



wwPDB EM Validation Summary Report ⓘ

Jul 8, 2025 – 03:40 PM JST

PDB ID : 9KNU / pdb_00009knu
EMDB ID : EMD-62462
Title : Neck structure of bacteriophage Mu in contracted state
Authors : Liu, H.R.; Zhou, J.Q.
Deposited on : 2024-11-19
Resolution : 3.60 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

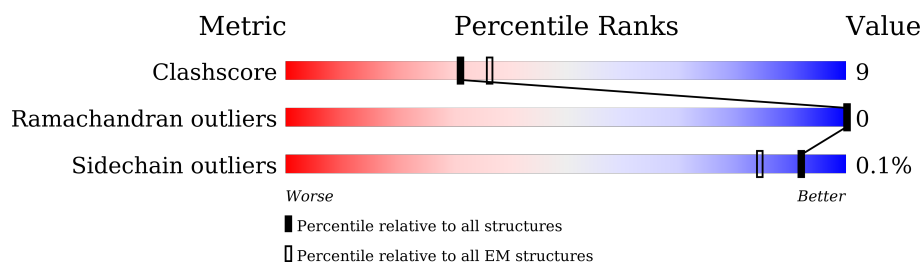
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	512	60% 15% 25%
1	B	512	60% 15% 25%
1	C	512	59% 16% 25%
1	D	512	59% 16% 25%
1	E	512	60% 15% 25%
1	F	512	59% 16% 25%
1	G	512	59% 15% 25%
1	H	512	60% 15% 25%
1	I	512	59% 15% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	512	
1	K	512	
1	L	512	
2	M	141	
2	N	141	
2	O	141	
2	P	141	
2	Q	141	
2	R	141	
2	S	141	
2	T	141	
2	U	141	
2	V	141	
2	W	141	
2	X	141	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 49248 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	B	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	C	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	D	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	E	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	F	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	G	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	H	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	I	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	J	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	K	383	Total 3009	C 1895	N 534	O 562	S 18	0	0
1	L	383	Total 3009	C 1895	N 534	O 562	S 18	0	0

- Molecule 2 is a protein called Gene product J.

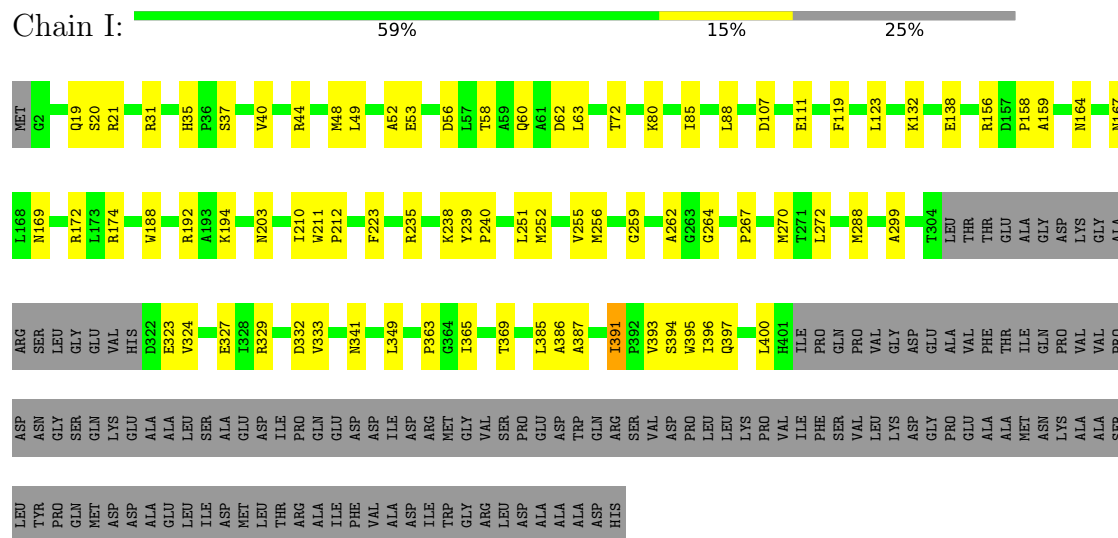
Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	M	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	N	140	Total 1095	C 686	N 192	O 214	S 3	0	0

Continued on next page...

