



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:27 PM UTC

PDB ID : 3FOQ / pdb_00003foq
Title : Crystal structure of N-acetylglucosamine-1-phosphate uridylyltransferase (GlmU) from Mycobacterium tuberculosis in a cubic space group.
Authors : Verma, S.K.; Prakash, B.
Deposited on : 2008-12-31
Resolution : 3.41 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
Mogul : 2022.3.0, CSD as543be (2022)
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

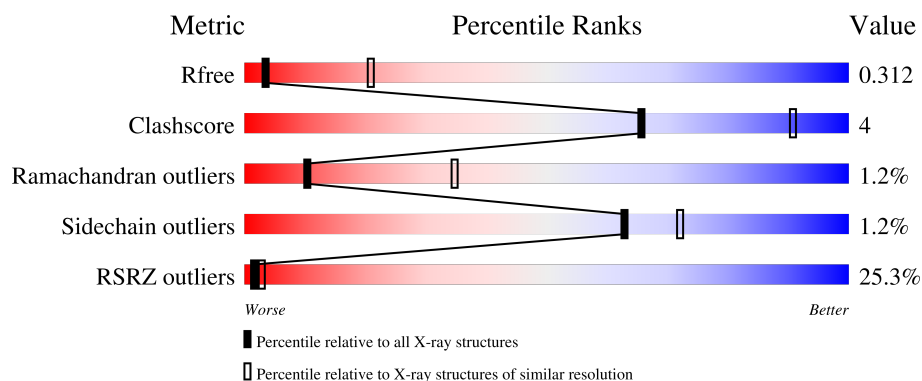
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	503	22% 77% 10% 13%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3186 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 Bifunctional protein glmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3166	1967	575	618	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P96382
A	-6	LYS	-	expression tag	UNP P96382
A	-5	HIS	-	expression tag	UNP P96382
A	-4	HIS	-	expression tag	UNP P96382
A	-3	HIS	-	expression tag	UNP P96382
A	-2	HIS	-	expression tag	UNP P96382
A	-1	HIS	-	expression tag	UNP P96382
A	0	HIS	-	expression tag	UNP P96382

