



## wwPDB EM Validation Summary Report ⓘ

Apr 23, 2025 – 05:28 PM EDT

PDB ID : 9C1K / pdb\_00009c1k  
EMDB ID : EMD-45122  
Title : Rhesus rotavirus (empty structure at 2.68 Angstrom resolution)  
Authors : Jenni, S.; Herrmann, T.; De Sautu, M.; Harrison, S.C.  
Deposited on : 2024-05-29  
Resolution : 2.68 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.42

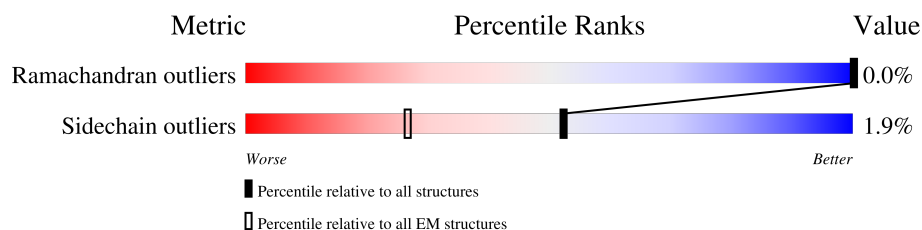
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.68 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.














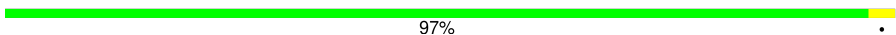
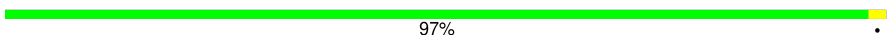
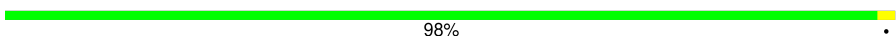

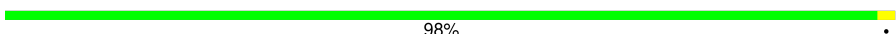
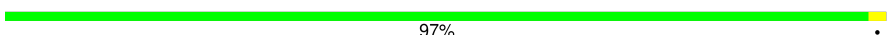
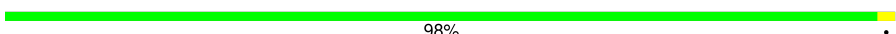
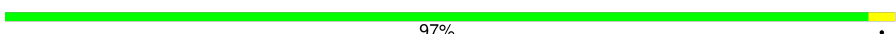
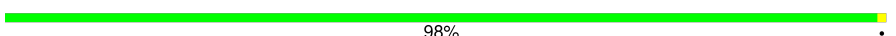



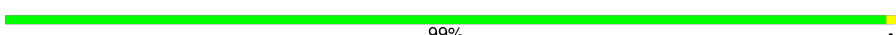

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	326	84% 15%
1	1	326	79% 19%
1	P	326	80% 19%
1	Q	326	83% 17%
1	R	326	83% 15%
1	S	326	80% 19%
1	T	326	84% 15%
1	U	326	83% 15%
1	V	326	83% 15%
1	W	326	84% 15%





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Mol	Chain	Length	Quality of chain
1	X	326	
1	Y	326	
1	Z	326	
1	t	326	
1	u	326	
1	v	326	
1	w	326	
1	x	326	
1	y	326	
2	A	887	
2	B	887	
3	C	397	
3	D	397	
3	E	397	
3	F	397	
3	G	397	
3	H	397	
3	I	397	
3	J	397	
3	K	397	
3	L	397	
3	M	397	
3	N	397	
3	O	397	
3	f	397	

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Mol	Chain	Length	Quality of chain
3	g	397	 98% •
3	h	397	 97% •
3	i	397	 98% •
3	j	397	 96% •
3	k	397	 98% •

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 226399 atoms, of which 112033 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 Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	1	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	P	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	Q	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	R	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	S	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	T	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	U	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	V	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	W	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	X	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	Y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	Z	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	t	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	u	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	v	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	w	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	x	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

- Molecule 2 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	779	Total	C	H	N	O	S	0	0
			12749	4041	6387	1098	1187	36		
2	B	799	Total	C	H	N	O	S	0	0
			13098	4154	6563	1126	1219	36		

- Molecule 3 is a protein called Intermediate capsid protein VP6.