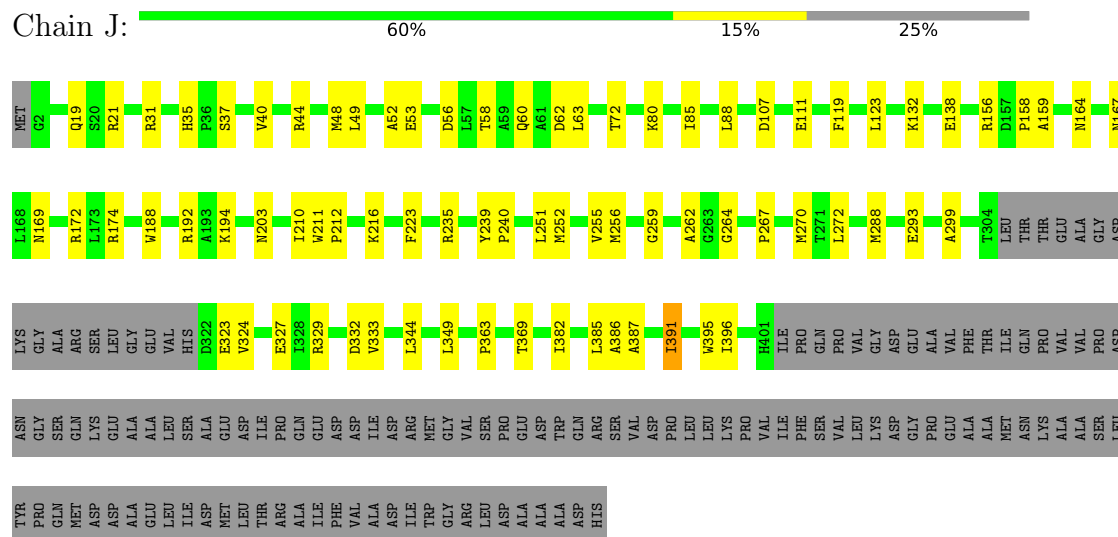
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	P	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	Q	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	R	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	S	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	T	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	U	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	V	140	Total 1095	C 686	N 192	O 214	S 3	0	0
2	W	140	Total 1095	C 686	N 192	O 214	S 3	0	0