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

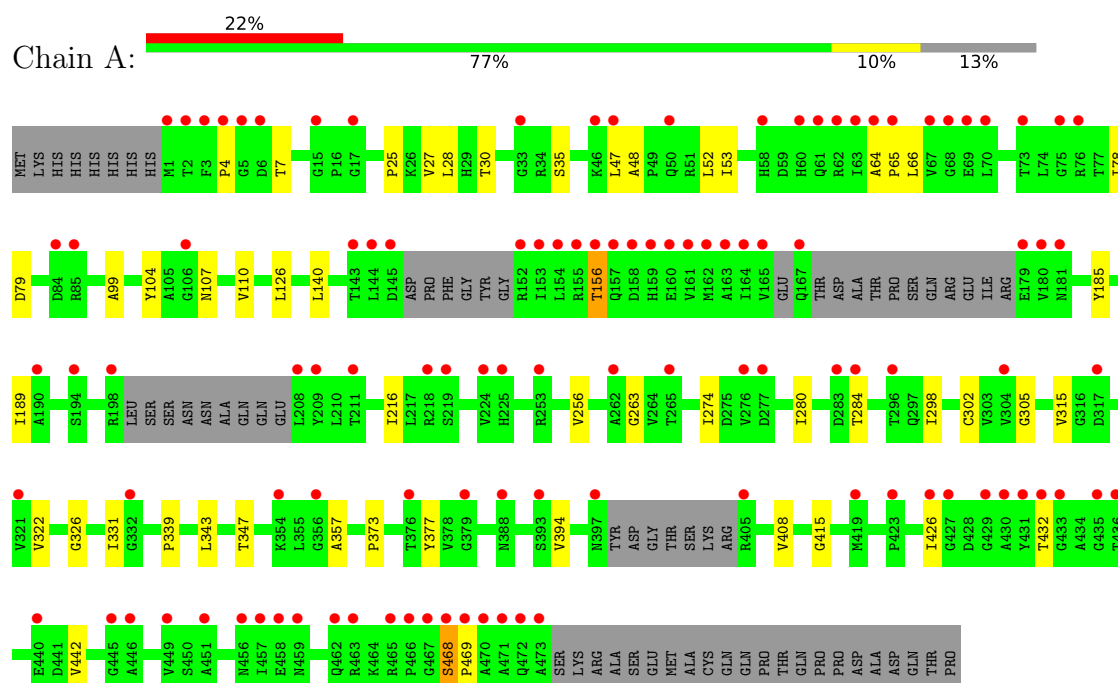


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional protein glmU



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	285.70Å 285.70Å 285.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.41 48.97 – 3.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.97-3.41) 98.9 (48.97-3.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.285 , 0.321 0.297 , 0.312	Depositor DCC
R_{free} test set	1349 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3186	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.46	0/3211	0.74	2/4391 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	442	VAL	CA-C-N	5.08	123.37	119.66
1	A	442	VAL	C-N-CA	5.08	123.37	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3166	0	3168	24	0
2	A	20	0	0	0	0
All	All	3186	0	3168	24	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 4.

All (24) 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:468:SER:CB	1:A:469:PRO:HD3	2.04	0.86
1:A:284:THR:HG22	1:A:302:CYS:H	1.60	0.66
1:A:468:SER:CB	1:A:469:PRO:CD	2.77	0.62
1:A:4:PRO:HD3	1:A:47:LEU:HB2	1.82	0.61
1:A:343:LEU:HD22	1:A:347:THR:HG21	1.86	0.58
1:A:25:PRO:HG2	1:A:28:LEU:HD12	1.87	0.56
1:A:126:LEU:HD13	1:A:140:LEU:HG	1.88	0.54
1:A:30:THR:HA	1:A:35:SER:HA	1.91	0.52
1:A:53:ILE:HG12	1:A:79:ASP:HB2	1.91	0.51
1:A:64:ALA:HB3	1:A:65:PRO:HD3	1.93	0.49
1:A:415:GLY:H	1:A:432:THR:HB	1.76	0.49
1:A:7:THR:HG22	1:A:107:ASN:HB2	1.97	0.47
1:A:408:VAL:HG22	1:A:426:ILE:HD12	1.98	0.46
1:A:326:GLY:HA2	1:A:343:LEU:HB2	1.98	0.45
1:A:339:PRO:O	1:A:357:ALA:HA	2.17	0.45
1:A:53:ILE:HD13	1:A:99:ALA:HB3	1.99	0.44
1:A:256:VAL:HG22	1:A:274:ILE:HD12	2.00	0.44
1:A:315:VAL:HG22	1:A:331:ILE:HD12	1.99	0.44
1:A:52:LEU:HD23	1:A:78:ILE:HG12	2.00	0.43
1:A:280:ILE:HA	1:A:298:ILE:HB	2.01	0.42
1:A:305:GLY:HA3	1:A:322:VAL:HG13	2.02	0.42
1:A:110:VAL:HB	1:A:185:TYR:HB2	2.03	0.41
1:A:104:TYR:HB3	1:A:189:ILE:HD13	2.03	0.41
1:A:377:TYR:HB3	1:A:394:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	428/503 (85%)	406 (95%)	17 (4%)	5 (1%)	10	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	A	156	THR
1	A	373	PRO
1	A	48	ALA
1	A	263	GLY

5.3.2 Protein sidechains ⓘ

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	333/396 (84%)	329 (99%)	4 (1%)	63 72

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	66	LEU
1	A	156	THR
1	A	216	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	181	ASN
1	A	225	HIS
1	A	291	GLN
1	A	454	GLN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	498	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	497	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	496	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	499	-	4,4,4	0.24	0	6,6,6	0.07	0

