



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2026 – 03:02 am BST

PDB ID : 30XJ / pdb_000030xj
Title : A C-terminal Processing Protease Links Flagellin Turnover to Developmental Progression in a Bacterial Predator
Authors : Harding, C.J.; Lovering, A.L.
Deposited on : 2026-05-15
Resolution : 2.58 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

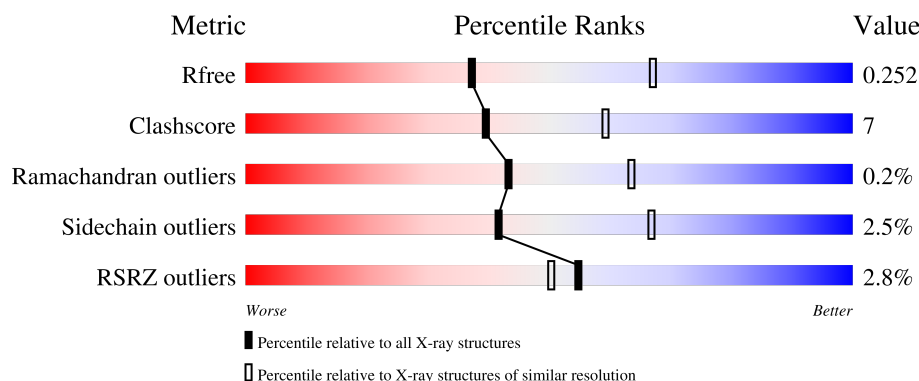
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

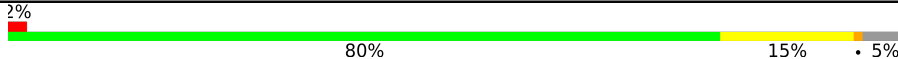
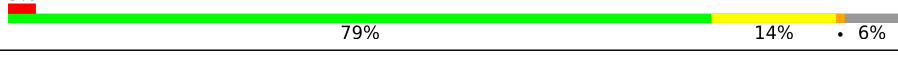
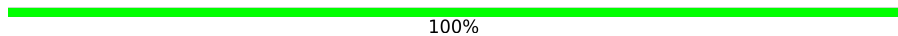
The reported resolution of this entry is 2.58 Å.

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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	668	 2% 80% 15% • 5%
1	B	668	 4% 80% 14% • 5%
1	C	668	 2% 78% 15% • 6%
1	D	668	 3% 79% 14% • 6%
2	E	4	 100%