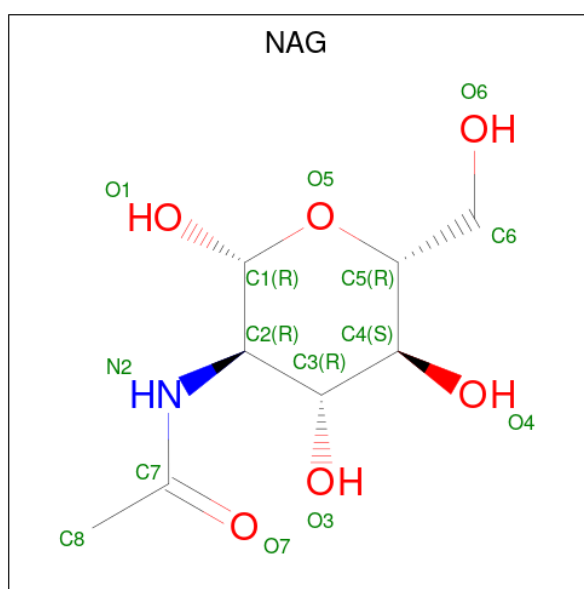
Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	397	Total	C	H	N	O	S	0	0
			6275	2005	3111	551	593	15		
3	D	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	E	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	F	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	G	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	H	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	I	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	J	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	K	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	L	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	M	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	N	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
3	O	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	f	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
3	g	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
3	h	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
3	i	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
3	j	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
3	k	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					AltConf
4	0	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	1	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	P	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	Q	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	R	1	Total	C	H	N	O	0
			28	8	14	1	5	

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Mol	Chain	Residues	Atoms					AltConf
4	S	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	T	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	U	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	V	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	W	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	X	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	Z	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	t	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	u	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	v	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	w	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	x	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	y	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	0	4	Total	Ca	0
			4	4	
5	1	4	Total	Ca	0
			4	4	
5	P	4	Total	Ca	0
			4	4	
5	Q	4	Total	Ca	0
			4	4	
5	R	4	Total	Ca	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
5	S	4	Total 4	Ca 4	0
5	T	4	Total 4	Ca 4	0
5	U	4	Total 4	Ca 4	0
5	V	4	Total 4	Ca 4	0
5	W	4	Total 4	Ca 4	0
5	X	4	Total 4	Ca 4	0
5	Y	4	Total 4	Ca 4	0
5	Z	4	Total 4	Ca 4	0
5	t	4	Total 4	Ca 4	0
5	u	4	Total 4	Ca 4	0
5	v	4	Total 4	Ca 4	0
5	w	4	Total 4	Ca 4	0
5	x	4	Total 4	Ca 4	0
5	y	4	Total 4	Ca 4	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total 2	Zn 2	0
6	D	1	Total 1	Zn 1	0
6	E	1	Total 1	Zn 1	0
6	F	2	Total 2	Zn 2	0
6	G	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
6	H	1	Total 1	Zn 1	0
6	I	2	Total 2	Zn 2	0
6	J	1	Total 1	Zn 1	0
6	K	1	Total 1	Zn 1	0
6	L	2	Total 2	Zn 2	0
6	M	1	Total 1	Zn 1	0
6	N	1	Total 1	Zn 1	0
6	O	2	Total 2	Zn 2	0
6	f	2	Total 2	Zn 2	0
6	g	1	Total 1	Zn 1	0
6	h	1	Total 1	Zn 1	0
6	i	2	Total 2	Zn 2	0
6	j	1	Total 1	Zn 1	0
6	k	1	Total 1	Zn 1	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total 1	Cl 1	0
7	F	1	Total 1	Cl 1	0
7	I	1	Total 1	Cl 1	0
7	N	1	Total 1	Cl 1	0
7	O	1	Total 1	Cl 1	0

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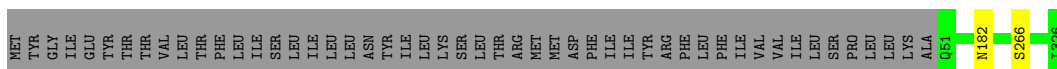
Mol	Chain	Residues	Atoms		AltConf
7	f	1	Total 1	Cl 1	0
7	i	1	Total 1	Cl 1	0

### 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.

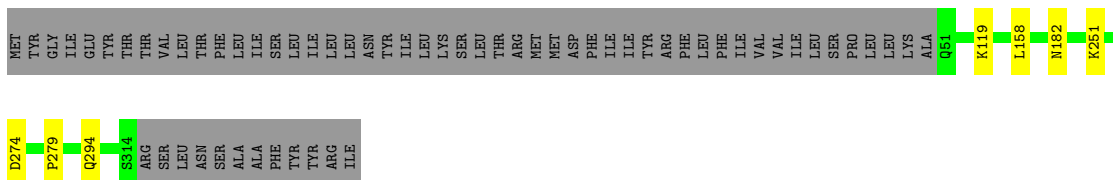
- Molecule 1: Outer capsid glycoprotein VP7

