



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:22 AM EDT

PDB ID : 4USX / pdb_00004usx
Title : The Structure of the C-terminal YadA-like domain of BPSL2063 from Burkholderia pseudomallei
Authors : Perletti, L.; Gourlay, L.J.; Peano, C.; Pietrelli, A.; DeBellis, G.; Deantonio, C.; Santoro, C.; Sblattero, D.; Bolognesi, M.
Deposited on : 2014-07-16
Resolution : 1.80 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

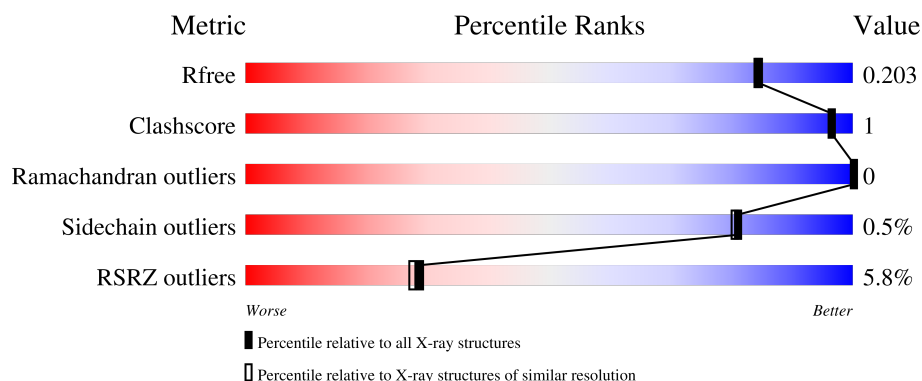
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	371	
1	B	371	
1	C	371	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4746 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 TRIMERIC AUTOTRANSPORTER ADHESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1415	860	247	307	1			
1	B	211	Total	C	N	O	S	0	0	0
			1431	870	250	310	1			
1	C	214	Total	C	N	O	S	0	1	0
			1445	875	254	315	1			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	641	MET	-	expression tag	UNP Q63TA4
A	642	ALA	-	expression tag	UNP Q63TA4
A	643	SER	-	expression tag	UNP Q63TA4
A	644	MET	-	expression tag	UNP Q63TA4
A	645	THR	-	expression tag	UNP Q63TA4
A	646	GLY	-	expression tag	UNP Q63TA4
A	647	GLY	-	expression tag	UNP Q63TA4
A	648	GLN	-	expression tag	UNP Q63TA4
A	649	GLN	-	expression tag	UNP Q63TA4
A	650	MET	-	expression tag	UNP Q63TA4
A	651	GLY	-	expression tag	UNP Q63TA4
A	652	ARG	-	expression tag	UNP Q63TA4
A	653	GLY	-	expression tag	UNP Q63TA4
A	654	SER	-	expression tag	UNP Q63TA4
A	655	MET	-	expression tag	UNP Q63TA4
A	656	ALA	-	expression tag	UNP Q63TA4
A	993	ASN	-	expression tag	UNP Q63TA4
A	994	SER	-	expression tag	UNP Q63TA4
A	995	SER	-	expression tag	UNP Q63TA4
A	996	SER	-	expression tag	UNP Q63TA4
A	997	VAL	-	expression tag	UNP Q63TA4
A	998	ASP	-	expression tag	UNP Q63TA4
A	999	LYS	-	expression tag	UNP Q63TA4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	LEU	-	expression tag	UNP Q63TA4
A	1001	ALA	-	expression tag	UNP Q63TA4
A	1002	ALA	-	expression tag	UNP Q63TA4
A	1003	ALA	-	expression tag	UNP Q63TA4
A	1004	LEU	-	expression tag	UNP Q63TA4
A	1005	GLU	-	expression tag	UNP Q63TA4
A	1006	HIS	-	expression tag	UNP Q63TA4
A	1007	HIS	-	expression tag	UNP Q63TA4
A	1008	HIS	-	expression tag	UNP Q63TA4
A	1009	HIS	-	expression tag	UNP Q63TA4
A	1010	HIS	-	expression tag	UNP Q63TA4
A	1011	HIS	-	expression tag	UNP Q63TA4
B	641	MET	-	expression tag	UNP Q63TA4
B	642	ALA	-	expression tag	UNP Q63TA4
B	643	SER	-	expression tag	UNP Q63TA4
B	644	MET	-	expression tag	UNP Q63TA4
B	645	THR	-	expression tag	UNP Q63TA4
B	646	GLY	-	expression tag	UNP Q63TA4
B	647	GLY	-	expression tag	UNP Q63TA4
