



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:10 AM UTC

PDB ID : 7LU4 / pdb_00007lu4
Title : Crystal structure of bacterial glycyl tRNA synthetase in complex with glycine
Authors : Torres-Larios, A.
Deposited on : 2021-02-20
Resolution : 2.50 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

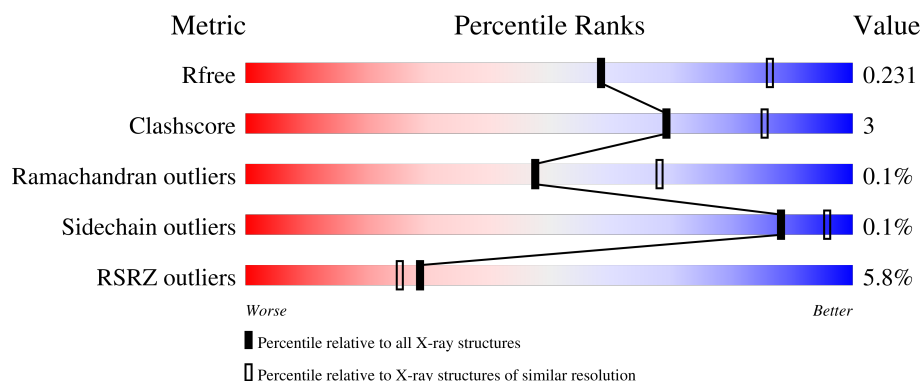
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1011	2% 88% 9% .
1	B	1011	9% 88% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14715 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 Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	978	Total	C	N	O	S	0	0	0
			7533	4815	1334	1366	18			
1	B	977	Total	C	N	O	S	0	0	0
			7177	4526	1302	1332	17			

There are 36 discrepancies between the modelled and reference sequences:

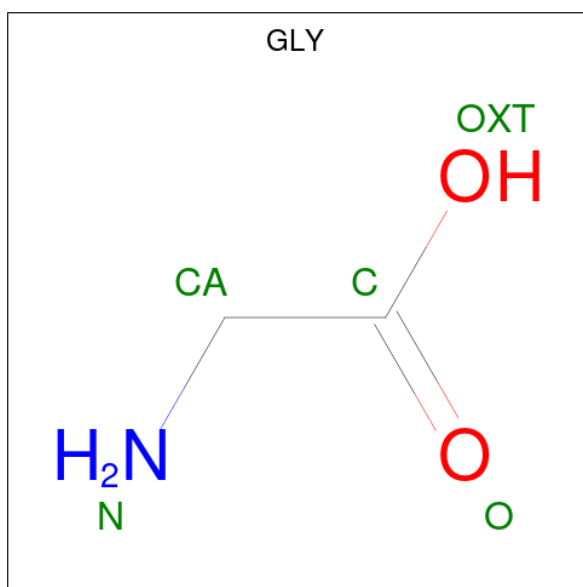
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
A	243	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
A	706	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
A	836	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
A	898	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
A	999	GLU	-	expression tag	UNP A0A0P6Y0P9
A	1000	ASN	-	expression tag	UNP A0A0P6Y0P9
A	1001	LEU	-	expression tag	UNP A0A0P6Y0P9
A	1002	TYR	-	expression tag	UNP A0A0P6Y0P9
A	1003	PHE	-	expression tag	UNP A0A0P6Y0P9
A	1004	GLN	-	expression tag	UNP A0A0P6Y0P9
A	1005	GLY	-	expression tag	UNP A0A0P6Y0P9
A	1006	HIS	-	expression tag	UNP A0A0P6Y0P9
A	1007	HIS	-	expression tag	UNP A0A0P6Y0P9
A	1008	HIS	-	expression tag	UNP A0A0P6Y0P9
A	1009	HIS	-	expression tag	UNP A0A0P6Y0P9
A	1010	HIS	-	expression tag	UNP A0A0P6Y0P9
A	1011	HIS	-	expression tag	UNP A0A0P6Y0P9
B	23	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
B	243	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
B	706	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
B	836	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
B	898	SER	CYS	engineered mutation	UNP A0A0P6Y0P9
B	999	GLU	-	expression tag	UNP A0A0P6Y0P9
B	1000	ASN	-	expression tag	UNP A0A0P6Y0P9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1001	LEU	-	expression tag	UNP A0A0P6Y0P9
B	1002	TYR	-	expression tag	UNP A0A0P6Y0P9
B	1003	PHE	-	expression tag	UNP A0A0P6Y0P9
B	1004	GLN	-	expression tag	UNP A0A0P6Y0P9
B	1005	GLY	-	expression tag	UNP A0A0P6Y0P9
B	1006	HIS	-	expression tag	UNP A0A0P6Y0P9
B	1007	HIS	-	expression tag	UNP A0A0P6Y0P9
B	1008	HIS	-	expression tag	UNP A0A0P6Y0P9
B	1009	HIS	-	expression tag	UNP A0A0P6Y0P9
B	1010	HIS	-	expression tag	UNP A0A0P6Y0P9
B	1011	HIS	-	expression tag	UNP A0A0P6Y0P9