Chain 0:  84% 15%




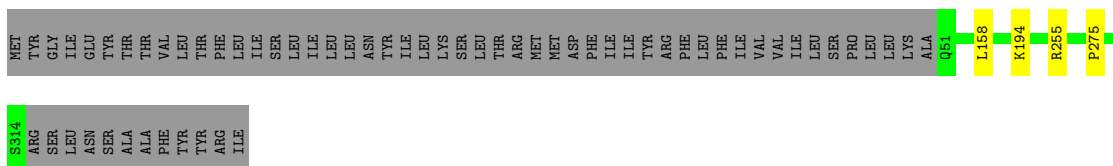
- Molecule 1: Outer capsid glycoprotein VP7

Chain 1:  79% 19%




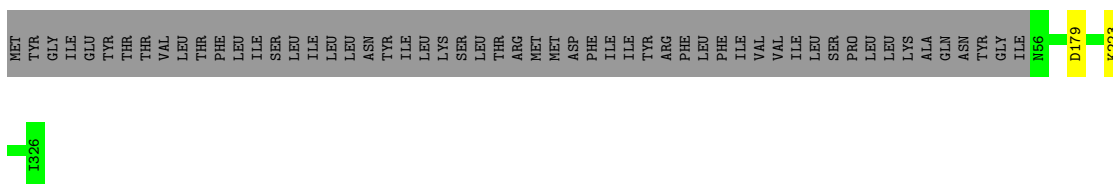
- Molecule 1: Outer capsid glycoprotein VP7

Chain P:  80% 19%




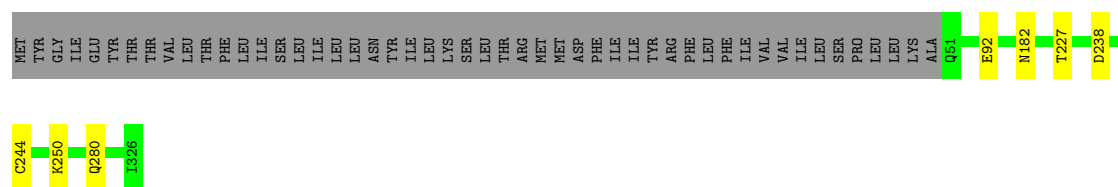
- Molecule 1: Outer capsid glycoprotein VP7

Chain Q:  83% 17%




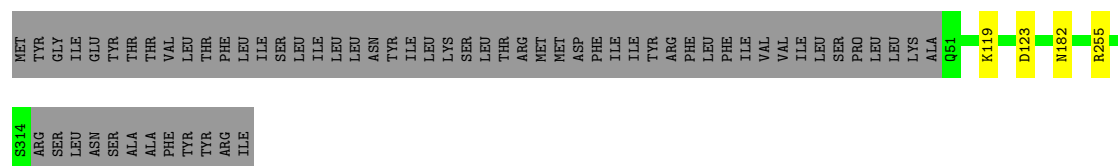
- Molecule 1: Outer capsid glycoprotein VP7

Chain R:  83% 15%




- Molecule 1: Outer capsid glycoprotein VP7

Chain S:  80% 19%




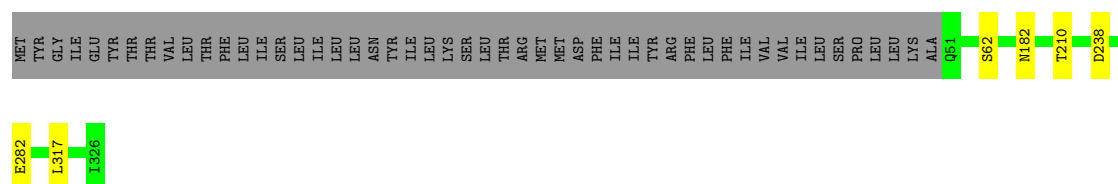
- Molecule 1: Outer capsid glycoprotein VP7

Chain T:  84% 15%




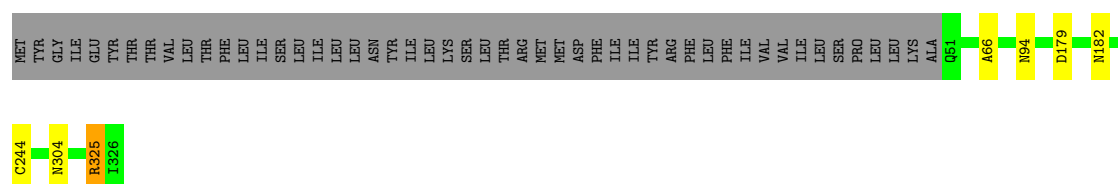
- Molecule 1: Outer capsid glycoprotein VP7