B	648	GLN	-	expression tag	UNP Q63TA4
B	649	GLN	-	expression tag	UNP Q63TA4
B	650	MET	-	expression tag	UNP Q63TA4
B	651	GLY	-	expression tag	UNP Q63TA4
B	652	ARG	-	expression tag	UNP Q63TA4
B	653	GLY	-	expression tag	UNP Q63TA4
B	654	SER	-	expression tag	UNP Q63TA4
B	655	MET	-	expression tag	UNP Q63TA4
B	656	ALA	-	expression tag	UNP Q63TA4
B	993	ASN	-	expression tag	UNP Q63TA4
B	994	SER	-	expression tag	UNP Q63TA4
B	995	SER	-	expression tag	UNP Q63TA4
B	996	SER	-	expression tag	UNP Q63TA4
B	997	VAL	-	expression tag	UNP Q63TA4
B	998	ASP	-	expression tag	UNP Q63TA4
B	999	LYS	-	expression tag	UNP Q63TA4
B	1000	LEU	-	expression tag	UNP Q63TA4
B	1001	ALA	-	expression tag	UNP Q63TA4
B	1002	ALA	-	expression tag	UNP Q63TA4
B	1003	ALA	-	expression tag	UNP Q63TA4
B	1004	LEU	-	expression tag	UNP Q63TA4
B	1005	GLU	-	expression tag	UNP Q63TA4
B	1006	HIS	-	expression tag	UNP Q63TA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1007	HIS	-	expression tag	UNP Q63TA4
B	1008	HIS	-	expression tag	UNP Q63TA4
B	1009	HIS	-	expression tag	UNP Q63TA4
B	1010	HIS	-	expression tag	UNP Q63TA4
B	1011	HIS	-	expression tag	UNP Q63TA4
C	641	MET	-	expression tag	UNP Q63TA4
C	642	ALA	-	expression tag	UNP Q63TA4
C	643	SER	-	expression tag	UNP Q63TA4
C	644	MET	-	expression tag	UNP Q63TA4
C	645	THR	-	expression tag	UNP Q63TA4
C	646	GLY	-	expression tag	UNP Q63TA4
C	647	GLY	-	expression tag	UNP Q63TA4
C	648	GLN	-	expression tag	UNP Q63TA4
C	649	GLN	-	expression tag	UNP Q63TA4
C	650	MET	-	expression tag	UNP Q63TA4
C	651	GLY	-	expression tag	UNP Q63TA4
C	652	ARG	-	expression tag	UNP Q63TA4
C	653	GLY	-	expression tag	UNP Q63TA4
C	654	SER	-	expression tag	UNP Q63TA4
C	655	MET	-	expression tag	UNP Q63TA4
C	656	ALA	-	expression tag	UNP Q63TA4
C	993	ASN	-	expression tag	UNP Q63TA4
C	994	SER	-	expression tag	UNP Q63TA4
C	995	SER	-	expression tag	UNP Q63TA4
C	996	SER	-	expression tag	UNP Q63TA4
C	997	VAL	-	expression tag	UNP Q63TA4
C	998	ASP	-	expression tag	UNP Q63TA4
C	999	LYS	-	expression tag	UNP Q63TA4
C	1000	LEU	-	expression tag	UNP Q63TA4
C	1001	ALA	-	expression tag	UNP Q63TA4
C	1002	ALA	-	expression tag	UNP Q63TA4
C	1003	ALA	-	expression tag	UNP Q63TA4
C	1004	LEU	-	expression tag	UNP Q63TA4
C	1005	GLU	-	expression tag	UNP Q63TA4
C	1006	HIS	-	expression tag	UNP Q63TA4
C	1007	HIS	-	expression tag	UNP Q63TA4
C	1008	HIS	-	expression tag	UNP Q63TA4
C	1009	HIS	-	expression tag	UNP Q63TA4
C	1010	HIS	-	expression tag	UNP Q63TA4
C	1011	HIS	-	expression tag	UNP Q63TA4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	4	Total 4	Mg 4	0	0
2	C	2	Total 2	Mg 2	0	0

