



Full wwPDB EM Validation Report ⓘ

Mar 16, 2025 – 03:13 pm GMT

PDB ID : 8QKM
EMDB ID : EMD-18466
Title : Symmetric structure of Satellite Tobacco Necrosis Virus-Like Particle with PS1-5 gRNA
Authors : Javed, A.; Mata, P.C.; Stockley, P.
Deposited on : 2023-09-15
Resolution : 2.39 Å(reported)
Based on initial model : 4bcu

This is a Full wwPDB EM Validation 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 : 4.02b-467
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) : 2.41

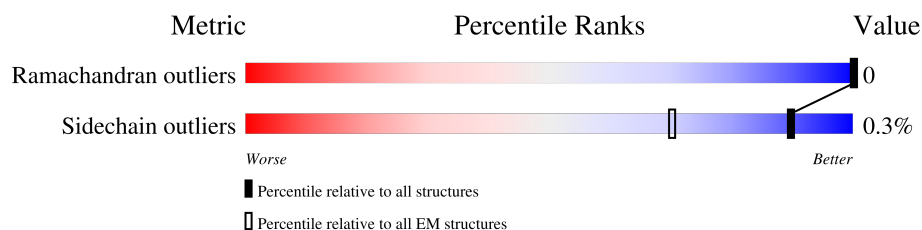
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 2.39 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.



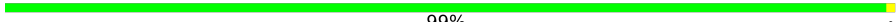














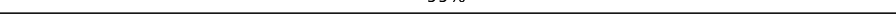
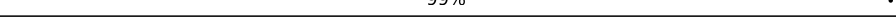
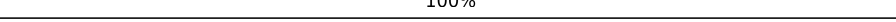

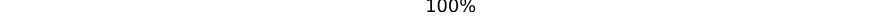
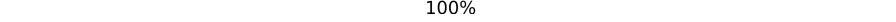
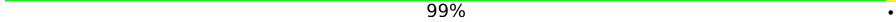
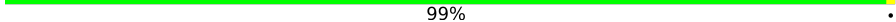


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	188	 100%
1	1	188	 99% .
1	2	188	 100%
1	3	188	 99% .
1	4	188	 100%
1	5	188	 100%
1	6	188	 100%
1	7	188	 100%
1	A	188	 99% .
1	B	188	 99% .


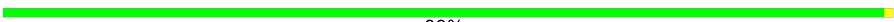












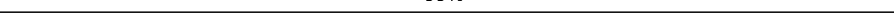
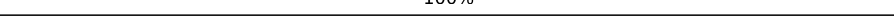
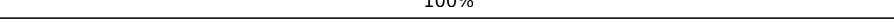
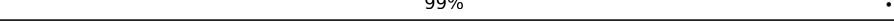
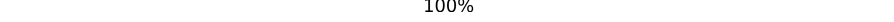
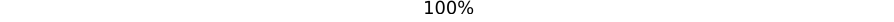
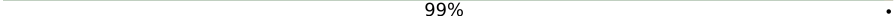
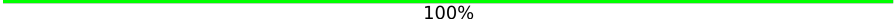
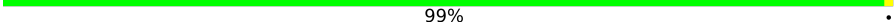
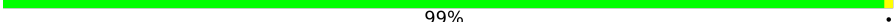

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Mol	Chain	Length	Quality of chain
1	C	188	 99% .
1	D	188	 100%
1	E	188	 100%
1	F	188	 99% .
1	G	188	 99% .
1	H	188	 100%
1	I	188	 99% .
1	J	188	 100%
1	K	188	 100%
1	L	188	 100%
1	M	188	 100%
1	N	188	 99% .
1	O	188	 99% .
1	P	188	 100%
1	Q	188	 99% .
1	R	188	 99% .
1	S	188	 100%
1	T	188	 100%
1	U	188	 100%
1	V	188	 100%
1	W	188	 99% .
1	X	188	 99% .
1	Y	188	 100%
1	Z	188	 100%
1	a	188	 99% .

