wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 02:16 AM EST

PDB ID	:	6WXG
EMDB ID	:	EMD-21957
Title	:	Cryo-EM reconstruction of VP5*/VP8* assembly from rhesus rotavirus particles - Reversed conformation
Authors	:	Herrmann, T.; Harrison, S.C.; Jenni, S.
Deposited on	:	2020-05-10
Resolution	:	3.30 Å(reported)
Based on initial models	:	4V7Q, 1SLQ

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

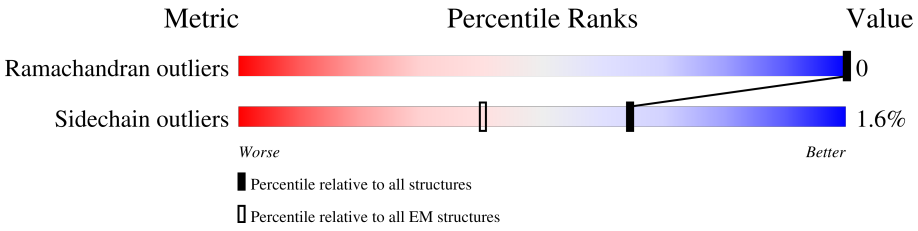
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.30 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	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	1	776	35% · 65%
1	2	776	35% · 65%
1	3	776	35% · 65%
2	A	397	99% ·
2	B	397	98% ·
2	C	397	98% ·
2	D	397	99% ·
2	E	397	99% ·
2	F	397	98% ·
2	G	397	98% ·

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Mol	Chain	Length	Quality of chain
2	H	397	98%
2	I	397	99%
2	J	397	99%
2	K	397	99%
2	L	397	98%
2	M	397	99%
2	N	397	99%
2	O	397	98%
2	P	397	98%
2	Q	397	99%
2	R	397	99%
3	a	326	79% 21%
3	b	326	83% 17%
3	c	326	79% 20%
3	d	326	80% 19%
3	e	326	79% 20%
3	f	326	80% 19%
3	g	326	82% 17%
3	h	326	79% 21%
3	i	326	82% 17%
3	j	326	81% 17%
3	k	326	80% 19%
3	l	326	79% 19%
3	m	326	82% 17%
3	n	326	80% 19%

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Mol	Chain	Length	Quality of chain
3	o	326	79% 19%
3	p	326	81% 17%
3	q	326	78% 21%
3	r	326	82% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 201212 atoms, of which 99503 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 protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
1	2	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
1	3	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	B	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	C	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	D	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	E	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	F	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	G	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	H	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	I	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	J	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	K	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	L	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	N	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	O	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	P	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	Q	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	R	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		

- Molecule 3 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
3	b	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
3	c	261	Total	C	H	N	O	S	0	0
			4074	1308	2011	327	412	16		
3	d	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	e	260	Total	C	H	N	O	S	0	0
			4050	1302	1998	323	411	16		
3	f	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	g	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
3	h	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
3	i	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
3	j	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
3	k	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	l	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	m	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		

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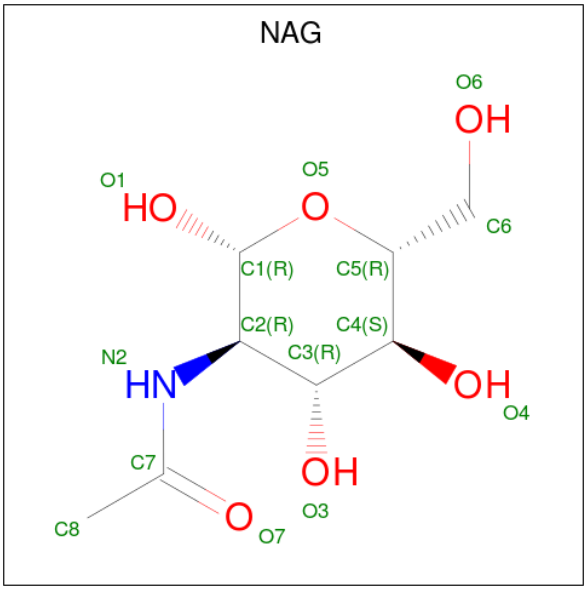
Mol	Chain	Residues	Atoms						AltConf	Trace
3	n	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	o	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
3	p	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
3	q	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
3	r	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		

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



Mol	Chain	Residues	Atoms					AltConf
4	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	b	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	d	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	e	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	f	1	Total	C	H	N	O	0
			28	8	14	1	5	

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Mol	Chain	Residues	Atoms					AltConf
4	g	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	h	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	i	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	j	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	k	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	l	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	m	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	n	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	o	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	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	a	5	Total	Ca	0
			5	5	
5	b	3	Total	Ca	0
			3	3	
5	c	1	Total	Ca	0
			1	1	
5	d	5	Total	Ca	0
			5	5	
5	e	3	Total	Ca	0
			3	3	
5	f	1	Total	Ca	0
			1	1	
5	g	5	Total	Ca	0
			5	5	

