



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:18 PM UTC

PDB ID : 4JBF / pdb_00004jbf
Title : Crystal structure of peptidoglycan glycosyltransferase from *Atopobium parvulum* DSM 20469.
Authors : Filippova, E.V.; Wawrzak, Z.; Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Babnigg, G.; Rubin, E.; Sacchettini, J.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG); Structures of Mtb Proteins Conferring Susceptibility to Known Mtb Inhibitors (MTBI)
Deposited on : 2013-02-19
Resolution : 1.92 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)

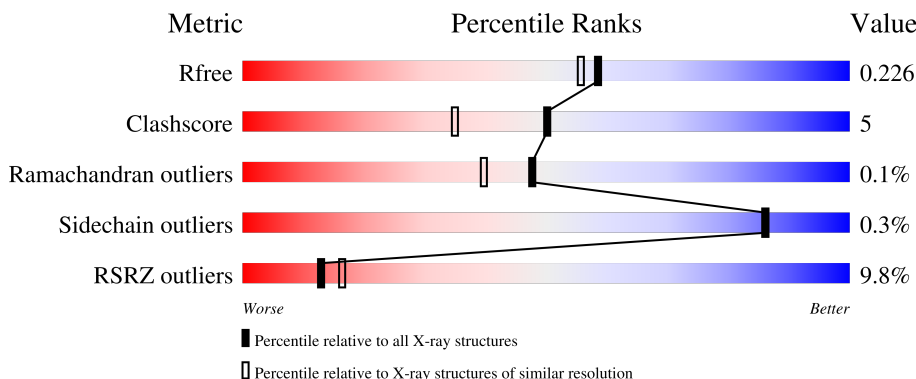
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	482	9% 76% 9% 15%
1	B	482	7% 74% 11% 15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6378 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 Peptidoglycan glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	Se	0	1	0
			2948	1833	499	601	2	13			
1	B	410	Total	C	N	O	S	Se	0	2	0
			2953	1832	501	605	2	13			

There are 64 discrepancies between the modelled and reference sequences:

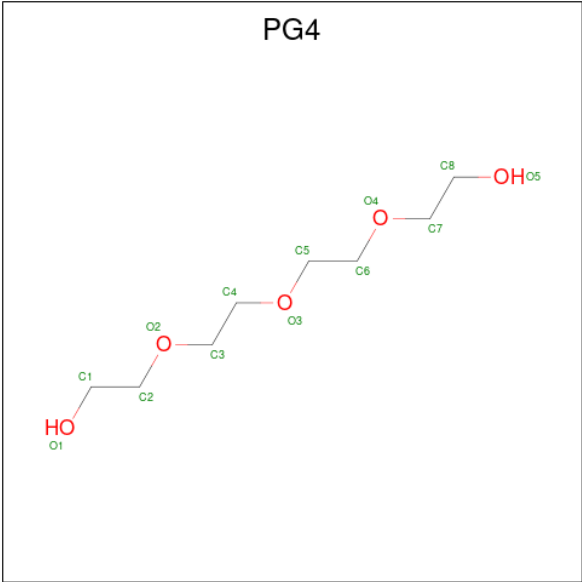
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	expression tag	UNP C8W8H7
A	474	HIS	-	expression tag	UNP C8W8H7
A	475	HIS	-	expression tag	UNP C8W8H7
A	476	HIS	-	expression tag	UNP C8W8H7
A	477	HIS	-	expression tag	UNP C8W8H7
A	478	HIS	-	expression tag	UNP C8W8H7
A	479	HIS	-	expression tag	UNP C8W8H7
A	480	SER	-	expression tag	UNP C8W8H7
A	481	SER	-	expression tag	UNP C8W8H7
A	482	GLY	-	expression tag	UNP C8W8H7
A	483	VAL	-	expression tag	UNP C8W8H7
A	484	ASP	-	expression tag	UNP C8W8H7
A	485	LEU	-	expression tag	UNP C8W8H7
A	486	TRP	-	expression tag	UNP C8W8H7
A	487	SER	-	expression tag	UNP C8W8H7
A	488	HIS	-	expression tag	UNP C8W8H7
A	489	PRO	-	expression tag	UNP C8W8H7
A	490	GLN	-	expression tag	UNP C8W8H7
A	491	PHE	-	expression tag	UNP C8W8H7
A	492	GLU	-	expression tag	UNP C8W8H7
A	493	LYS	-	expression tag	UNP C8W8H7
A	494	GLY	-	expression tag	UNP C8W8H7
A	495	THR	-	expression tag	UNP C8W8H7
A	496	GLU	-	expression tag	UNP C8W8H7
A	497	ASN	-	expression tag	UNP C8W8H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP C8W8H7
A	499	TYR	-	expression tag	UNP C8W8H7
A	500	PHE	-	expression tag	UNP C8W8H7
A	501	GLN	-	expression tag	UNP C8W8H7
A	502	SER	-	expression tag	UNP C8W8H7
A	503	ASN	-	expression tag	UNP C8W8H7
A	504	ALA	-	expression tag	UNP C8W8H7
B	473	MSE	-	expression tag	UNP C8W8H7
B	474	HIS	-	expression tag	UNP C8W8H7
B	475	HIS	-	expression tag	UNP C8W8H7
B	476	HIS	-	expression tag	UNP C8W8H7
B	477	HIS	-	expression tag	UNP C8W8H7
B	478	HIS	-	expression tag	UNP C8W8H7
B	479	HIS	-	expression tag	UNP C8W8H7
B	480	SER	-	expression tag	UNP C8W8H7
B	481	SER	-	expression tag	UNP C8W8H7
B	482	GLY	-	expression tag	UNP C8W8H7
B	483	VAL	-	expression tag	UNP C8W8H7
B	484	ASP	-	expression tag	UNP C8W8H7
B	485	LEU	-	expression tag	UNP C8W8H7
B	486	TRP	-	expression tag	UNP C8W8H7
B	487	SER	-	expression tag	UNP C8W8H7
B	488	HIS	-	expression tag	UNP C8W8H7
B	489	PRO	-	expression tag	UNP C8W8H7
B	490	GLN	-	expression tag	UNP C8W8H7
B	491	PHE	-	expression tag	UNP C8W8H7
B	492	GLU	-	expression tag	UNP C8W8H7
B	493	LYS	-	expression tag	UNP C8W8H7
B	494	GLY	-	expression tag	UNP C8W8H7
B	495	THR	-	expression tag	UNP C8W8H7
B	496	GLU	-	expression tag	UNP C8W8H7
B	497	ASN	-	expression tag	UNP C8W8H7
B	498	LEU	-	expression tag	UNP C8W8H7
B	499	TYR	-	expression tag	UNP C8W8H7
B	500	PHE	-	expression tag	UNP C8W8H7
B	501	GLN	-	expression tag	UNP C8W8H7
B	502	SER	-	expression tag	UNP C8W8H7
B	503	ASN	-	expression tag	UNP C8W8H7
B	504	ALA	-	expression tag	UNP C8W8H7