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Mol	Chain	Length	Quality of chain
2	F	4	100%
2	H	4	100%
2	L	4	100%
2	M	4	75%25%
2	N	4	75%25%
2	U	4	75%25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20122 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 Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4966	3123	863	967	13			
1	B	633	Total	C	N	O	S	0	0	0
			4962	3121	862	966	13			
1	C	629	Total	C	N	O	S	0	0	0
			4925	3100	853	959	13			
1	D	629	Total	C	N	O	S	0	0	0
			4929	3103	854	959	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP Q6MP94
A	7	GLY	-	expression tag	UNP Q6MP94
A	8	SER	-	expression tag	UNP Q6MP94
A	9	SER	-	expression tag	UNP Q6MP94
A	10	HIS	-	expression tag	UNP Q6MP94
A	11	HIS	-	expression tag	UNP Q6MP94
A	12	HIS	-	expression tag	UNP Q6MP94
A	13	HIS	-	expression tag	UNP Q6MP94
A	14	HIS	-	expression tag	UNP Q6MP94
A	15	HIS	-	expression tag	UNP Q6MP94
A	16	SER	-	expression tag	UNP Q6MP94
A	17	SER	-	expression tag	UNP Q6MP94
A	18	GLY	-	expression tag	UNP Q6MP94
A	19	LEU	-	expression tag	UNP Q6MP94
A	20	VAL	-	expression tag	UNP Q6MP94
A	21	PRO	-	expression tag	UNP Q6MP94
A	22	ARG	-	expression tag	UNP Q6MP94
A	23	GLY	-	expression tag	UNP Q6MP94
A	24	SER	-	expression tag	UNP Q6MP94
A	25	HIS	-	expression tag	UNP Q6MP94
A	457	ALA	SER	engineered mutation	UNP Q6MP94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	MET	-	initiating methionine	UNP Q6MP94
B	7	GLY	-	expression tag	UNP Q6MP94
B	8	SER	-	expression tag	UNP Q6MP94
B	9	SER	-	expression tag	UNP Q6MP94
B	10	HIS	-	expression tag	UNP Q6MP94
B	11	HIS	-	expression tag	UNP Q6MP94
B	12	HIS	-	expression tag	UNP Q6MP94
B	13	HIS	-	expression tag	UNP Q6MP94
B	14	HIS	-	expression tag	UNP Q6MP94
B	15	HIS	-	expression tag	UNP Q6MP94
B	16	SER	-	expression tag	UNP Q6MP94
B	17	SER	-	expression tag	UNP Q6MP94
B	18	GLY	-	expression tag	UNP Q6MP94
B	19	LEU	-	expression tag	UNP Q6MP94
B	20	VAL	-	expression tag	UNP Q6MP94
B	21	PRO	-	expression tag	UNP Q6MP94
B	22	ARG	-	expression tag	UNP Q6MP94
B	23	GLY	-	expression tag	UNP Q6MP94
B	24	SER	-	expression tag	UNP Q6MP94
B	25	HIS	-	expression tag	UNP Q6MP94
B	457	ALA	SER	engineered mutation	UNP Q6MP94
C	6	MET	-	initiating methionine	UNP Q6MP94
C	7	GLY	-	expression tag	UNP Q6MP94
C	8	SER	-	expression tag	UNP Q6MP94
C	9	SER	-	expression tag	UNP Q6MP94
C	10	HIS	-	expression tag	UNP Q6MP94
C	11	HIS	-	expression tag	UNP Q6MP94
C	12	HIS	-	expression tag	UNP Q6MP94
C	13	HIS	-	expression tag	UNP Q6MP94
C	14	HIS	-	expression tag	UNP Q6MP94
C	15	HIS	-	expression tag	UNP Q6MP94
C	16	SER	-	expression tag	UNP Q6MP94
C	17	SER	-	expression tag	UNP Q6MP94
C	18	GLY	-	expression tag	UNP Q6MP94
C	19	LEU	-	expression tag	UNP Q6MP94
C	20	VAL	-	expression tag	UNP Q6MP94
C	21	PRO	-	expression tag	UNP Q6MP94
C	22	ARG	-	expression tag	UNP Q6MP94
C	23	GLY	-	expression tag	UNP Q6MP94
C	24	SER	-	expression tag	UNP Q6MP94
C	25	HIS	-	expression tag	UNP Q6MP94
C	457	ALA	SER	engineered mutation	UNP Q6MP94

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	MET	-	initiating methionine	UNP Q6MP94
D	7	GLY	-	expression tag	UNP Q6MP94
D	8	SER	-	expression tag	UNP Q6MP94
D	9	SER	-	expression tag	UNP Q6MP94
D	10	HIS	-	expression tag	UNP Q6MP94
D	11	HIS	-	expression tag	UNP Q6MP94
D	12	HIS	-	expression tag	UNP Q6MP94
D	13	HIS	-	expression tag	UNP Q6MP94
D	14	HIS	-	expression tag	UNP Q6MP94
D	15	HIS	-	expression tag	UNP Q6MP94
D	16	SER	-	expression tag	UNP Q6MP94
D	17	SER	-	expression tag	UNP Q6MP94
D	18	GLY	-	expression tag	UNP Q6MP94
D	19	LEU	-	expression tag	UNP Q6MP94
D	20	VAL	-	expression tag	UNP Q6MP94
D	21	PRO	-	expression tag	UNP Q6MP94
D	22	ARG	-	expression tag	UNP Q6MP94
D	23	GLY	-	expression tag	UNP Q6MP94
D	24	SER	-	expression tag	UNP Q6MP94
D	25	HIS	-	expression tag	UNP Q6MP94
D	457	ALA	SER	engineered mutation	UNP Q6MP94

- Molecule 2 is a protein called UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	U	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	F	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	H	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	L	4	Total	C	N	O	0	0	0
			20	12	4	4			
2	M	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	N	4	Total	C	N	O	0	0	0
			20	12	4	4			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0