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).

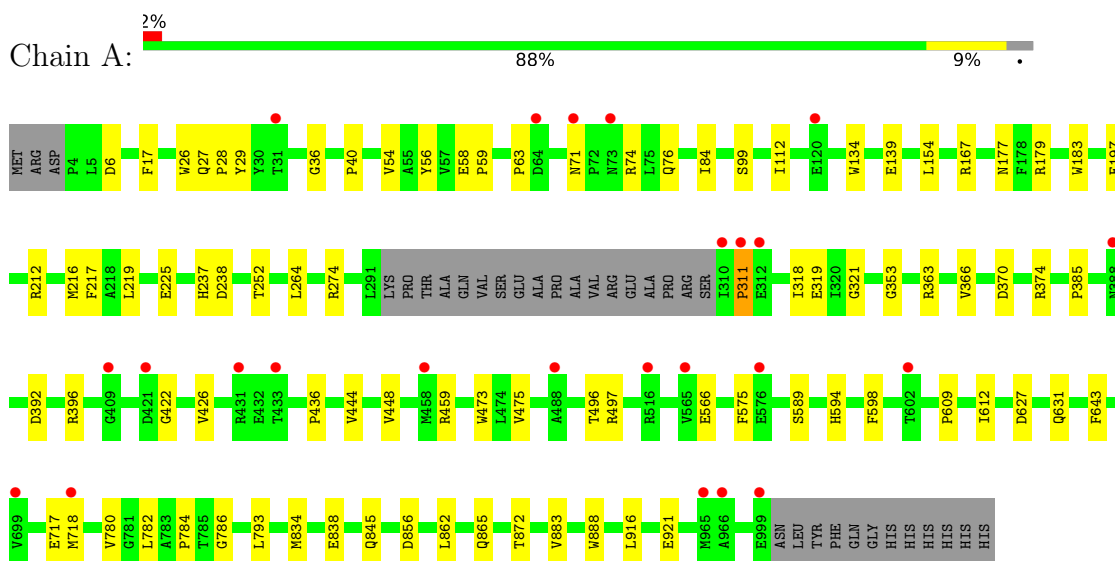


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

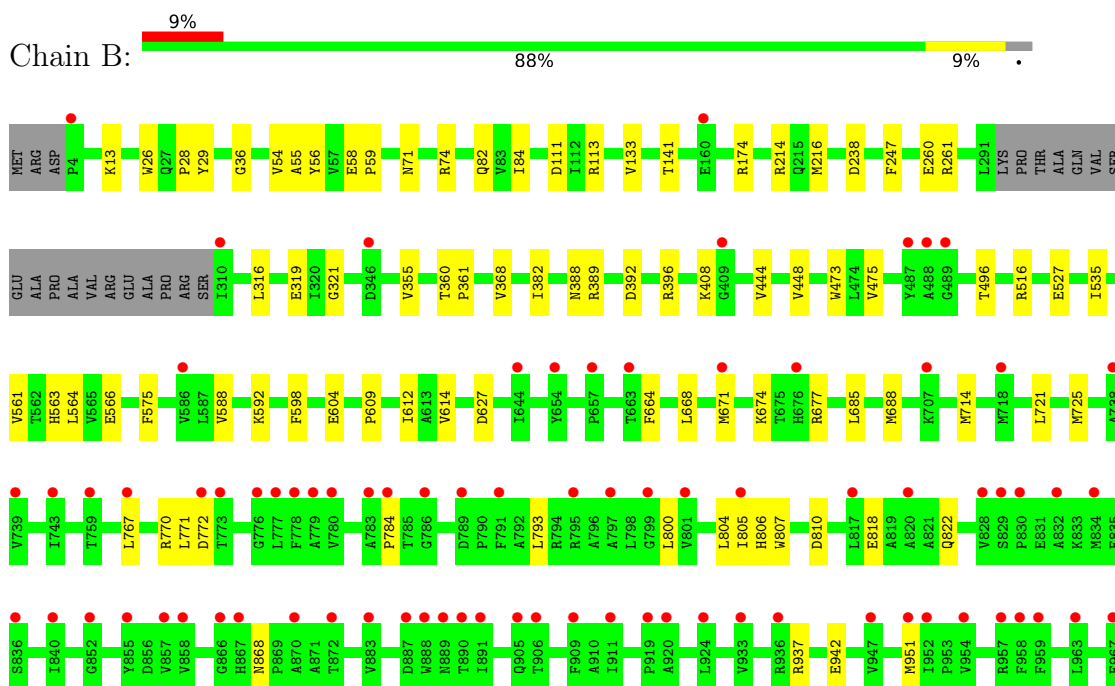
3 Residue-property plots [i](#)

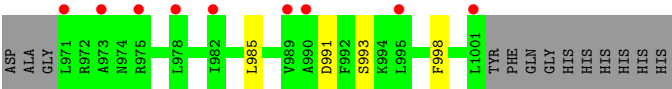
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multifunctional fusion protein



• Molecule 1: Multifunctional fusion protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.58Å 127.86Å 133.06Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	35.74 – 2.50 35.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.74-2.50) 99.1 (35.74-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.207 , 0.228 0.209 , 0.231	Depositor DCC
R_{free} test set	6485 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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](#)

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	0/7713	0.39	1/10501 (0.0%)
1	B	0.23	0/7349	0.44	0/9968
All	All	0.21	0/15062	0.41	1/20469 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	N-CA-CB	8.41	112.08	103.25

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	7533	0	7322	48	1
1	B	7177	0	6506	52	1
2	B	5	0	2	0	0
All	All	14715	0	13830	99	1

