



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:04 AM UTC

PDB ID : 8QJA / pdb_00008qja
Title : T6SS-linked Rhs repeat protein - Advenella mimigardefordensis VgrG-Rhs core
Authors : Kielkopf, C.S.; Shneider, M.M.; Leiman, P.G.; Taylor, N.M.I.
Deposited on : 2023-09-13
Resolution : 3.36 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

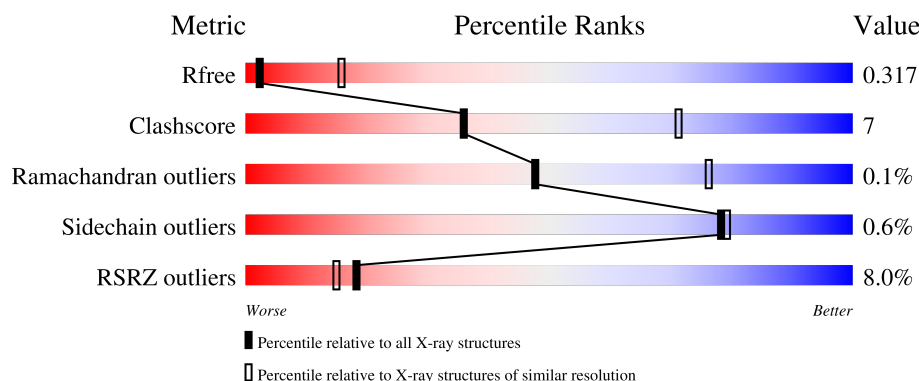
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1879	5% 43% 11% 46%
1	B	1879	4% 44% 11% 45%
1	C	1879	4% 44% 11% 46%
1	D	1879	4% 44% 10% 46%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33470 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 Putative type VI secretion system YD repeat-containing Rhs element Vgr protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0	0
			8365	5240	1479	1631	15			
1	B	1026	Total	C	N	O	S	0	0	0
			8390	5255	1484	1636	15			
1	C	1020	Total	C	N	O	S	0	0	0
			8355	5233	1478	1629	15			
1	D	1021	Total	C	N	O	S	0	0	0
			8360	5236	1479	1630	15			