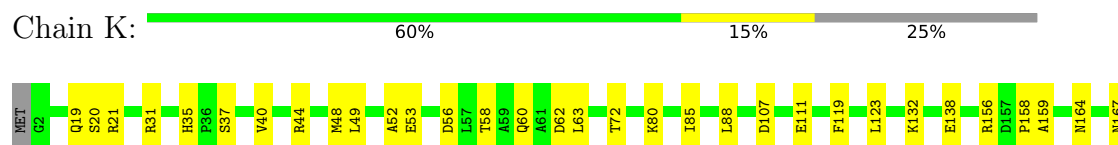
- Molecule 1: Portal protein

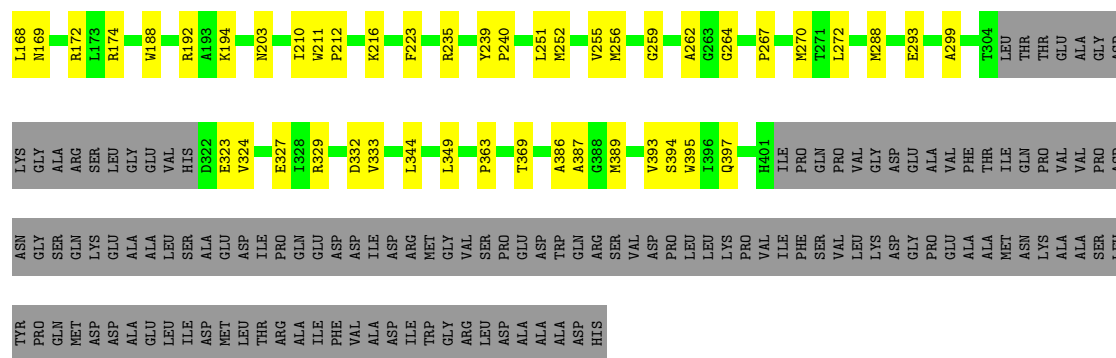


- Molecule 1: Portal protein

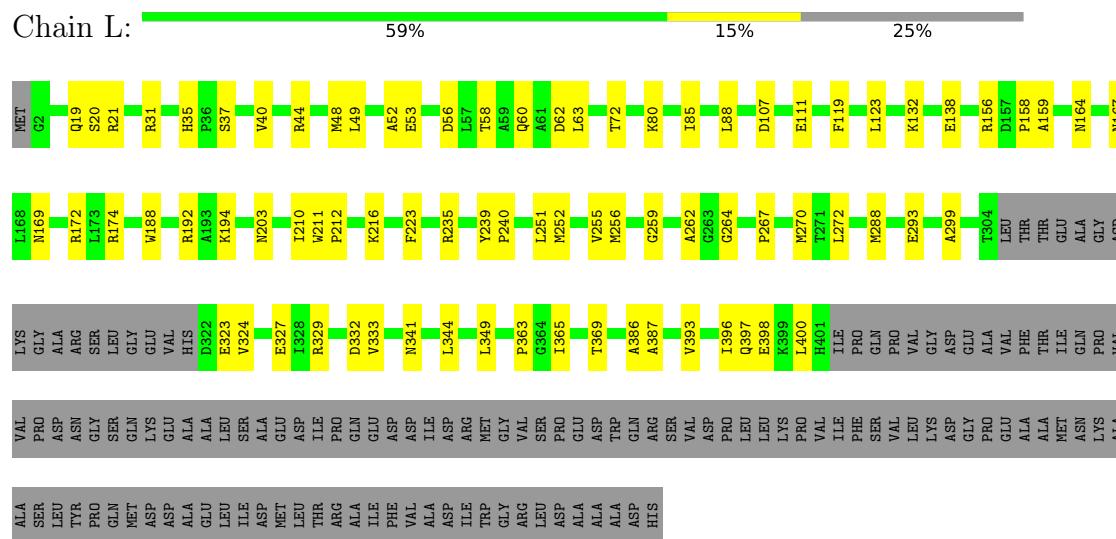


- Molecule 1: Portal protein

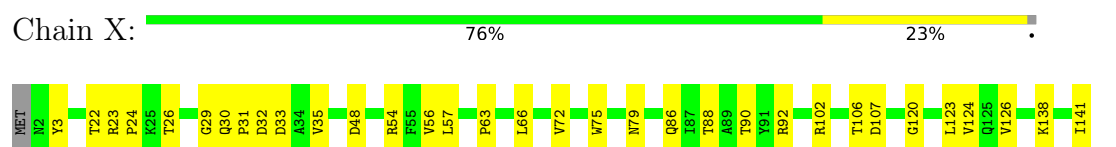




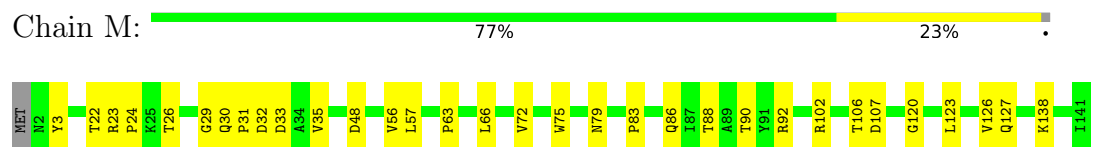
- Molecule 1: Portal protein



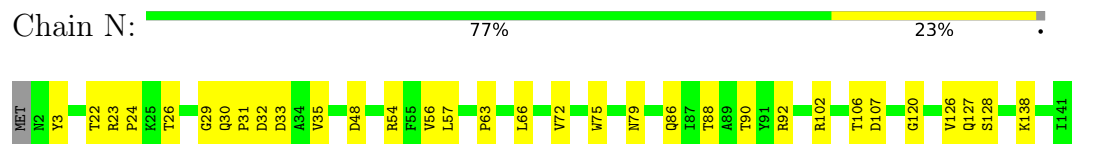
- Molecule 2: Gene product J



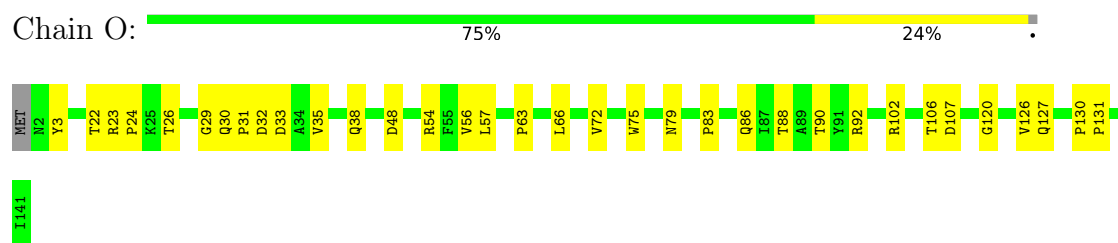
- Molecule 2: Gene product J



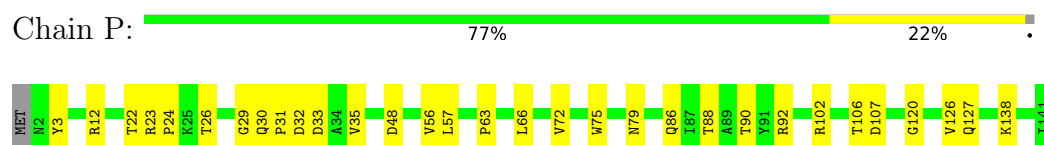
- Molecule 2: Gene product J



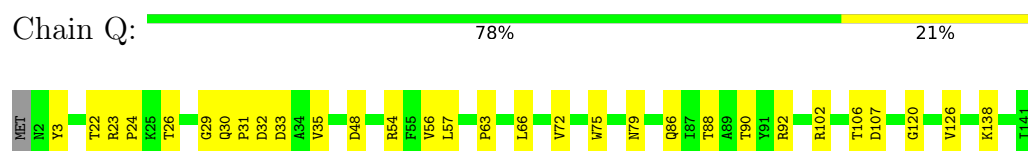
- Molecule 2: Gene product J



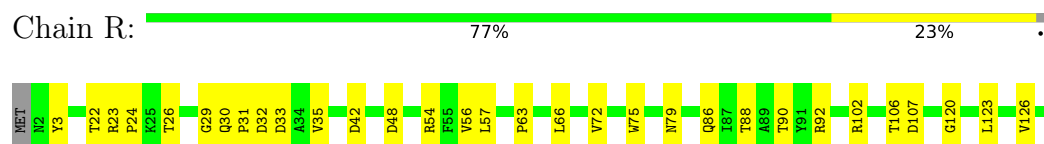
- Molecule 2: Gene product J



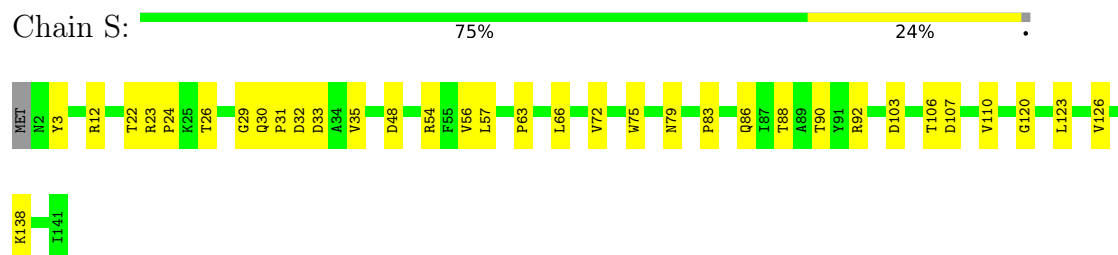
- Molecule 2: Gene product J



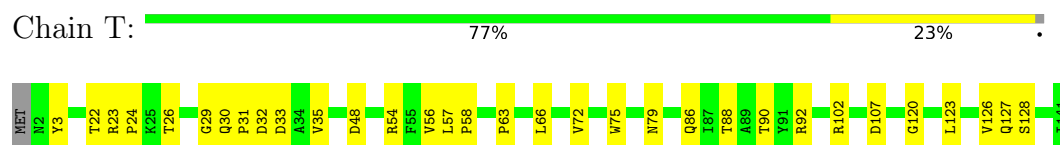
- Molecule 2: Gene product J




- Molecule 2: Gene product J



- Molecule 2: Gene product J




- Molecule 2: Gene product J

Chain U:  77% 23%




• Molecule 2: Gene product J

