

Feb 24, 2024 – 11:22 PM EST

PDB ID	:	7LNK
EMDB ID	:	EMD-23460
Title	:	Gorilla Bocavirus 1 Capsid
Authors	:	Yu, J.C.; Mietzsch, M.; Agbandje-McKenna, M.
Deposited on		
Resolution	:	2.76 Å(reported)

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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

#### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 Å.

Sidechain outliers

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		Percentile Ranks	Value
Ramachandran outliers			0
Sidechain outliers			0
Wors	е		Better
Per	centile relati	ve to all structures	
Per	centile relati	ve to all EM structures	
Matria		Whole archive	EM structures
Metric		$(\# {\rm Entries})$	(# Entries)
Ramachandran ou	tliers	154571	4023

154315

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  $\leq 5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

3826

Mol	Chain	Length	Quality of chain
1	1	510	100%
1	2	510	100%
1	3	510	100%
1	4	510	100%
1	5	510	100%
1	6	510	100%
1	7	510	100%
1	8	510	100%
1	А	510	



Mol	Chain	Length	Quality of chain
1	В	510	100%
1	С	510	100%
1	D	510	100%
1	Е	510	100%
1	F	510	100%
1	G	510	100%
1	Н	510	100%
1	Ι	510	100%
1	J	510	100%
1	K	510	100%
1	L	510	100%
1	M	510	100%
1	N	510	100%
1	0	510	•
			100%
1	P	510	100%
1	Q	510	100%
1	R	510	100%
1	S	510	100%
1	Т	510	100%
1	U	510	100%
1	V	510	100%
1	W	510	100%
1	Х	510	100%
1	Y	510	100%
1	Ζ	510	100%



Mol	Chain	Length	Quality of chain
1	a	510	100%
1	b	510	100%
1	с	510	100%
1	d	510	100%
1	е	510	100%
1	f	510	100%
1	g	510	100%
1	h	510	100%
1	i	510	100%
1	j	510	100%
1	k	510	100%
1	1	510	•
1		510	100%
	m		100%
1	n	510	100%
1	0	510	100%
1	р	510	100%
1	q	510	100%
1	r	510	100%
1	S	510	100%
1	t	510	100%
1	u	510	100%
1	V	510	100%
1	W	510	100%
1	х	510	100%
1	У	510	100%



N	Mol	Chain	Length	Quality of chain
	1		F10	
	T	$\mathbf{Z}$	510	100%



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 243540 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	٨	510	Total	С	Ν	0	S	1	0
1	А	510	4059	2575	691	771	22	1	0
1	D	510	Total	С	Ν	0	S	1	0
1	В	510	4059	2575	691	771	22	1	0
1	С	510	Total	С	Ν	0	S	1	0
1	C	510	4059	2575	691	771	22	L	0
1	D	510	Total	С	Ν	0	S	1	0
	D	510	4059	2575	691	771	22	L	0
1	Е	510	Total	С	Ν	0	S	1	0
	E	510	4059	2575	691	771	22	L	0
1	F	510	Total	С	Ν	0	S	1	0
	Г	510	4059	2575	691	771	22	L	0
1	G	510	Total	С	Ν	0	S	1	0
	G	510	4059	2575	691	771	22	L	0
1	Н	510	Total	С	Ν	0	S	1	0
	11	510	4059	2575	691	771	22	T	0
1	Ι	510	Total	С	Ν	0	S	1	0
	1	510	4059	2575	691	771	22	I	0
1	J	510	Total	С	Ν	0	S	1	0
	J	510	4059	2575	691	771	22	I	0
1	K	510	Total	С	Ν	0	S	1	0
	Γ	510	4059	2575	691	771	22	L	0
1	L	510	Total	С	Ν	0	S	1	0
		510	4059	2575	691	771	22	I	0
1	М	510	Total	$\mathbf{C}$	Ν	0	$\mathbf{S}$	1	0
	111	510	4059	2575	691	771	22	I	0
1	Ν	510	Total	С	Ν	0	S	1	0
	11	510	4059	2575	691	771	22	I	0
1	Ο	510	Total	С	Ν	0	S	1	0
		510	4059	2575	691	771	22		U
1	Р	510	Total	С	Ν	0	S	1	0
	1	510	4059	2575	691	771	22		U
1	0	510	Total	С	Ν	Ο	S	1	0
	Q	510	4059	2575	691	771	22		U

• Molecule 1 is a protein called Capsid protein.



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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Residues	5	At	oms			AltConf	Trace
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	п	F10	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	1	К	510	4059	2575	691	771	22	1	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	C	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	S	510	4059	2575	691	771	22	1	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	т	510	Total	С	Ν	0	S	1	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	1	1	510	4059	2575	691	771	22	L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	T	510	Total	С	Ν	Ο	S	1	0
1         V         510         4059         2575         691         771         22         1         0           1         W         510         Total         C         N         0         S         1         0           1         X         510         Total         C         N         0         S         1         0           1         X         510         Total         C         N         0         S         1         0           1         Y         510         Total         C         N         0         S         1         0           1         Y         510         Total         C         N         0         S         1         0           1         Z         510         Total         C         N         0         S         1         0           1         a         510         Total         C         N         0         S         1         0           1         b         510         Total         C         N         0         S         1         0           1         b         510         Total <td< td=""><td></td><td>U</td><td>510</td><td>4059</td><td>2575</td><td>691</td><td>771</td><td></td><td>L</td><td>0</td></td<>		U	510	4059	2575	691	771		L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	V	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	v	510	4059	2575	691	771	22	L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	117	510	Total	С	Ν	0	S	1	0
1         X         510         4059         2575         691         771         22         1         0           1         Y         510         Total         C         N         O         S         1         0           1         Y         510         Total         C         N         O         S         1         0           1         Z         510         Total         C         N         O         S         1         0           1         a         510         Total         C         N         O         S         1         0           1         a         510         Total         C         N         O         S         1         0           1         b         510         Total         C         N         O         S         1         0           1         c         510         Total         C         N         O         S         1         0           1         d         510         Total         C         N         O         S         1         0           1         f         510         Total <td< td=""><td>1</td><td>vv</td><td>510</td><td>4059</td><td>2575</td><td>691</td><td>771</td><td>22</td><td>L</td><td>0</td></td<>	1	vv	510	4059	2575	691	771	22	L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	v	510	Total	С	Ν	0	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Λ	510	4059	2575	691	771	22	L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	V	510	Total	С	Ν	0	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	I	510	4059	2575	691	771	22	L	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	1	7	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		510	4059	2575	691	771	22	L	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		a	510	4059	2575	691	771	22		0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	h	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	510	4059	2575	691	771	22	L	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		510	Total	С	Ν	0	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	C	510	4059	2575	691	771		L	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	d	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	u	510	4059	2575	691	771		I	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	0	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	е	510	4059	2575	691	771	22	I	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	f	510	Total	С	Ν	Ο	S	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	L	L	510	4059	2575	691	771	22	T	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	ſ	510	Total	С	Ν	Ο	$\mathbf{S}$	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	T	5	510	4059	2575	691	771		I	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	h	510	Total	С	Ν	Ο	$\mathbf{S}$	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	T	11	510	4059	2575		771		I	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	i	510	Total	С	Ν	Ο	$\mathbf{S}$	1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	1	510						1 	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	i	510						1	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		J	010						1	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	k	510			Ν		S	1	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	n.	010						1 	0
4059 2575 691 771 22	1	1	510						1	0
		1	010	4059	2575	691	771			0