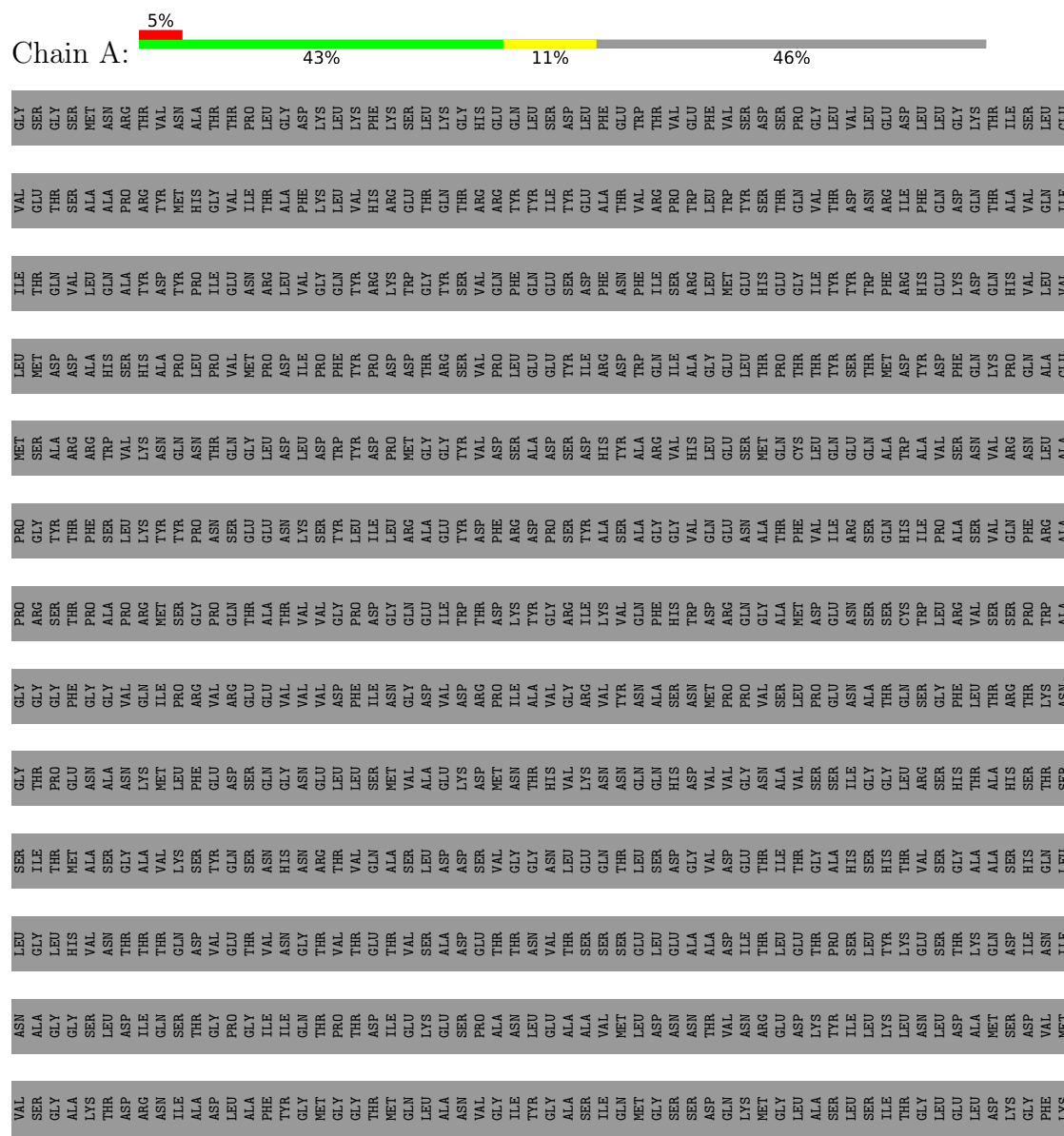
There are 16 discrepancies between the modelled and reference sequences:

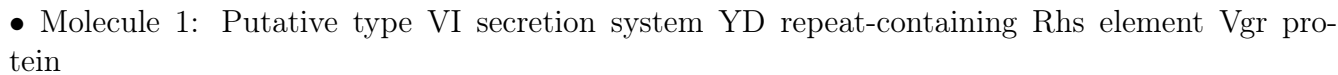
Chain	Residue	Modelled	Actual	Comment	Reference
A	-802	GLY	-	expression tag	UNP W0PIA9
A	-801	SER	-	expression tag	UNP W0PIA9
A	-800	GLY	-	expression tag	UNP W0PIA9
A	-799	SER	-	expression tag	UNP W0PIA9
B	-802	GLY	-	expression tag	UNP W0PIA9
B	-801	SER	-	expression tag	UNP W0PIA9
B	-800	GLY	-	expression tag	UNP W0PIA9
B	-799	SER	-	expression tag	UNP W0PIA9
C	-802	GLY	-	expression tag	UNP W0PIA9
C	-801	SER	-	expression tag	UNP W0PIA9
C	-800	GLY	-	expression tag	UNP W0PIA9
C	-799	SER	-	expression tag	UNP W0PIA9
D	-802	GLY	-	expression tag	UNP W0PIA9
D	-801	SER	-	expression tag	UNP W0PIA9
D	-800	GLY	-	expression tag	UNP W0PIA9
D	-799	SER	-	expression tag	UNP W0PIA9

3 Residue-property plots

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: Putative type VI secretion system YD repeat-containing Rhs element Vgr protein