Chain U:  83% 15%




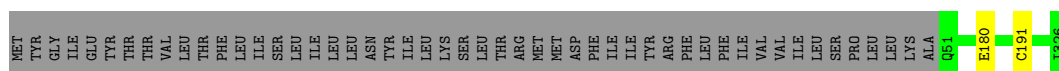
- Molecule 1: Outer capsid glycoprotein VP7

Chain V:  83% 15%



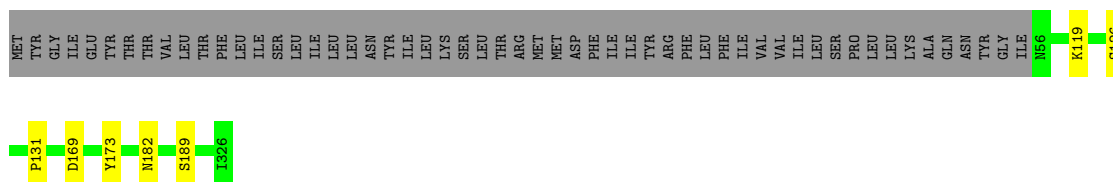
- Molecule 1: Outer capsid glycoprotein VP7

Chain W:  84% 15%



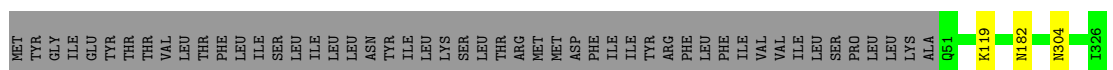
- Molecule 1: Outer capsid glycoprotein VP7

Chain X: 81% 17%



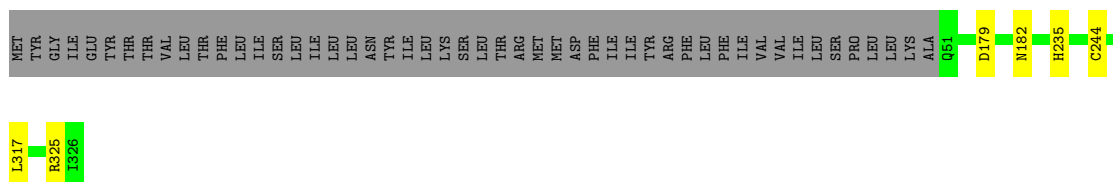
- Molecule 1: Outer capsid glycoprotein VP7

Chain Y: 84% 15%



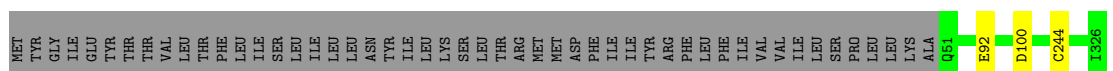
- Molecule 1: Outer capsid glycoprotein VP7

Chain Z: 83% 15%



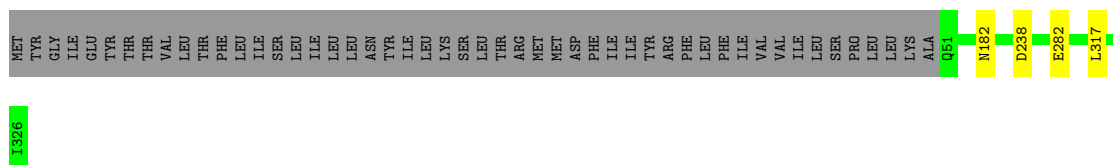
- Molecule 1: Outer capsid glycoprotein VP7

Chain t: 84% 15%




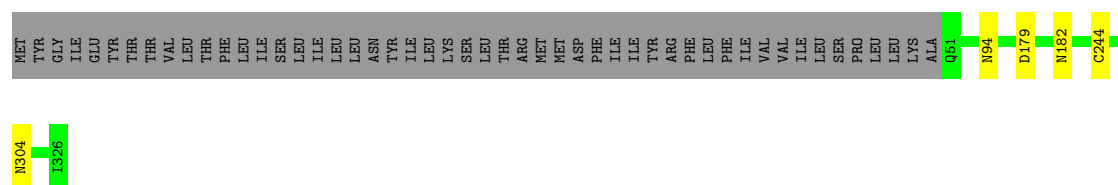
- Molecule 1: Outer capsid glycoprotein VP7

