



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2025 – 08:32 AM JST

PDB ID : 9K0L / pdb\_00009k0l  
Title : crystal structure Rtk's of F222  
Authors : Xu, M.; Ran, T.; Wang, W.  
Deposited on : 2024-10-15  
Resolution : 2.46 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](mailto: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>.

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

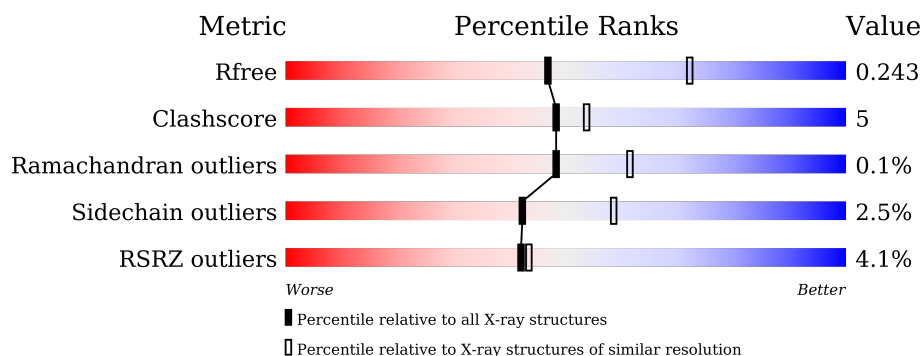
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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  $\geq 3$ , 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	227	<div> <div>3%</div> <div>78% 14% • 7%</div> </div>
1	B	227	<div> <div>4%</div> <div>79% 12% 8%</div> </div>
1	C	227	<div> <div>4%</div> <div>78% 13% • 8%</div> </div>
1	D	227	<div> <div>4%</div> <div>77% 15% • 7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6319 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 Type VI secretion system-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1586	1007	279	296	4			
1	B	208	Total	C	N	O	S	0	0	0
			1559	988	276	291	4			
1	C	208	Total	C	N	O	S	0	0	0
			1549	982	272	291	4			
1	D	210	Total	C	N	O	S	0	0	0
			1564	993	274	293	4			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP A0A2V4GN18
A	-11	PHE	-	expression tag	UNP A0A2V4GN18
A	-10	ALA	-	expression tag	UNP A0A2V4GN18
A	-9	LYS	-	expression tag	UNP A0A2V4GN18
A	-8	ILE	-	expression tag	UNP A0A2V4GN18
A	-7	GLU	-	expression tag	UNP A0A2V4GN18
A	-6	GLU	-	expression tag	UNP A0A2V4GN18
A	-5	GLY	-	expression tag	UNP A0A2V4GN18
A	-4	LYS	-	expression tag	UNP A0A2V4GN18
A	-3	LEU	-	expression tag	UNP A0A2V4GN18
A	-2	VAL	-	expression tag	UNP A0A2V4GN18
A	-1	ILE	-	expression tag	UNP A0A2V4GN18
A	0	HIS	-	expression tag	UNP A0A2V4GN18
A	1	MET	ILE	conflict	UNP A0A2V4GN18
A	14	SER	THR	conflict	UNP A0A2V4GN18
A	40	SER	ALA	conflict	UNP A0A2V4GN18
A	87	VAL	ILE	conflict	UNP A0A2V4GN18
A	105	ILE	VAL	conflict	UNP A0A2V4GN18
A	120	THR	SER	conflict	UNP A0A2V4GN18
A	124	GLN	LYS	conflict	UNP A0A2V4GN18
A	147	THR	ASN	conflict	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	153	VAL	LEU	conflict	UNP A0A2V4GN18
A	199	LEU	-	expression tag	UNP A0A2V4GN18
A	200	GLU	-	expression tag	UNP A0A2V4GN18
A	201	GLY	-	expression tag	UNP A0A2V4GN18
A	202	SER	-	expression tag	UNP A0A2V4GN18
A	203	GLU	-	expression tag	UNP A0A2V4GN18
A	204	PHE	-	expression tag	UNP A0A2V4GN18
A	205	LYS	-	expression tag	UNP A0A2V4GN18
A	206	LEU	-	expression tag	UNP A0A2V4GN18
A	207	VAL	-	expression tag	UNP A0A2V4GN18