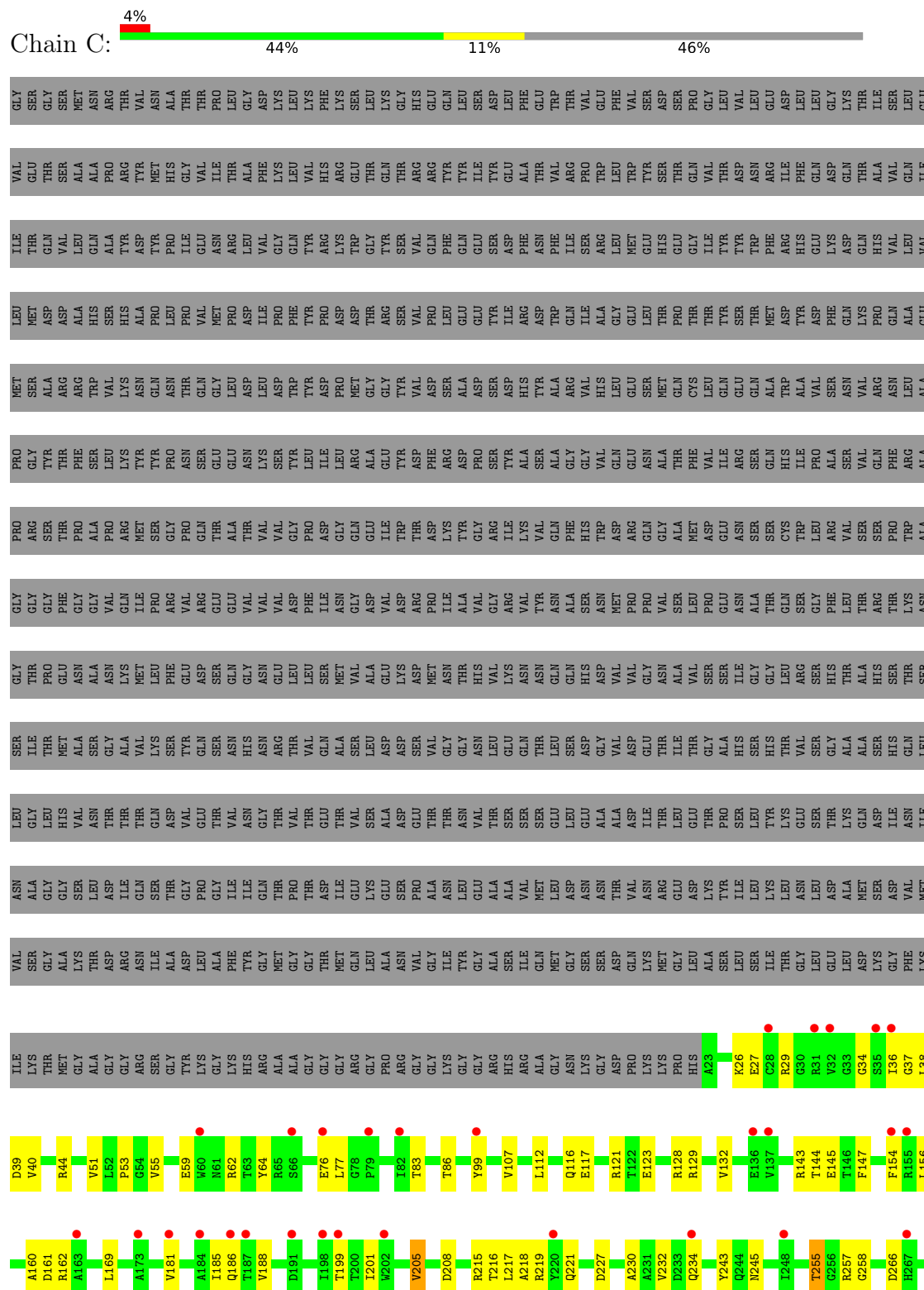


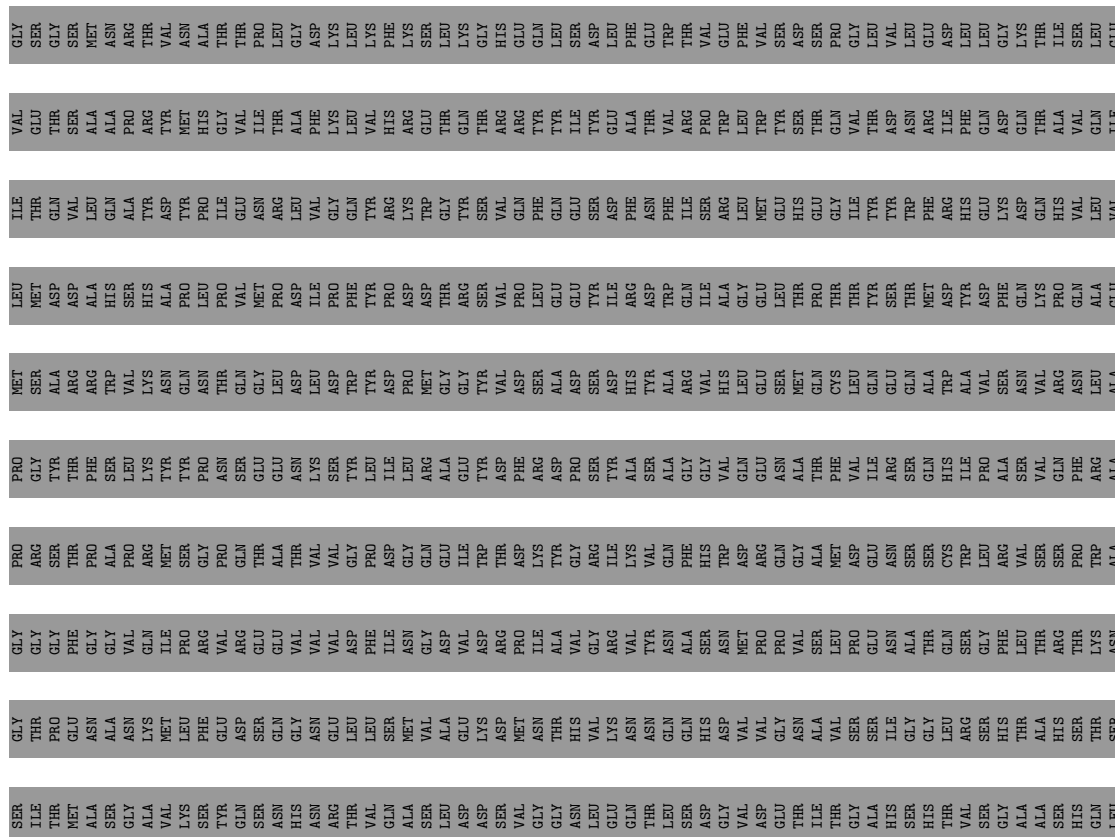






- Molecule 1: Putative type VI secretion system YD repeat-containing Rhs element Vgr protein





F1036	R1037	P1041	D1050	P1051	I1052	G1053	L1054	F1055	G1056	F1060	A1064	P1065	N1066	T1067	A1068	N1069	W1070	I1071	D1072	P1073	F1074	G1075	L1076																																
E926	D931	P940	F945	I949	Q950	Y951	Q952	TYR	SER	ALA	ASP	ASN	THR	PHE	ILE	N1069	GLU	GLY	ARG	ASN	H965	L966	Y971	Q972	H975	Q984	I976	L981	S996	A997	L998	G999	K1000	Q1001	L1002	D1003	SER	ILE	GLY	GLY	ASP	ALA	VAL	A1012	C1019	Y1020	Q1021	N1034	R1035						
E799	D804	P805	S684	P685	G686	S689	Y693	G694	A695	V698	L702	E707	R721	K722	R723	L729	D735	V736	W737	G738	R739	N746	L747	A748	Q749	L755	R756	S757	R758	D765	G766	S767	L768	I771	E772	S774	N903	Q904	Q905	S908	Q909	T913													
D499	E500	G502	R503	A518	R527	K543	L546	L549	Q556	D562	R566	V571	D574	D594	A595	L610	K611	R612	R613	N634	C637	E642	Y643	D644	N647	I650	R651	N657	N662	R663	E664	V665	V666																						