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Mol	Chain	Residues	0	At	oms			AltConf	Trace
1		<b>F10</b>	Total	С	Ν	Ο	S	1	0
1	m	510	4059	2575	691	771	22	1	0
1		F10	Total	С	Ν	0	S	1	0
1	n	510	4059	2575	691	771	22	1	0
1		510	Total	С	Ν	Ο	S	1	0
1	0	510	4059	2575	691	771	22	1	0
1	n	510	Total	С	Ν	Ο	S	1	0
1	р	510	4059	2575	691	771	22	1	0
1		510	Total	С	Ν	0	S	1	0
1	q	510	4059	2575	691	771	22	L	0
1		510	Total	С	Ν	0	S	1	0
1	r	510	4059	2575	691	771	22	L	0
1	G	510	Total	С	Ν	Ο	S	1	0
1	S	510	4059	2575	691	771	22	L	0
1	t	510	Total	С	Ν	Ο	S	1	0
1	U	510	4059	2575	691	771	22	L	0
1		510	Total	С	Ν	Ο	S	1	0
1	u	510	4059	2575	691	771	22	L	0
1		510	Total	С	Ν	Ο	S	1	0
1	V	510	4059	2575	691	771	22		0
1		510	Total	С	Ν	0	S	1	0
1	W	510	4059	2575	691	771	22	1	0
1		F10	Total	С	Ν	0	S	1	0
1	X	510	4059	2575	691	771	22	1	0
1		510	Total	С	Ν	0	S	1	0
1	У	510	4059	2575	691	771	22	L	0
1	_	F10	Total	С	Ν	0	S	1	0
1	Z	510	4059	2575	691	771	22	1	0
1	1	510	Total	С	Ν	Ο	S	1	0
1	1	510	4059	2575	691	771	22	L	0
1	2	510	Total	С	Ν	0	S	1	0
1		510	4059	2575	691	771	22	L	0
1	3	510	Total	С	Ν	Ο	S	1	0
1	3	510	4059	2575	691	771	22	L	0
1	4	510	Total	С	Ν	Ο	S	1	0
1	4	510	4059	2575	691	771	22	1	0
1	5	510	Total	С	Ν	Ο	S	1	0
T	J	510	4059	2575	691	771	22		U
1	6	510	Total	С	Ν	Ο	$\mathbf{S}$	1	0
1	U	510	4059	2575	691	771	22	1	U
1	7	510	Total	С	Ν	Ο	S	1	0
1	(	510	4059	2575	691	771	22		0
		•					<u>a .</u> :	ned on ner	,

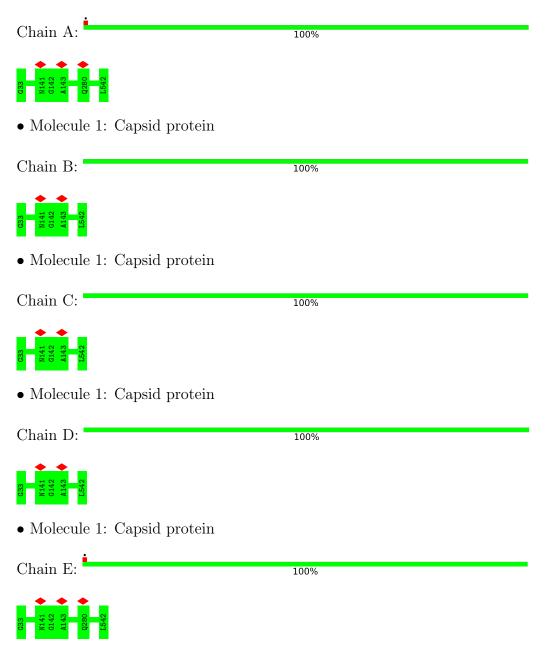


Mol	Chain	Residues		At	oms			AltConf	Trace
1	8	510	Total 4059	C 2575	N 691	0 771	S 22	1	0



## 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.





100%
100%
100%
100%
100%
100%
100%





Chain M:	100%
G33 6141 6143 280 4143 143 143 143 143 143 143 143 143 14	
• Molecule 1: Capsid protein	
Chain N:	100%
G33 6142 143 143 1542	
• Molecule 1: Capsid protein	
Chain O:	100%
G3 3 01 42 01 43 0280 0280 0280 0280 0280 0280 0280 028	
• Molecule 1: Capsid protein	
Chain P:	100%
G33 6141 6142 L542 L542	
• Molecule 1: Capsid protein	
Chain Q:	100%
G33 G142 A143 L542 L542	
• Molecule 1: Capsid protein	
Chain R:	100%
G133 G142 A143 L542 L542	



Chain S:	100%	•
G33 C142 L542 L542		
• Molecule 1: Capsid protein		
Chain T:	100%	•
G33 6142 A143 L542 L542		
• Molecule 1: Capsid protein		
Chain U:	100%	•
G33 M141 6142 A143 L542		
• Molecule 1: Capsid protein		
Chain V:	100%	•
G33 N141 A143 L542 L542		
• Molecule 1: Capsid protein		
Chain W:	100%	-
G33 N141 G142 A143 L542		
• Molecule 1: Capsid protein		
Chain X:	100%	•
G33 142 A142 C580 ♦ L542		
• Molecule 1: Capsid protein		
Chain Y:	100%	•
633 N141 A143 L542 L542		



• Molecule 1: Capsid protein	
Chain Z:	100%
G33 C142 A143 C142 L542 L542	
• Molecule 1: Capsid protein	
Chain a:	100%
G33 N141 C142 A143 L542 L542	
• Molecule 1: Capsid protein	
Chain b:	100%
G133 0141 6142 1384 1542 L542	
• Molecule 1: Capsid protein	
Chain c:	100%
G33 M141 ← C142 A143 ← C280 ← L542	
• Molecule 1: Capsid protein	
Chain d:	100%
G33 N141 C142 L542 L542	
• Molecule 1: Capsid protein	
Chain e:	100%
633 0141 143 1542 1542	
• Molecule 1: Capsid protein	
Chain f:	100%





Chain g:	100%
G33 N141 ♦ A143 ♦ L542 L542	
• Molecule 1: Capsid protein	
Chain h:	100%
G33 N141 G142 A143 Q280 Q280 Q280 Q280	
• Molecule 1: Capsid protein	
Chain i:	100%
G33 N141 G142 A143 L542 L542	
• Molecule 1: Capsid protein	
Chain j:	100%
633 1141 6142 A143 L542	
• Molecule 1: Capsid protein	
Chain k:	100%
G33 N141 A143 A143 L542	
• Molecule 1: Capsid protein	
Chain l:	100%
G33 142 142 142 1542 1542	
• Molecule 1: Capsid protein	



