



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 02:04 pm BST

PDB ID : 28JF / pdb_000028jf
Title : BKP_yV VP1 IN COMPLEX WITH VHH016
Authors : Akkermans, O.; Ubeda Nicolau, C.; Sienaert, S.; De Graef, S.; Munawar, A.;
Weeks, S.D.
Deposited on : 2026-02-03
Resolution : 2.59 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

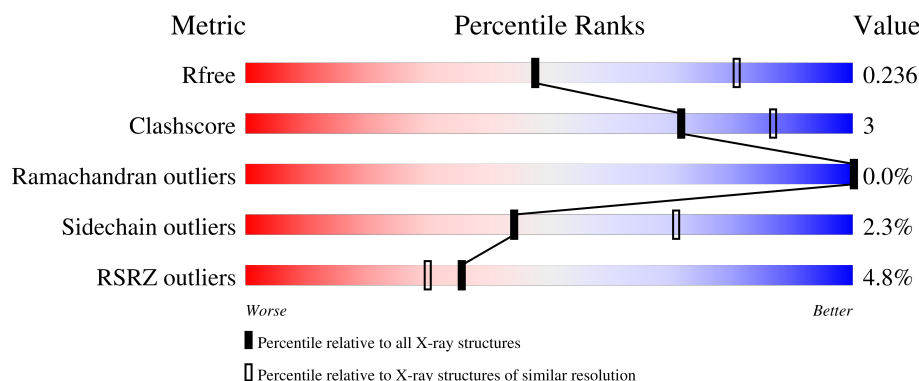
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	273	2% 88% 9% .
1	B	273	5% 87% 9% ..
1	C	273	5% 85% 8% 6%
1	D	273	4% 86% 6% 7%
1	E	273	4% 92% 5% ..

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Mol	Chain	Length	Quality of chain
1	L	273	
1	M	273	
1	N	273	
1	O	273	
1	P	273	
2	F	124	
2	G	124	
2	H	124	
2	I	124	
2	J	124	
2	Q	124	
2	R	124	
2	S	124	
2	T	124	
2	U	124	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 58145 atoms, of which 28565 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	H	N	O	S	61	1	0
			4107	1299	2041	359	396	12			
1	B	264	Total	C	H	N	O	S	61	0	0
			4064	1288	2016	353	395	12			
1	C	257	Total	C	H	N	O	S	63	0	0
			3936	1250	1946	343	385	12			
1	D	253	Total	C	H	N	O	S	60	0	0
			3900	1238	1932	340	378	12			
1	E	267	Total	C	H	N	O	S	61	0	0
			4101	1299	2034	357	399	12			
1	L	265	Total	C	H	N	O	S	61	0	0
			4072	1290	2022	354	394	12			
1	M	257	Total	C	H	N	O	S	61	0	0
			3949	1253	1955	344	385	12			
1	N	251	Total	C	H	N	O	S	60	0	0
			3875	1230	1921	338	374	12			
1	O	256	Total	C	H	N	O	S	61	0	0
			3935	1249	1949	342	383	12			
1	P	267	Total	C	H	N	O	S	61	0	0
			4101	1299	2034	357	399	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP A0A3G2SFE7
A	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
B	25	GLY	-	expression tag	UNP A0A3G2SFE7
B	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
C	25	GLY	-	expression tag	UNP A0A3G2SFE7
C	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
D	25	GLY	-	expression tag	UNP A0A3G2SFE7
D	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
E	25	GLY	-	expression tag	UNP A0A3G2SFE7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
L	25	GLY	-	expression tag	UNP A0A3G2SFE7
L	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
M	25	GLY	-	expression tag	UNP A0A3G2SFE7
M	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
N	25	GLY	-	expression tag	UNP A0A3G2SFE7
N	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
O	25	GLY	-	expression tag	UNP A0A3G2SFE7
O	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7
P	25	GLY	-	expression tag	UNP A0A3G2SFE7
P	104	SER	CYS	engineered mutation	UNP A0A3G2SFE7