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 (99) 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:363:ARG:NH2	1:A:497:ARG:O	2.13	0.82
1:B:516:ARG:NH2	1:B:527:GLU:OE2	2.23	0.71
1:A:363:ARG:NH1	1:A:566:GLU:OE2	2.25	0.69
1:A:598:PHE:HB2	1:A:612:ILE:HB	1.78	0.66
1:B:111:ASP:OD2	1:B:113:ARG:NH2	2.29	0.65
1:A:26:TRP:HB3	1:A:56:TYR:HB3	1.79	0.65
1:B:382:ILE:HG21	1:B:408:LYS:HE2	1.78	0.65
1:A:784:PRO:HD3	1:A:793:LEU:HD12	1.80	0.63
1:A:154:LEU:O	1:A:459:ARG:NH2	2.35	0.59
1:A:916:LEU:HD22	1:A:921:GLU:HB3	1.83	0.59
1:B:598:PHE:HB2	1:B:612:ILE:HB	1.85	0.57
1:A:780:VAL:HG23	1:A:782:LEU:HD23	1.87	0.57
1:A:589:SER:HB3	1:A:718:MET:HE2	1.87	0.56
1:B:54:VAL:HG12	1:B:84:ILE:HB	1.87	0.56
1:B:685:LEU:HD13	1:B:688:MET:HE3	1.87	0.56
1:A:54:VAL:HG12	1:A:84:ILE:HB	1.88	0.56
1:B:174:ARG:NH1	1:B:627:ASP:OD2	2.38	0.55
1:B:991:ASP:OD2	1:B:993:SER:OG	2.23	0.55
1:B:805:ILE:C	1:B:807:TRP:H	2.15	0.54
1:B:28:PRO:HB3	1:B:59:PRO:HD2	1.90	0.54
1:B:604:GLU:N	1:B:604:GLU:OE2	2.41	0.53
1:A:643:PHE:CE2	1:A:717:GLU:HG3	2.45	0.51
1:B:664:PHE:HB2	1:B:671:MET:HE2	1.92	0.51
1:A:865:GLN:O	1:A:872:THR:OG1	2.30	0.50
1:B:993:SER:HA	1:B:998:PHE:CD1	2.47	0.50
1:A:76:GLN:HG3	1:A:197:GLU:OE1	2.13	0.49
1:A:319:GLU:OE1	1:A:496:THR:OG1	2.21	0.49
1:A:883:VAL:HG12	1:A:888:TRP:CE2	2.48	0.49
1:B:674:LYS:NZ	1:B:772:ASP:OD2	2.43	0.49
1:A:29:TYR:OH	1:A:238:ASP:OD1	2.21	0.49
1:A:225:GLU:OE2	1:A:274:ARG:NH2	2.37	0.49
1:B:767:LEU:HD11	1:B:804:LEU:HD21	1.93	0.49
1:B:818:GLU:O	1:B:822:GLN:OE1	2.32	0.48
1:A:318:ILE:HB	1:A:366:VAL:HB	1.96	0.48
1:B:214:ARG:NH1	1:B:260:GLU:OE2	2.37	0.47
1:B:784:PRO:HD3	1:B:793:LEU:HD12	1.95	0.47
1:A:177:ASN:HD21	1:A:179:ARG:NE	2.13	0.47
1:B:321:GLY:HA3	1:B:473:TRP:CD2	2.49	0.47
1:A:28:PRO:HB3	1:A:59:PRO:HD2	1.96	0.47
1:B:319:GLU:HB3	1:B:475:VAL:HB	1.96	0.47
1:B:360:THR:HB	1:B:566:GLU:HG2	1.95	0.47
1:A:392:ASP:OD1	1:A:396:ARG:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:PHE:CZ	1:A:609:PRO:HA	2.50	0.46
1:A:26:TRP:CG	1:A:27:GLN:H	2.34	0.46
1:B:36:GLY:HA2	1:B:58:GLU:HG2	1.98	0.46
1:B:133:VAL:HB	1:B:141:THR:HB	1.98	0.45
1:A:845:GLN:HB3	1:A:862:LEU:HD11	1.97	0.45
1:B:810:ASP:HB3	1:B:868:ASN:HD21	1.81	0.45
1:B:247:PHE:HZ	1:B:261:ARG:HG3	1.82	0.45
