



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 05:46 PM UTC

PDB ID : 5V8Y / pdb_00005v8y
Title : Mutant Structures of Streptococcus Agalactiae GBS Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH)
Authors : Schormann, N.; Ulett, G.C.; Chattopadhyay, D.
Deposited on : 2017-03-22
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

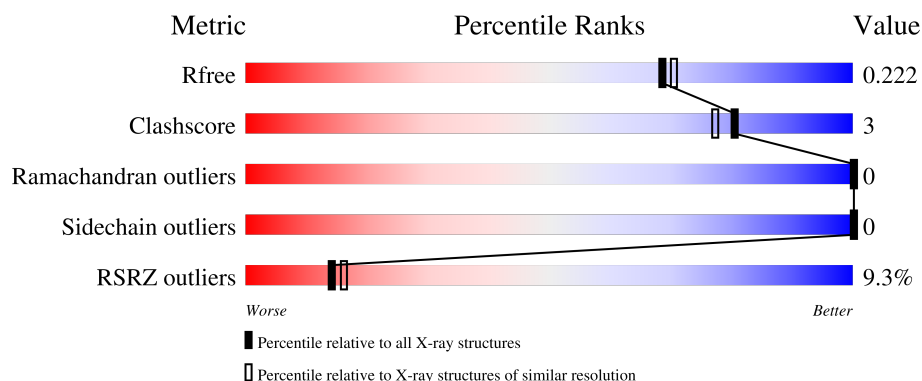
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	355	11% 84% 9% 7%
1	B	355	6% 92% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5472 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2478	1544	431	495	8			
1	B	335	Total	C	N	O	S	0	2	0
			2540	1586	441	504	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9ALW2
A	-18	GLY	-	expression tag	UNP Q9ALW2
A	-17	SER	-	expression tag	UNP Q9ALW2
A	-16	SER	-	expression tag	UNP Q9ALW2
A	-15	HIS	-	expression tag	UNP Q9ALW2
A	-14	HIS	-	expression tag	UNP Q9ALW2
A	-13	HIS	-	expression tag	UNP Q9ALW2
A	-12	HIS	-	expression tag	UNP Q9ALW2
A	-11	HIS	-	expression tag	UNP Q9ALW2
A	-10	HIS	-	expression tag	UNP Q9ALW2
A	-9	SER	-	expression tag	UNP Q9ALW2
A	-8	SER	-	expression tag	UNP Q9ALW2
A	-7	GLY	-	expression tag	UNP Q9ALW2
A	-6	LEU	-	expression tag	UNP Q9ALW2
A	-5	VAL	-	expression tag	UNP Q9ALW2
A	-4	PRO	-	expression tag	UNP Q9ALW2
A	-3	ARG	-	expression tag	UNP Q9ALW2
A	-2	GLY	-	expression tag	UNP Q9ALW2
A	-1	SER	-	expression tag	UNP Q9ALW2
A	0	HIS	-	expression tag	UNP Q9ALW2
A	298	ILE	LYS	engineered mutation	UNP Q9ALW2
B	-19	MET	-	expression tag	UNP Q9ALW2
B	-18	GLY	-	expression tag	UNP Q9ALW2
B	-17	SER	-	expression tag	UNP Q9ALW2
B	-16	SER	-	expression tag	UNP Q9ALW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q9ALW2
B	-14	HIS	-	expression tag	UNP Q9ALW2
B	-13	HIS	-	expression tag	UNP Q9ALW2
B	-12	HIS	-	expression tag	UNP Q9ALW2
B	-11	HIS	-	expression tag	UNP Q9ALW2
B	-10	HIS	-	expression tag	UNP Q9ALW2
B	-9	SER	-	expression tag	UNP Q9ALW2
B	-8	SER	-	expression tag	UNP Q9ALW2
B	-7	GLY	-	expression tag	UNP Q9ALW2
B	-6	LEU	-	expression tag	UNP Q9ALW2
B	-5	VAL	-	expression tag	UNP Q9ALW2
B	-4	PRO	-	expression tag	UNP Q9ALW2
B	-3	ARG	-	expression tag	UNP Q9ALW2
B	-2	GLY	-	expression tag	UNP Q9ALW2
B	-1	SER	-	expression tag	UNP Q9ALW2
B	0	HIS	-	expression tag	UNP Q9ALW2
B	298	ILE	LYS	engineered mutation	UNP Q9ALW2

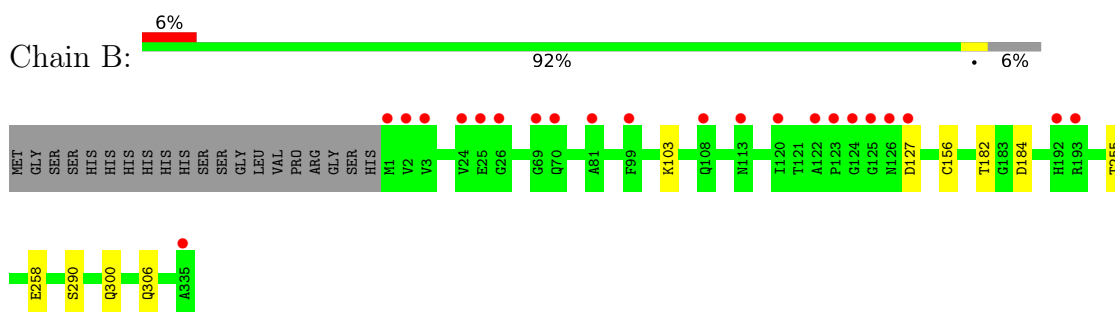
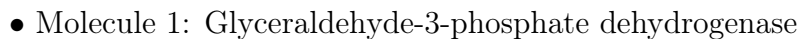
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	221	Total O 221 221	0	0
3	B	232	Total O 232 232	0	0