A	208	ASP	-	expression tag	UNP A0A2V4GN18
A	209	HIS	-	expression tag	UNP A0A2V4GN18
A	210	HIS	-	expression tag	UNP A0A2V4GN18
A	211	HIS	-	expression tag	UNP A0A2V4GN18
A	212	HIS	-	expression tag	UNP A0A2V4GN18
A	213	HIS	-	expression tag	UNP A0A2V4GN18
A	214	HIS	-	expression tag	UNP A0A2V4GN18
B	-12	ALA	-	expression tag	UNP A0A2V4GN18
B	-11	PHE	-	expression tag	UNP A0A2V4GN18
B	-10	ALA	-	expression tag	UNP A0A2V4GN18
B	-9	LYS	-	expression tag	UNP A0A2V4GN18
B	-8	ILE	-	expression tag	UNP A0A2V4GN18
B	-7	GLU	-	expression tag	UNP A0A2V4GN18
B	-6	GLU	-	expression tag	UNP A0A2V4GN18
B	-5	GLY	-	expression tag	UNP A0A2V4GN18
B	-4	LYS	-	expression tag	UNP A0A2V4GN18
B	-3	LEU	-	expression tag	UNP A0A2V4GN18
B	-2	VAL	-	expression tag	UNP A0A2V4GN18
B	-1	ILE	-	expression tag	UNP A0A2V4GN18
B	0	HIS	-	expression tag	UNP A0A2V4GN18
B	1	MET	ILE	conflict	UNP A0A2V4GN18
B	14	SER	THR	conflict	UNP A0A2V4GN18
B	40	SER	ALA	conflict	UNP A0A2V4GN18
B	87	VAL	ILE	conflict	UNP A0A2V4GN18
B	105	ILE	VAL	conflict	UNP A0A2V4GN18
B	120	THR	SER	conflict	UNP A0A2V4GN18
B	124	GLN	LYS	conflict	UNP A0A2V4GN18
B	147	THR	ASN	conflict	UNP A0A2V4GN18
B	153	VAL	LEU	conflict	UNP A0A2V4GN18
B	199	LEU	-	expression tag	UNP A0A2V4GN18
B	200	GLU	-	expression tag	UNP A0A2V4GN18
B	201	GLY	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
B	202	SER	-	expression tag	UNP A0A2V4GN18
B	203	GLU	-	expression tag	UNP A0A2V4GN18
B	204	PHE	-	expression tag	UNP A0A2V4GN18
B	205	LYS	-	expression tag	UNP A0A2V4GN18
B	206	LEU	-	expression tag	UNP A0A2V4GN18
B	207	VAL	-	expression tag	UNP A0A2V4GN18
B	208	ASP	-	expression tag	UNP A0A2V4GN18
B	209	HIS	-	expression tag	UNP A0A2V4GN18
B	210	HIS	-	expression tag	UNP A0A2V4GN18
B	211	HIS	-	expression tag	UNP A0A2V4GN18
B	212	HIS	-	expression tag	UNP A0A2V4GN18
B	213	HIS	-	expression tag	UNP A0A2V4GN18
B	214	HIS	-	expression tag	UNP A0A2V4GN18
C	-12	ALA	-	expression tag	UNP A0A2V4GN18
C	-11	PHE	-	expression tag	UNP A0A2V4GN18
C	-10	ALA	-	expression tag	UNP A0A2V4GN18
C	-9	LYS	-	expression tag	UNP A0A2V4GN18
C	-8	ILE	-	expression tag	UNP A0A2V4GN18
C	-7	GLU	-	expression tag	UNP A0A2V4GN18
C	-6	GLU	-	expression tag	UNP A0A2V4GN18
C	-5	GLY	-	expression tag	UNP A0A2V4GN18
C	-4	LYS	-	expression tag	UNP A0A2V4GN18
C	-3	LEU	-	expression tag	UNP A0A2V4GN18
C	-2	VAL	-	expression tag	UNP A0A2V4GN18
C	-1	ILE	-	expression tag	UNP A0A2V4GN18
C	0	HIS	-	expression tag	UNP A0A2V4GN18
C	1	MET	ILE	conflict	UNP A0A2V4GN18
C	14	SER	THR	conflict	UNP A0A2V4GN18