Chain m:	100%
C33 C142 L143 L542	
• Molecule 1: Capsid protein	
Chain n:	100%
G33 1141 6142 143 143 143 143 143 143 143	
• Molecule 1: Capsid protein	
Chain o:	100%
G33 N1 41 C1 42 A1 43 A1 43 C1 42 L5 42	
• Molecule 1: Capsid protein	
Chain p:	100%
C 33 N 141 6 142 1542 1542	
• Molecule 1: Capsid protein	
Chain q:	100%
G33 6142 1542 L542	
• Molecule 1: Capsid protein	
Chain r:	100%
G33 1141 6142 1143 1143	
• Molecule 1: Capsid protein	
Chain s:	100%





Chain t:	100%
G33           N141           G142           A143           Q280           Q280	
• Molecule 1: Capsid protein	
Chain u:	100%
G33 C142 L542 L542	
• Molecule 1: Capsid protein	
Chain v:	100%
G33       N141       G142       A143       Q280       Q242	
• Molecule 1: Capsid protein	
Chain w:	100%
G33 N141 C142 A143 Q280 Q280 Q280 Q280 Q280	
• Molecule 1: Capsid protein	
Chain x:	100%
G33           0142           A143           L542	
• Molecule 1: Capsid protein	
Chain y:	100%
G33           N141           G142           A143           Q280           Q280           L542	
• Molecule 1: Capsid protein	



Chain z:	100%
G1142 61143 1143 1144	
• Molecule 1: Capsid protein	
Chain 1:	100%
G33 C1441 C1443 A143 L542 L542	
• Molecule 1: Capsid protein	
Chain 2:	100%
G33 M141 6142 A143 L542	
• Molecule 1: Capsid protein	
Chain 3:	100%
G33 N141 G142 A143 Q280 Q280 L542	
• Molecule 1: Capsid protein	
Chain 4:	100%
G33 N141 A143 L542 L542	
• Molecule 1: Capsid protein	
Chain 5:	100%
033 M141 0142 A143 L542	
• Molecule 1: Capsid protein	
Chain 6:	100%
633 1414 1413 1413 1413 1542	



Chain 7:

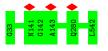
100%



• Molecule 1: Capsid protein

Chain 8:

100%





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	168565	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 $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	18.198	Depositor
Minimum map value	-11.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^{\circ}$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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	l angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	1	0.50	0/4187	0.56	0/5712
1	2	0.50	0/4187	0.56	0/5712
1	3	0.50	0/4187	0.56	0/5712
1	4	0.50	0/4187	0.56	0/5712
1	5	0.50	0/4187	0.56	0/5712
1	6	0.50	0/4187	0.56	0/5712
1	7	0.50	0/4187	0.56	0/5712
1	8	0.50	0/4187	0.56	0/5712
1	А	0.50	0/4187	0.56	0/5712
1	В	0.50	0/4187	0.56	0/5712
1	С	0.50	0/4187	0.56	0/5712
1	D	0.50	0/4187	0.56	0/5712
1	Е	0.50	0/4187	0.56	0/5712
1	F	0.50	0/4187	0.56	0/5712
1	G	0.50	0/4187	0.56	0/5712
1	Н	0.50	0/4187	0.56	0/5712
1	Ι	0.50	0/4187	0.56	0/5712
1	J	0.50	0/4187	0.56	0/5712
1	Κ	0.50	0/4187	0.56	0/5712
1	L	0.50	0/4187	0.56	0/5712
1	М	0.50	0/4187	0.56	0/5712
1	Ν	0.50	0/4187	0.56	0/5712
1	0	0.50	0/4187	0.56	0/5712
1	Р	0.50	0/4187	0.56	0/5712
1	Q	0.50	0/4187	0.56	0/5712
1	R	0.50	0/4187	0.56	0/5712
1	S	0.50	0/4187	0.56	0/5712
1	Т	0.50	0/4187	0.56	0/5712
1	U	0.50	0/4187	0.56	0/5712
1	V	0.50	0/4187	0.56	0/5712
1	W	0.50	0/4187	0.56	0/5712
1	Х	0.50	0/4187	0.56	0/5712
1	Y	0.50	0/4187	0.56	0/5712
1	Ζ	0.50	0/4187	0.56	0/5712



Mol	Chain	Bond lengths Bond an		l angles	
WIOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	а	0.50	0/4187	0.56	0/5712
1	b	0.50	0/4187	0.56	0/5712
1	с	0.50	0/4187	0.56	0/5712
1	d	0.50	0/4187	0.56	0/5712
1	е	0.50	0/4187	0.56	0/5712
1	f	0.50	0/4187	0.56	0/5712
1	g	0.50	0/4187	0.56	0/5712
1	h	0.50	0/4187	0.56	0/5712
1	i	0.50	0/4187	0.56	0/5712
1	j	0.50	0/4187	0.56	0/5712
1	k	0.50	0/4187	0.56	0/5712
1	1	0.50	0/4187	0.56	0/5712
1	m	0.50	0/4187	0.56	0/5712
1	n	0.50	0/4187	0.56	0/5712
1	0	0.50	0/4187	0.56	0/5712
1	р	0.50	0/4187	0.56	0/5712
1	q	0.50	0/4187	0.56	0/5712
1	r	0.50	0/4187	0.56	0/5712
1	s	0.50	0/4187	0.56	0/5712
1	t	0.50	0/4187	0.56	0/5712
1	u	0.50	0/4187	0.56	0/5712
1	V	0.50	0/4187	0.56	0/5712
1	W	0.50	0/4187	0.56	0/5712
1	Х	0.50	0/4187	0.56	0/5712
1	У	0.50	0/4187	0.56	0/5712
1	Z	0.50	0/4187	0.56	0/5712
All	All	0.50	0/251220	0.56	0/342720

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 (i)

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



### 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	Perce	ntiles
1	1	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	2	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	3	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	4	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	5	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	6	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	7	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	8	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	А	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	В	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	С	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	D	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Ε	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	F	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	G	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Н	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Ι	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	J	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	K	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	L	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	М	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Ν	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	0	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Р	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Q	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
	1			1	Continued a	on next	page



1	R						entiles
	п	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	S	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	Т	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	U	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	V	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	W	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	Х	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	Y	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	Ζ	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	a	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	b	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	с	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	d	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	е	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	f	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	g	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	h	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	i	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	j	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	k	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	1	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	m	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	n	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	0	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	р	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	q	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	r	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	s	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	t	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	u	509/510~(100%)	501 (98%)	8 (2%)	0	100	100
1	V	509/510~(100%)	501 (98%)	8 (2%)	0	100	100