Chain u: 83% 15%




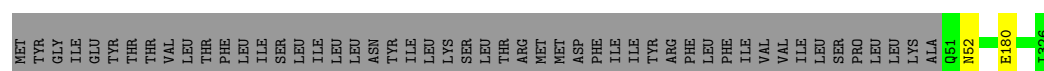
- Molecule 1: Outer capsid glycoprotein VP7

Chain v:  83% 15%




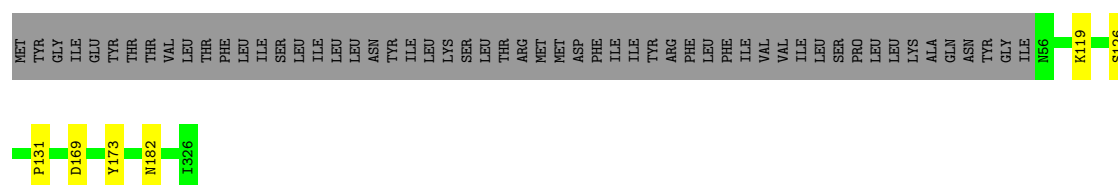
- Molecule 1: Outer capsid glycoprotein VP7

Chain w:  84% 15%




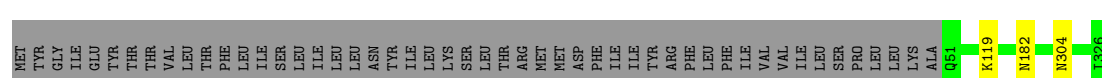
- Molecule 1: Outer capsid glycoprotein VP7

Chain x:  81% 17%




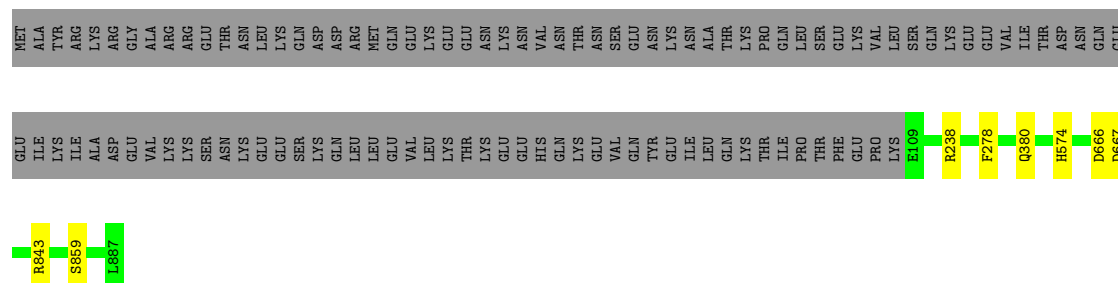
- Molecule 1: Outer capsid glycoprotein VP7

Chain y:  84% 15%



- Molecule 2: Inner capsid protein VP2

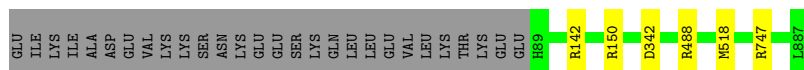
Chain A:  87% 12%



- Molecule 2: Inner capsid protein VP2

Chain B:  89% 10%





Chain C:  97%



Chain D:  97%



Chain E:  98%



Chain F:  98%



Chain G:  98%



Chain H:  97%





Chain I:  98% .



- Molecule 3: Intermediate capsid protein VP6

Chain J:  97% .



- Molecule 3: Intermediate capsid protein VP6

Chain K:  98% .



- Molecule 3: Intermediate capsid protein VP6

Chain L:  97% .



- Molecule 3: Intermediate capsid protein VP6

Chain M:  97% .



- Molecule 3: Intermediate capsid protein VP6

Chain N:  97% .



- Molecule 3: Intermediate capsid protein VP6

Chain O:  99% .



- Molecule 3: Intermediate capsid protein VP6

Chain f:  98%



- Molecule 3: Intermediate capsid protein VP6

Chain g:  98%



- Molecule 3: Intermediate capsid protein VP6

Chain h:  97%



- Molecule 3: Intermediate capsid protein VP6

Chain i:  98%



- Molecule 3: Intermediate capsid protein VP6

Chain j:  96%



- Molecule 3: Intermediate capsid protein VP6

Chain k:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1970094	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: FME, CL, NAG, CA, ZN