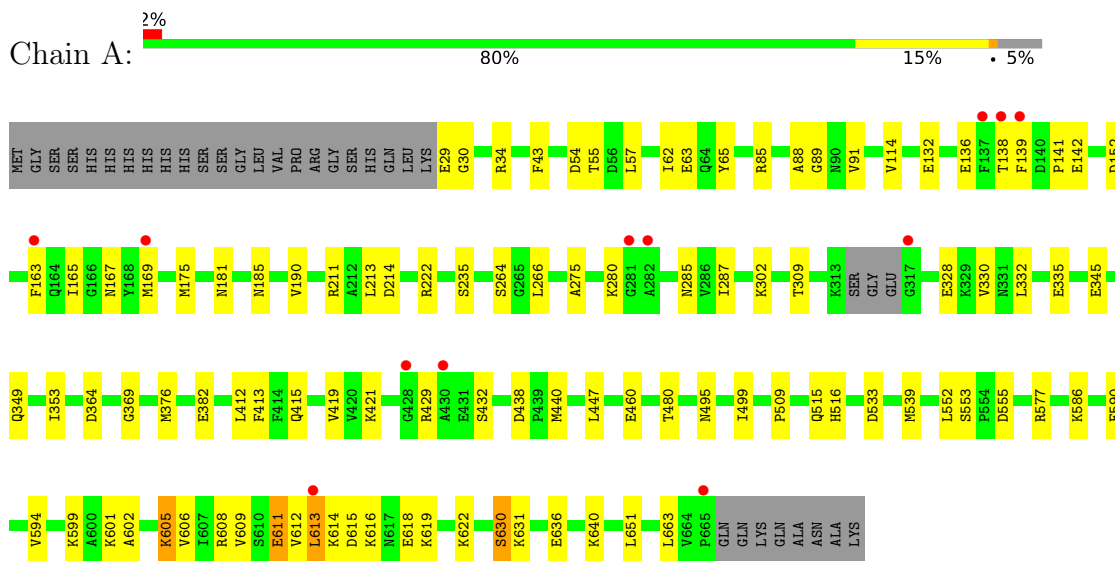
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	52	Total 52	O 52	0	0
4	U	1	Total 1	O 1	0	0
4	C	55	Total 55	O 55	0	0
4	F	2	Total 2	O 2	0	0
4	H	1	Total 1	O 1	0	0
4	D	49	Total 49	O 49	0	0

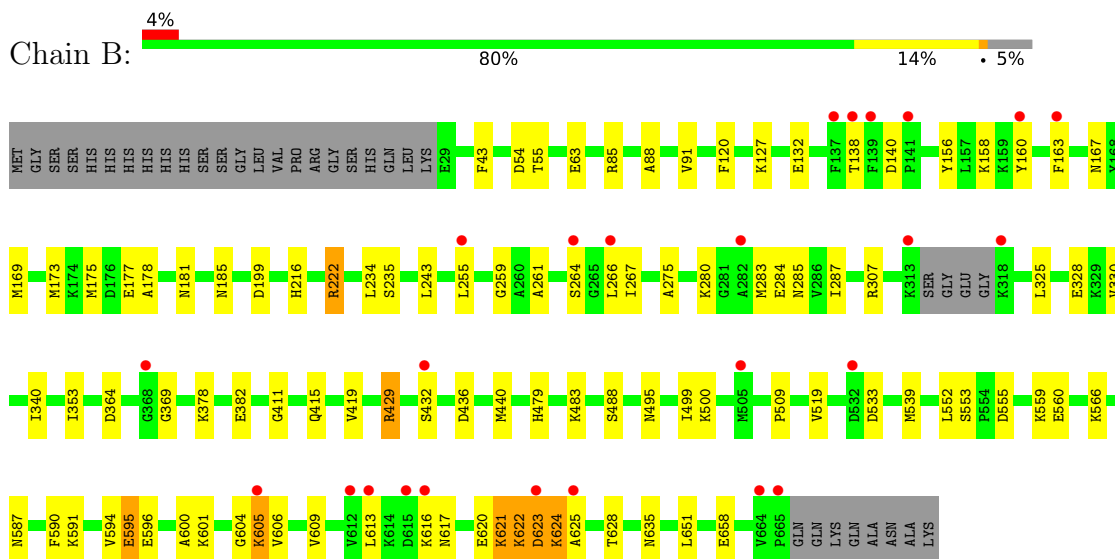
3 Residue-property plots [i](#)

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.