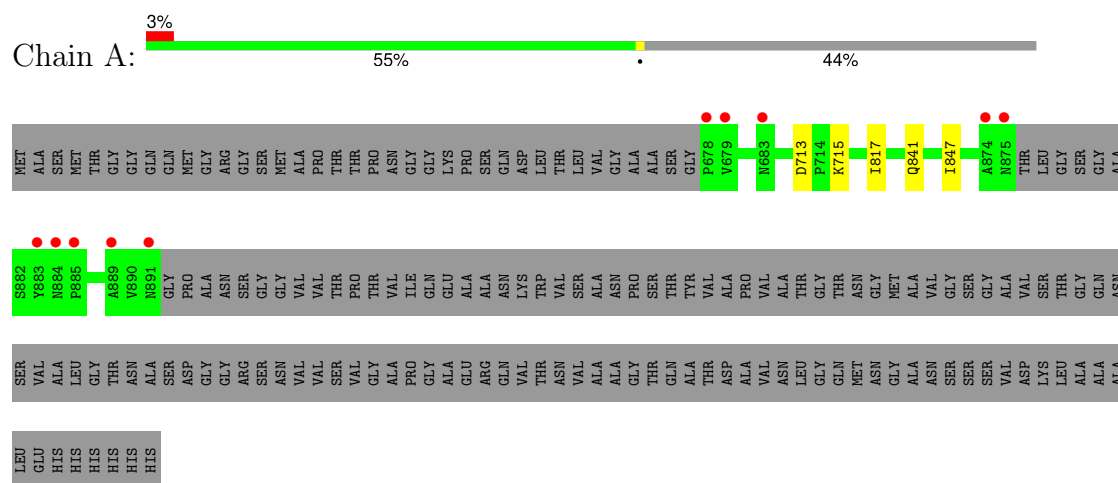
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total 184	O 184	0	0
3	B	150	Total 150	O 150	0	0
3	C	114	Total 114	O 114	0	0

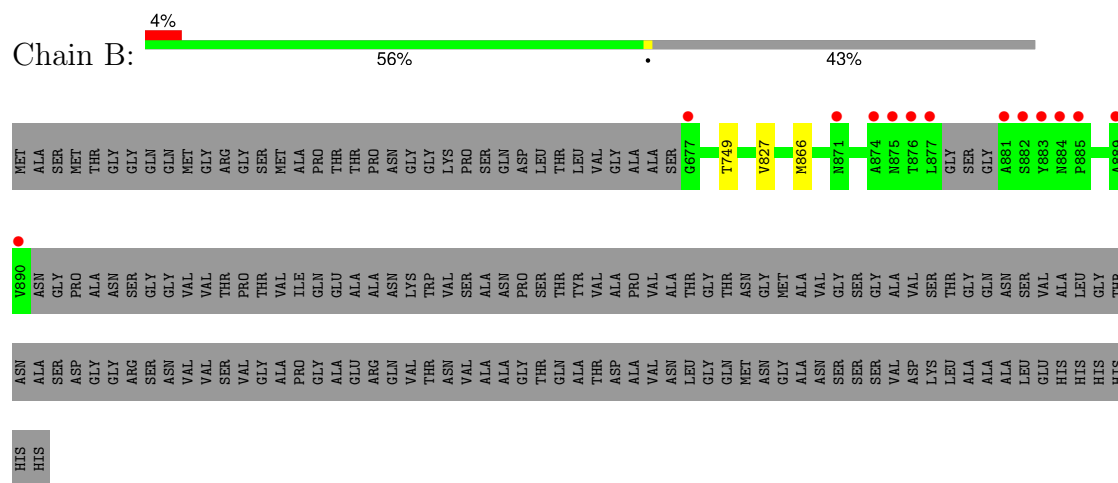
3 Residue-property plots [i](#)