R362	A363	V368	D383	P384	N387	P405	H408	Q413	E417	T421	Q422	N423	V424	N425	P426	V430	S431	T432	L433	S434	L441	T442	R443	S448	N449	K450	E455	Y456	D457	L458	L459	K464	D467	M471	M478	N484	E485	G491	T495																
W202	H203	G207	D208	D209	P212	L213	R214	T215	R216	L217	A218	R219	Q221	A230	Q234	Y235	E236	H246	L247	T248	K254	T255	L261	D299	T308	T315	I316	H317	T324	D331	E332	F333	P342	E347	K348	D352	E353	F354	L358	T361															
R44	L48	D49	F50	V51	E59	R62	T63	Y64	L77	R80	T83	G95	R105	Q116	E117	W118	Y119	D120	R121	T122	E123	L124	I126	F136	V137	S138	Q139	Q142	R143	T144	E148	R149	S150	R155	A160	D161	R162	V181	V188	D191															
VAL	SER	GLY	ALA	THR	GLY	ARG	ASN	GLN	ILE	SER	GLY	TYR	ALA	PRO	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	MET	GLY	ASN	LYS	GLY	ASP	PRO	LYS	LYS	PRO	ALA	TYR	SER	ILE	LEU	LYS	TYR	LYS	ASN	GLY	THR	LEU	ASP	ALA	MET	GLN	ASP	ILE	ASN	VAL	MET