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	W	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	х	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	У	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
1	Z	509/510~(100%)	501~(98%)	8 (2%)	0	100	100
All	All	30540/30600~(100%)	30060 (98%)	480 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	445/444~(100%)	445 (100%)	0	100 100
1	2	445/444~(100%)	445 (100%)	0	100 100
1	3	445/444~(100%)	445 (100%)	0	100 100
1	4	445/444~(100%)	445 (100%)	0	100 100
1	5	445/444~(100%)	445 (100%)	0	100 100
1	6	445/444~(100%)	445 (100%)	0	100 100
1	7	445/444~(100%)	445 (100%)	0	100 100
1	8	445/444~(100%)	445 (100%)	0	100 100
1	А	445/444~(100%)	445 (100%)	0	100 100
1	В	445/444~(100%)	445 (100%)	0	100 100
1	С	445/444 (100%)	445 (100%)	0	100 100
1	D	445/444~(100%)	445 (100%)	0	100 100
1	Ε	445/444~(100%)	445 (100%)	0	100 100
1	F	445/444~(100%)	445 (100%)	0	100 100
1	G	445/444 (100%)	445 (100%)	0	100 100
1	Н	445/444~(100%)	445 (100%)	0	100 100
1	Ι	445/444~(100%)	445 (100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	J	445/444~(100%)	445 (100%)	0	100	100
1	Κ	445/444~(100%)	445 (100%)	0	100	100
1	L	445/444 (100%)	445 (100%)	0	100	100
1	М	445/444 (100%)	445 (100%)	0	100	100
1	Ν	445/444 (100%)	445 (100%)	0	100	100
1	Ο	445/444 (100%)	445 (100%)	0	100	100
1	Р	445/444 (100%)	445 (100%)	0	100	100
1	Q	445/444 (100%)	445 (100%)	0	100	100
1	R	445/444 (100%)	445 (100%)	0	100	100
1	S	445/444 (100%)	445 (100%)	0	100	100
1	Т	445/444 (100%)	445 (100%)	0	100	100
1	U	445/444 (100%)	445 (100%)	0	100	100
1	V	445/444 (100%)	445 (100%)	0	100	100
1	W	445/444 (100%)	445 (100%)	0	100	100
1	Х	445/444 (100%)	445 (100%)	0	100	100
1	Y	445/444 (100%)	445 (100%)	0	100	100
1	Ζ	445/444~(100%)	445 (100%)	0	100	100
1	a	445/444~(100%)	445 (100%)	0	100	100
1	b	445/444~(100%)	445 (100%)	0	100	100
1	с	445/444~(100%)	445 (100%)	0	100	100
1	d	445/444~(100%)	445 (100%)	0	100	100
1	е	445/444~(100%)	445 (100%)	0	100	100
1	f	445/444~(100%)	445 (100%)	0	100	100
1	g	445/444~(100%)	445 (100%)	0	100	100
1	h	445/444~(100%)	445 (100%)	0	100	100
1	i	445/444~(100%)	445 (100%)	0	100	100
1	j	445/444 (100%)	445 (100%)	0	100	100
1	k	445/444 (100%)	445 (100%)	0	100	100
1	1	445/444~(100%)	445 (100%)	0	100	100
1	m	445/444~(100%)	445 (100%)	0	100	100
1	n	445/444~(100%)	445 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	О	445/444~(100%)	445 (100%)	0	100	100
1	р	445/444~(100%)	445 (100%)	0	100	100
1	q	445/444~(100%)	445 (100%)	0	100	100
1	r	445/444~(100%)	445 (100%)	0	100	100
1	$\mathbf{S}$	445/444~(100%)	445 (100%)	0	100	100
1	t	445/444~(100%)	445 (100%)	0	100	100
1	u	445/444~(100%)	445 (100%)	0	100	100
1	v	445/444~(100%)	445 (100%)	0	100	100
1	W	445/444~(100%)	445 (100%)	0	100	100
1	х	445/444~(100%)	445 (100%)	0	100	100
1	У	445/444~(100%)	445 (100%)	0	100	100
1	Z	445/444~(100%)	445 (100%)	0	100	100
All	All	26700/26640~(100%)	26700 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (744) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	58	ASN
1	А	67	GLN
1	А	68	ASN
1	А	109	GLN
1	А	163	HIS
1	А	189	GLN
1	А	197	ASN
1	А	230	HIS
1	А	251	ASN
1	А	358	GLN
1	А	443	HIS
1	А	537	ASN
1	В	58	ASN
1	В	67	GLN
1	В	68	ASN
1	В	101	GLN
1	В	109	GLN
1	В	163	HIS
1	В	189	GLN



Mol	Chain	Res	Type
1	В	197	ASN
1	В	230	HIS
1	В	251	ASN
1	В	358	GLN
1	В	443	HIS
1	В	537	ASN
1	С	58	ASN
1	С	67	GLN
1	С	68	ASN
1	С	101	GLN
1	С	109	GLN
1	С	163	HIS
1	С	189	GLN
1	С	197	ASN
1	C C C C C C C C C C C C C D D	230	HIS
1	С	251	ASN
1	С	358	GLN
1	С	443	HIS
1	С	537	ASN
1	D	58	ASN
1	D	67	GLN
1	D	68	ASN
1	D	109	GLN
1	D	163	HIS
1	D D D	189	GLN
1	D	197	ASN
1	D	230	HIS
1	D	251	ASN
1	D	358	GLN
1	D	443	HIS
1	D	537	ASN
1	Е	58	ASN
1	Е	67	GLN
1	Е	68	ASN
1	Е	109	GLN
1	Е	137	GLN
1	Е	163	HIS
1	Е	189	GLN
1	Е	197	ASN
1	Е	230	HIS
1	Е	251	ASN
1	Е	358	GLN



Mol	Chain	Res	Type
1	Е	443	HIS
1	Е	537	ASN
1	F	58	ASN
1	F	67	GLN
1	F	68	ASN
1	F	109	GLN
1	F	137	GLN
1	F	163	HIS
1	F	189	GLN
1	F	197	ASN
1	F	230	HIS
1	F F	251	ASN
1	F	358	GLN
1	F	443	HIS
1	F	537	ASN
1	G	58	ASN
1	G	67	GLN
1	G	68	ASN
1	G	101	GLN
1	G	109	GLN
1	G	137	GLN
1	G	163	HIS
1	G	189	GLN
1	G	197	ASN
1	G	230	HIS
1	G	251	ASN
1	G	358	GLN
1	G	443	HIS
1	G	537	ASN
1	Н	58	ASN
1	Н	67	GLN
1	Н	68	ASN
1	Н	109	GLN
1	Н	137	GLN
1	Н	163	HIS
1	Н	189	GLN
1	Н	197	ASN
1	Н	230	HIS
1	Н	251	ASN
1	Н	358	GLN
1	Н	443	HIS
1	Н	537	ASN