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		

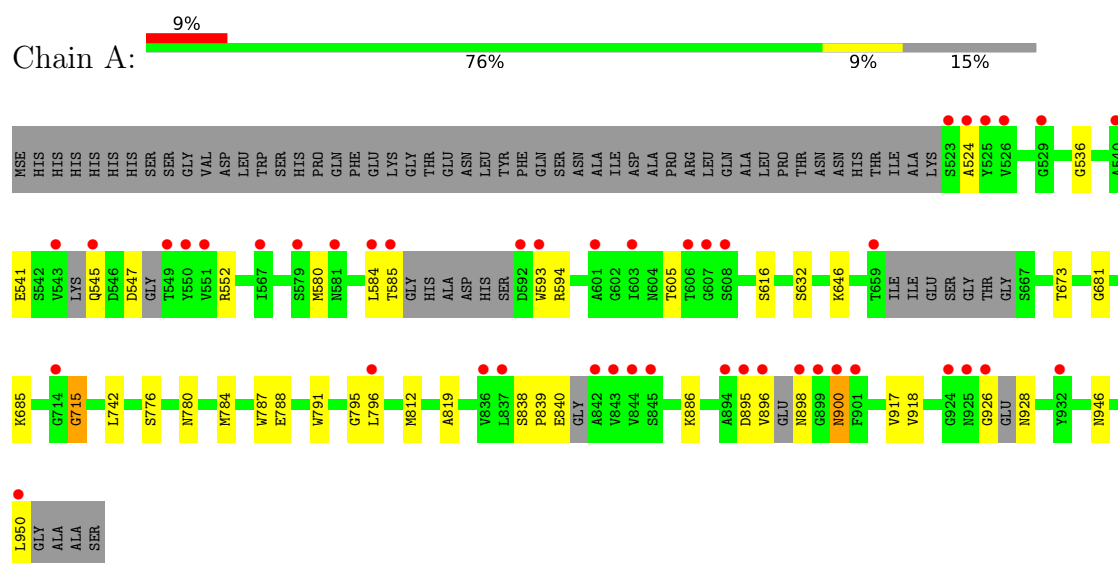
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total	O	0	4
			222	222		
3	B	247	Total	O	0	1
			248	248		

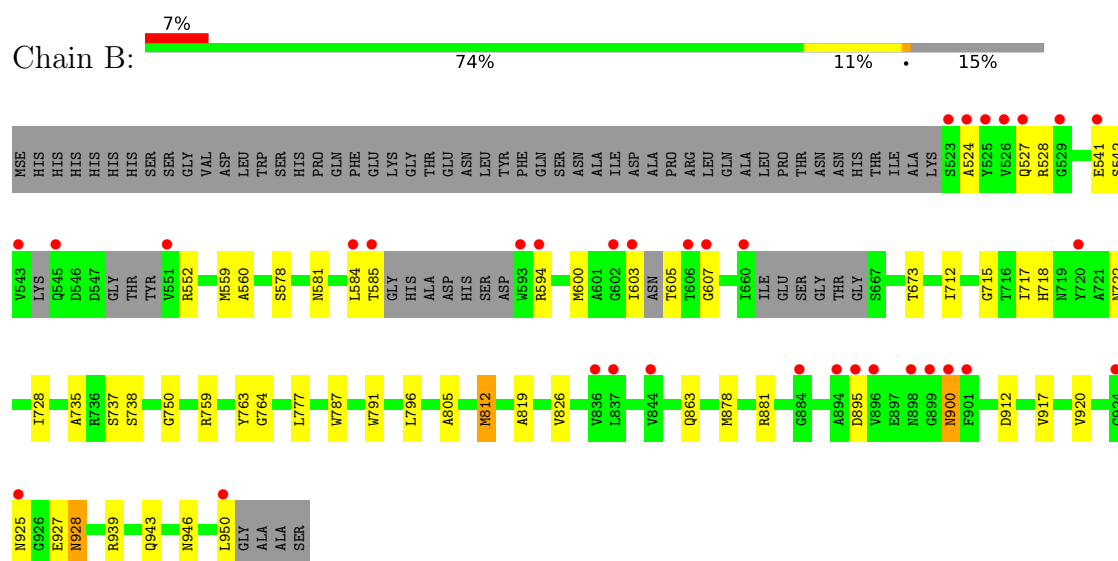
3 Residue-property plots [i](#)

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: Peptidoglycan glycosyltransferase



• Molecule 1: Peptidoglycan glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.93Å 70.17Å 114.82Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	29.48 – 1.92 29.48 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.48-1.92) 98.8 (29.48-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.237 0.192 , 0.226	Depositor DCC
R_{free} test set	5211 reflections (6.42%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: PG4