- Molecule 2 is a protein called VHH016.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	120	Total	C	H	N	O	S	36	1	0
			1793	565	880	165	179	4			
2	G	118	Total	C	H	N	O	S	34	1	0
			1776	560	872	165	175	4			
2	H	122	Total	C	H	N	O	S	34	0	0
			1814	572	888	169	181	4			
2	I	117	Total	C	H	N	O	S	32	1	0
			1758	554	864	162	174	4			
2	J	116	Total	C	H	N	O	S	31	1	0
			1747	551	859	161	172	4			
2	Q	118	Total	C	H	N	O	S	32	0	0
			1761	555	864	163	175	4			
2	R	118	Total	C	H	N	O	S	30	0	0
			1760	554	864	161	177	4			
2	S	118	Total	C	H	N	O	S	30	0	0
			1760	554	864	161	177	4			
2	T	121	Total	C	H	N	O	S	36	0	0
			1814	572	888	170	180	4			
2	U	118	Total	C	H	N	O	S	32	1	0
			1775	559	872	163	177	4			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	C	2	Total 2	Na 2	0	0
3	D	2	Total 2	Na 2	0	0
3	E	1	Total 1	Na 1	0	0
3	L	3	Total 3	Na 3	0	0
3	M	2	Total 2	Na 2	0	0
3	N	1	Total 1	Na 1	0	0
3	O	2	Total 2	Na 2	0	0
3	P	2	Total 2	Na 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	38	Total 38	O 38	0	0
4	C	26	Total 26	O 26	0	0
4	D	28	Total 28	O 28	0	0
4	E	41	Total 41	O 41	0	0
4	F	7	Total 7	O 7	0	0
4	G	3	Total 3	O 3	0	0
4	H	4	Total 4	O 4	0	0
4	I	2	Total 2	O 2	0	0
4	J	2	Total 2	O 2	0	0

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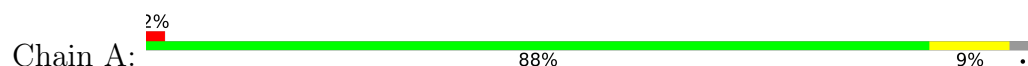
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	29	Total 29	O 29	0	0
4	M	20	Total 20	O 20	0	0
4	N	18	Total 18	O 18	0	0
4	O	24	Total 24	O 24	0	0
4	P	33	Total 33	O 33	0	0
4	Q	4	Total 4	O 4	0	0
4	R	6	Total 6	O 6	0	0
4	S	2	Total 2	O 2	0	0
4	T	6	Total 6	O 6	0	0
4	U	5	Total 5	O 5	0	0

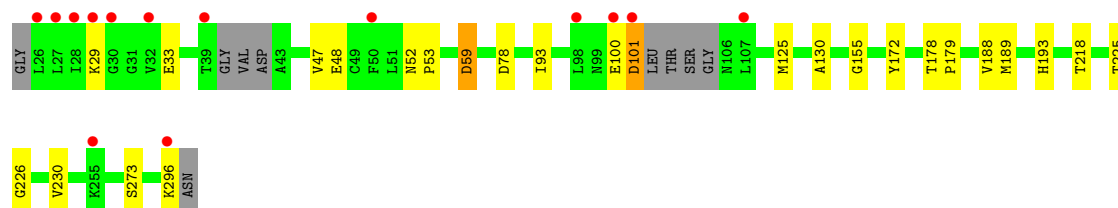
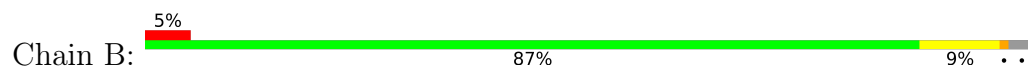
3 Residue-property plots [i](#)

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.