Mol	Chain	Res	Type
1	Ι	58	ASN
1	Ι	67	GLN
1	Ι	68	ASN
1	Ι	109	GLN
1	Ι	163	HIS
1	Ι	189	GLN
1	Ι	197	ASN
1	Ι	230	HIS
1	Ι	251	ASN
1	Ι	358	GLN
1	Ι	443	HIS
1	Ι	537	ASN
1	J	58	ASN
1	J	67	GLN
1	J	68	ASN
1	J	109	GLN
1	J	163	HIS
1	J	189	GLN
1	J	197	ASN
1	J	230	HIS
1	J	251	ASN
1	J	358	GLN
1	J	443	HIS
1	J	537	ASN
1	K	58	ASN
1	K	67	GLN
1	K	68	ASN
1	K	109	GLN
1	K	163	HIS
1	K	189	GLN
1	K	197	ASN
1	K	230	HIS
1	K	251	ASN
1	K	358	GLN
1	K	443	HIS
1	K	537	ASN
1	L	58	ASN
1	L	67	GLN
1	L	68	ASN
1	L	109	GLN
1	L	163	HIS
1	L	189	GLN



Mol	Chain	Res	Type
1	L	197	ASN
1	L	230	HIS
1	L	251	ASN
1	L	358	GLN
1	L	443	HIS
1	L	537	ASN
1	М	58	ASN
1	М	67	GLN
1	М	68	ASN
1	М	109	GLN
1	М	163	HIS
1	М	189	GLN
1	М	197	ASN
1	М	230	HIS
1	М	251	ASN
1	М	358	GLN
1	М	443	HIS
1	М	537	ASN
1	Ν	58	ASN
1	Ν	67	GLN
1	Ν	68	ASN
1	N	109	GLN
1	Ν	163	HIS
1	N	189	GLN
1	Ν	197	ASN
1	N	230	HIS
1	N	251	ASN
1	N	358	GLN
1	N	443	HIS
1	Ν	537	ASN
1	0	58	ASN
1	0	67	GLN
1	0 0 0 0 0 0 0 0 0 0	68	ASN
1	0	101	GLN
1	0	109	GLN
1	0	137	GLN GLN
1	0	163	HIS
1	0	189	GLN
1	0	197	ASN
1	0	230	HIS
1	0	251	ASN
1			



Mol	Chain	Res	Type
1	0	443	HIS
1	0	537	ASN
1	Р	58	ASN
1	Р	67	GLN
1	P P P P P	68	ASN
1	Р	109	GLN
1	Р	163	HIS
1	Р	189	GLN
1	Р	197	ASN
1	Р	230	HIS
1	Р	251	ASN
1	Р	358	GLN HIS
1	Р	443	HIS
1	Р	537	ASN
1	Q	58	ASN ASN
1	Q	67	GLN ASN
1	P           P           P           P           P           Q	68	
1	Q	109	GLN
1	Q	163	HIS
1	Q	189	GLN
1	Q	197	ASN
1	Q	230	HIS
1	Q	251	ASN
1	Q	358	GLN
1	Q	443	HIS
1	Q	537	ASN
1	R	58	ASN
1	R	67	GLN
1	R	68	ASN
1	R	109	GLN
1	R	163	HIS
1	R	189	GLN
1	R	197	ASN
1	R	230	HIS
1	R	251	ASN
1	R	358	GLN
1	R	443	HIS
1	R	537	ASN
1	S	58	ASN
1	S	67	GLN
1	S	68	ASN
1	S	101	GLN



Mol	Chain	Res	Type
1	S	109	GLN
1	S	163	HIS
1	S	189	GLN
1	S	197	ASN
1	S S S S	230	HIS
1	S	251	ASN
1	S	358	GLN
1	S	443	HIS
1	S	537	ASN
1	Т	58	ASN
1	Т	67	GLN
1	Т	68	ASN
1	S T T T T	109	GLN
1	Т	163	HIS
1	Т	189	GLN
1	T T T T T T	197	ASN
1	Т	230	HIS
1	Т	251	ASN
1	Т	358	GLN
1	Т	443	HIS
1	Т	537	ASN
1	U	58	ASN
1	U	67	GLN
1	U	68	ASN
1	U	109	GLN
1	U	163	HIS
1	U	189	GLN
1	U	197	ASN
1	U	230	HIS
1	U	251	ASN
1	U	358	GLN
1	U	443	HIS
1	U	537	ASN
1	V	58	ASN
1	V	67	GLN
1	V	68	ASN
1	V	109	GLN
1	V	163	HIS
1	V	189	GLN
1	V	197	ASN
1	V	230	HIS
	· V		
1	V	251	ASN



Mol	Chain	Res	Type
1	V	358	GLN
1	V	443	HIS
1	V	537	ASN
1	W	58	ASN
1	W	67	GLN
1	W	68	ASN
1	W	109	GLN
1	W	163	HIS
1	W	189	GLN
1	W	197	ASN
1	W	230	HIS
1	W	251	ASN
1	W	358	GLN
1	W	443	HIS
1	W	537	ASN
1	Х	58	ASN
1	Х	67	GLN
1	Х	68	ASN
1	Х	109	GLN
1	Х	163	HIS
1	Х	189	GLN
1	Х	197	ASN
1	X	230	HIS
1	X	251	ASN
1	Х	358	GLN
1	X	443	HIS
1	Х	537	ASN
1	Y	58	ASN
1	Y	67	GLN
1	Y	68	ASN
1	Y	109	GLN
1	Y	163	HIS
1	Y	189	GLN
1	Y	197	ASN
1	Y Y	230	HIS
1	Y	251	ASN
1	Y	358	GLN
1	Y	443	HIS
1	Y	537	ASN
1	Z	58	ASN
1	Z Z	67	GLN
1	Z	68	ASN



Mol	Chain	Res	Type
1	Ζ	109	GLN
1	Ζ	163	HIS
1	Ζ	189	GLN
1	Ζ	197	ASN
1	Ζ	230	HIS
1	Ζ	251	ASN
1	Ζ	358	GLN
1	Ζ	443	HIS
1	Ζ	537	ASN
1	a	58	ASN
1	a	67	GLN
1	a	68	ASN
1	a	109	GLN
1	a	163	HIS
1	a	189	GLN
1	a	197	ASN
1	a	230	HIS
1	a	251	ASN
1	a	358	GLN
1	a	443	HIS
1	a	537	ASN
1	b	58	ASN
1	b	67	GLN
1	b	68	ASN
1	b	101	GLN
1	b	109	GLN
1	b	163	HIS
1	b	189	GLN
1	b	197	ASN
1	b	230	HIS
1	b	251	ASN
1	b	358	GLN
1	b	443	HIS
1	b	537	ASN
1	С	58	ASN
1	c	67	GLN
1	c	68	ASN
1	c	109	GLN
1	c	163	HIS
1	c	189	GLN
1	c	197	ASN
1	c	230	HIS