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	1.03	2/2982 (0.1%)	1.15	7/4044 (0.2%)
1	B	1.14	9/2985 (0.3%)	1.18	6/4047 (0.1%)
All	All	1.09	11/5967 (0.2%)	1.16	13/8091 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	812	MSE	N-CA	9.08	1.57	1.46
1	B	738	SER	N-CA	6.34	1.53	1.46
1	B	826	VAL	CA-CB	6.20	1.61	1.54
1	A	812	MSE	N-CA	6.18	1.53	1.46
1	B	920	VAL	N-CA	-5.50	1.39	1.46
1	B	673	THR	CA-CB	5.36	1.62	1.53
1	B	750	GLY	C-O	5.32	1.29	1.23
1	B	737	SER	CA-C	5.12	1.59	1.53
1	B	735	ALA	N-CA	5.08	1.52	1.46
1	A	918	VAL	N-CA	-5.05	1.40	1.46
1	B	863	GLN	N-CA	5.01	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ALA	N-CA-C	-8.24	103.26	112.57
1	B	524	ALA	N-CA-C	-7.22	104.49	112.72
1	A	776	SER	N-CA-C	-6.34	101.09	110.48
1	B	805	ALA	N-CA-C	-5.97	102.09	110.50
1	B	728	ILE	N-CA-C	5.95	115.73	109.01
1	B	928	ASN	N-CA-C	-5.84	99.77	109.46
1	A	715	GLY	N-CA-C	-5.80	102.62	111.10
1	A	605	THR	N-CA-C	5.80	118.92	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	920	VAL	CB-CA-C	-5.75	100.77	110.71
1	B	777	LEU	N-CA-C	5.65	118.68	109.24
1	A	780	ASN	N-CA-C	-5.50	101.28	109.42
1	A	616	SER	N-CA-C	5.07	117.55	111.71
1	A	536	GLY	N-CA-C	5.07	122.71	114.90

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	2948	0	2863	24	0
1	B	2953	0	2874	38	0
2	B	7	0	9	0	0
3	A	222	0	0	4	0
3	B	248	0	0	4	0
All	All	6378	0	5746	62	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 5.