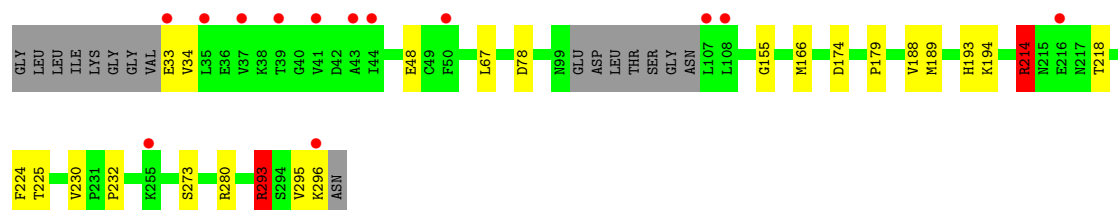
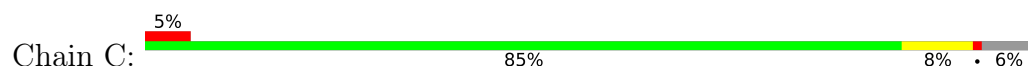
- Molecule 1: Capsid protein VP1



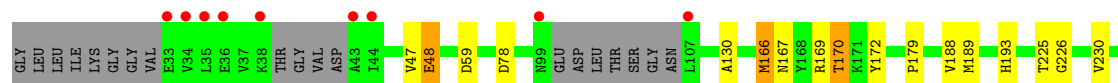
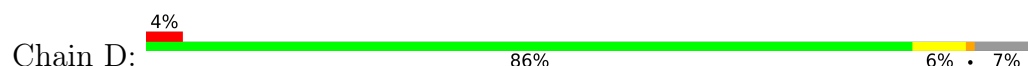
- Molecule 1: Capsid protein VP1

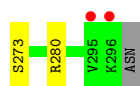


- Molecule 1: Capsid protein VP1

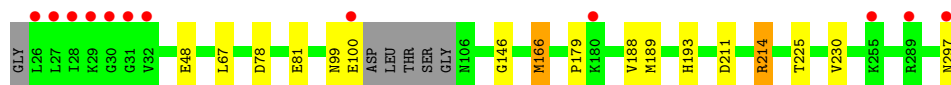


- Molecule 1: Capsid protein VP1

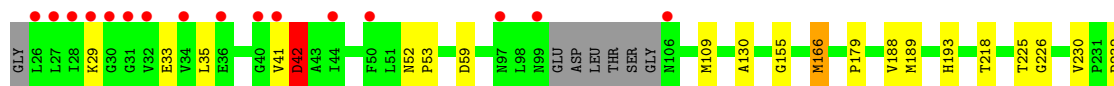
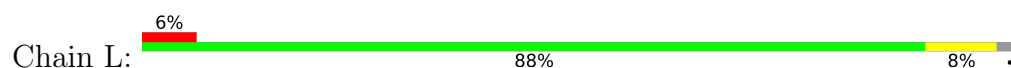




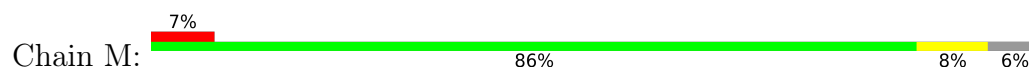
- Molecule 1: Capsid protein VP1



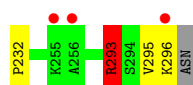
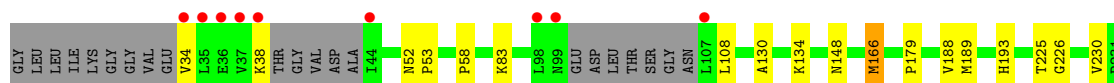
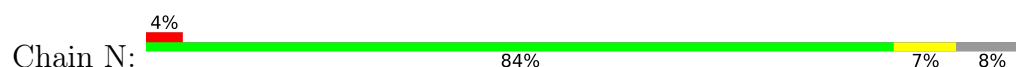
- Molecule 1: Capsid protein VP1