Mol	Chain	Res	Type
1	с	251	ASN
1	с	358	GLN
1	с	443	HIS
1	с	537	ASN
1	d	58	ASN
1	d	67	GLN
1	d	68	ASN
1	d	109	GLN
1	d	137	GLN
1	d	163	HIS
1	d	189	GLN
1	d	197	ASN
1	d	230	HIS
1	d	251	ASN
1	d	358	GLN
1	d	443	HIS
1	d	537	ASN
1	е	58	ASN
1	е	67	GLN
1	е	68	ASN
1	е	109	GLN
1	е	163	HIS
1	е	189	GLN
1	е	197	ASN
1	е	230	HIS
1	е	251	ASN
1	е	358	GLN
1	е	443	HIS
1	е	537	ASN
1	f	58	ASN
1	f	67	GLN
1	f	68	ASN
1	f	101	GLN
1	f	109	GLN
1	f	163	HIS
1	f	189	GLN
1	f	197	ASN
1	f	230	HIS
1	f	251	ASN
1	f	358	GLN
1	f	443	HIS
1	f	537	ASN



Mol	Chain	Res	Type
1	g	58	ASN
1	g	67	GLN
1	g	68	ASN
1	g	101	GLN
1	g	109	GLN
1	g	163	HIS
1	g	189	GLN
1	g	197	ASN
1	g	230	HIS
1	g	251	ASN
1	g	358	GLN
1	g	443	HIS
1	g	537	ASN
1	h	58	ASN
1	h	67	GLN
1	h	68	ASN
1	h	109	GLN
1	h	163	HIS
1	h	189	GLN
1	h	197	ASN
1	h	230	HIS
1	h	251	ASN
1	h	358	GLN
1	h	443	HIS
1	h	537	ASN
1	i	58	ASN
1	i	67	GLN
1	i	68	ASN
1	i	109	GLN
1	i	163	HIS
1	i	189	GLN
1	i	197	ASN
1	i	230	HIS
1	i	251	ASN
1	i	358	GLN
1	i	443	HIS
1	i	537	ASN
1		58	ASN
1	j	67	GLN
1	j	68	ASN
1	j j j j	109	GLN
1	i	163	HIS



Mol	Chain	Res	Type
1	j	189	GLN
1	j j j j j j k	197	ASN
1	j	230	HIS
1	j	251	ASN
1	j	358	GLN
1	j	443	HIS
1	j	537	ASN
1	k	58	ASN
1	k	67	GLN
1	k	68	ASN
1	k	109	GLN
1	k	163	HIS
1	k	189	GLN
1	k	197	ASN
1	k	230	HIS
1	k	251	ASN
1	k	358	GLN
1	k	443	HIS
1	k	537	ASN
1	1	58	ASN
1	1	67	GLN
1	1	68	ASN
1	1	101	GLN
1	1	109	GLN
1	1	163	HIS
1	1	189	GLN
1	1	197	ASN
1	1	230	HIS
1	1	251	ASN
1	1	358	GLN
1	1	443	HIS
1	1	537	ASN
1	m	58	ASN
1	m	67	GLN
1	m	68	ASN
1	m	109	GLN
1	m	163	HIS
1	m	189	GLN
1	m	197	ASN
1	m	230	HIS
1	m	250 251	ASN
1	m	358	GLN
-	Continuu		



Mol	Chain	Res	Type
1	m	443	HIS
1	m	537	ASN
1	n	58	ASN
1	n	67	GLN
1	n	68	ASN
1	n	109	GLN
1	n	137	GLN
1	n	163	HIS
1	n	189	GLN
1	n	197	ASN
1	n	230	HIS
1	n	251	ASN
1	n	358	GLN
1	n	443	HIS
1	n	537	ASN
1	0	58	ASN
1	0	67	GLN
1	0	68	ASN
1	0	109	GLN
1	0	163	HIS
1	0	189	GLN
1	0	197	ASN
1	0	230	HIS
1	0	251	ASN
1	0	358	GLN
1	0	443	HIS
1	0	537	ASN
1	р	58	ASN
1	p	67	GLN
1	p	68	ASN
1	p	109	GLN
1	p	163	HIS
1	p	189	GLN
1	p	197	ASN
1	p	230	HIS
1	p	251	ASN
1	p	358	GLN
1	p p	443	HIS
1	p p	537	ASN
	q	58	ASN
1	q	67	GLN



Mol	Chain	Res	Type
1	q	109	GLN
1	q	163	HIS
1	q	189	GLN
1	q	197	ASN
1	q	230	HIS
1	q	251	ASN
1	q	358	GLN
1	q	443	HIS
1	q	537	ASN
1	r	58	ASN
1	r	67	GLN
1	r	68	ASN
1	r	109	GLN
1	r	137	GLN
1	r	163	HIS
1	r	189	GLN
1	r	197	ASN
1	r	230	HIS
1	r	251	ASN
1	r	358	GLN
1	r	443	HIS
1	r	537	ASN
1	s	58	ASN
1	s	67	GLN
1	S	68	ASN
1	S	101	GLN
1	S	109	GLN
1	S	163	HIS
1	S	189	GLN
1	S	197	ASN
1	S	230	HIS
1	s	251	ASN
1	S	358	GLN
1	S	443	HIS
1	S	537	ASN
1	t	58	ASN
1	t	67	GLN
1	t	68	ASN
1	t	101	GLN
1	t	109	GLN
1	t	137	GLN
1	t	163	HIS



Mol	Chain	Res	Type
1	t	189	GLN
1	t	197	ASN
1	t	230	HIS
1	t	251	ASN
1	t	358	GLN
1	t	443	HIS
1	t	537	ASN
1	u	58	ASN
1	u	67	GLN
1	u	68	ASN
1	u	109	GLN
1	u	163	HIS
1	u	189	GLN
1	u	197	ASN
1	u	230	HIS
1	u	251	ASN
1	u	358	GLN
1	u	443	HIS
1	u	537	ASN
1	V	58	ASN
1	V	67	GLN
1	V	68	ASN
1	V	109	GLN
1	V	163	HIS
1	V	189	GLN
1	V	197	ASN
1	V	230	HIS
1	V	251	ASN
1	v	358	GLN
1	V	443	HIS
1	V	537	ASN
1	W	58	ASN
1	W	67	GLN
1	W	68	ASN
1	W	109	GLN
1	W	137	GLN
1	W	163	HIS
1	W	189	GLN
1	W	197	ASN
1	W	230	HIS
1	W	250	ASN
-	••		~-



Mol	Chain	Res	Type
1	W	443	HIS
1	W	537	ASN
1	Х	58	ASN
1	Х	67	GLN
1	Х	68	ASN
1	Х	109	GLN
1	Х	163	HIS
1	Х	189	GLN
1	Х	197	ASN
1	Х	230	HIS
1	х	251	ASN
1	Х	358	GLN
1	х	443	HIS
1	X	537	ASN
1	У	58	ASN
1	У	67	GLN
1	y	68	ASN
1	у	109	GLN
1	У	137	GLN
1	У	163	HIS
1	У	189	GLN
1	У	197	ASN
1	У	230	HIS
1	У	251	ASN
1	У	358	GLN
1	У	443	HIS
1	y	537	ASN
1	Z	58	ASN
1	Z	67	GLN
1	Z	68	ASN
1	Z	109	GLN
1	Z	163	HIS
1	Z	189	GLN
1	Z	197	ASN
1	Z	230	HIS
1	Z	251	ASN
1	Z	358	GLN
1	Z	443	HIS
1	Z	537	ASN
1	1	58	ASN
1	1	67	GLN
1	1	68	ASN