All (62) 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:B:759[C]:ARG:HH21	1:B:759[C]:ARG:HG2	1.27	0.98
1:B:878:MSE:CE	1:B:881:ARG:HH11	1.90	0.84
1:B:759[C]:ARG:HH21	1:B:759[C]:ARG:CG	1.90	0.84
1:B:878:MSE:HE2	1:B:881:ARG:HH11	1.45	0.80
1:A:545:GLN:HA	3:A:1146:HOH:O	1.83	0.77
1:B:759[C]:ARG:HG2	1:B:759[C]:ARG:NH2	2.04	0.69
1:B:912:ASP:HB2	3:B:1288:HOH:O	1.93	0.69
1:A:547:ASP:HB2	3:A:1145:HOH:O	1.93	0.68
1:A:946:ASN:O	1:A:950:LEU:HD13	1.93	0.68
1:B:759[C]:ARG:NH2	1:B:763:TYR:HB3	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:MSE:CE	1:B:881:ARG:NH1	2.58	0.66
1:A:545:GLN:N	3:A:1146:HOH:O	2.27	0.66
1:B:541:GLU:O	1:B:552:ARG:NH1	2.27	0.65
1:A:715:GLY:HA3	1:A:787:TRP:CD1	2.34	0.62
1:A:886:LYS:NZ	3:A:1078:HOH:O	2.33	0.61
1:B:715:GLY:HA3	1:B:787:TRP:CD1	2.35	0.60
1:B:939:ARG:HD3	3:B:1319:HOH:O	2.01	0.59
1:A:632:SER:HB2	1:A:673:THR:HG22	1.85	0.58
1:A:681:GLY:O	1:A:795:GLY:HA3	2.04	0.58
1:B:878:MSE:HE3	1:B:881:ARG:NH1	2.19	0.57
1:B:878:MSE:HE3	1:B:881:ARG:HH11	1.67	0.56
1:B:878:MSE:HE2	1:B:881:ARG:NH1	2.18	0.56
1:B:759[C]:ARG:NH2	1:B:763:TYR:C	2.67	0.53
1:B:895:ASP:OD1	1:B:900:ASN:ND2	2.41	0.52
1:B:946:ASN:O	1:B:950:LEU:HD13	2.08	0.52
1:A:646:LYS:HE2	1:A:673:THR:OG1	2.11	0.51
1:B:759[C]:ARG:HH22	1:B:763:TYR:HB3	1.75	0.50
1:B:594:ARG:HB3	1:B:600:MSE:HE3	1.94	0.49
1:B:541:GLU:O	1:B:552:ARG:HD2	2.13	0.49
1:A:541:GLU:O	1:A:552:ARG:HD2	2.14	0.48
1:B:578:SER:O	1:B:581:ASN:HB2	2.13	0.48
1:A:791:TRP:CE3	1:A:796:LEU:HD12	2.49	0.47
1:A:593:TRP:CE2	1:A:594:ARG:CG	2.98	0.47
1:A:584:LEU:O	1:A:585:THR:C	2.58	0.46
1:B:927:GLU:HG2	1:B:928:ASN:O	2.15	0.46
1:A:819:ALA:HA	1:A:917:VAL:HG21	1.97	0.46
1:B:819:ALA:HA	1:B:917:VAL:HG21	1.97	0.46
1:B:528:ARG:HA	1:B:584:LEU:O	2.16	0.45
1:A:900:ASN:O	1:A:900:ASN:ND2	2.50	0.45
1:A:926:GLY:O	1:A:928:ASN:N	2.51	0.44
1:B:759[C]:ARG:HH22	1:B:764:GLY:N	2.14	0.44
1:A:838:SER:O	1:A:839:PRO:C	2.60	0.44
1:B:585:THR:O	1:B:607:GLY:HA2	2.18	0.44
1:A:685:LYS:HD3	1:A:742:LEU:HG	2.00	0.44
1:A:895:ASP:OD1	1:A:900:ASN:ND2	2.51	0.43
1:A:580:MSE:O	1:A:584:LEU:HG	2.19	0.43
1:B:791:TRP:CE3	1:B:796:LEU:HD12	2.54	0.42
1:B:943:GLN:NE2	3:B:1242:HOH:O	2.52	0.42
1:B:603:ILE:C	3:B:1250:HOH:O	2.62	0.42
1:B:718:HIS:HB2	1:B:722:ASN:HD22	1.85	0.42
1:A:838:SER:C	1:A:840:GLU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:GLU:HB3	1:B:542:SER:H	1.64	0.42
1:A:896:VAL:O	1:A:898:ASN:N	2.53	0.42
1:B:812:MSE:HE2	1:B:812:MSE:HB2	1.92	0.42
1:B:718:HIS:HB2	1:B:722:ASN:ND2	2.35	0.41
1:B:527:GLN:CG	1:B:528:ARG:N	2.84	0.41
1:B:759[C]:ARG:NH2	1:B:764:GLY:N	2.69	0.41
1:A:784:MSE:HA	1:A:788:GLU:OE1	2.20	0.41
1:B:559:MSE:O	1:B:560:ALA:C	2.63	0.41
1:B:712:ILE:HD12	1:B:717:ILE:HG13	2.03	0.40
1:A:928:ASN:OD1	1:A:928:ASN:C	2.65	0.40
1:B:603:ILE:O	1:B:605:THR:N	2.55	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	395/482 (82%)	385 (98%)	10 (2%)	0	100	100
1	B	400/482 (83%)	384 (96%)	15 (4%)	1 (0%)	36	26
All	All	795/964 (82%)	769 (97%)	25 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	925	ASN