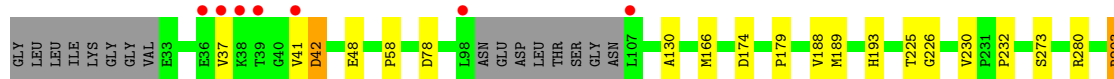
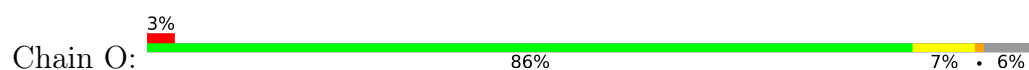
- Molecule 1: Capsid protein VP1



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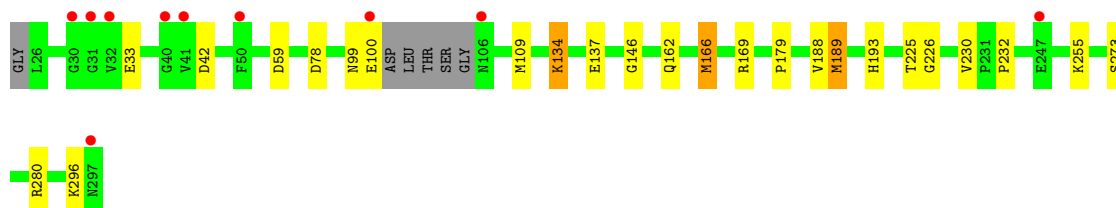
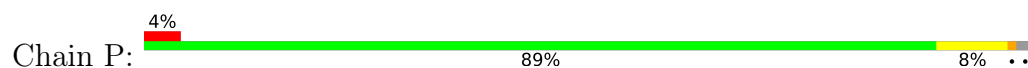


- Molecule 1: Capsid protein VP1

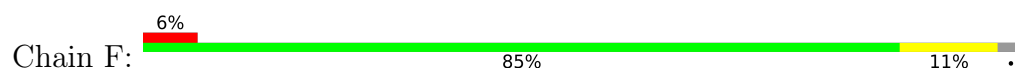




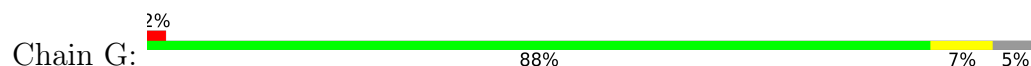
- Molecule 1: Capsid protein VP1



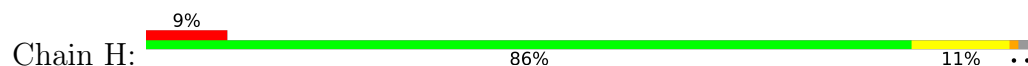
- Molecule 2: VHH016



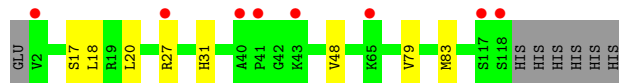
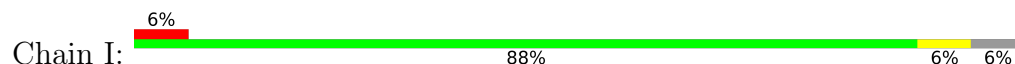
- Molecule 2: VHH016



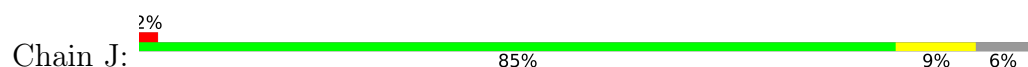
- Molecule 2: VHH016



- Molecule 2: VHH016



- Molecule 2: VHH016



● Molecule 2: VHH016

Chain Q:  4% 85% 9% 5%



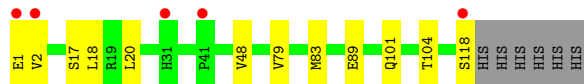
● Molecule 2: VHH016

Chain R:  6% 85% 10% 5%



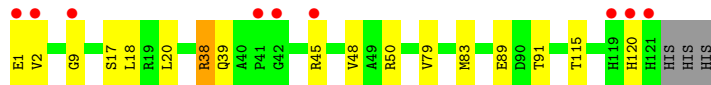
● Molecule 2: VHH016

Chain S:  4% 85% 10% 5%



● Molecule 2: VHH016

Chain T:  7% 84% 13% 5%



● Molecule 2: VHH016

Chain U:  2% 85% 10% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.58Å 135.27Å 167.83Å 90.00° 97.79° 90.00°	Depositor
Resolution (Å)	116.77 – 2.59 116.77 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (116.77-2.59) 99.8 (116.77-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.211 , 0.236 0.211 , 0.236	Depositor DCC
R_{free} test set	8025 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	58145	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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:
NA