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.

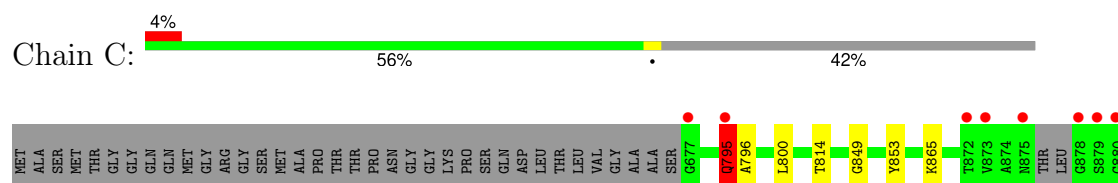
• Molecule 1: TRIMERIC AUTOTRANSPORTER ADHESIN



• Molecule 1: TRIMERIC AUTOTRANSPORTER ADHESIN



• Molecule 1: TRIMERIC AUTOTRANSPORTER ADHESIN



LEU	SER	A861
GLU	VAL	S882
HIS	LEU	Y883
HIS	GLY	G886
HIS	THR	A889
HIS	ASN	V890
HIS	ALA	N891
HIS	SER	G892
	ASP	PRO
	GLY	ALA
	GLY	ASN
	ARG	SER
	SER	GLY
	ASN	GLY
	VAL	VAL
	VAL	THR
	SER	PRO
	VAL	THR
	GLY	VAL
	ALA	ILE
	PRO	GLN
	GLY	GLU
	GLU	ALA
	GLU	ALA
	ARG	ASN
	GLN	ASN
	VAL	LYS
	THR	TRP
	ASN	VAL
	VAL	SER
	ALA	ALA
	ALA	ASN
	GLY	PRO
	THR	SER
	GLN	THR
	ALA	TYR
	THR	VAL
	ASP	ALA
	ALA	PRO
	VAL	VAL
	ASN	ALA
	LEU	THR
	GLY	GLY
	GLN	THR
	MET	ASN
	ASN	GLY
	GLY	MET
	ALA	ALA
	ASN	VAL
	SER	GLY
	SER	SER
	SER	GLY
	VAL	ALA
	ASP	VAL
	LYS	SER
	LEU	THR
	ALA	GLY
	ALA	GLN
	ALA	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 58.85Å 74.41Å 90.00° 104.65° 90.00°	Depositor
Resolution (Å)	39.69 – 1.80 39.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.69-1.80) 93.9 (39.69-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.204 0.169 , 0.203	Depositor DCC
R_{free} test set	2462 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	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	4746	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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: 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	0.49	0/1435	0.75	0/1966
1	B	0.49	0/1448	0.74	0/1985
1	C	0.50	0/1465	0.79	1/2006 (0.0%)
All	All	0.49	0/4348	0.76	1/5957 (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	C	795	GLN	CA-CB-CG	-6.27	101.56	114.10

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	1415	0	1370	5	0
1	B	1431	0	1388	3	0
1	C	1445	0	1395	5	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
3	A	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	150	0	0	0	0
3	C	114	0	0	0	0
All	All	4746	0	4153	8	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 1.