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	311/356 (87%)	310 (100%)	1 (0%)	86	86
1	B	311/356 (87%)	310 (100%)	1 (0%)	86	86
All	All	622/712 (87%)	620 (100%)	2 (0%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	B	900	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	A	722	ASN
1	A	898	ASN
1	A	913	HIS
1	A	925	ASN
1	A	943	GLN
1	A	948	GLN
1	B	527	GLN
1	B	570	GLN
1	B	696	HIS
1	B	722	ASN
1	B	753	ASN
1	B	863	GLN
1	B	913	HIS
1	B	925	ASN
1	B	943	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	PG4	B	1001	-	6,6,12	0.51	0	5,5,11	0.76	0

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	PG4	B	1001	-	-	1/4/4/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	PG4	O1-C1-C2-O2

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	397/482 (82%)	0.58	44 (11%)	10 13	21, 37, 81, 125	1 (0%)
1	B	397/482 (82%)	0.44	34 (8%)	16 19	14, 34, 77, 97	2 (0%)
All	All	794/964 (82%)	0.51	78 (9%)	13 16	14, 35, 79, 125	3 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	6.1
1	A	593	TRP	5.8
1	B	543	VAL	5.6
1	A	551	VAL	5.3
1	B	525	TYR	5.3
1	B	593	TRP	5.1
1	B	603	ILE	5.0
1	B	551	VAL	5.0
1	B	660	ILE	4.6
1	A	525	TYR	4.6
1	A	603	ILE	4.5
1	A	549	THR	4.5
1	A	585	THR	4.3
1	B	545	GLN	4.2
1	A	550	TYR	3.8
1	A	606	THR	3.8
1	B	607	GLY	3.7
1	B	894	ALA	3.7
1	B	896	VAL	3.5
1	A	925	ASN	3.5
1	A	896	VAL	3.5
1	A	894	ALA	3.4
1	A	524	ALA	3.3
1	A	842	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	844	VAL	3.3
1	A	932	TYR	3.2
1	B	526	VAL	3.2
1	A	581	ASN	3.2
1	A	529	GLY	3.1
1	B	585	THR	3.1
1	A	901	PHE	3.0
1	A	601	ALA	3.0
1	B	584	LEU	2.9
1	B	950	LEU	2.9
1	A	545	GLN	2.8
1	A	950	LEU	2.8
1	B	901	PHE	2.8
1	A	607	GLY	2.8
1	A	584	LEU	2.8
1	B	524	ALA	2.7
1	B	529	GLY	2.7
1	A	659	THR	2.7
1	A	924	GLY	2.6
1	B	606	THR	2.6
1	A	900	ASN	2.5
1	A	843	VAL	2.5
1	A	608	SER	2.4
1	B	895	ASP	2.4
1	A	836	VAL	2.4
1	B	900	ASN	2.4
1	A	899	GLY	2.4
1	A	523	SER	2.4
1	A	837	LEU	2.3
1	B	925	ASN	2.3
1	A	526	VAL	2.3
1	B	837	LEU	2.3
1	A	898	ASN	2.3
1	B	836	VAL	2.3
1	B	720	TYR	2.3
1	B	924	GLY	2.3
1	A	895	ASP	2.3
1	B	602	GLY	2.2
1	A	796	LEU	2.2
1	B	541	GLU	2.2
1	A	926	GLY	2.2
1	A	845	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	527	GLN	2.2
1	A	592	ASP	2.1
1	B	594	ARG	2.1
1	B	523	SER	2.1
1	B	899	GLY	2.1
1	A	540	ALA	2.1
1	B	884	GLY	2.0
1	A	579	SER	2.0
1	A	567	ILE	2.0
1	A	714	GLY	2.0
1	B	898	ASN	2.0
1	B	844	VAL	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	PG4	B	1001	7/13	0.81	0.12	42,44,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.