1:A:219:LEU:HD13	1:B:216:MET:HG3	1.99	0.45
1:B:26:TRP:HB3	1:B:56:TYR:HB3	1.99	0.45
1:A:36:GLY:HA2	1:A:58:GLU:HG2	1.99	0.45
1:B:535:ILE:HD13	1:B:561:VAL:HG12	1.98	0.45
1:B:319:GLU:OE1	1:B:496:THR:OG1	2.30	0.44
1:A:321:GLY:HA3	1:A:473:TRP:CD2	2.52	0.44
1:A:834:MET:O	1:A:838:GLU:HG3	2.16	0.44
1:B:355:VAL:HG22	1:B:368:VAL:HG22	1.99	0.44
1:A:112:ILE:HA	1:A:134:TRP:O	2.18	0.44
1:A:6:ASP:HB3	1:A:183:TRP:O	2.18	0.44
1:A:385:PRO:O	1:A:426:VAL:HG12	2.18	0.44
1:B:29:TYR:OH	1:B:238:ASP:OD1	2.35	0.44
1:A:217:PHE:CE2	1:A:264:LEU:HD22	2.53	0.43
1:B:444:VAL:O	1:B:448:VAL:HG23	2.18	0.43
1:A:74:ARG:NH2	1:A:717:GLU:OE1	2.51	0.43
1:A:856:ASP:OD1	1:A:856:ASP:N	2.50	0.43
1:A:177:ASN:HD21	1:A:179:ARG:CZ	2.31	0.43
1:B:721:LEU:HB3	1:B:725:MET:HG2	2.00	0.42
1:B:937:ARG:HE	1:B:937:ARG:HB2	1.68	0.42
1:A:319:GLU:HB3	1:A:475:VAL:HB	2.00	0.42
1:B:668:LEU:O	1:B:677:ARG:NH2	2.53	0.42
1:A:40:PRO:HG3	1:A:237:HIS:CD2	2.54	0.42
1:B:388:ASN:OD1	1:B:389:ARG:N	2.53	0.42
1:B:55:ALA:HA	1:B:82:GLN:O	2.20	0.42
1:B:316:LEU:HB3	1:B:368:VAL:HB	2.02	0.42
1:A:71:ASN:HB3	1:A:74:ARG:HB2	2.01	0.42
1:A:353:GLY:N	1:A:370:ASP:O	2.44	0.42
1:A:444:VAL:O	1:A:448:VAL:HG23	2.20	0.42
1:A:627:ASP:O	1:A:631:GLN:HG2	2.20	0.42
1:B:561:VAL:HG11	1:B:614:VAL:HG21	2.01	0.42
1:A:177:ASN:ND2	1:A:179:ARG:HB2	2.35	0.41
1:B:805:ILE:O	1:B:806:HIS:HB3	2.18	0.41
1:B:951:MET:HE1	1:B:985:LEU:HD11	2.03	0.41
1:A:374:ARG:HA	1:A:436:PRO:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLY:HA3	1:B:473:TRP:CE2	2.55	0.41
1:A:139:GLU:O	1:A:167:ARG:HD3	2.21	0.41
1:B:392:ASP:OD1	1:B:396:ARG:N	2.52	0.41
1:B:714:MET:HG3	1:B:725:MET:HE2	2.01	0.41
1:A:212:ARG:O	1:A:216:MET:HG3	2.21	0.41
1:B:575:PHE:CZ	1:B:609:PRO:HA	2.56	0.40
1:B:113:ARG:HD3	1:B:564:LEU:O	2.20	0.40
1:B:588:VAL:HG13	1:B:592:LYS:HD3	2.03	0.40
1:B:770:ARG:HD3	1:B:800:LEU:HB2	2.03	0.40
1:A:63:PRO:HB2	1:A:252:THR:HG21	2.02	0.40
1:B:13:LYS:HD2	1:B:13:LYS:HA	1.95	0.40
1:A:17:PHE:CE2	1:A:99:SER:HB3	2.57	0.40
1:A:594:HIS:NE2	1:A:718:MET:SD	2.94	0.40
1:B:71:ASN:OD1	1:B:74:ARG:N	2.50	0.40
1:B:361:PRO:HG3	1:B:563:HIS:O	2.21	0.40
1:B:805:ILE:C	1:B:807:TRP:N	2.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:GLY:N	1:B:942:GLU:OE1[4_556]	2.08	0.12