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	0.55	0/2114	0.90	1/2870 (0.0%)
1	B	0.53	0/2092	0.91	3/2839 (0.1%)
1	C	0.54	0/2035	0.95	4/2766 (0.1%)
1	D	0.53	0/2012	0.90	4/2731 (0.1%)
1	E	0.55	0/2112	0.93	1/2868 (0.0%)
1	L	0.52	0/2095	0.87	2/2845 (0.1%)
1	M	0.52	0/2039	0.89	2/2770 (0.1%)
1	N	0.52	0/1998	0.91	1/2712 (0.0%)
1	O	0.54	0/2031	0.93	3/2759 (0.1%)
1	P	0.56	0/2112	0.92	3/2868 (0.1%)
2	F	0.54	0/933	0.88	0/1260
2	G	0.53	0/925	0.85	0/1249
2	H	0.55	0/944	0.91	0/1275
2	I	0.53	0/914	0.85	0/1234
2	J	0.52	0/908	0.86	0/1226
2	Q	0.51	0/914	0.93	3/1234 (0.2%)
2	R	0.57	0/912	0.92	1/1231 (0.1%)
2	S	0.51	0/912	0.86	0/1231
2	T	0.54	0/945	0.95	2/1276 (0.2%)
2	U	0.56	0/923	0.94	1/1246 (0.1%)
All	All	0.54	0/29870	0.91	31/40490 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Q	0	2
2	R	0	1
2	T	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	293	ARG	CG-CD-NE	14.29	143.43	112.00
1	C	293	ARG	CB-CG-CD	8.06	129.85	111.30
1	N	293	ARG	CB-CG-CD	8.00	129.71	111.30
1	A	60	GLU	CB-CA-C	-7.68	95.56	110.46
1	P	189	MET	CG-SD-CE	-6.79	85.96	100.90

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ARG	Sidechain
1	C	214	ARG	Sidechain
1	C	293	ARG	Sidechain
1	N	293	ARG	Sidechain
2	Q	38	ARG	Sidechain

5.2 Too-close contacts

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	2066	2041	2033	19	1
1	B	2048	2016	2007	21	0
1	C	1990	1946	1936	19	0
1	D	1968	1932	1923	13	0
1	E	2067	2034	2026	13	0
1	L	2050	2022	2014	21	0
1	M	1994	1955	1947	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1954	1921	1912	23	0
1	O	1986	1949	1941	15	0
1	P	2067	2034	2026	18	0
2	F	913	880	874	8	0
2	G	904	872	868	4	0
2	H	926	888	881	10	0
2	I	894	864	861	7	0
2	J	888	859	856	5	0
2	Q	897	864	861	4	0
2	R	896	864	863	3	1
2	S	896	864	863	4	0
2	T	926	888	884	6	0
2	U	903	872	870	11	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	L	3	0	0	0	0
3	M	2	0	0	0	0
3	N	1	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	30	0	0	0	0
4	B	38	0	0	0	0
4	C	26	0	0	2	0
4	D	28	0	0	3	0
4	E	41	0	0	1	0
4	F	7	0	0	2	0
4	G	3	0	0	0	0
4	H	4	0	0	1	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	L	29	0	0	0	0
4	M	20	0	0	0	0
4	N	18	0	0	1	0
4	O	24	0	0	0	0
4	P	33	0	0	2	0
4	Q	4	0	0	0	0
4	R	6	0	0	0	0
4	S	2	0	0	0	0
4	T	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	5	0	0	1	0
All	All	29580	28565	28446	190	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.