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.24Å 97.78Å 215.01Å 85.69° 89.99° 76.89°	Depositor
Resolution (Å)	48.48 – 3.36 48.48 – 3.36	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.48-3.36) 93.9 (48.48-3.36)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.20.1_4487, BUSTER	Depositor
R, R_{free}	0.257 , 0.317 0.257 , 0.317	Depositor DCC
R_{free} test set	3510 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33470	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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	0.10	0/8565	0.34	0/11607
1	B	0.10	0/8590	0.34	0/11641
1	C	0.11	0/8555	0.33	0/11593
1	D	0.11	0/8560	0.34	0/11600
All	All	0.10	0/34270	0.33	0/46441

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 [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	8365	0	7857	127	0
1	B	8390	0	7882	121	0
1	C	8355	0	7844	118	0
1	D	8360	0	7849	115	0
All	All	33470	0	31432	475	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 7.

The worst 5 of 475 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:29:ARG:NH2	1:B:121:ARG:O	2.09	0.85
1:B:55:VAL:HG11	1:B:417:GLU:HB3	1.57	0.84
1:D:299:ASP:HB2	1:D:543:LYS:HE3	1.59	0.83
1:A:219:ARG:HH22	1:A:236:GLU:HG2	1.47	0.80
1:C:117:GLU:HG2	1:C:128:ARG:HG2	1.65	0.79

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	1013/1879 (54%)	969 (96%)	44 (4%)	0	100	100
1	B	1018/1879 (54%)	971 (95%)	47 (5%)	0	100	100
1	C	1012/1879 (54%)	966 (96%)	45 (4%)	1 (0%)	48	76
1	D	1013/1879 (54%)	968 (96%)	43 (4%)	2 (0%)	43	70
All	All	4056/7516 (54%)	3874 (96%)	179 (4%)	3 (0%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	694	GLY
1	D	694	GLY
1	D	95	GLY

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	889/1607 (55%)	883 (99%)	6 (1%)	76	77
1	B	890/1607 (55%)	886 (100%)	4 (0%)	84	82
1	C	887/1607 (55%)	881 (99%)	6 (1%)	76	77
1	D	887/1607 (55%)	883 (100%)	4 (0%)	81	80
All	All	3553/6428 (55%)	3533 (99%)	20 (1%)	78	79

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	442	ILE
1	D	255	THR
1	D	1021	GLN
1	D	421	ILE
1	B	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1001	GLN
1	D	796	ASN
1	D	116	GLN
1	D	657	ASN
1	D	972	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1021/1879 (54%)	0.84	95 (9%) 14 13	30, 56, 98, 228	0
1	B	1026/1879 (54%)	0.80	80 (7%) 19 15	30, 56, 99, 175	0
1	C	1020/1879 (54%)	0.80	70 (6%) 23 18	39, 68, 108, 156	0
1	D	1021/1879 (54%)	0.82	81 (7%) 18 15	38, 69, 111, 201	0
All	All	4088/7516 (54%)	0.82	326 (7%) 18 15	30, 62, 107, 228	0

The worst 5 of 326 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1035	ARG	6.6
1	D	1067	THR	5.7
1	D	1020	TYR	5.5
1	A	1073	PRO	5.3
1	A	574	ASP	4.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.