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Mol	Chain	Length	Quality of chain
1	b	188	 100%
1	c	188	 99%
1	d	188	 99%
1	e	188	 100%
1	f	188	 100%
1	g	188	 99%
1	h	188	 99%
1	i	188	 100%
1	j	188	 99%
1	k	188	 99%
1	l	188	 100%
1	m	188	 99%
1	n	188	 99%
1	o	188	 99%
1	p	188	 100%
1	q	188	 100%
1	r	188	 99%
1	s	188	 100%
1	t	188	 100%
1	u	188	 99%
1	v	188	 100%
1	w	188	 99%
1	x	188	 99%
1	y	188	 100%
1	z	188	 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 87512 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	B	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	C	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	D	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	E	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	F	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	G	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	H	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	I	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	J	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	K	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	L	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	M	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	N	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	O	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	P	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	Q	188	Total 1457	C 907	N 268	O 276	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	S	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	T	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	U	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	V	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	W	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	X	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	Y	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	Z	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	a	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	b	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	c	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	d	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	e	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	f	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	g	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	h	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	i	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	j	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	k	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	l	188	Total 1457	C 907	N 268	O 276	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	n	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	o	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	p	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	q	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	r	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	s	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	t	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	u	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	v	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	w	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	x	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	y	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	z	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	0	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	1	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	2	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	3	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	4	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	5	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	6	188	Total 1457	C 907	N 268	O 276	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	
2	B	2	Total	Ca	0
			2	2	
2	C	1	Total	Ca	0
			1	1	
2	D	2	Total	Ca	0
			2	2	
2	E	2	Total	Ca	0
			2	2	
2	F	2	Total	Ca	0
			2	2	
2	G	2	Total	Ca	0
			2	2	
2	H	2	Total	Ca	0
			2	2	
2	I	2	Total	Ca	0
			2	2	
2	J	1	Total	Ca	0
			1	1	
2	K	2	Total	Ca	0
			2	2	
2	L	1	Total	Ca	0
			1	1	
2	M	2	Total	Ca	0
			2	2	
2	N	1	Total	Ca	0
			1	1	
2	O	2	Total	Ca	0
			2	2	
2	P	2	Total	Ca	0
			2	2	
2	Q	2	Total	Ca	0
			2	2	
2	R	2	Total	Ca	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
2	S	2	Total 2	Ca 2	0
2	T	1	Total 1	Ca 1	0
2	U	1	Total 1	Ca 1	0
2	V	1	Total 1	Ca 1	0
2	W	2	Total 2	Ca 2	0
2	X	2	Total 2	Ca 2	0
2	Y	1	Total 1	Ca 1	0
2	Z	2	Total 2	Ca 2	0
2	a	1	Total 1	Ca 1	0
2	b	1	Total 1	Ca 1	0
2	c	1	Total 1	Ca 1	0
2	d	1	Total 1	Ca 1	0
2	e	1	Total 1	Ca 1	0
2	f	1	Total 1	Ca 1	0
2	g	1	Total 1	Ca 1	0
2	h	1	Total 1	Ca 1	0
2	i	2	Total 2	Ca 2	0
2	j	1	Total 1	Ca 1	0
2	k	1	Total 1	Ca 1	0
2	l	1	Total 1	Ca 1	0
2	m	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	n	1	Total 1	Ca 1	0
2	o	1	Total 1	Ca 1	0
2	p	1	Total 1	Ca 1	0
2	q	1	Total 1	Ca 1	0
2	r	1	Total 1	Ca 1	0
2	s	1	Total 1	Ca 1	0
2	t	3	Total 3	Ca 3	0
2	u	1	Total 1	Ca 1	0
2	v	1	Total 1	Ca 1	0
2	w	2	Total 2	Ca 2	0
2	x	1	Total 1	Ca 1	0
2	y	2	Total 2	Ca 2	0
2	z	1	Total 1	Ca 1	0
2	0	2	Total 2	Ca 2	0
2	1	2	Total 2	Ca 2	0
2	2	2	Total 2	Ca 2	0
2	3	2	Total 2	Ca 2	0
2	4	2	Total 2	Ca 2	0
2	5	2	Total 2	Ca 2	0
2	6	3	Total 3	Ca 3	0
2	7	2	Total 2	Ca 2	0

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. 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. 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

Chain A:  99% .



- Molecule 1: Capsid protein

Chain B:  99% .



- Molecule 1: Capsid protein

Chain C:  99% .



- Molecule 1: Capsid protein

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain F:  99% .



- Molecule 1: Capsid protein

Chain G:  99%



- Molecule 1: Capsid protein

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain I:  99%



- Molecule 1: Capsid protein

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain L:  100%

There are no outlier residues recorded for this chain.

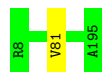
- Molecule 1: Capsid protein

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain N:  99%



- Molecule 1: Capsid protein

Chain O:  99% .



- Molecule 1: Capsid protein

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain Q:  99% .



- Molecule 1: Capsid protein

Chain R:  99% .



- Molecule 1: Capsid protein

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain W:  99% .