The worst 5 of 190 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:P:169:ARG:HH22	2:U:31[A]:HIS:HE1	1.18	0.88
1:A:63[B]:ARG:CG	1:A:63[B]:ARG:HH11	1.88	0.85
1:C:67:LEU:HD11	2:I:27:ARG:HG3	1.60	0.83
1:D:169:ARG:HH22	2:I:31[B]:HIS:HE1	1.28	0.79
1:D:78:ASP:OD2	1:D:170:THR:HG22	1.83	0.77

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:213:SER:HG	2:R:42:GLY:HA3[2_546]	1.19	0.41

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	263/273 (96%)	254 (97%)	9 (3%)	0	100	100
1	B	258/273 (94%)	250 (97%)	8 (3%)	0	100	100
1	C	253/273 (93%)	244 (96%)	9 (4%)	0	100	100
1	D	247/273 (90%)	239 (97%)	8 (3%)	0	100	100
1	E	263/273 (96%)	254 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	261/273 (96%)	252 (97%)	9 (3%)	0	100	100
1	M	253/273 (93%)	243 (96%)	10 (4%)	0	100	100
1	N	245/273 (90%)	237 (97%)	8 (3%)	0	100	100
1	O	252/273 (92%)	243 (96%)	9 (4%)	0	100	100
1	P	263/273 (96%)	255 (97%)	8 (3%)	0	100	100
2	F	119/124 (96%)	116 (98%)	3 (2%)	0	100	100
2	G	117/124 (94%)	114 (97%)	3 (3%)	0	100	100
2	H	120/124 (97%)	115 (96%)	4 (3%)	1 (1%)	16	34
2	I	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
2	J	115/124 (93%)	112 (97%)	3 (3%)	0	100	100
2	Q	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
2	R	116/124 (94%)	114 (98%)	2 (2%)	0	100	100
2	S	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
2	T	119/124 (96%)	115 (97%)	4 (3%)	0	100	100
2	U	117/124 (94%)	114 (97%)	3 (3%)	0	100	100
All	All	3729/3970 (94%)	3610 (97%)	118 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	120	HIS

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	230/234 (98%)	227 (99%)	3 (1%)	61	82
1	B	228/234 (97%)	226 (99%)	2 (1%)	70	87
1	C	221/234 (94%)	218 (99%)	3 (1%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	219/234 (94%)	215 (98%)	4 (2%)	51	76
1	E	230/234 (98%)	228 (99%)	2 (1%)	70	87
1	L	228/234 (97%)	226 (99%)	2 (1%)	70	87
1	M	222/234 (95%)	221 (100%)	1 (0%)	81	92
1	N	218/234 (93%)	216 (99%)	2 (1%)	70	87
1	O	221/234 (94%)	215 (97%)	6 (3%)	39	67
1	P	230/234 (98%)	226 (98%)	4 (2%)	53	78
2	F	94/99 (95%)	89 (95%)	5 (5%)	20	43
2	G	94/99 (95%)	91 (97%)	3 (3%)	34	62
2	H	95/99 (96%)	90 (95%)	5 (5%)	20	43
2	I	93/99 (94%)	90 (97%)	3 (3%)	34	62
2	J	92/99 (93%)	88 (96%)	4 (4%)	26	51
2	Q	93/99 (94%)	87 (94%)	6 (6%)	15	35
2	R	93/99 (94%)	89 (96%)	4 (4%)	26	51
2	S	93/99 (94%)	88 (95%)	5 (5%)	20	42
2	T	96/99 (97%)	90 (94%)	6 (6%)	16	36
2	U	94/99 (95%)	90 (96%)	4 (4%)	26	51
All	All	3184/3330 (96%)	3110 (98%)	74 (2%)	44	71

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	79	VAL
2	U	77	ASN
2	S	17	SER
2	T	39	GLN
2	H	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	77	ASN
2	S	113	GLN
1	L	278	GLN
2	U	77	ASN

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Mol	Chain	Res	Type
1	P	272	ASN