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.08Å 147.08Å 72.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 1.95 34.67 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.2 (34.67-1.95) 90.2 (34.67-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, R_{free}	0.192 , 0.219 0.194 , 0.222	Depositor DCC
R_{free} test set	2739 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5472	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/2513	0.40	0/3411
1	B	0.18	0/2578	0.42	0/3499
All	All	0.18	0/5091	0.41	0/6910

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2478	0	2457	21	0
1	B	2540	0	2519	5	0
2	A	1	0	0	0	0
3	A	221	0	0	2	0
3	B	232	0	0	0	0
All	All	5472	0	4976	26	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HG3	1:A:105:LYS:H	1.53	0.72
1:A:101:ALA:HA	1:A:105:LYS:HE3	1.80	0.64
1:A:3:VAL:N	3:A:505:HOH:O	2.36	0.59
1:A:94:LEU:HD13	1:A:328:LEU:HD11	1.85	0.58
1:A:112:GLU:CD	1:A:113:ASN:H	2.13	0.57
1:A:103:LYS:HZ2	1:A:104:GLU:H	1.55	0.55
1:A:162:LYS:NZ	3:A:506:HOH:O	2.42	0.53
1:B:103:LYS:HD2	1:B:127:ASP:HB2	1.91	0.52
1:A:182:THR:OG1	1:A:184:ASP:OD1	2.28	0.52
1:A:103:LYS:HG3	1:A:104:GLU:N	2.26	0.51
1:A:103:LYS:HB3	1:A:105:LYS:HE2	1.94	0.49
1:A:117:LYS:HD2	1:A:331:PHE:CZ	2.47	0.49
1:A:64:GLY:HA2	1:A:74:VAL:HB	1.94	0.49
1:B:255:THR:OG1	1:B:258:GLU:HG3	2.13	0.48
1:B:156:CYS:HA	1:B:290:SER:HB2	1.96	0.46
1:B:182:THR:OG1	1:B:184:ASP:OD1	2.34	0.45
1:A:85:TRP:HB3	1:A:90:VAL:HB	2.00	0.44
1:A:177:THR:HG22	1:A:179:HIS:HB2	2.00	0.43
1:A:24:VAL:HG23	1:A:27:VAL:HB	2.00	0.43
1:A:21:ILE:HA	1:A:24:VAL:HG22	2.00	0.43
1:A:300:GLN:O	1:A:306:GLN:HA	2.19	0.43
1:B:300:GLN:O	1:B:306:GLN:HA	2.19	0.43
1:A:181:TYR:HD2	1:A:237:PRO:HA	1.84	0.42
1:A:91:GLU:H	1:A:91:GLU:HG2	1.64	0.42
1:A:106:ALA:HB1	1:A:118:VAL:HG11	2.03	0.41
1:A:156:CYS:HA	1:A:290:SER:HB2	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/355 (92%)	308 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	335/355 (94%)	322 (96%)	13 (4%)	0	100	100
All	All	661/710 (93%)	630 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/286 (93%)	265 (100%)	0	100	100
1	B	271/286 (95%)	271 (100%)	0	100	100
All	All	536/572 (94%)	536 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	113	ASN
1	A	260	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/355 (92%)	0.40	40 (12%) 8 10	16, 29, 67, 92	0
1	B	335/355 (94%)	0.19	22 (6%) 24 28	12, 26, 60, 90	2 (0%)
All	All	665/710 (93%)	0.29	62 (9%) 14 16	12, 28, 64, 92	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ALA	5.1
1	A	101	ALA	4.6
1	A	124	GLY	4.5
1	B	124	GLY	4.5
1	A	115	ALA	4.0
1	B	1	MET	4.0
1	A	3	VAL	4.0
1	A	24	VAL	4.0
1	B	2	VAL	3.8
1	A	113	ASN	3.7
1	B	126	ASN	3.6
1	A	81	ALA	3.6
1	A	116	LYS	3.6
1	B	123	PRO	3.6
1	B	125	GLY	3.5
1	A	83	ILE	3.5
1	A	98	GLY	3.3
1	A	125	GLY	3.3
1	B	99	PHE	3.2
1	B	192	HIS	3.2
1	A	105	LYS	3.1
1	A	126	ASN	3.0
1	A	102	SER	3.0
1	A	106	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	3.0
1	A	91	GLU	2.9
1	A	111	HIS	2.8
1	A	110	ILE	2.8
1	A	112	GLU	2.7
1	A	114	GLY	2.7
1	A	192	HIS	2.7
1	A	69	GLY	2.6
1	A	27	VAL	2.6
1	A	86	ALA	2.6
1	A	334	ILE	2.5
1	B	113	ASN	2.5
1	A	5	VAL	2.5
1	A	108	GLN	2.5
1	A	77	GLU	2.5
1	A	127	ASP	2.4
1	B	127	ASP	2.4
1	A	23	ASN	2.4
1	A	103	LYS	2.4
1	B	120	ILE	2.4
1	B	122	ALA	2.4
1	A	25	GLU	2.4
1	B	24	VAL	2.4
1	A	104	GLU	2.3
1	B	26	GLY	2.3
1	A	78	ARG	2.3
1	B	108	GLN	2.3
1	A	80	PRO	2.3
1	B	193	ARG	2.3
1	B	3	VAL	2.3
1	B	25	GLU	2.2
1	A	122	ALA	2.2
1	A	30	THR	2.2
1	B	70	GLN	2.1
1	B	69	GLY	2.1
1	A	90	VAL	2.1
1	B	81	ALA	2.1
1	A	193	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	401	1/1	0.97	0.11	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.