C	40	SER	ALA	conflict	UNP A0A2V4GN18
C	87	VAL	ILE	conflict	UNP A0A2V4GN18
C	105	ILE	VAL	conflict	UNP A0A2V4GN18
C	120	THR	SER	conflict	UNP A0A2V4GN18
C	124	GLN	LYS	conflict	UNP A0A2V4GN18
C	147	THR	ASN	conflict	UNP A0A2V4GN18
C	153	VAL	LEU	conflict	UNP A0A2V4GN18
C	199	LEU	-	expression tag	UNP A0A2V4GN18
C	200	GLU	-	expression tag	UNP A0A2V4GN18
C	201	GLY	-	expression tag	UNP A0A2V4GN18
C	202	SER	-	expression tag	UNP A0A2V4GN18
C	203	GLU	-	expression tag	UNP A0A2V4GN18
C	204	PHE	-	expression tag	UNP A0A2V4GN18
C	205	LYS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	LEU	-	expression tag	UNP A0A2V4GN18
C	207	VAL	-	expression tag	UNP A0A2V4GN18
C	208	ASP	-	expression tag	UNP A0A2V4GN18
C	209	HIS	-	expression tag	UNP A0A2V4GN18
C	210	HIS	-	expression tag	UNP A0A2V4GN18
C	211	HIS	-	expression tag	UNP A0A2V4GN18
C	212	HIS	-	expression tag	UNP A0A2V4GN18
C	213	HIS	-	expression tag	UNP A0A2V4GN18
C	214	HIS	-	expression tag	UNP A0A2V4GN18
D	-12	ALA	-	expression tag	UNP A0A2V4GN18
D	-11	PHE	-	expression tag	UNP A0A2V4GN18
D	-10	ALA	-	expression tag	UNP A0A2V4GN18
D	-9	LYS	-	expression tag	UNP A0A2V4GN18
D	-8	ILE	-	expression tag	UNP A0A2V4GN18
D	-7	GLU	-	expression tag	UNP A0A2V4GN18
D	-6	GLU	-	expression tag	UNP A0A2V4GN18
D	-5	GLY	-	expression tag	UNP A0A2V4GN18
D	-4	LYS	-	expression tag	UNP A0A2V4GN18
D	-3	LEU	-	expression tag	UNP A0A2V4GN18
D	-2	VAL	-	expression tag	UNP A0A2V4GN18
D	-1	ILE	-	expression tag	UNP A0A2V4GN18
D	0	HIS	-	expression tag	UNP A0A2V4GN18
D	1	MET	ILE	conflict	UNP A0A2V4GN18
D	14	SER	THR	conflict	UNP A0A2V4GN18
D	40	SER	ALA	conflict	UNP A0A2V4GN18
D	87	VAL	ILE	conflict	UNP A0A2V4GN18
D	105	ILE	VAL	conflict	UNP A0A2V4GN18
D	120	THR	SER	conflict	UNP A0A2V4GN18
D	124	GLN	LYS	conflict	UNP A0A2V4GN18
D	147	THR	ASN	conflict	UNP A0A2V4GN18
D	153	VAL	LEU	conflict	UNP A0A2V4GN18
D	199	LEU	-	expression tag	UNP A0A2V4GN18
D	200	GLU	-	expression tag	UNP A0A2V4GN18
D	201	GLY	-	expression tag	UNP A0A2V4GN18
D	202	SER	-	expression tag	UNP A0A2V4GN18
D	203	GLU	-	expression tag	UNP A0A2V4GN18
D	204	PHE	-	expression tag	UNP A0A2V4GN18
D	205	LYS	-	expression tag	UNP A0A2V4GN18
D	206	LEU	-	expression tag	UNP A0A2V4GN18
D	207	VAL	-	expression tag	UNP A0A2V4GN18
D	208	ASP	-	expression tag	UNP A0A2V4GN18
D	209	HIS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
D	210	HIS	-	expression tag	UNP A0A2V4GN18
D	211	HIS	-	expression tag	UNP A0A2V4GN18
D	212	HIS	-	expression tag	UNP A0A2V4GN18
D	213	HIS	-	expression tag	UNP A0A2V4GN18
D	214	HIS	-	expression tag	UNP A0A2V4GN18