5.3.3 RNA [i](#)

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](#)

Of 19 ligands modelled in this entry, 19 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	266/273 (97%)	-0.20	5 (1%) 66 61	25, 41, 84, 120	1 (0%)
1	B	264/273 (96%)	-0.03	14 (5%) 32 26	31, 44, 91, 132	0
1	C	257/273 (94%)	0.13	13 (5%) 33 28	32, 45, 93, 126	0
1	D	253/273 (92%)	0.06	11 (4%) 40 34	31, 44, 87, 122	0
1	E	267/273 (97%)	-0.12	12 (4%) 38 32	30, 41, 86, 146	0
1	L	265/273 (97%)	0.19	16 (6%) 27 22	35, 48, 112, 192	0
1	M	257/273 (94%)	0.23	19 (7%) 20 16	34, 51, 111, 135	0
1	N	251/273 (91%)	0.12	12 (4%) 35 30	34, 49, 92, 123	0
1	O	256/273 (93%)	0.03	8 (3%) 51 45	31, 44, 90, 125	0
1	P	267/273 (97%)	-0.08	10 (3%) 45 39	31, 45, 80, 118	0
2	F	120/124 (96%)	0.25	7 (5%) 29 23	18, 47, 81, 97	1 (0%)
2	G	118/124 (95%)	0.26	3 (2%) 58 52	17, 52, 87, 118	1 (0%)
2	H	122/124 (98%)	0.30	11 (9%) 15 11	34, 47, 85, 104	0
2	I	117/124 (94%)	0.38	8 (6%) 23 19	20, 54, 88, 117	1 (0%)
2	J	116/124 (93%)	0.30	3 (2%) 57 51	21, 56, 93, 108	1 (0%)
2	Q	118/124 (95%)	0.30	5 (4%) 40 35	38, 52, 83, 114	0
2	R	118/124 (95%)	0.20	7 (5%) 28 23	35, 46, 71, 115	0
2	S	118/124 (95%)	0.48	5 (4%) 40 35	40, 57, 94, 137	0
2	T	121/124 (97%)	0.46	9 (7%) 20 16	40, 53, 97, 121	0
2	U	118/124 (95%)	0.07	3 (2%) 58 52	19, 46, 72, 98	1 (0%)
All	All	3789/3970 (95%)	0.12	181 (4%) 35 30	17, 47, 91, 192	6 (0%)

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	2	VAL	7.6
2	Q	2	VAL	6.9
2	G	2	VAL	6.3
2	I	2	VAL	6.1
2	R	118	SER	6.0

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
3	NA	M	302	1/1	0.81	0.28	56,56,56,56	0
3	NA	P	302	1/1	0.81	0.28	50,50,50,50	0
3	NA	B	301	1/1	0.82	0.27	44,44,44,44	0
3	NA	A	303	1/1	0.83	0.25	51,51,51,51	0
3	NA	N	301	1/1	0.88	0.25	51,51,51,51	0
3	NA	L	303	1/1	0.89	0.24	45,45,45,45	0
3	NA	D	302	1/1	0.90	0.17	36,36,36,36	0
3	NA	L	302	1/1	0.93	0.16	43,43,43,43	0
3	NA	P	301	1/1	0.94	0.28	46,46,46,46	0
3	NA	O	302	1/1	0.94	0.19	37,37,37,37	0
3	NA	L	301	1/1	0.95	0.36	49,49,49,49	0
3	NA	O	301	1/1	0.95	0.34	56,56,56,56	0
3	NA	C	302	1/1	0.95	0.19	42,42,42,42	0
3	NA	A	302	1/1	0.95	0.32	46,46,46,46	0
3	NA	E	301	1/1	0.95	0.34	52,52,52,52	0
3	NA	M	301	1/1	0.96	0.32	52,52,52,52	0
3	NA	C	301	1/1	0.97	0.26	39,39,39,39	0
3	NA	A	301	1/1	0.97	0.29	40,40,40,40	0
3	NA	D	301	1/1	0.97	0.33	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.