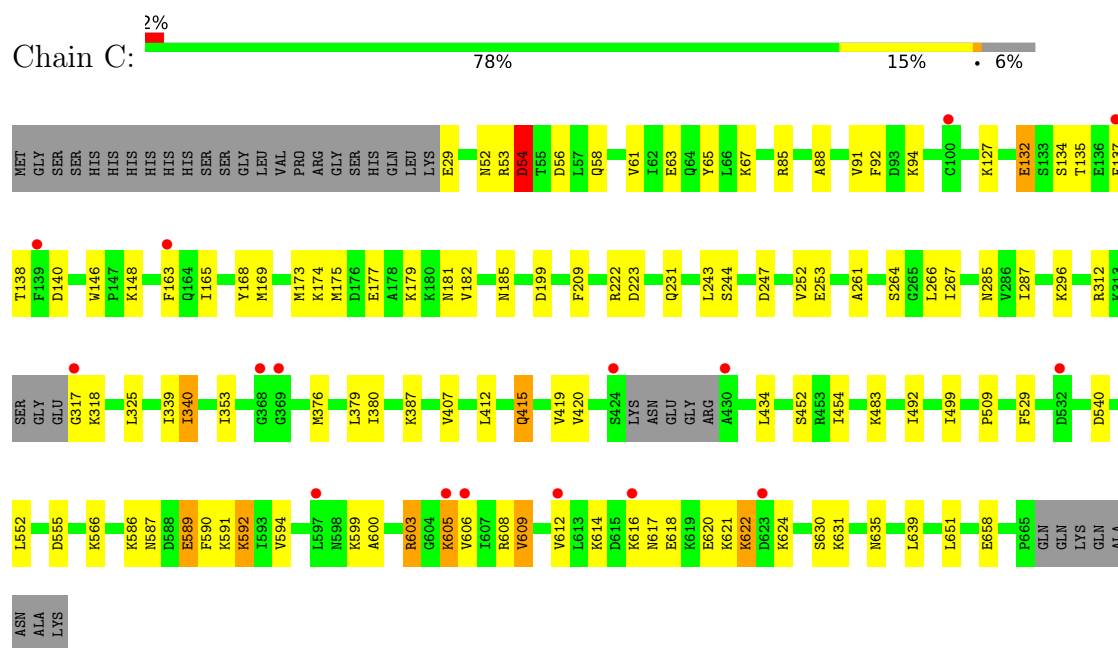
- Molecule 1: Tail-specific protease



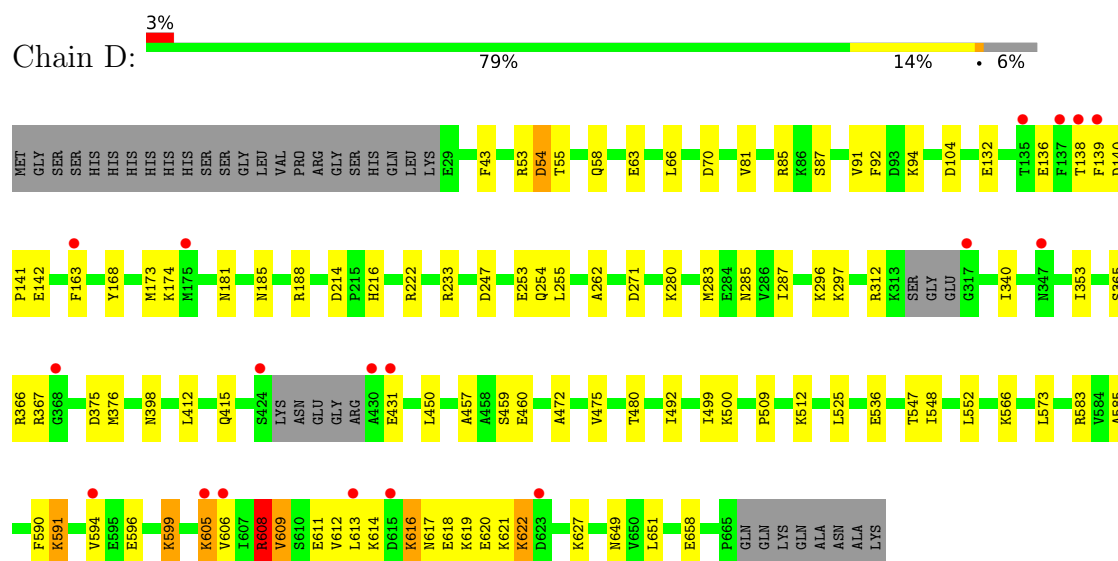
- Molecule 1: Tail-specific protease



- Molecule 1: Tail-specific protease



- Molecule 1: Tail-specific protease



- Molecule 2: UNK-UNK-UNK-UNK

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: UNK-UNK-UNK-UNK

Chain U: 75% 25%



- Molecule 2: UNK-UNK-UNK-UNK

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: UNK-UNK-UNK-UNK

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: UNK-UNK-UNK-UNK

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: UNK-UNK-UNK-UNK

Chain M:  75% 25%



- Molecule 2: UNK-UNK-UNK-UNK

Chain N:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.88Å 95.02Å 113.26Å 77.68° 71.80° 81.94°	Depositor
Resolution (Å)	38.42 – 2.58 38.42 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.42-2.58) 98.5 (38.42-2.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.212 , 0.252 0.212 , 0.252	Depositor DCC
R_{free} test set	4359 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20122	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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:
CA