Chain V:  78% 21%



• Molecule 2: Gene product J

Chain W:  76% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.21	0/3072	0.40	1/4150 (0.0%)
1	B	0.22	0/3072	0.41	0/4150
1	C	0.22	0/3072	0.40	0/4150
1	D	0.22	0/3072	0.40	1/4150 (0.0%)
1	E	0.22	0/3072	0.40	0/4150
1	F	0.22	0/3072	0.39	0/4150
1	G	0.22	0/3072	0.40	0/4150
1	H	0.22	0/3072	0.40	0/4150
1	I	0.22	0/3072	0.39	0/4150
1	J	0.22	0/3072	0.40	0/4150
1	K	0.22	0/3072	0.40	0/4150
1	L	0.22	0/3072	0.40	0/4150
2	M	0.16	0/1117	0.33	0/1524
2	N	0.16	0/1117	0.33	0/1524
2	O	0.16	0/1117	0.32	0/1524
2	P	0.16	0/1117	0.32	0/1524
2	Q	0.16	0/1117	0.32	0/1524
2	R	0.16	0/1117	0.33	0/1524
2	S	0.18	0/1117	0.34	0/1524
2	T	0.16	0/1117	0.33	0/1524
2	U	0.18	0/1117	0.34	0/1524
2	V	0.16	0/1117	0.33	0/1524
2	W	0.16	0/1117	0.32	0/1524
2	X	0.16	0/1117	0.33	0/1524
All	All	0.20	0/50268	0.38	2/68088 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	VAL	N-CA-C	-5.08	105.59	110.72
1	D	393	VAL	N-CA-C	-5.06	105.61	110.72

There are no chirality outliers.

