR121	B
N7N	3.29	ND2	ASN316	B
O7N	3.30	O	HOH410	B
O2D	3.31	O	HOH430	B
O3B	3.37	OD1	ASP34	B

C5N	3.40	CD2	TYR320	B
C4A	3.45	CG2	THR97	B
C8A	3.49	CE2	PHE99	B

NAD401: Chain C

Atom	Distance [Å]	Atom	Residue/Water/EDO	Chain
O3D	2.32	O2	EDO402	C
O2B	2.54	OD1	ASP34	C
O2N	2.67	O	HOH410	C
O2A	2.68	O	HOH443	D
N6A	2.91*	O	ARG78	C
O2A	2.92*	N	ARG12	C
O3B	2.92	OD2	ASP34	C
O2N	3.06*	N	ARG12	C
O2N	3.14*	N	ILE13	C
O4D	3.15*	OG1	THR121	C
O7N	3.23*	ND2	ASN316	C
O4D	3.35	O	THR121	C
O3B	3.36	OD1	ASP34	C
C4A	3.40	CG2	THR97	C
O5B	3.45	O	HOH410	C
C4N	3.50	CB	CYS152	C

NAD401: Chain D

Atom	Distance [Å]	Atom	Residue/Water	Chain
O2B	2.52	OD1	ASP34	D
O2N	2.64	O	HOH408	D
O2A	2.67	O	HOH405	C
O2N	2.93*	N	ARG12	D
N1A	2.93	O	HOH422	D
N6A	2.94*	O	ARG78	D
O3B	2.96	OD2	ASP34	D
O2N	2.99*	N	ILE13	D
O4D	3.08*	OG1	THR121	D
O2A	3.10*	N	ARG12	D
N7N	3.19	ND2	ASN316	D
O4D	3.26	O	THR121	D
N7N	3.41*	O	ASN316	D
C5N	3.42	CD2	TYR320	D
O3D	3.44	O	HOH441	D

Distances up to 3.5 Å are shown.

*Hydrogen bonds with protein residues

Extracted from: Quality Control Check v3.0 (http://smb.slac.stanford.edu/jcsg/QC/); PDBePISA (https://www.ebi.ac.uk/msd-srv/prot_int/cgi-bin/piserver)