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	0.26	0/2234	0.50	0/3051
1	1	0.26	0/2128	0.48	0/2908
1	P	0.26	0/2128	0.48	0/2908
1	Q	0.26	0/2192	0.49	0/2994
1	R	0.26	0/2234	0.48	0/3051
1	S	0.26	0/2128	0.48	0/2908
1	T	0.26	0/2234	0.49	0/3051
1	U	0.26	0/2234	0.50	0/3051
1	V	0.26	0/2234	0.49	0/3051
1	W	0.25	0/2234	0.48	0/3051
1	X	0.26	0/2192	0.48	0/2994
1	Y	0.26	0/2234	0.48	0/3051
1	Z	0.26	0/2234	0.50	1/3051 (0.0%)
1	t	0.26	0/2234	0.50	0/3051
1	u	0.26	0/2234	0.50	0/3051
1	v	0.26	0/2234	0.48	0/3051
1	w	0.26	0/2234	0.48	0/3051
1	x	0.26	0/2192	0.48	0/2994
1	y	0.26	0/2234	0.48	0/3051
2	A	0.27	0/6477	0.51	0/8788
2	B	0.27	0/6655	0.51	0/9029
3	C	0.27	0/3224	0.53	0/4387
3	D	0.27	0/3215	0.54	0/4376
3	E	0.27	0/3215	0.53	0/4376
3	F	0.27	0/3215	0.53	0/4376
3	G	0.27	0/3215	0.52	0/4376
3	H	0.27	0/3215	0.53	0/4376
3	I	0.26	0/3215	0.53	0/4376
3	J	0.27	0/3215	0.53	0/4376
3	K	0.26	0/3215	0.52	0/4376
3	L	0.27	0/3215	0.53	0/4376
3	M	0.27	0/3215	0.53	0/4376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	N	0.26	0/3215	0.53	0/4376
3	O	0.27	0/3215	0.54	0/4376
3	f	0.27	0/3215	0.54	0/4376
3	g	0.26	0/3215	0.52	0/4376
3	h	0.27	0/3215	0.53	0/4376
3	i	0.26	0/3215	0.53	0/4376
3	j	0.27	0/3215	0.54	0/4376
3	k	0.26	0/3215	0.52	0/4376
All	All	0.26	0/116228	0.51	1/158341 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	317	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V	325	ARG	Sidechain

## 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	Percentiles	
1	0	274/326 (84%)	265 (97%)	9 (3%)	0	100	100
1	1	262/326 (80%)	257 (98%)	5 (2%)	0	100	100
1	P	262/326 (80%)	258 (98%)	4 (2%)	0	100	100
1	Q	269/326 (82%)	266 (99%)	3 (1%)	0	100	100
1	R	274/326 (84%)	268 (98%)	6 (2%)	0	100	100
1	S	262/326 (80%)	255 (97%)	7 (3%)	0	100	100
1	T	274/326 (84%)	271 (99%)	3 (1%)	0	100	100
1	U	274/326 (84%)	265 (97%)	9 (3%)	0	100	100
1	V	274/326 (84%)	265 (97%)	8 (3%)	1 (0%)	30	52
1	W	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	X	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	Y	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	Z	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	t	274/326 (84%)	269 (98%)	5 (2%)	0	100	100
1	u	274/326 (84%)	262 (96%)	12 (4%)	0	100	100
1	v	274/326 (84%)	262 (96%)	12 (4%)	0	100	100
1	w	274/326 (84%)	267 (97%)	7 (3%)	0	100	100
1	x	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	y	274/326 (84%)	269 (98%)	5 (2%)	0	100	100
2	A	777/887 (88%)	764 (98%)	13 (2%)	0	100	100
2	B	797/887 (90%)	786 (99%)	11 (1%)	0	100	100
3	C	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	D	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
3	E	394/397 (99%)	389 (99%)	5 (1%)	0	100	100
3	F	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
3	G	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
3	H	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
3	I	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
3	J	394/397 (99%)	384 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
3	L	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
3	M	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
3	N	394/397 (99%)	389 (99%)	5 (1%)	0	100	100
3	O	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
3	f	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
3	g	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
3	h	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
3	i	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
3	j	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
3	k	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
All	All	14216/15511 (92%)	13908 (98%)	307 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	66	ALA