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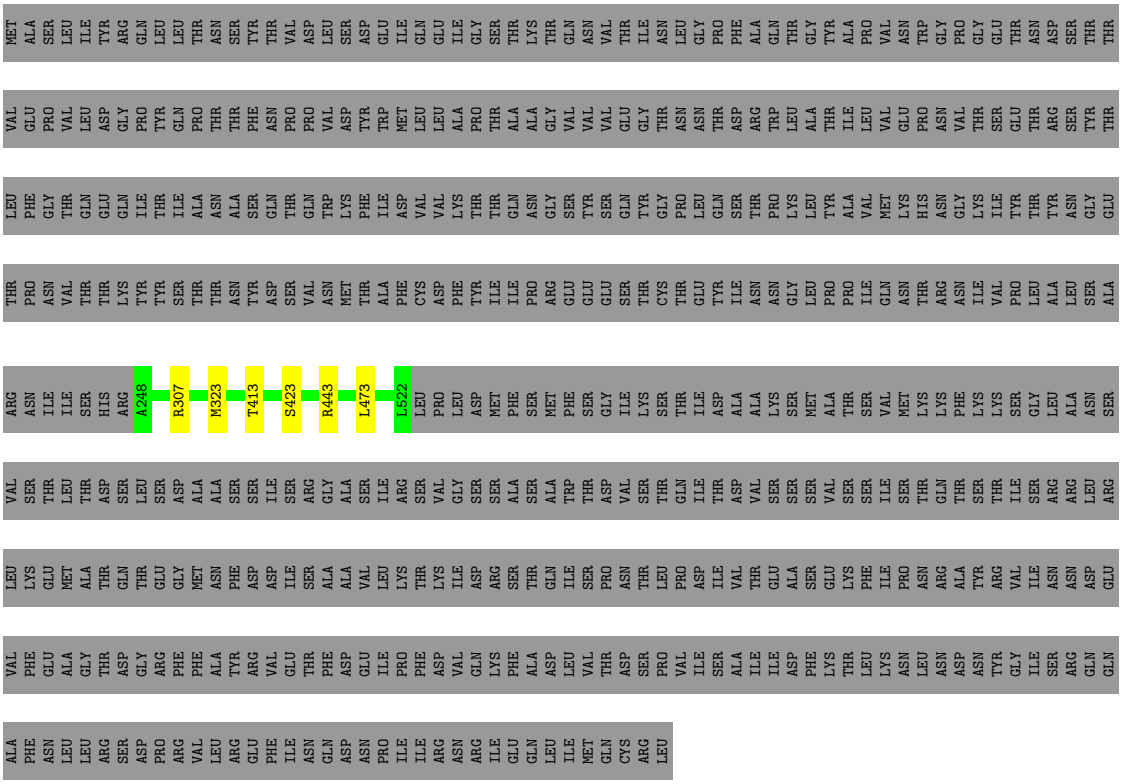
Mol	Chain	Residues	Atoms	AltConf
5	h	3	Total Ca 3 3	0
5	i	1	Total Ca 1 1	0
5	j	5	Total Ca 5 5	0
5	k	3	Total Ca 3 3	0
5	l	1	Total Ca 1 1	0
5	m	5	Total Ca 5 5	0
5	n	3	Total Ca 3 3	0
5	o	1	Total Ca 1 1	0
5	p	5	Total Ca 5 5	0
5	q	3	Total Ca 3 3	0
5	r	1	Total Ca 1 1	0

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. 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.

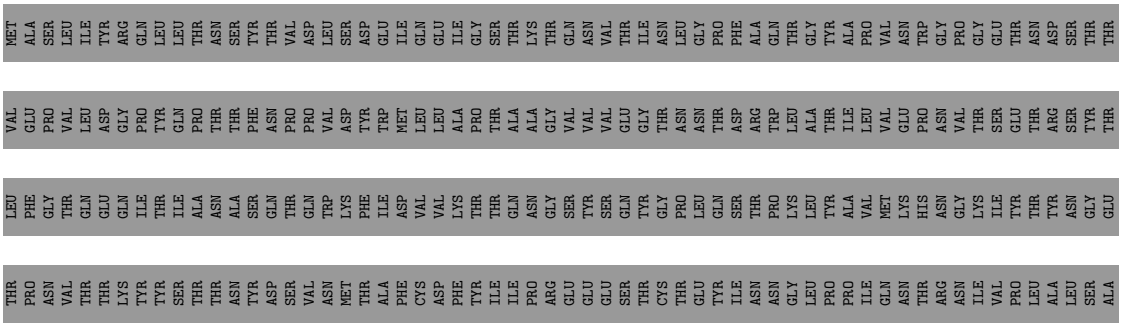
- Molecule 1: Outer capsid protein VP4

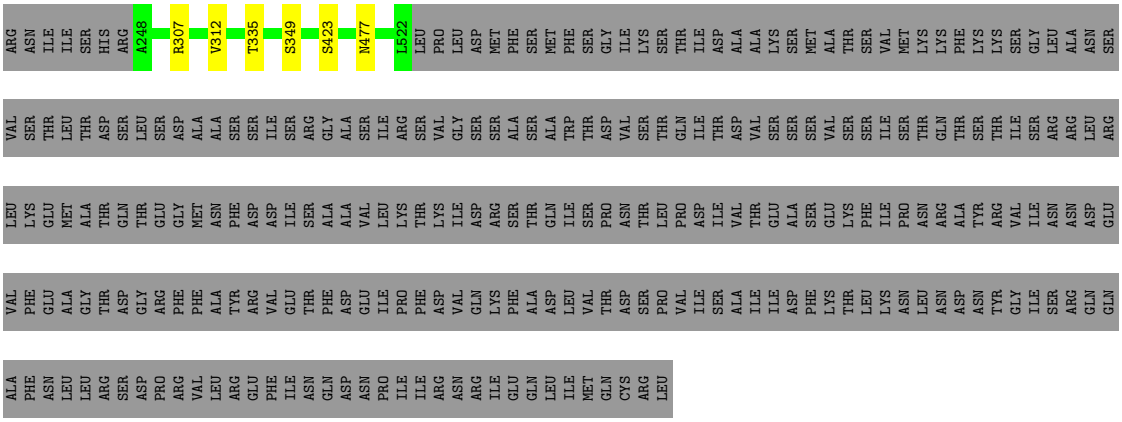
Chain 1:



- Molecule 1: Outer capsid protein VP4

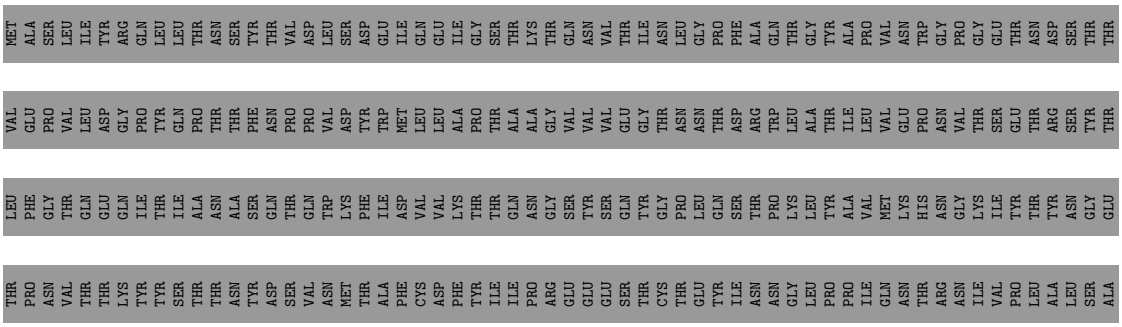
Chain 2:

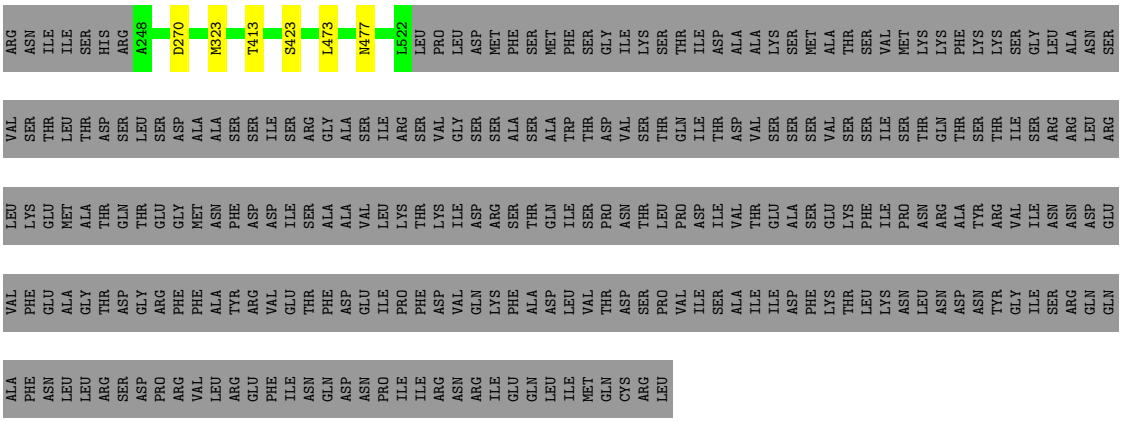




• Molecule 1: Outer capsid protein VP4

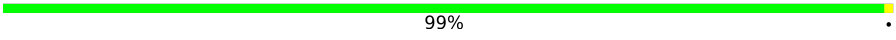
Chain 3:





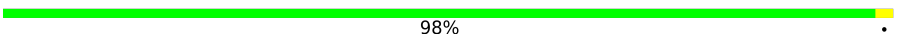
• Molecule 2: Intermediate capsid protein VP6

Chain A:



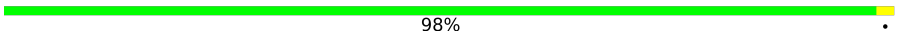
• Molecule 2: Intermediate capsid protein VP6

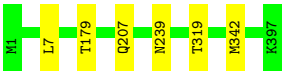
Chain B:



• Molecule 2: Intermediate capsid protein VP6

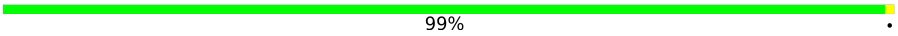
Chain C:

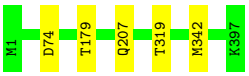




• Molecule 2: Intermediate capsid protein VP6

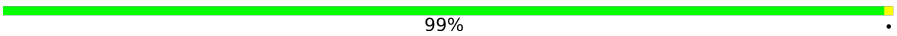
Chain D:

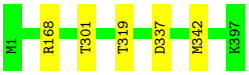




• Molecule 2: Intermediate capsid protein VP6

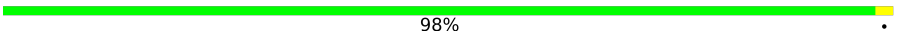
Chain E:





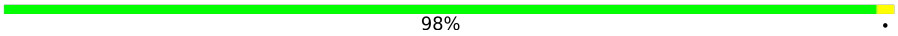
• Molecule 2: Intermediate capsid protein VP6

Chain F:



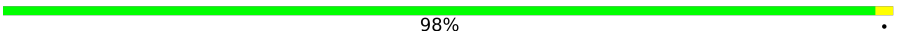
• Molecule 2: Intermediate capsid protein VP6

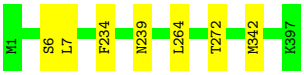
Chain G:



• Molecule 2: Intermediate capsid protein VP6

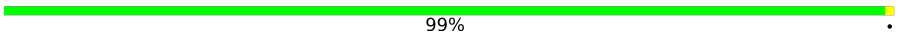
Chain H:

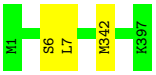




• Molecule 2: Intermediate capsid protein VP6

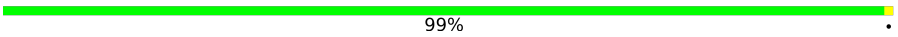
Chain I:

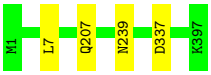




• Molecule 2: Intermediate capsid protein VP6

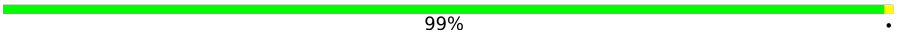
Chain J:

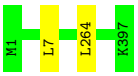




• Molecule 2: Intermediate capsid protein VP6

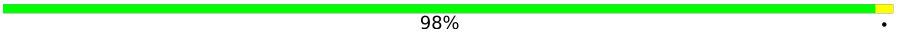
Chain K:





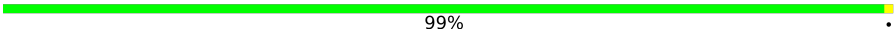
• Molecule 2: Intermediate capsid protein VP6

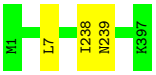
Chain L:



• Molecule 2: Intermediate capsid protein VP6

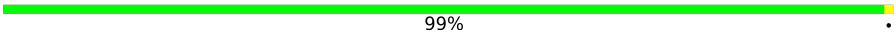
Chain M:

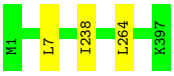




• Molecule 2: Intermediate capsid protein VP6

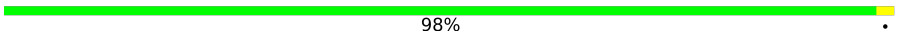
Chain N:





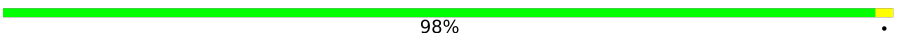
• Molecule 2: Intermediate capsid protein VP6

Chain O:



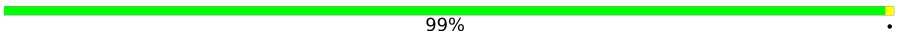
• Molecule 2: Intermediate capsid protein VP6

Chain P:



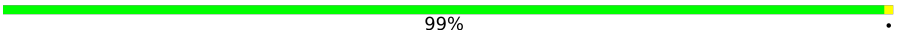
• Molecule 2: Intermediate capsid protein VP6

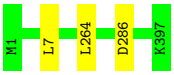
Chain Q:



• Molecule 2: Intermediate capsid protein VP6

Chain R:





• Molecule 3: Outer capsid glycoprotein VP7

Chain a:

• Molecule 3: Outer capsid glycoprotein VP7

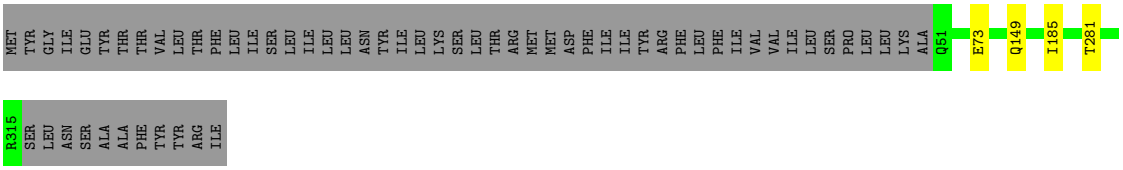
Chain b:

• Molecule 3: Outer capsid glycoprotein VP7

Chain c:

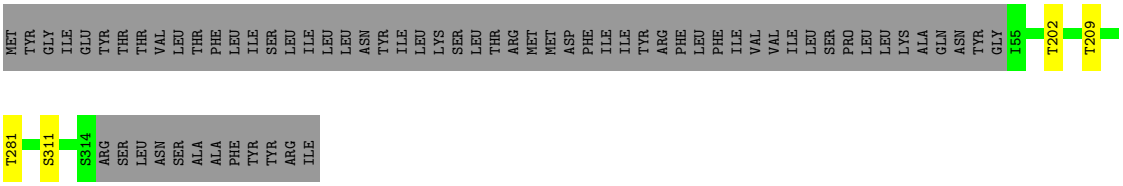
• Molecule 3: Outer capsid glycoprotein VP7

Chain d:



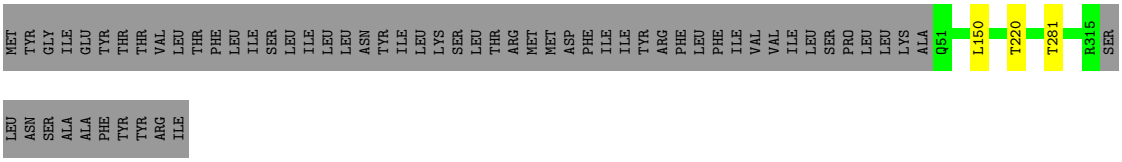
• Molecule 3: Outer capsid glycoprotein VP7

Chain e:



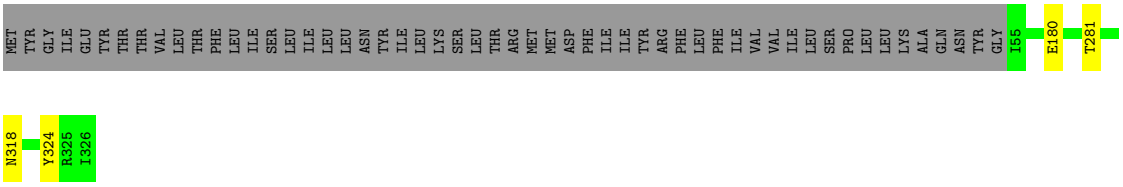
• Molecule 3: Outer capsid glycoprotein VP7

Chain f:



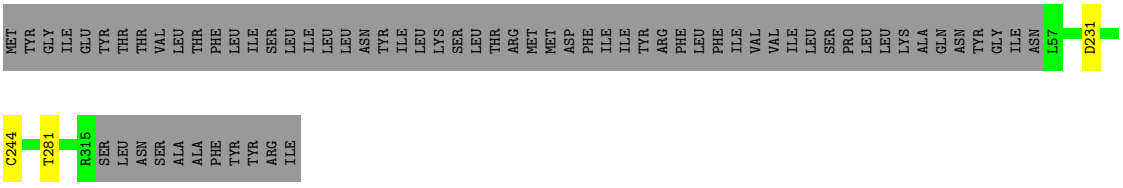
• Molecule 3: Outer capsid glycoprotein VP7

Chain g:



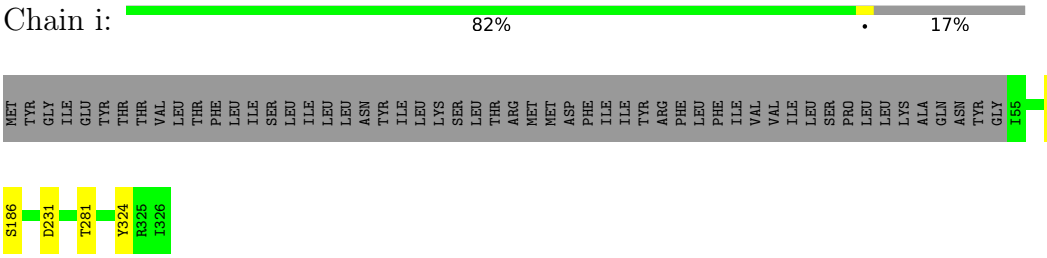
• Molecule 3: Outer capsid glycoprotein VP7

Chain h:



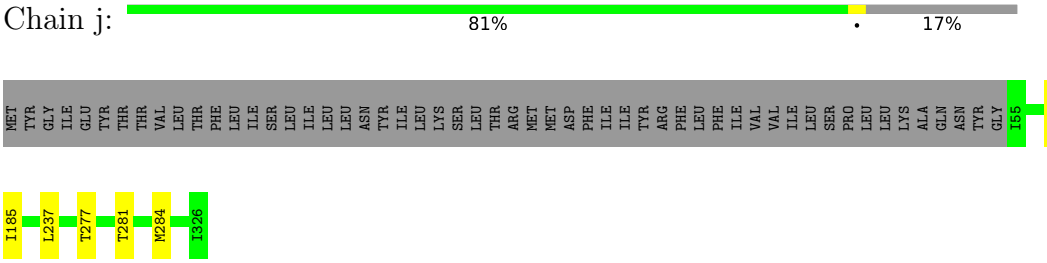
• Molecule 3: Outer capsid glycoprotein VP7

Chain i:



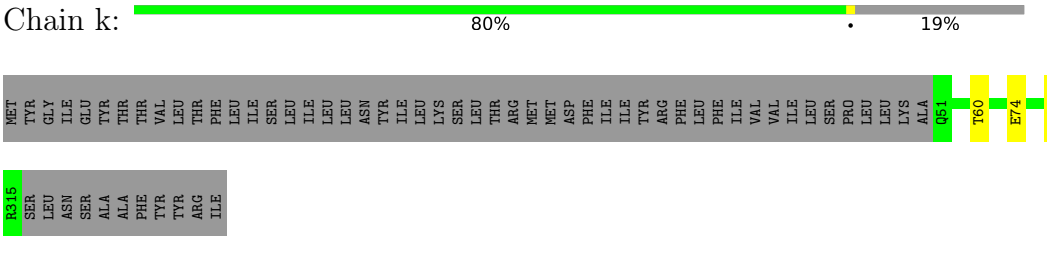
• Molecule 3: Outer capsid glycoprotein VP7

Chain j:



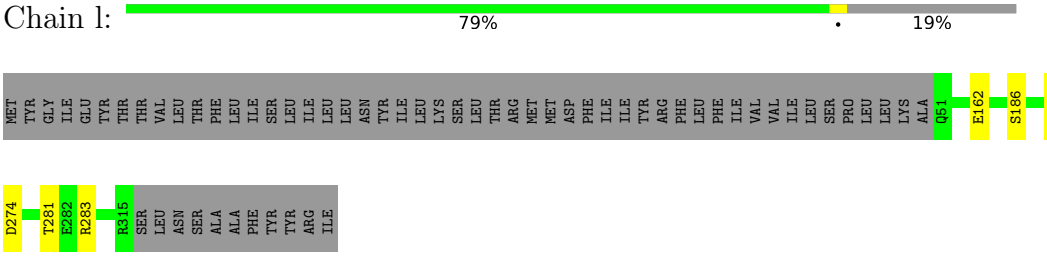
• Molecule 3: Outer capsid glycoprotein VP7

Chain k:



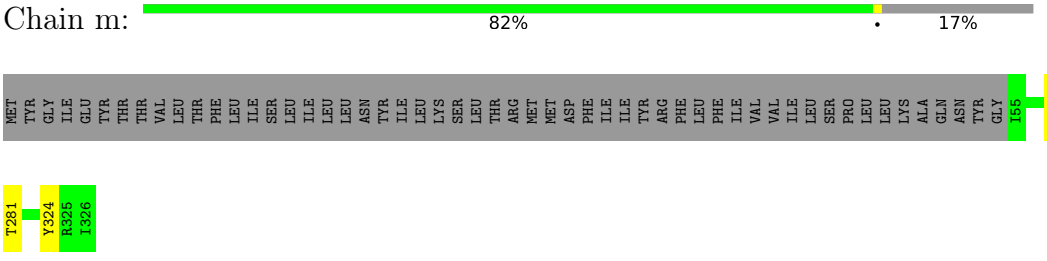
• Molecule 3: Outer capsid glycoprotein VP7

Chain l:



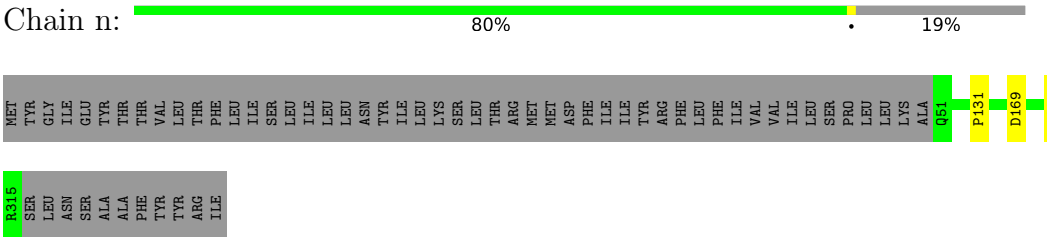
• Molecule 3: Outer capsid glycoprotein VP7

Chain m:



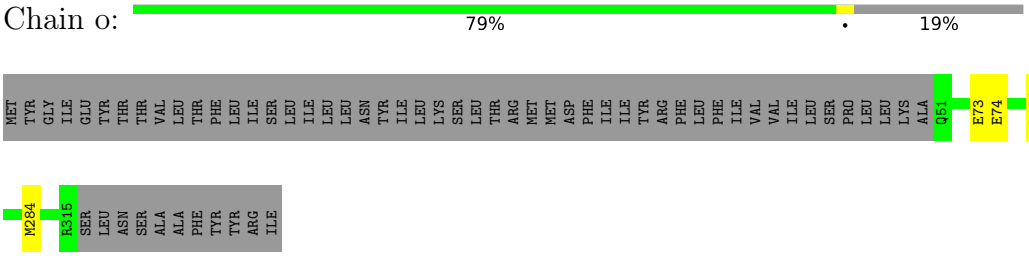
• Molecule 3: Outer capsid glycoprotein VP7

Chain n:



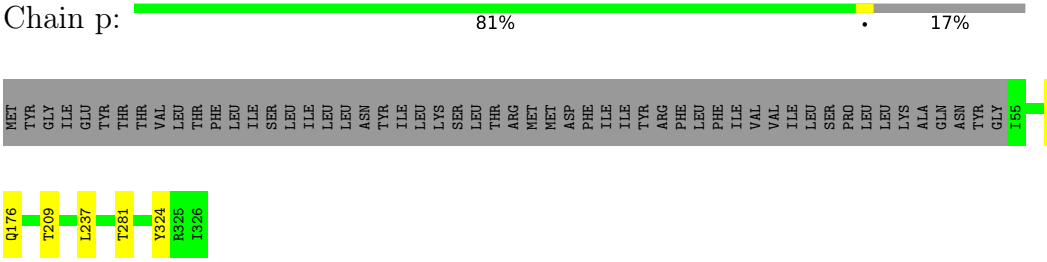
• Molecule 3: Outer capsid glycoprotein VP7

Chain o:



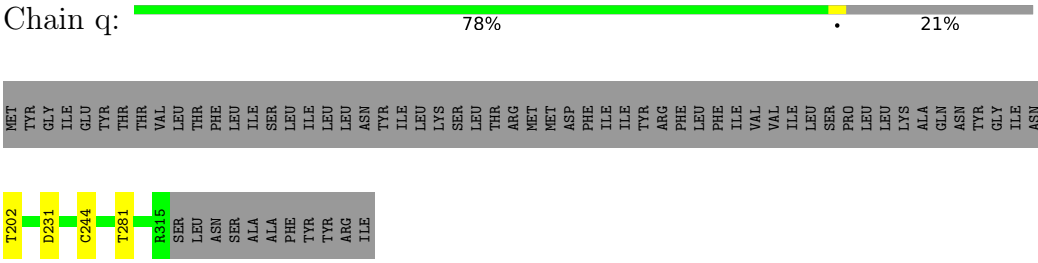
• Molecule 3: Outer capsid glycoprotein VP7

Chain p:



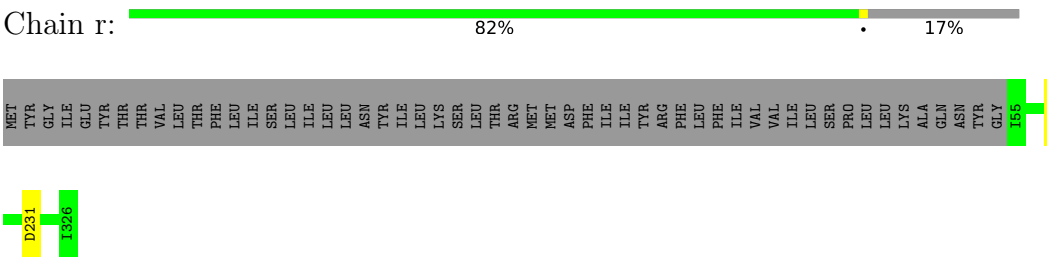
• Molecule 3: Outer capsid glycoprotein VP7