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	974/1011 (96%)	954 (98%)	18 (2%)	2 (0%)	43	63
1	B	971/1011 (96%)	936 (96%)	35 (4%)	0	100	100
All	All	1945/2022 (96%)	1890 (97%)	53 (3%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
1	A	422	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	749/827 (91%)	749 (100%)	0	100	100
1	B	659/827 (80%)	658 (100%)	1 (0%)	87	95
All	All	1408/1654 (85%)	1407 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	771	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	27	GLN
1	A	142	GLN
1	A	215	GLN
1	A	245	HIS
1	A	704	HIS
1	A	806	HIS
1	B	78	HIS
1	B	215	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](#)

1 ligand is 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	GLY	B	1101	-	4,4,4	1.14	1 (25%)	3,4,4	1.57	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLY	B	1101	-	-	0/2/2/2	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	GLY	OXT-C	-2.16	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	GLY	OXT-C-O	-2.01	118.16	123.33

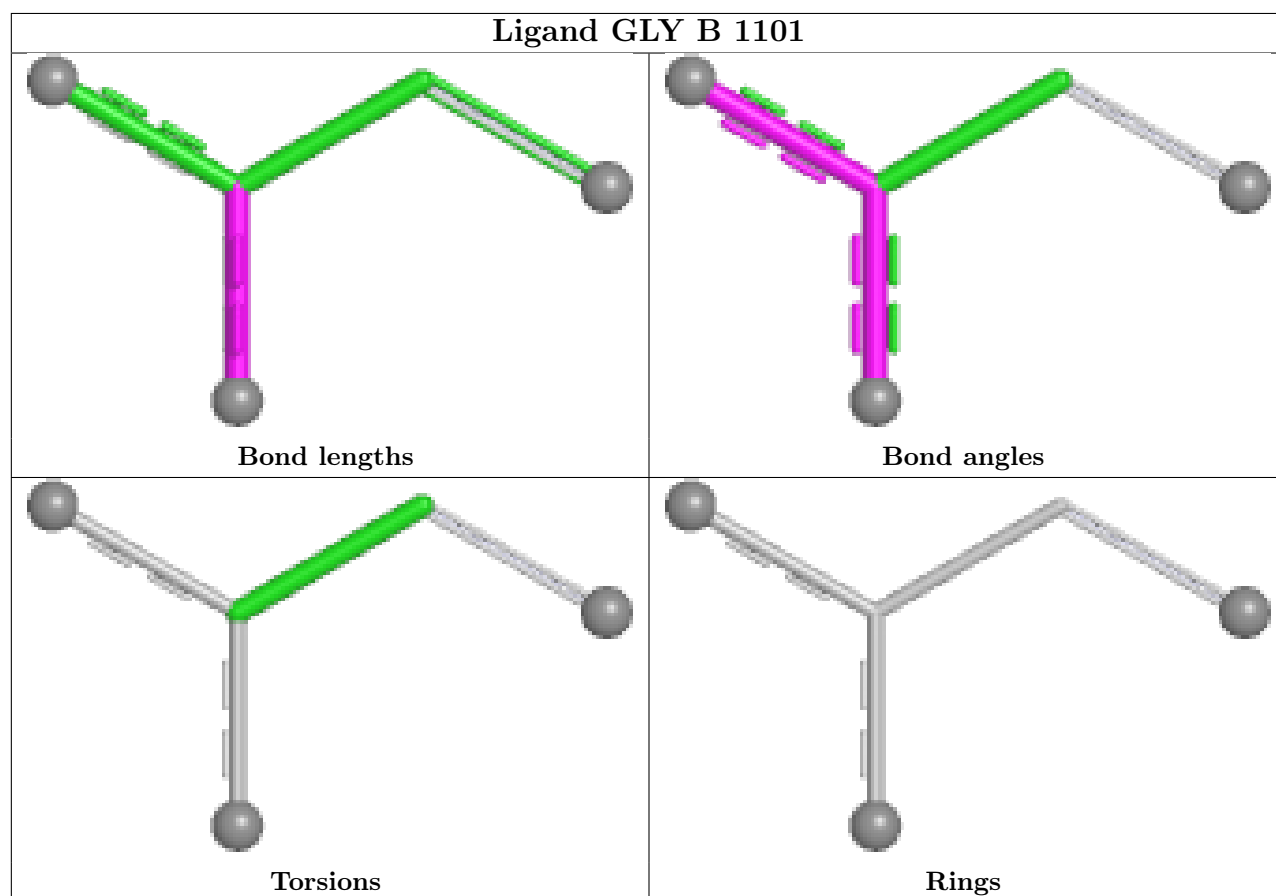
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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	978/1011 (96%)	0.27	24 (2%)	58	54	50, 78, 105, 139	0
1	B	977/1011 (96%)	0.63	89 (9%)	15	13	50, 85, 122, 140	0
All	All	1955/2022 (96%)	0.45	113 (5%)	29	25	50, 80, 115, 140	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	971	LEU	5.4
1	B	911	ILE	4.9
1	B	743	ILE	4.4
1	A	310	ILE	4.1
1	A	312	GLU	4.0
1	B	780	VAL	4.0
1	A	999	GLU	3.9
1	A	965	MET	3.9
1	B	777	LEU	3.8
1	B	989	VAL	3.7
1	B	409	GLY	3.7
1	B	1001	LEU	3.7
1	B	905	GLN	3.6
1	B	889	ASN	3.6
1	A	565	VAL	3.5
1	B	982	ILE	3.5
1	B	779	ALA	3.4
1	B	739	VAL	3.4
1	B	958	PHE	3.3