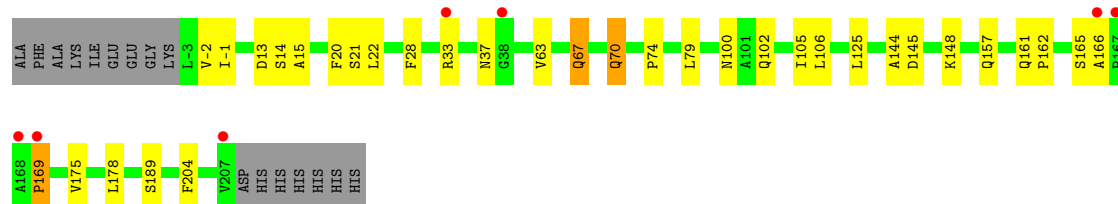
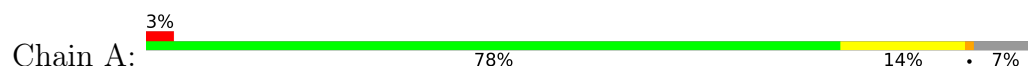
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	20	Total O 20 20	0	0
2	C	11	Total O 11 11	0	0
2	D	7	Total O 7 7	0	0

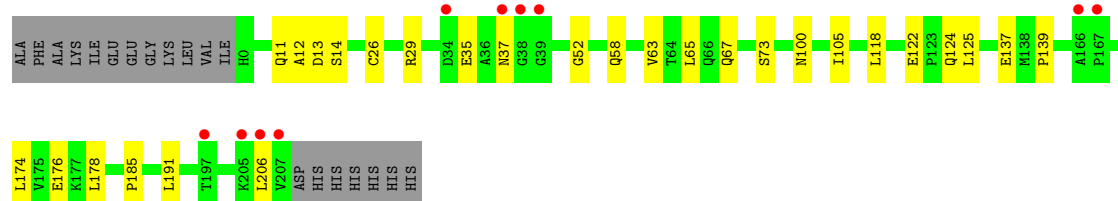
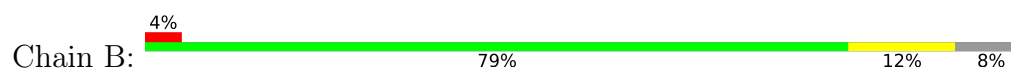
### 3 Residue-property plots [i](#)

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.

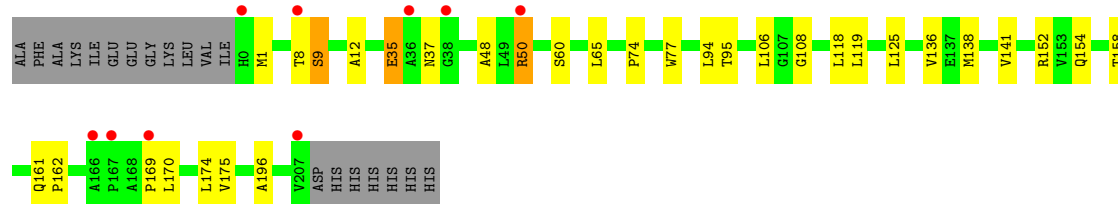
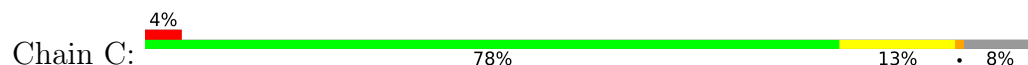
- Molecule 1: Type VI secretion system-associated protein