### 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	247/295 (84%)	245 (99%)	2 (1%)	79	91
1	1	237/295 (80%)	230 (97%)	7 (3%)	36	63
1	P	237/295 (80%)	233 (98%)	4 (2%)	56	79
1	Q	243/295 (82%)	241 (99%)	2 (1%)	79	91
1	R	247/295 (84%)	240 (97%)	7 (3%)	38	65
1	S	237/295 (80%)	233 (98%)	4 (2%)	56	79
1	T	247/295 (84%)	244 (99%)	3 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	247/295 (84%)	241 (98%)	6 (2%)	44	70
1	V	247/295 (84%)	241 (98%)	6 (2%)	44	70
1	W	247/295 (84%)	245 (99%)	2 (1%)	79	91
1	X	243/295 (82%)	236 (97%)	7 (3%)	37	64
1	Y	247/295 (84%)	244 (99%)	3 (1%)	67	85
1	Z	247/295 (84%)	242 (98%)	5 (2%)	50	76
1	t	247/295 (84%)	244 (99%)	3 (1%)	67	85
1	u	247/295 (84%)	243 (98%)	4 (2%)	58	80
1	v	247/295 (84%)	242 (98%)	5 (2%)	50	76
1	w	247/295 (84%)	245 (99%)	2 (1%)	79	91
1	x	243/295 (82%)	237 (98%)	6 (2%)	42	69
1	y	247/295 (84%)	244 (99%)	3 (1%)	67	85
2	A	715/818 (87%)	707 (99%)	8 (1%)	70	86
2	B	735/818 (90%)	729 (99%)	6 (1%)	79	91
3	C	349/349 (100%)	339 (97%)	10 (3%)	37	64
3	D	348/349 (100%)	340 (98%)	8 (2%)	45	72
3	E	348/349 (100%)	342 (98%)	6 (2%)	56	79
3	F	348/349 (100%)	343 (99%)	5 (1%)	62	82
3	G	348/349 (100%)	341 (98%)	7 (2%)	50	76
3	H	348/349 (100%)	340 (98%)	8 (2%)	45	72
3	I	348/349 (100%)	341 (98%)	7 (2%)	50	76
3	J	348/349 (100%)	337 (97%)	11 (3%)	34	60
3	K	348/349 (100%)	344 (99%)	4 (1%)	70	86
3	L	348/349 (100%)	338 (97%)	10 (3%)	37	64
3	M	348/349 (100%)	338 (97%)	10 (3%)	37	64
3	N	348/349 (100%)	338 (97%)	10 (3%)	37	64
3	O	348/349 (100%)	345 (99%)	3 (1%)	75	89
3	f	348/349 (100%)	342 (98%)	6 (2%)	56	79
3	g	348/349 (100%)	342 (98%)	6 (2%)	56	79
3	h	348/349 (100%)	340 (98%)	8 (2%)	45	72
3	i	348/349 (100%)	342 (98%)	6 (2%)	56	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	j	348/349 (100%)	336 (97%)	12 (3%)	32	58
3	k	348/349 (100%)	344 (99%)	4 (1%)	70	86
All	All	12714/13872 (92%)	12478 (98%)	236 (2%)	52	77

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	299	ASN
1	v	179	ASP
1	U	182	ASN
1	u	317	LEU
3	j	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	u	305	GLN
1	y	305	GLN
1	w	305	GLN
1	W	305	GLN
1	t	305	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

19 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FME	E	1	3	8,9,10	0.38	0	8,9,11	1.01	1 (12%)
3	FME	L	1	3	8,9,10	0.38	0	8,9,11	1.02	1 (12%)
3	FME	k	1	3	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
3	FME	H	1	3	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
3	FME	I	1	3	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
3	FME	C	1	3	8,9,10	0.37	0	8,9,11	1.12	1 (12%)
3	FME	f	1	3	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
3	FME	F	1	3	8,9,10	0.37	0	8,9,11	1.07	1 (12%)
3	FME	K	1	3	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
3	FME	g	1	3	8,9,10	0.37	0	8,9,11	1.08	1 (12%)
3	FME	O	1	3	8,9,10	0.37	0	8,9,11	1.05	1 (12%)
3	FME	J	1	3	8,9,10	0.37	0	8,9,11	1.00	1 (12%)
3	FME	j	1	3	8,9,10	0.37	0	8,9,11	0.97	1 (12%)
3	FME	G	1	3	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
3	FME	D	1	3	8,9,10	0.37	0	8,9,11	1.02	1 (12%)
3	FME	i	1	3	8,9,10	0.37	0	8,9,11	1.04	1 (12%)
3	FME	N	1	3	8,9,10	0.39	0	8,9,11	1.03	1 (12%)
3	FME	h	1	3	8,9,10	0.37	0	8,9,11	1.03	1 (12%)
3	FME	M	1	3	8,9,10	0.37	0	8,9,11	1.07	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FME	E	1	3	-	1/7/9/11	-
3	FME	L	1	3	-	1/7/9/11	-
3	FME	k	1	3	-	1/7/9/11	-
3	FME	H	1	3	-	1/7/9/11	-
3	FME	I	1	3	-	1/7/9/11	-
3	FME	C	1	3	-	1/7/9/11	-
3	FME	f	1	3	-	1/7/9/11	-
3	FME	F	1	3	-	1/7/9/11	-
3	FME	K	1	3	-	1/7/9/11	-
3	FME	g	1	3	-	1/7/9/11	-
3	FME	O	1	3	-	1/7/9/11	-
3	FME	J	1	3	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FME	j	1	3	-	1/7/9/11	-
3	FME	G	1	3	-	1/7/9/11	-
3	FME	D	1	3	-	1/7/9/11	-
3	FME	i	1	3	-	1/7/9/11	-
3	FME	N	1	3	-	1/7/9/11	-
3	FME	h	1	3	-	1/7/9/11	-
3	FME	M	1	3	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.57	126.77	122.82
3	g	1	FME	CA-N-CN	2.42	126.55	122.82
3	F	1	FME	CA-N-CN	2.37	126.46	122.82
3	I	1	FME	CA-N-CN	2.36	126.45	122.82
3	i	1	FME	CA-N-CN	2.35	126.44	122.82