1	B	891	ILE	3.2
1	B	738	ALA	3.1
1	B	906	THR	3.1
1	A	699	VAL	3.1
1	B	857	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	783	ALA	3.1
1	B	805	ILE	3.1
1	B	817	LEU	3.0
1	B	310	ILE	2.9
1	A	602	THR	2.9
1	B	872	THR	2.9
1	B	767	LEU	2.8
1	B	866	GLY	2.8
1	B	952	ILE	2.8
1	B	786	GLY	2.8
1	A	71	ASN	2.8
1	B	663	THR	2.8
1	B	967	GLU	2.8
1	B	488	ALA	2.8
1	B	671	MET	2.8
1	B	801	VAL	2.7
1	B	978	LEU	2.7
1	B	832	ALA	2.7
1	B	990	ALA	2.7
1	B	909	PHE	2.7
1	A	73	ASN	2.7
1	B	820	ALA	2.7
1	B	799	GLY	2.7
1	B	883	VAL	2.7
1	B	951	MET	2.7
1	B	954	VAL	2.7
1	A	421	ASP	2.6
1	B	776	GLY	2.6
1	A	311	PRO	2.6
1	B	840	ILE	2.6
1	B	834	MET	2.6
1	A	458	MET	2.6
1	B	947	VAL	2.6
1	B	829	SER	2.6
1	B	489	GLY	2.6
1	B	797	ALA	2.6
1	B	657	PRO	2.5
1	B	867	HIS	2.5
1	B	870	ALA	2.5
1	B	920	ALA	2.5
1	B	975	ARG	2.5
1	B	4	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	995	LEU	2.4
1	B	773	THR	2.4
1	B	789	ASP	2.4
1	A	409	GLY	2.4
1	A	576	GLU	2.4
1	B	919	PRO	2.4
1	A	488	ALA	2.3
1	A	431	ARG	2.3
1	B	718	MET	2.3
1	B	778	PHE	2.3
1	B	791	PHE	2.3
1	A	31	THR	2.3
1	B	858	VAL	2.3
1	B	676	HIS	2.2
1	A	718	MET	2.2
1	B	924	LEU	2.2
1	B	836	SER	2.2
1	B	830	PRO	2.2
1	B	759	THR	2.2
1	B	855	TYR	2.2
1	B	852	GLY	2.2
1	B	957	ARG	2.2
1	A	388	ASN	2.2
1	A	966	ALA	2.2
1	B	654	TYR	2.2
1	B	890	THR	2.2
1	B	586	VAL	2.1
1	B	933	VAL	2.1
1	B	795	ARG	2.1
1	B	346	ASP	2.1
1	B	707	LYS	2.1
1	B	784	PRO	2.1
1	A	516	ARG	2.1
1	B	160	GLU	2.1
1	B	959	PHE	2.1
1	A	433	THR	2.1
1	B	828	VAL	2.0
1	B	973	ALA	2.0
1	A	120	GLU	2.0
1	B	644	ILE	2.0
1	A	64	ASP	2.0
1	B	887	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	936	ARG	2.0
1	B	963	LEU	2.0
1	B	888	TRP	2.0
1	B	772	ASP	2.0
1	B	487	TYR	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](#)