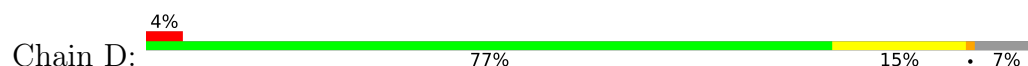
- Molecule 1: Type VI secretion system-associated protein

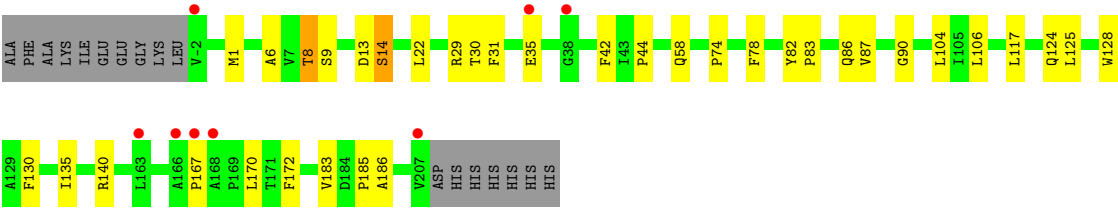


- Molecule 1: Type VI secretion system-associated protein



- Molecule 1: Type VI secretion system-associated protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.44Å 150.81Å 228.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.49 – 2.46 20.49 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.49-2.46) 95.0 (20.49-2.46)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.206 , 0.240 0.214 , 0.243	Depositor DCC
$R_{free}$ test set	1987 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.50	0/1626	0.69	3/2219 (0.1%)
1	B	0.52	0/1599	0.70	2/2182 (0.1%)
1	C	0.55	0/1589	0.70	3/2171 (0.1%)
1	D	0.40	0/1604	0.63	1/2192 (0.0%)
All	All	0.50	0/6418	0.68	9/8764 (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	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	169	PRO	N-CA-C	-7.38	100.95	113.12
1	B	26	CYS	N-CA-C	6.39	118.77	110.53
1	D	167	PRO	N-CA-C	-6.11	99.89	112.47
1	A	21	SER	N-CA-C	5.80	119.09	109.46
1	C	12	ALA	N-CA-C	5.56	118.06	110.55
1	A	28	PHE	N-CA-C	-5.53	100.76	109.50
1	A	169	PRO	N-CA-C	-5.34	101.46	112.47
1	B	29	ARG	N-CA-C	5.27	116.99	108.34
1	C	9	SER	N-CA-C	5.00	115.72	109.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	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	1586	0	1554	18	0
1	B	1559	0	1519	15	0
1	C	1549	0	1497	17	0
1	D	1564	0	1517	18	0
2	A	23	0	0	0	0
2	B	20	0	0	0	0
2	C	11	0	0	0	0
2	D	7	0	0	1	0
All	All	6319	0	6087	66	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 (66) 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:139:PRO:HA	1:B:176:GLU:HG3	1.65	0.77
1:C:1:MET:HE2	1:C:141:VAL:HA	1.69	0.75
1:A:67:GLN:NE2	1:A:70:GLN:OE1	2.26	0.68
1:B:124:GLN:H	1:B:124:GLN:CD	2.03	0.67
1:A:157:GLN:NE2	1:A:161:GLN:OE1	2.28	0.64
1:B:122:GLU:OE2	1:B:124:GLN:NE2	2.31	0.63
1:B:118:LEU:HD11	1:B:185:PRO:HD2	1.83	0.61
1:C:95:THR:HG23	1:C:108:GLY:HA3	1.82	0.60
1:B:65:LEU:HD13	1:B:125:LEU:HA	1.83	0.60
1:D:124:GLN:HG3	1:D:125:LEU:HD12	1.83	0.59
1:A:161:GLN:HG2	1:A:162:PRO:HD3	1.85	0.58
1:A:37:ASN:HB3	1:A:67:GLN:HG3	1.87	0.57
1:A:-1:ILE:HD13	1:A:144:ALA:HB1	1.88	0.56
1:C:65:LEU:HD13	1:C:125:LEU:HA	1.87	0.56