Mol	Chain	Res	Type
1	1	101	GLN
1	1	109	GLN
1	1	137	GLN
1	1	163	HIS
1	1	189	GLN
1	1	197	ASN
1	1	230	HIS
1	1	251	ASN
1	1	358	GLN
1	1	443	HIS
1	1	537	ASN
1	2	58	ASN
1	2	67	GLN
1	2 2 2 2 2 2	68	ASN
1	2	109	GLN
1	2	163	HIS
1	2	189	GLN
1	2 2 2	197	ASN
1	2	230	HIS
1		251	ASN
1	2	358	GLN
1	2	443	HIS
1	23	537	ASN
1		58	ASN
1	3	67	GLN
1	3	68	ASN
1	3	109	GLN HIS
1	3	163	
1	3	189	GLN
1	3	197	ASN
1	3	230	HIS
1	3	251	ASN
1	3	358	GLN
1	3	443	HIS
1	3	537	ASN
1	4	58	ASN
1	4	67	GLN
1	4	68	ASN
1	4	109	GLN
1	4	163	HIS
1	4	189	GLN
1	4	197	ASN



Mol	Chain	Res	Type
1	4	230	HIS
1	4	251	ASN
1	4	358	GLN
1	4	443	HIS
1	4	537	ASN
1	5	58	ASN
1	5	67	GLN
1	5	68	ASN
1	5	109	GLN
1	5	163	HIS
1	5	189	GLN
1	5	197	ASN
1	5	230	HIS
1	5	251	ASN
1	5	358	GLN
1	5	443	HIS
1	5	537	ASN
1	6	58	ASN
1	6	67	GLN
1	6	68	ASN
1	6	109	GLN
1	6	163	HIS
1	6	189	GLN
1	6	197	ASN
1	6	230	HIS
1	6	251	ASN
1	6	358	GLN
1	6	443	HIS
1	6	537	ASN
1	7	58	ASN
1	7	67	GLN
1	7	68	ASN
1	7	109	GLN HIS
1	7	163	HIS
1	7	189	GLN
1	7	197	ASN
1	7	230	HIS
1	7	251	ASN
1	7	358	GLN
1	7	443	HIS
1	7	537	ASN
1	8	58	ASN



$\mathbf{Mol}$	Chain	Res	Type
1	8	67	GLN
1	8	68	ASN
1	8	109	GLN
1	8	163	HIS
1	8	189	GLN
1	8	197	ASN
1	8	230	HIS
1	8	251	ASN
1	8	358	GLN
1	8	443	HIS
1	8	537	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 monosaccharides 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.



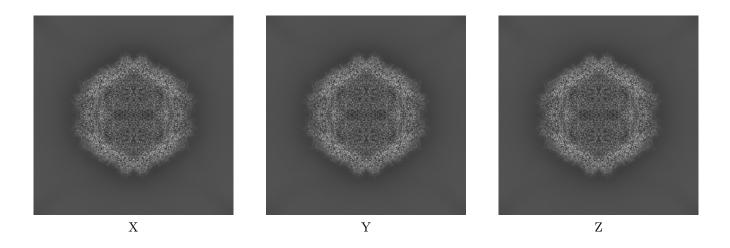
#### Map visualisation (i) 6

This section contains visualisations of the EMDB entry EMD-23460. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### Orthogonal projections (i) 6.1

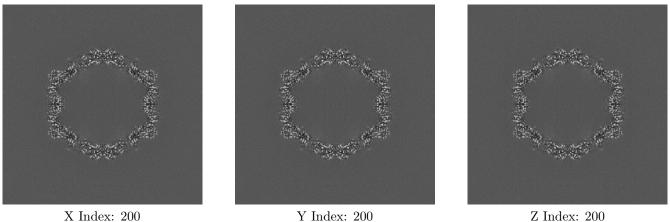
#### 6.1.1Primary map



The images above show the map projected in three orthogonal directions.

#### 6.2Central slices (i)

#### 6.2.1Primary map



X Index: 200

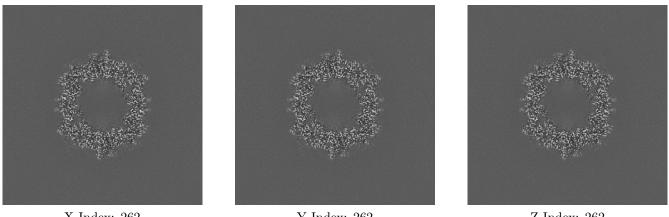




The images above show central slices of the map in three orthogonal directions.

#### Largest variance slices (i) 6.3

#### 6.3.1**Primary** map



X Index: 262

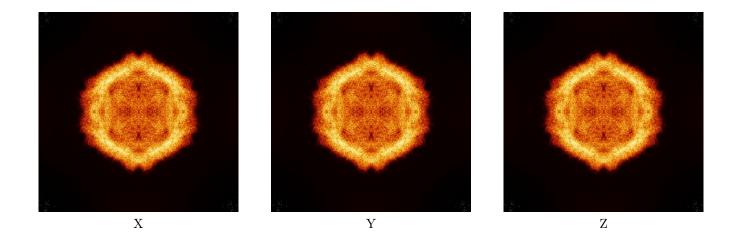
Y Index: 262

Z Index: 262

The images above show the largest variance slices of the map in three orthogonal directions.

#### Orthogonal standard-deviation projections (False-color) (i) 6.4

#### 6.4.1Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.6 Mask visualisation (i)

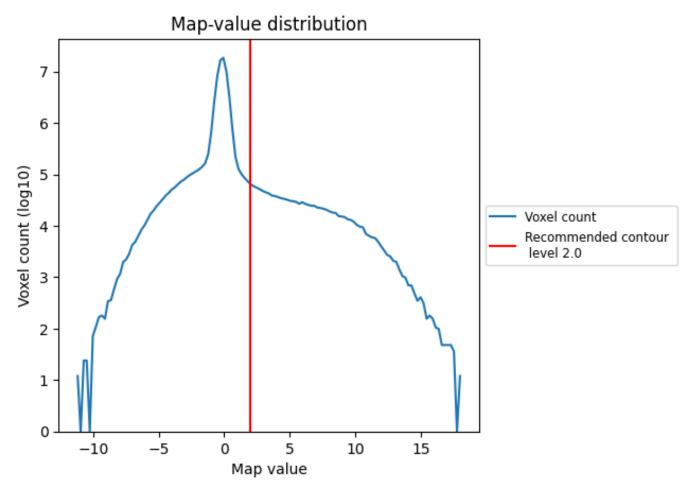
This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