Chain q:



• Molecule 3: Outer capsid glycoprotein VP7

Chain r:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40605	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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	1	0.27	0/2232	0.57	0/3032
1	2	0.27	0/2232	0.57	0/3032
1	3	0.27	0/2232	0.56	0/3032
2	A	0.28	0/3233	0.59	0/4397
2	B	0.28	0/3233	0.59	0/4397
2	C	0.27	0/3233	0.59	0/4397
2	D	0.28	0/3233	0.59	0/4397
2	E	0.28	0/3233	0.59	1/4397 (0.0%)
2	F	0.28	0/3233	0.59	0/4397
2	G	0.28	0/3233	0.60	1/4397 (0.0%)
2	H	0.28	0/3233	0.59	0/4397
2	I	0.28	0/3233	0.59	0/4397
2	J	0.28	0/3233	0.58	0/4397
2	K	0.28	0/3233	0.59	0/4397
2	L	0.28	0/3233	0.59	0/4397
2	M	0.28	0/3233	0.59	0/4397
2	N	0.27	0/3233	0.58	0/4397
2	O	0.28	0/3233	0.59	1/4397 (0.0%)
2	P	0.28	0/3233	0.59	0/4397
2	Q	0.28	0/3233	0.60	0/4397
2	R	0.27	0/3233	0.58	0/4397
3	a	0.27	0/2089	0.55	0/2854
3	b	0.26	0/2200	0.54	0/3005
3	c	0.27	0/2105	0.54	0/2876
3	d	0.27	0/2139	0.54	0/2922
3	e	0.27	0/2094	0.54	0/2862
3	f	0.27	0/2139	0.54	0/2922
3	g	0.27	0/2200	0.55	0/3005
3	h	0.26	0/2089	0.54	0/2854
3	i	0.28	0/2200	0.55	0/3005
3	j	0.27	0/2200	0.54	0/3005
3	k	0.27	0/2139	0.55	0/2922

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	l	0.27	0/2139	0.55	0/2922
3	m	0.27	0/2200	0.55	0/3005
3	n	0.26	0/2139	0.55	0/2922
3	o	0.27	0/2139	0.54	0/2922
3	p	0.27	0/2200	0.55	0/3005
3	q	0.26	0/2089	0.54	0/2854
3	r	0.27	0/2200	0.55	0/3005
All	All	0.27	0/103590	0.57	3/141109 (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
3	e	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	168	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	G	168	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	O	168	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	e	311	SER	Peptide

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	1	273/776 (35%)	273 (100%)	0	0	100	100
1	2	273/776 (35%)	273 (100%)	0	0	100	100
1	3	273/776 (35%)	273 (100%)	0	0	100	100
2	A	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	B	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	C	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	D	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	E	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	F	395/397 (100%)	391 (99%)	4 (1%)	0	100	100
2	G	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	H	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	I	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	J	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	K	395/397 (100%)	391 (99%)	4 (1%)	0	100	100
2	L	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	M	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	N	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	O	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	P	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	Q	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	R	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
3	a	257/326 (79%)	257 (100%)	0	0	100	100
3	b	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
3	c	259/326 (79%)	258 (100%)	1 (0%)	0	100	100
3	d	263/326 (81%)	263 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	e	258/326 (79%)	257 (100%)	1 (0%)	0	100	100
3	f	263/326 (81%)	263 (100%)	0	0	100	100
3	g	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
3	h	257/326 (79%)	257 (100%)	0	0	100	100
3	i	270/326 (83%)	270 (100%)	0	0	100	100
3	j	270/326 (83%)	268 (99%)	2 (1%)	0	100	100
3	k	263/326 (81%)	263 (100%)	0	0	100	100
3	l	263/326 (81%)	263 (100%)	0	0	100	100
3	m	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
3	n	263/326 (81%)	263 (100%)	0	0	100	100
3	o	263/326 (81%)	263 (100%)	0	0	100	100
3	p	270/326 (83%)	270 (100%)	0	0	100	100
3	q	257/326 (79%)	257 (100%)	0	0	100	100
3	r	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
All	All	12685/15342 (83%)	12626 (100%)	59 (0%)	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 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	1	241/688 (35%)	235 (98%)	6 (2%)	47	72
1	2	241/688 (35%)	235 (98%)	6 (2%)	47	72
1	3	241/688 (35%)	235 (98%)	6 (2%)	47	72
2	A	350/350 (100%)	347 (99%)	3 (1%)	78	87
2	B	350/350 (100%)	344 (98%)	6 (2%)	60	78
2	C	350/350 (100%)	344 (98%)	6 (2%)	60	78
2	D	350/350 (100%)	345 (99%)	5 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	350/350 (100%)	346 (99%)	4 (1%)	73 85
2	F	350/350 (100%)	343 (98%)	7 (2%)	55 76
2	G	350/350 (100%)	345 (99%)	5 (1%)	67 82
2	H	350/350 (100%)	343 (98%)	7 (2%)	55 76
2	I	350/350 (100%)	347 (99%)	3 (1%)	78 87
2	J	350/350 (100%)	346 (99%)	4 (1%)	73 85
2	K	350/350 (100%)	348 (99%)	2 (1%)	86 91
2	L	350/350 (100%)	343 (98%)	7 (2%)	55 76
2	M	350/350 (100%)	347 (99%)	3 (1%)	78 87
2	N	350/350 (100%)	347 (99%)	3 (1%)	78 87
2	O	350/350 (100%)	343 (98%)	7 (2%)	55 76
2	P	350/350 (100%)	344 (98%)	6 (2%)	60 78
2	Q	350/350 (100%)	347 (99%)	3 (1%)	78 87
2	R	350/350 (100%)	347 (99%)	3 (1%)	78 87
3	a	233/295 (79%)	230 (99%)	3 (1%)	69 82
3	b	244/295 (83%)	241 (99%)	3 (1%)	71 83
3	c	235/295 (80%)	232 (99%)	3 (1%)	69 82
3	d	238/295 (81%)	234 (98%)	4 (2%)	60 78
3	e	234/295 (79%)	231 (99%)	3 (1%)	69 82
3	f	238/295 (81%)	235 (99%)	3 (1%)	69 82
3	g	244/295 (83%)	240 (98%)	4 (2%)	62 79
3	h	233/295 (79%)	230 (99%)	3 (1%)	69 82
3	i	244/295 (83%)	238 (98%)	6 (2%)	47 72
3	j	244/295 (83%)	237 (97%)	7 (3%)	42 69
3	k	238/295 (81%)	234 (98%)	4 (2%)	60 78
3	l	238/295 (81%)	231 (97%)	7 (3%)	42 69
3	m	244/295 (83%)	240 (98%)	4 (2%)	62 79
3	n	238/295 (81%)	234 (98%)	4 (2%)	60 78
3	o	238/295 (81%)	232 (98%)	6 (2%)	47 72
3	p	244/295 (83%)	237 (97%)	7 (3%)	42 69
3	q	233/295 (79%)	228 (98%)	5 (2%)	53 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	r	244/295 (83%)	240 (98%)	4 (2%)	62 79
All	All	11327/13674 (83%)	11145 (98%)	182 (2%)	64 79