1:A:20:PHE:HE1	1:B:206:LEU:HD11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:HB1	1:B:100:ASN:ND2	2.22	0.54
1:D:90:GLY:HA2	2:D:306:HOH:O	2.08	0.53
1:B:124:GLN:OE1	1:B:124:GLN:N	2.42	0.53
1:C:154:GLN:O	1:C:158:THR:HG23	2.09	0.52
1:D:29:ARG:O	1:D:83:PRO:HD3	2.11	0.51
1:C:77:TRP:HH2	1:C:94:LEU:HD12	1.75	0.50
1:A:13:ASP:OD1	1:A:14:SER:N	2.45	0.50
1:D:135:ILE:HD11	1:D:186:ALA:HB2	1.94	0.49
1:D:30:THR:OG1	1:D:31:PHE:N	2.45	0.49
1:D:170:LEU:HD23	1:D:172:PHE:CZ	2.48	0.49
1:C:48:ALA:HB1	1:C:60:SER:O	2.13	0.48
1:B:174:LEU:HD22	1:B:191:LEU:HD23	1.96	0.47
1:D:74:PRO:HG3	1:D:125:LEU:HD23	1.97	0.47
1:A:145:ASP:OD2	1:A:148:LYS:HG3	2.15	0.47
1:C:8:THR:HG23	1:C:9:SER:N	2.29	0.47
1:C:136:VAL:HB	1:C:174:LEU:HD22	1.97	0.46
1:A:-1:ILE:C	1:A:-1:ILE:HD12	2.40	0.46
1:D:78:PHE:HA	1:D:82:TYR:O	2.16	0.46
1:A:63:VAL:O	1:A:74:PRO:HD2	2.16	0.45
1:C:138:MET:N	1:C:175:VAL:O	2.41	0.44
1:B:35:GLU:C	1:B:37:ASN:N	2.74	0.44
1:D:9:SER:OG	1:D:183:VAL:HG22	2.18	0.44
1:C:106:LEU:HD12	1:C:106:LEU:HA	1.89	0.43
1:A:79:LEU:HD23	1:A:106:LEU:HD11	2.00	0.43
1:D:13:ASP:OD1	1:D:14:SER:N	2.52	0.43
1:C:35:GLU:HG3	1:C:37:ASN:HB3	2.01	0.43
1:D:1:MET:HE3	1:D:140:ARG:NH1	2.34	0.43
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.82	0.42
1:A:175:VAL:HG12	1:A:189:SER:HA	2.01	0.42
1:B:63:VAL:O	1:B:73:SER:HA	2.19	0.42
1:C:74:PRO:HG3	1:C:125:LEU:HD22	2.00	0.42
1:D:42:PHE:O	1:D:44:PRO:HD3	2.19	0.42
1:A:165:SER:OG	1:A:166:ALA:N	2.52	0.42
1:B:52:GLY:HA3	1:B:58:GLN:NE2	2.35	0.42
1:D:6:ALA:O	1:D:8:THR:HG22	2.20	0.42
1:D:106:LEU:HB3	1:D:117:LEU:HB2	2.02	0.42
1:A:204:PHE:CZ	1:C:196:ALA:HB2	2.55	0.42
1:B:105:ILE:HG21	1:B:178:LEU:HD21	2.01	0.41
1:C:161:GLN:HG2	1:C:162:PRO:HD3	2.02	0.41
1:C:77:TRP:CH2	1:C:94:LEU:HD12	2.56	0.41
1:A:105:ILE:HG21	1:A:178:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:ND2	1:A:102:GLN:OE1	2.46	0.41
1:B:37:ASN:HB2	1:B:67:GLN:CG	2.51	0.41
1:D:104:LEU:HB2	1:D:128:TRP:CD1	2.56	0.41
1:A:15:ALA:CB	1:A:33:ARG:HH22	2.34	0.41
1:A:74:PRO:HG3	1:A:125:LEU:HD22	2.03	0.40
1:B:13:ASP:OD1	1:B:14:SER:N	2.54	0.40
1:D:117:LEU:HD13	1:D:130:PHE:CE1	2.55	0.40
1:C:138:MET:HG3	1:C:152:ARG:NH1	2.36	0.40
1:D:183:VAL:O	1:D:185:PRO:HD3	2.22	0.40
1:C:118:LEU:HD23	1:C:119:LEU:N	2.36	0.40