- Molecule 1: Capsid protein

Chain X:  99%



- Molecule 1: Capsid protein

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain a:  99%



- Molecule 1: Capsid protein

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain c:  99%



- Molecule 1: Capsid protein

Chain d:  99%



- Molecule 1: Capsid protein

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain g:  99%



- Molecule 1: Capsid protein

Chain h:  99%



- Molecule 1: Capsid protein

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain j:  99%



- Molecule 1: Capsid protein

Chain k:  99%



- Molecule 1: Capsid protein

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain m:  99%



- Molecule 1: Capsid protein

Chain n:  99%



- Molecule 1: Capsid protein

Chain o:  99%



- Molecule 1: Capsid protein

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain r:  99%



- Molecule 1: Capsid protein

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain u:  99%



- Molecule 1: Capsid protein

Chain v:  100%

There are no outlier residues recorded for this chain.

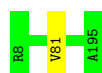
- Molecule 1: Capsid protein

Chain w:  99%



- Molecule 1: Capsid protein

Chain x:  99%



- Molecule 1: Capsid protein

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 1:  99%



- Molecule 1: Capsid protein

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 3:  99%



- Molecule 1: Capsid protein

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein

Chain 7:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	78988	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	178000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	0	0.34	0/1479	0.53	0/2004
1	1	0.35	0/1479	0.53	0/2004
1	2	0.35	0/1479	0.52	0/2004
1	3	0.35	0/1479	0.54	0/2004
1	4	0.35	0/1479	0.54	0/2004
1	5	0.35	0/1479	0.53	0/2004
1	6	0.34	0/1479	0.53	0/2004
1	7	0.35	0/1479	0.53	0/2004
1	A	0.35	0/1479	0.53	0/2004
1	B	0.34	0/1479	0.54	0/2004
1	C	0.35	0/1479	0.54	0/2004
1	D	0.35	0/1479	0.55	0/2004
1	E	0.34	0/1479	0.54	0/2004
1	F	0.35	0/1479	0.53	0/2004
1	G	0.34	0/1479	0.54	0/2004
1	H	0.35	0/1479	0.55	0/2004
1	I	0.35	0/1479	0.53	0/2004
1	J	0.35	0/1479	0.54	0/2004
1	K	0.34	0/1479	0.55	0/2004
1	L	0.34	0/1479	0.54	0/2004
1	M	0.34	0/1479	0.53	0/2004
1	N	0.35	0/1479	0.54	0/2004
1	O	0.34	0/1479	0.53	0/2004
1	P	0.34	0/1479	0.54	0/2004
1	Q	0.35	0/1479	0.53	0/2004
1	R	0.35	0/1479	0.53	0/2004
1	S	0.34	0/1479	0.53	0/2004
1	T	0.35	0/1479	0.53	0/2004
1	U	0.35	0/1479	0.54	0/2004
1	V	0.35	0/1479	0.54	0/2004
1	W	0.35	0/1479	0.54	0/2004
1	X	0.34	0/1479	0.53	0/2004

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.34	0/1479	0.54	0/2004
1	Z	0.35	0/1479	0.55	0/2004
1	a	0.35	0/1479	0.54	0/2004
1	b	0.35	0/1479	0.55	0/2004
1	c	0.35	0/1479	0.54	0/2004
1	d	0.34	0/1479	0.54	0/2004
1	e	0.34	0/1479	0.54	0/2004
1	f	0.34	0/1479	0.54	0/2004
1	g	0.34	0/1479	0.53	0/2004
1	h	0.34	0/1479	0.53	0/2004
1	i	0.35	0/1479	0.54	0/2004
1	j	0.35	0/1479	0.55	0/2004
1	k	0.34	0/1479	0.53	0/2004
1	l	0.35	0/1479	0.54	0/2004
1	m	0.35	0/1479	0.55	0/2004
1	n	0.35	0/1479	0.53	0/2004
1	o	0.34	0/1479	0.54	0/2004
1	p	0.34	0/1479	0.54	0/2004
1	q	0.35	0/1479	0.55	0/2004
1	r	0.34	0/1479	0.54	0/2004
1	s	0.34	0/1479	0.55	0/2004
1	t	0.35	0/1479	0.55	0/2004
1	u	0.35	0/1479	0.55	0/2004
1	v	0.35	0/1479	0.55	0/2004
1	w	0.35	0/1479	0.53	0/2004
1	x	0.35	0/1479	0.55	0/2004
1	y	0.35	0/1479	0.54	0/2004
1	z	0.35	0/1479	0.53	0/2004
All	All	0.35	0/88740	0.54	0/120240