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	O1-CN-N-CA
3	D	1	FME	O1-CN-N-CA
3	E	1	FME	O1-CN-N-CA
3	F	1	FME	O1-CN-N-CA
3	G	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 109 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	X	401	1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	P	401	1	14,14,15	0.71	0	17,19,21	0.95	0
4	NAG	R	401	1	14,14,15	0.72	0	17,19,21	0.89	0
4	NAG	V	401	1	14,14,15	0.73	0	17,19,21	0.98	0
4	NAG	S	401	1	14,14,15	0.72	0	17,19,21	0.93	0
4	NAG	Y	401	1	14,14,15	0.70	0	17,19,21	0.98	0
4	NAG	U	401	1	14,14,15	0.70	0	17,19,21	1.04	1 (5%)
4	NAG	Z	401	1	14,14,15	0.67	0	17,19,21	1.08	0
4	NAG	t	401	1	14,14,15	0.70	0	17,19,21	0.95	0
4	NAG	y	401	1	14,14,15	0.69	0	17,19,21	0.96	0
4	NAG	Q	401	1	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
4	NAG	l	401	1	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	x	401	1	14,14,15	0.71	0	17,19,21	0.90	0
4	NAG	v	401	1	14,14,15	0.74	0	17,19,21	0.90	0
4	NAG	T	401	1	14,14,15	0.70	0	17,19,21	0.93	0
4	NAG	u	401	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
4	NAG	w	401	1	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
4	NAG	o	401	1	14,14,15	0.69	0	17,19,21	1.16	3 (17%)
4	NAG	W	401	1	14,14,15	0.70	0	17,19,21	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	401	1	-	4/6/23/26	0/1/1/1
4	NAG	P	401	1	-	3/6/23/26	0/1/1/1
4	NAG	R	401	1	-	2/6/23/26	0/1/1/1
4	NAG	V	401	1	-	4/6/23/26	0/1/1/1
4	NAG	S	401	1	-	2/6/23/26	0/1/1/1
4	NAG	Y	401	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	401	1	-	2/6/23/26	0/1/1/1
4	NAG	Z	401	1	-	2/6/23/26	0/1/1/1
4	NAG	t	401	1	-	2/6/23/26	0/1/1/1
4	NAG	y	401	1	-	2/6/23/26	0/1/1/1
4	NAG	Q	401	1	-	4/6/23/26	0/1/1/1
4	NAG	l	401	1	-	2/6/23/26	0/1/1/1
4	NAG	x	401	1	-	4/6/23/26	0/1/1/1
4	NAG	v	401	1	-	4/6/23/26	0/1/1/1
4	NAG	T	401	1	-	2/6/23/26	0/1/1/1
4	NAG	u	401	1	-	2/6/23/26	0/1/1/1
4	NAG	w	401	1	-	4/6/23/26	0/1/1/1
4	NAG	0	401	1	-	2/6/23/26	0/1/1/1
4	NAG	W	401	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	u	401	NAG	C2-N2-C7	2.33	126.02	122.90
4	U	401	NAG	C2-N2-C7	2.32	126.01	122.90
4	0	401	NAG	C2-N2-C7	2.20	125.85	122.90
4	W	401	NAG	C2-N2-C7	2.19	125.84	122.90
4	w	401	NAG	C2-N2-C7	2.16	125.80	122.90

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	401	NAG	C1-C2-N2-C7
4	Q	401	NAG	C1-C2-N2-C7
4	U	401	NAG	C1-C2-N2-C7
4	V	401	NAG	C1-C2-N2-C7
4	W	401	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45122. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.