There are no symmetry-related clashes.

## 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	209/227 (92%)	203 (97%)	5 (2%)	1 (0%)	25	32
1	B	206/227 (91%)	193 (94%)	13 (6%)	0	100	100
1	C	206/227 (91%)	199 (97%)	7 (3%)	0	100	100
1	D	208/227 (92%)	197 (95%)	11 (5%)	0	100	100
All	All	829/908 (91%)	792 (96%)	36 (4%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	PRO

### 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	162/176 (92%)	158 (98%)	4 (2%)	42	58
1	B	158/176 (90%)	156 (99%)	2 (1%)	65	78
1	C	156/176 (89%)	153 (98%)	3 (2%)	52	67
1	D	158/176 (90%)	151 (96%)	7 (4%)	24	36
All	All	634/704 (90%)	618 (98%)	16 (2%)	42	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	VAL
1	A	22	LEU
1	A	67	GLN
1	A	70	GLN
1	B	11	GLN
1	B	137	GLU
1	C	35	GLU
1	C	50	ARG
1	C	170	LEU
1	D	8	THR
1	D	14	SER
1	D	22	LEU
1	D	35	GLU
1	D	58	GLN
1	D	86	GLN
1	D	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	198	HIS
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	80	GLN
1	B	86	GLN
1	C	37	ASN
1	C	66	GLN
1	C	131	ASN
1	C	194	ASN
1	D	66	GLN
1	D	126	HIS
1	D	157	GLN

### 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](#)

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	211/227 (92%)	0.04	7 (3%)	49	51	51, 67, 103, 127	0
1	B	208/227 (91%)	0.29	10 (4%)	36	37	30, 73, 98, 125	0
1	C	208/227 (91%)	0.23	9 (4%)	40	41	59, 77, 106, 128	0
1	D	210/227 (92%)	0.26	8 (3%)	44	46	64, 80, 110, 135	0
All	All	837/908 (92%)	0.20	34 (4%)	42	43	30, 75, 106, 135	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	GLY	10.6
1	A	38	GLY	4.9
1	A	167	PRO	4.7
1	D	207	VAL	4.5
1	A	207	VAL	4.1
1	A	168	ALA	4.0
1	A	166	ALA	3.7
1	C	36	ALA	3.6
1	C	167	PRO	3.4
1	B	167	PRO	3.2
1	B	207	VAL	3.2
1	B	206	LEU	3.1
1	D	167	PRO	3.0
1	B	166	ALA	2.9
1	A	169	PRO	2.9
1	C	207	VAL	2.9
1	B	39	GLY	2.8
1	C	8	THR	2.8
1	C	166	ALA	2.7
1	D	38	GLY	2.7
1	D	163	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	168	ALA	2.7
1	C	38	GLY	2.6
1	D	166	ALA	2.6
1	C	169	PRO	2.6
1	C	50	ARG	2.6
1	B	205	LYS	2.5
1	B	37	ASN	2.4
1	C	0	HIS	2.4
1	D	-2	VAL	2.4
1	A	33	ARG	2.3
1	B	34	ASP	2.3
1	B	197	THR	2.2
1	D	35	GLU	2.2

## 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.