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 ⓘ

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	439/503 (87%)	1.52	111 (25%) 1 3	9, 37, 122, 195	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	THR	15.7
1	A	165	VAL	14.9
1	A	208	LEU	10.8
1	A	155	ARG	9.4
1	A	154	LEU	9.1
1	A	167	GLN	9.0
1	A	473	ALA	8.2
1	A	153	ILE	7.1
1	A	67	VAL	6.7
1	A	471	ALA	6.6
1	A	160	GLU	6.4
1	A	159	HIS	6.3
1	A	472	GLN	6.2
1	A	152	ARG	6.0
1	A	164	ILE	5.8
1	A	157	GLN	5.6
1	A	68	GLY	5.5
1	A	397	ASN	5.5
1	A	469	PRO	5.5
1	A	1	MET	5.2
1	A	163	ALA	5.2
1	A	466	PRO	4.9
1	A	161	VAL	4.9
1	A	63	ILE	4.9
1	A	468	SER	4.9
1	A	209	TYR	4.7
1	A	162	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLU	4.7
1	A	158	ASP	4.5
1	A	462	GLN	4.3
1	A	198	ARG	4.0
1	A	467	GLY	3.9
1	A	2	THR	3.9
1	A	423	PRO	3.9
1	A	284	THR	3.9
1	A	143	THR	3.8
1	A	64	ALA	3.8
1	A	465	ARG	3.7
1	A	470	ALA	3.7
1	A	356	GLY	3.6
1	A	181	ASN	3.6
1	A	60	HIS	3.5
1	A	405	ARG	3.5
1	A	225	HIS	3.4
1	A	4	PRO	3.4
1	A	58	HIS	3.4
1	A	179	GLU	3.3
1	A	449	VAL	3.3
1	A	5	GLY	3.2
1	A	144	LEU	3.2
1	A	145	ASP	3.2
1	A	304	VAL	3.2
1	A	445	GLY	3.2
1	A	85	ARG	3.2
1	A	440	GLU	3.1
1	A	62	ARG	3.1
1	A	276	VAL	3.0
1	A	253	ARG	3.0
1	A	218	ARG	3.0
1	A	106	GLY	3.0
1	A	84	ASP	2.9
1	A	463	ARG	2.9
1	A	76	ARG	2.8
1	A	3	PHE	2.8
1	A	17	GLY	2.8
1	A	432	THR	2.8
1	A	354	LYS	2.8
1	A	376	THR	2.7
1	A	379	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	VAL	2.6
1	A	446	ALA	2.6
1	A	219	SER	2.6
1	A	75	GLY	2.6
1	A	426	ILE	2.6
1	A	61	GLN	2.6
1	A	73	THR	2.6
1	A	431	TYR	2.5
1	A	47	LEU	2.5
1	A	419	MET	2.5
1	A	190	ALA	2.5
1	A	50	GLN	2.5
1	A	457	ILE	2.4
1	A	6	ASP	2.4
1	A	456	ASN	2.4
1	A	427	GLY	2.4
1	A	393	SER	2.4
1	A	388	ASN	2.4
1	A	70	LEU	2.4
1	A	211	THR	2.3
1	A	46	LYS	2.3
1	A	224	VAL	2.3
1	A	194	SER	2.2
1	A	277	ASP	2.2
1	A	435	GLY	2.2
1	A	65	PRO	2.2
1	A	458	GLU	2.2
1	A	33	GLY	2.2
1	A	332	GLY	2.2
1	A	262	ALA	2.1
1	A	430	ALA	2.1
1	A	433	GLY	2.1
1	A	265	THR	2.1
1	A	436	THR	2.1
1	A	321	VAL	2.1
1	A	459	ASN	2.1
1	A	429	GLY	2.1
1	A	283	ASP	2.1
1	A	451	ALA	2.1
1	A	15	GLY	2.1
1	A	296	THR	2.0
1	A	317	ASP	2.0

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

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	SO4	A	498	5/5	0.78	0.39	109,111,116,119	1
2	SO4	A	496	5/5	0.86	0.21	89,94,96,96	0
2	SO4	A	499	5/5	0.90	0.13	55,61,63,67	0
2	SO4	A	497	5/5	0.92	0.22	240,241,242,242	0

6.5 Other polymers [i](#)

There are no such residues in this entry.