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	0	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	1	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	2	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	3	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	4	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	5	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	6	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	7	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	A	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	B	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	C	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	D	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	E	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	F	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	G	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	H	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	I	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	J	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	K	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	L	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	M	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	N	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	O	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	P	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	Q	186/188 (99%)	183 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	S	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	T	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	U	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	V	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	W	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	X	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	Y	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	Z	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	a	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	b	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	c	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	d	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	e	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	f	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	g	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	h	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	i	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	j	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	k	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	l	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	m	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	n	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	o	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	p	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	q	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	r	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	s	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
1	t	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	u	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	v	186/188 (99%)	184 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	x	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
1	y	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	z	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
All	All	11160/11280 (99%)	11010 (99%)	150 (1%)	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	0	160/160 (100%)	160 (100%)	0	100	100
1	1	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	2	160/160 (100%)	160 (100%)	0	100	100
1	3	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	4	160/160 (100%)	160 (100%)	0	100	100
1	5	160/160 (100%)	160 (100%)	0	100	100
1	6	160/160 (100%)	160 (100%)	0	100	100
1	7	160/160 (100%)	160 (100%)	0	100	100
1	A	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	B	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	C	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	D	160/160 (100%)	160 (100%)	0	100	100
1	E	160/160 (100%)	160 (100%)	0	100	100
1	F	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	G	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	H	160/160 (100%)	160 (100%)	0	100	100
1	I	160/160 (100%)	159 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	160/160 (100%)	160 (100%)	0	100	100
1	K	160/160 (100%)	160 (100%)	0	100	100
1	L	160/160 (100%)	160 (100%)	0	100	100
1	M	160/160 (100%)	160 (100%)	0	100	100
1	N	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	O	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	P	160/160 (100%)	160 (100%)	0	100	100
1	Q	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	R	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	S	160/160 (100%)	160 (100%)	0	100	100
1	T	160/160 (100%)	160 (100%)	0	100	100
1	U	160/160 (100%)	160 (100%)	0	100	100
1	V	160/160 (100%)	160 (100%)	0	100	100
1	W	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	X	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	Y	160/160 (100%)	160 (100%)	0	100	100
1	Z	160/160 (100%)	160 (100%)	0	100	100
1	a	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	b	160/160 (100%)	160 (100%)	0	100	100
1	c	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	d	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	e	160/160 (100%)	160 (100%)	0	100	100
1	f	160/160 (100%)	160 (100%)	0	100	100
1	g	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	h	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	i	160/160 (100%)	160 (100%)	0	100	100
1	j	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	k	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	l	160/160 (100%)	160 (100%)	0	100	100
1	m	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	n	160/160 (100%)	159 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	p	160/160 (100%)	160 (100%)	0	100	100
1	q	160/160 (100%)	160 (100%)	0	100	100
1	r	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	s	160/160 (100%)	160 (100%)	0	100	100
1	t	160/160 (100%)	160 (100%)	0	100	100
1	u	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	v	160/160 (100%)	160 (100%)	0	100	100
1	w	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	x	160/160 (100%)	159 (99%)	1 (1%)	84	92
1	y	160/160 (100%)	160 (100%)	0	100	100
1	z	160/160 (100%)	160 (100%)	0	100	100
All	All	9600/9600 (100%)	9572 (100%)	28 (0%)	90	96

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	B	8	ARG
1	C	81	VAL
1	F	8	ARG
1	G	8	ARG
1	I	8	ARG
1	N	81	VAL
1	O	8	ARG
1	Q	8	ARG
1	R	8	ARG
1	W	8	ARG
1	X	8	ARG
1	a	8	ARG
1	c	81	VAL
1	d	8	ARG
1	g	8	ARG
1	h	8	ARG
1	j	8	ARG
1	k	8	ARG
1	m	8	ARG
1	n	8	ARG

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Mol	Chain	Res	Type
1	o	8	ARG
1	r	8	ARG
1	u	81	VAL
1	w	8	ARG
1	x	81	VAL
1	1	8	ARG
1	3	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	122	GLN
1	A	148	ASN
1	B	59	GLN
1	B	122	GLN
1	C	59	GLN
1	C	73	HIS
1	C	122	GLN
1	D	36	ASN
1	D	45	GLN
1	D	59	GLN
1	D	122	GLN
1	D	148	ASN
1	E	45	GLN
1	E	59	GLN
1	E	122	GLN
1	F	59	GLN
1	F	122	GLN
1	G	59	GLN
1	G	122	GLN
1	H	59	GLN
1	H	73	HIS
1	H	122	GLN
1	I	59	GLN
1	I	122	GLN
1	J	59	GLN
1	J	73	HIS
1	J	122	GLN
1	K	45	GLN
1	K	59	GLN
1	K	73	HIS