There are no planarity outliers.

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	3009	0	2948	54	0
1	B	3009	0	2948	52	0
1	C	3009	0	2948	55	0
1	D	3009	0	2948	57	0
1	E	3009	0	2948	54	0
1	F	3009	0	2948	57	0
1	G	3009	0	2948	53	0
1	H	3009	0	2948	51	0
1	I	3009	0	2948	57	0
1	J	3009	0	2948	54	0
1	K	3009	0	2948	55	0
1	L	3009	0	2948	56	0
2	M	1095	0	1071	24	0
2	N	1095	0	1071	25	0
2	O	1095	0	1071	25	0
2	P	1095	0	1071	23	0
2	Q	1095	0	1071	21	0
2	R	1095	0	1071	24	0
2	S	1095	0	1071	26	0
2	T	1095	0	1071	28	0
2	U	1095	0	1071	24	0
2	V	1095	0	1071	21	0
2	W	1095	0	1071	25	0
2	X	1095	0	1071	26	0
All	All	49248	0	48228	839	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 9.

The worst 5 of 839 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)
2:R:102:ARG:NH1	2:S:106:THR:OG1	2.20	0.74
1:K:235:ARG:NH1	1:K:255:VAL:O	2.25	0.70
1:A:235:ARG:NH1	1:A:255:VAL:O	2.25	0.70
1:C:235:ARG:NH1	1:C:255:VAL:O	2.25	0.69
1:I:235:ARG:NH1	1:I:255:VAL:O	2.25	0.69

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 PDB entries followed by that with respect to all EM entries.

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	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	B	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	C	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	D	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	E	379/512 (74%)	372 (98%)	7 (2%)	0	100	100
1	F	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	G	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	H	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	I	379/512 (74%)	370 (98%)	9 (2%)	0	100	100
1	J	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	K	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
1	L	379/512 (74%)	371 (98%)	8 (2%)	0	100	100
2	M	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	N	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	O	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	P	138/141 (98%)	135 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	R	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	S	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	T	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	U	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	W	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
2	X	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
All	All	6204/7836 (79%)	6072 (98%)	132 (2%)	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 PDB entries followed by that with respect to all EM entries.

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	310/418 (74%)	310 (100%)	0	100	100
1	B	310/418 (74%)	309 (100%)	1 (0%)	91	96
1	C	310/418 (74%)	310 (100%)	0	100	100
1	D	310/418 (74%)	310 (100%)	0	100	100
1	E	310/418 (74%)	310 (100%)	0	100	100
1	F	310/418 (74%)	309 (100%)	1 (0%)	91	96
1	G	310/418 (74%)	309 (100%)	1 (0%)	91	96
1	H	310/418 (74%)	310 (100%)	0	100	100
1	I	310/418 (74%)	309 (100%)	1 (0%)	91	96
1	J	310/418 (74%)	309 (100%)	1 (0%)	91	96
1	K	310/418 (74%)	310 (100%)	0	100	100
1	L	310/418 (74%)	310 (100%)	0	100	100
2	M	118/120 (98%)	118 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	118/120 (98%)	118 (100%)	0	100	100
2	O	118/120 (98%)	118 (100%)	0	100	100
2	P	118/120 (98%)	118 (100%)	0	100	100
2	Q	118/120 (98%)	118 (100%)	0	100	100
2	R	118/120 (98%)	118 (100%)	0	100	100
2	S	118/120 (98%)	118 (100%)	0	100	100
2	T	118/120 (98%)	118 (100%)	0	100	100
2	U	118/120 (98%)	118 (100%)	0	100	100
2	V	118/120 (98%)	118 (100%)	0	100	100
2	W	118/120 (98%)	118 (100%)	0	100	100
2	X	118/120 (98%)	118 (100%)	0	100	100
All	All	5136/6456 (80%)	5131 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	393	VAL
1	F	391	ILE
1	G	393	VAL
1	I	391	ILE
1	J	391	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	7	ASN
2	U	86	GLN
2	Q	86	GLN
2	S	7	ASN
2	W	7	ASN

5.3.3 RNA ⓘ

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.