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	0.48	0/5040	0.87	3/6769 (0.0%)
1	B	0.51	0/5036	0.86	2/6764 (0.0%)
1	C	0.49	0/4998	0.84	4/6713 (0.1%)
1	D	0.49	0/5002	0.81	3/6717 (0.0%)
All	All	0.49	0/20076	0.84	12/26963 (0.0%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	54	ASP	N-CA-CB	-8.31	98.43	111.56
1	C	589	GLU	CB-CG-CD	7.74	125.75	112.60
1	D	54	ASP	N-CA-CB	-7.25	99.56	111.66
1	C	94	LYS	CA-CB-CG	6.66	127.41	114.10
1	B	621	LYS	CB-CG-CD	-6.62	96.07	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	ARG	Sidechain
1	B	429	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	4966	0	5017	69	0
1	B	4962	0	5014	66	0
1	C	4925	0	4975	70	0
1	D	4929	0	4986	62	0
2	E	21	0	6	0	0
2	F	21	0	6	0	0
2	H	21	0	6	0	0
2	L	20	0	6	0	0
2	M	15	0	5	0	0
2	N	20	0	6	1	0
2	U	21	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	37	0	0	11	1
4	B	52	0	0	5	0
4	C	55	0	0	8	1
4	D	49	0	0	9	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
4	U	1	0	0	0	0
All	All	20122	0	20033	267	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 7.

The worst 5 of 267 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:440:MET:SD	4:B:851:HOH:O	2.27	0.90
1:D:617:ASN:O	1:D:620:GLU:HG3	1.71	0.90
1:D:608:ARG:NH1	1:D:611:GLU:OE2	2.05	0.88
1:D:188:ARG:HD2	4:D:809:HOH:O	1.72	0.88
1:B:264:SER:HB2	1:B:266:LEU:HD12	1.57	0.87

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)
4:A:833:HOH:O	4:C:822:HOH:O[1_556]	2.12	0.08

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	630/668 (94%)	612 (97%)	17 (3%)	1 (0%)	43	63
1	B	629/668 (94%)	608 (97%)	20 (3%)	1 (0%)	43	63
1	C	623/668 (93%)	605 (97%)	17 (3%)	1 (0%)	43	63
1	D	623/668 (93%)	604 (97%)	18 (3%)	1 (0%)	43	63
All	All	2505/2672 (94%)	2429 (97%)	72 (3%)	4 (0%)	43	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	B	415	GLN
1	C	415	GLN
1	D	415	GLN

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	538/569 (95%)	531 (99%)	7 (1%)	61	81
1	B	538/569 (95%)	526 (98%)	12 (2%)	45	70
1	C	534/569 (94%)	517 (97%)	17 (3%)	34	59
1	D	535/569 (94%)	517 (97%)	18 (3%)	32	58
All	All	2145/2276 (94%)	2091 (98%)	54 (2%)	42	67

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	605	LYS
1	C	624	LYS
1	D	614	LYS
1	C	608	ARG
1	C	616	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	GLN
1	C	495	ASN
1	C	397	ASN
1	D	78	GLN
1	B	97	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 4 ligands modelled in this entry, 4 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 [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	634/668 (94%)	0.27	12 (1%) 66 62	38, 62, 104, 125	0
1	B	633/668 (94%)	0.32	25 (3%) 43 39	38, 58, 106, 139	0
1	C	629/668 (94%)	0.18	16 (2%) 58 54	36, 56, 102, 120	0
1	D	629/668 (94%)	0.18	18 (2%) 53 49	37, 57, 104, 128	0
2	E	0/4	-	-	-	-
2	F	0/4	-	-	-	-
2	H	0/4	-	-	-	-
2	L	0/4	-	-	-	-
2	M	0/4	-	-	-	-
2	N	0/4	-	-	-	-
2	U	0/4	-	-	-	-
All	All	2525/2700 (93%)	0.24	71 (2%) 55 50	36, 58, 104, 139	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	GLY	4.4
1	B	163	PHE	4.4
1	C	139	PHE	3.9
1	B	160	TYR	3.8
1	D	138	THR	3.3

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	CA	A	701	1/1	0.99	0.02	55,55,55,55	0
3	CA	C	701	1/1	0.99	0.02	45,45,45,45	0
3	CA	B	701	1/1	1.00	0.04	41,41,41,41	0
3	CA	D	701	1/1	1.00	0.01	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.