All (8) 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:C:795:GLN:HG3	1:C:796:ALA:N	2.10	0.67
1:A:847:ILE:HD11	1:C:849:GLY:HA2	1.88	0.55
1:A:841:GLN:HG3	1:C:853:TYR:CE2	2.44	0.53
1:C:800:LEU:HD23	1:C:814:THR:HB	1.90	0.53
1:A:817:ILE:HG21	1:B:827:VAL:HG12	1.91	0.52
1:B:866:MET:HE1	1:C:865:LYS:HE2	1.92	0.51
1:A:713:ASP:OD1	1:A:715:LYS:HB3	2.19	0.42
1:A:817:ILE:HG12	1:B:827:VAL:HB	2.02	0.41

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	205/371 (55%)	203 (99%)	2 (1%)	0	100	100
1	B	207/371 (56%)	204 (99%)	3 (1%)	0	100	100
1	C	211/371 (57%)	207 (98%)	4 (2%)	0	100	100
All	All	623/1113 (56%)	614 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	147/259 (57%)	147 (100%)	0	100	100
1	B	148/259 (57%)	147 (99%)	1 (1%)	76	73
1	C	149/259 (58%)	148 (99%)	1 (1%)	76	73
All	All	444/777 (57%)	442 (100%)	2 (0%)	81	80

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

Mol	Chain	Res	Type
1	B	749	THR
1	C	795	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	795	GLN
1	B	833	ASN
1	B	841	GLN
1	C	764	GLN
1	C	805	ASN
1	C	833	ASN
1	C	857	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](#)

Of 7 ligands modelled in this entry, 7 are 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	208/371 (56%)	-0.10	10 (4%)	35 34	8, 17, 42, 50	1 (0%)
1	B	211/371 (56%)	0.01	13 (6%)	26 25	11, 17, 47, 57	0
1	C	214/371 (57%)	-0.04	14 (6%)	25 23	9, 17, 40, 57	1 (0%)
All	All	633/1113 (56%)	-0.04	37 (5%)	29 27	8, 17, 43, 57	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	881	ALA	4.2
1	B	889	ALA	4.0
1	A	678	PRO	3.9
1	B	890	VAL	3.7
1	B	883	TYR	3.5
1	A	889	ALA	3.5
1	A	891	ASN	3.4
1	B	874	ALA	3.4
1	C	875	ASN	3.1
1	A	883	TYR	2.8
1	B	882	SER	2.8
1	C	892	GLY	2.8
1	B	885	PRO	2.8
1	C	888	GLY	2.7
1	C	878	GLY	2.6
1	A	885	PRO	2.6
1	A	874	ALA	2.6
1	C	873	VAL	2.6
1	C	879	SER	2.6
1	A	679	VAL	2.5
1	A	884	ASN	2.4
1	B	877	LEU	2.4
1	C	881	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	677	GLY	2.3
1	B	871	ASN	2.3
1	C	872	THR	2.2
1	B	884	ASN	2.1
1	C	883	TYR	2.1
1	A	875	ASN	2.1
1	B	875	ASN	2.1
1	C	795	GLN	2.1
1	C	677	GLY	2.1
1	C	880	GLY	2.1
1	B	876	THR	2.0
1	A	683	ASN	2.0
1	C	889	ALA	2.0
1	C	891	ASN	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	MG	B	1894	1/1	0.94	0.08	31,31,31,31	0
2	MG	B	1893	1/1	0.96	0.08	28,28,28,28	0
2	MG	C	1894	1/1	0.98	0.05	23,23,23,23	0
2	MG	A	1892	1/1	0.99	0.05	21,21,21,21	0
2	MG	B	1891	1/1	0.99	0.06	20,20,20,20	0
2	MG	C	1893	1/1	0.99	0.07	21,21,21,21	0
2	MG	B	1892	1/1	0.99	0.08	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.