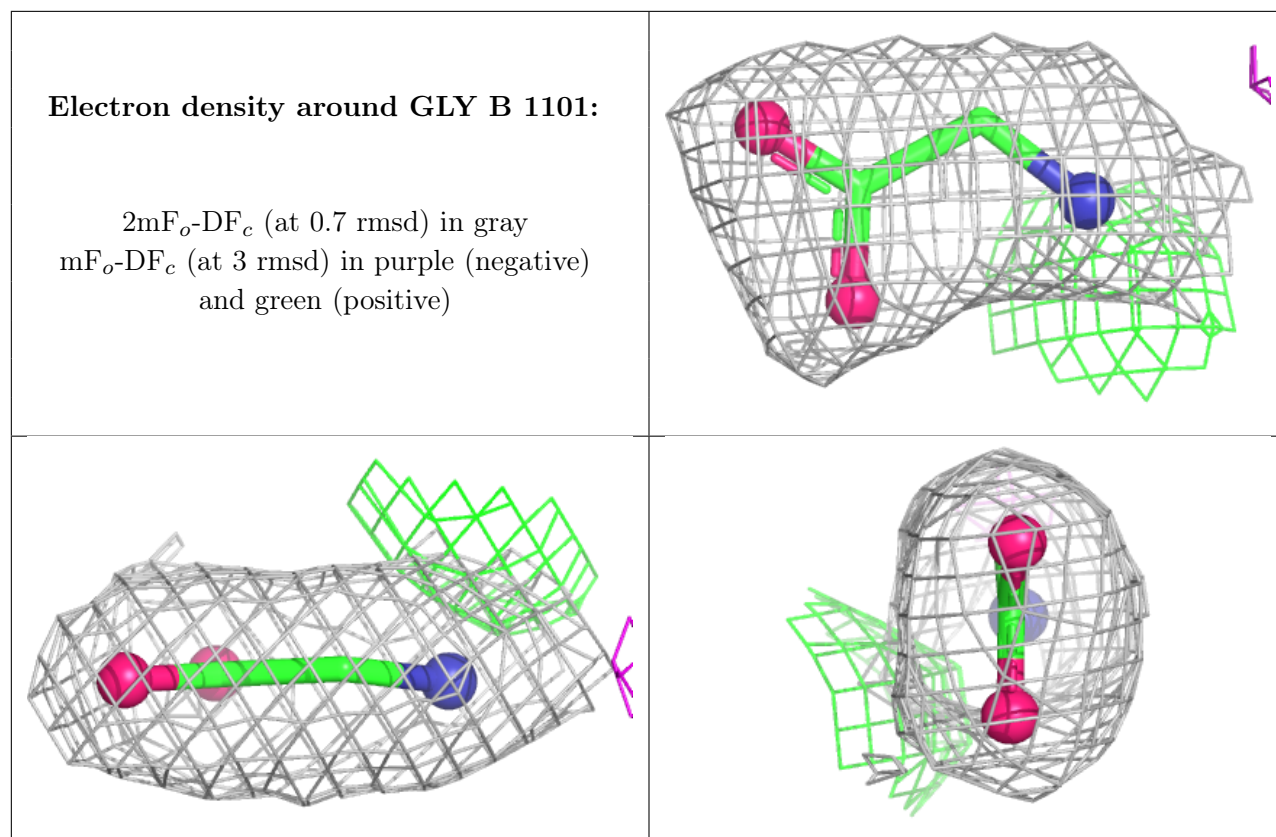
There are no oligosaccharides in this entry.

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	GLY	B	1101	5/5	0.90	0.13	67,72,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.