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Mol	Chain	Res	Type
1	K	122	GLN
1	K	148	ASN
1	L	45	GLN
1	L	59	GLN
1	L	73	HIS
1	L	122	GLN
1	M	59	GLN
1	M	122	GLN
1	N	59	GLN
1	N	73	HIS
1	N	122	GLN
1	O	59	GLN
1	O	122	GLN
1	P	45	GLN
1	P	59	GLN
1	P	122	GLN
1	P	148	ASN
1	Q	59	GLN
1	Q	73	HIS
1	Q	122	GLN
1	R	59	GLN
1	R	122	GLN
1	R	148	ASN
1	S	59	GLN
1	S	122	GLN
1	T	45	GLN
1	T	59	GLN
1	T	122	GLN
1	T	148	ASN
1	U	59	GLN
1	U	73	HIS
1	U	122	GLN
1	V	59	GLN
1	V	73	HIS
1	V	122	GLN
1	W	45	GLN
1	W	59	GLN
1	W	73	HIS
1	W	122	GLN
1	W	148	ASN
1	X	59	GLN
1	X	122	GLN

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Mol	Chain	Res	Type
1	Y	45	GLN
1	Y	59	GLN
1	Y	122	GLN
1	Z	45	GLN
1	Z	59	GLN
1	Z	122	GLN
1	Z	148	ASN
1	a	45	GLN
1	a	59	GLN
1	a	122	GLN
1	a	148	ASN
1	b	45	GLN
1	b	59	GLN
1	b	122	GLN
1	c	59	GLN
1	c	73	HIS
1	c	122	GLN
1	d	59	GLN
1	d	122	GLN
1	e	45	GLN
1	e	59	GLN
1	e	122	GLN
1	f	45	GLN
1	f	59	GLN
1	f	122	GLN
1	f	148	ASN
1	g	59	GLN
1	g	122	GLN
1	h	59	GLN
1	h	122	GLN
1	i	45	GLN
1	i	59	GLN
1	i	122	GLN
1	j	45	GLN
1	j	59	GLN
1	j	73	HIS
1	j	122	GLN
1	j	148	ASN
1	k	59	GLN
1	k	122	GLN
1	l	45	GLN
1	l	59	GLN

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Mol	Chain	Res	Type
1	l	122	GLN
1	m	45	GLN
1	m	59	GLN
1	m	122	GLN
1	m	148	ASN
1	n	59	GLN
1	n	122	GLN
1	n	148	ASN
1	o	59	GLN
1	o	122	GLN
1	p	45	GLN
1	p	59	GLN
1	p	73	HIS
1	p	122	GLN
1	p	148	ASN
1	q	45	GLN
1	q	59	GLN
1	q	73	HIS
1	q	122	GLN
1	q	148	ASN
1	r	59	GLN
1	r	122	GLN
1	s	45	GLN
1	s	59	GLN
1	s	122	GLN
1	t	45	GLN
1	t	59	GLN
1	t	73	HIS
1	t	122	GLN
1	t	148	ASN
1	u	59	GLN
1	u	73	HIS
1	u	122	GLN
1	v	59	GLN
1	v	73	HIS
1	v	122	GLN
1	w	59	GLN
1	w	73	HIS
1	w	122	GLN
1	x	59	GLN
1	x	73	HIS
1	x	122	GLN

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Mol	Chain	Res	Type
1	y	36	ASN
1	y	45	GLN
1	y	59	GLN
1	y	122	GLN
1	y	148	ASN
1	z	59	GLN
1	z	122	GLN
1	z	148	ASN
1	0	59	GLN
1	0	73	HIS
1	0	122	GLN
1	0	148	ASN
1	1	45	GLN
1	1	59	GLN
1	1	122	GLN
1	2	59	GLN
1	2	122	GLN
1	3	59	GLN
1	3	73	HIS
1	3	122	GLN
1	4	59	GLN
1	4	73	HIS
1	4	122	GLN
1	5	45	GLN
1	5	59	GLN
1	5	122	GLN
1	5	148	ASN
1	6	59	GLN
1	6	122	GLN
1	7	59	GLN
1	7	122	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 92 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.