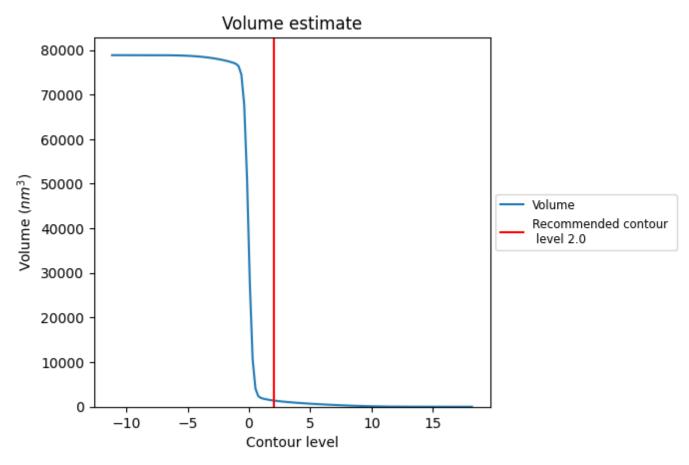
### 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



### 7.2 Volume estimate (i)

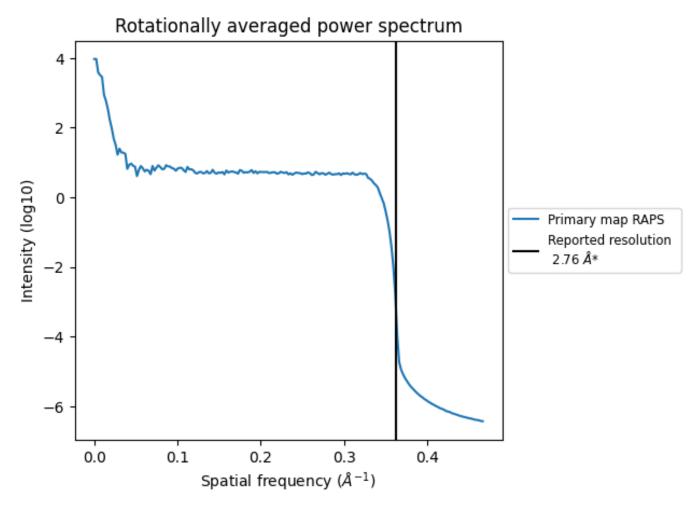


The volume at the recommended contour level is  $1405 \text{ nm}^3$ ; this corresponds to an approximate mass of 1269 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.362  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

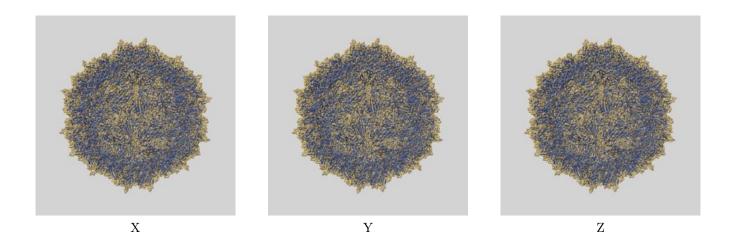
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23460 and PDB model 7LNK. Per-residue inclusion information can be found in section 3 on page 10.

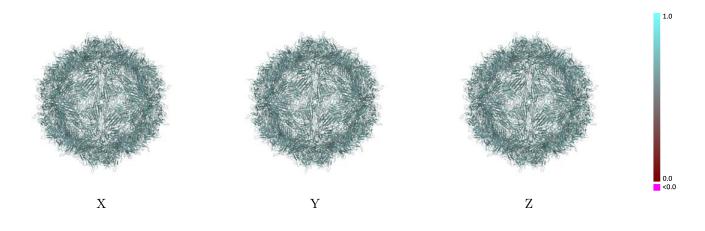
### 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

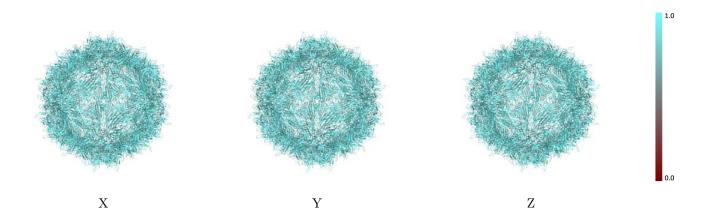


#### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

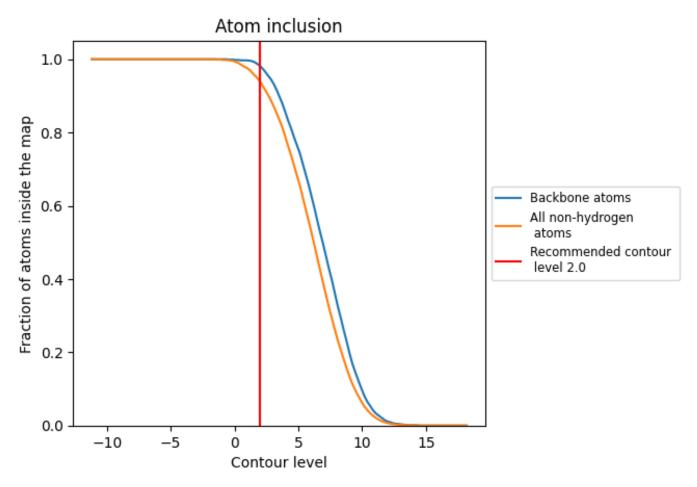
#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).



### 9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.6350
1	0.9410	0.6350
2	0.9410	0.6360
3	0.9400	0.6350
4	0.9390	0.6360
5	0.9380	0.6360
6	0.9380	0.6350
7	0.9380	0.6350
8	0.9400	0.6350
А	0.9400	0.6340
В	0.9410	0.6360
С	0.9390	0.6360
D	0.9380	0.6340
Е	0.9400	0.6350
F	0.9400	0.6340
G	0.9400	0.6340
Н	0.9380	0.6350
Ι	0.9390	0.6360
J	0.9410	0.6360
К	0.9390	0.6360
L	0.9410	0.6350
М	0.9400	0.6350
Ν	0.9380	0.6360
0	0.9400	0.6350
Р	0.9380	0.6360
Q	0.9390	0.6360
R	0.9410	0.6350
S	0.9410	0.6350
Т	0.9390	0.6360
U	0.9410	0.6360
V	0.9390	0.6350
W	0.9380	0.6360
Х	0.9390	0.6350
Y	0.9380	0.6360
Ζ	0.9400	0.6340



Chain	Atom inclusion	Q-score
a	0.9400	0.6340
b	0.9400	0.6350
с	0.9400	0.6350
d	0.9410	0.6350
e	0.9410	0.6350
f	0.9400	0.6350
g	0.9390	0.6350
h	0.9400	0.6350
i	0.9380	0.6360
j	0.9380	0.6350
k	0.9380	0.6350
1	0.9400	0.6350
m	0.9390	0.6360
n	0.9400	0.6350
0	0.9400	0.6340
р	0.9390	0.6350
q	0.9410	0.6340
r	0.9410	0.6360
S	0.9410	0.6360
t	0.9400	0.6340
u	0.9390	0.6370
V	0.9400	0.6350
W	0.9400	0.6340
X	0.9390	0.6360
У	0.9400	0.6340
Z	0.9410	0.6350