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	202	THR
3	k	208	LEU
3	f	220	THR
3	i	186	SER
3	l	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	n	288	ASN
3	n	305	GLN
3	d	149	GLN
3	c	305	GLN
3	r	182	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)

Of 72 ligands modelled in this entry, 54 are monoatomic - leaving 18 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	g	401	3	14,14,15	0.44	0	17,19,21	0.44	0
4	NAG	b	401	-	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	h	401	3	14,14,15	0.59	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	d	401	3	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	m	401	3	14,14,15	0.57	0	17,19,21	0.71	1 (5%)
4	NAG	k	401	3	14,14,15	0.60	1 (7%)	17,19,21	0.79	1 (5%)
4	NAG	p	401	3	14,14,15	0.51	0	17,19,21	0.74	1 (5%)
4	NAG	o	401	3	14,14,15	0.49	0	17,19,21	0.45	0
4	NAG	a	401	3	14,14,15	0.63	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	f	401	3	14,14,15	0.38	0	17,19,21	0.43	0
4	NAG	q	401	3	14,14,15	0.43	0	17,19,21	0.70	1 (5%)
4	NAG	j	401	3	14,14,15	0.35	0	17,19,21	0.36	0
4	NAG	l	401	3	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	r	401	3	14,14,15	0.60	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	n	401	3	14,14,15	0.30	0	17,19,21	0.34	0
4	NAG	i	401	3	14,14,15	0.60	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	e	401	3	14,14,15	0.20	0	17,19,21	0.56	0
4	NAG	c	401	3	14,14,15	0.58	0	17,19,21	0.70	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	g	401	3	-	0/6/23/26	0/1/1/1
4	NAG	b	401	-	-	0/6/23/26	0/1/1/1
4	NAG	h	401	3	-	0/6/23/26	0/1/1/1
4	NAG	d	401	3	-	0/6/23/26	0/1/1/1
4	NAG	m	401	3	-	0/6/23/26	0/1/1/1
4	NAG	k	401	3	-	0/6/23/26	0/1/1/1
4	NAG	p	401	3	-	2/6/23/26	0/1/1/1
4	NAG	o	401	3	-	0/6/23/26	0/1/1/1
4	NAG	a	401	3	-	0/6/23/26	0/1/1/1
4	NAG	f	401	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	q	401	3	-	0/6/23/26	0/1/1/1
4	NAG	j	401	3	-	0/6/23/26	0/1/1/1
4	NAG	l	401	3	-	0/6/23/26	0/1/1/1
4	NAG	r	401	3	-	0/6/23/26	0/1/1/1
4	NAG	n	401	3	-	0/6/23/26	0/1/1/1
4	NAG	i	401	3	-	0/6/23/26	0/1/1/1
4	NAG	e	401	3	-	0/6/23/26	0/1/1/1
4	NAG	c	401	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	401	NAG	C1-C2	2.11	1.55	1.52
4	r	401	NAG	C1-C2	2.03	1.55	1.52
4	h	401	NAG	C1-C2	2.02	1.55	1.52
4	k	401	NAG	C1-C2	2.02	1.55	1.52
4	i	401	NAG	C1-C2	2.00	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	k	401	NAG	C1-O5-C5	2.84	116.04	112.19
4	r	401	NAG	C1-O5-C5	2.72	115.88	112.19
4	a	401	NAG	C1-O5-C5	2.69	115.83	112.19
4	p	401	NAG	C1-O5-C5	2.58	115.68	112.19
4	i	401	NAG	C1-O5-C5	2.55	115.65	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	c	401	NAG	C4-C5-C6-O6
4	c	401	NAG	O5-C5-C6-O6
4	p	401	NAG	O5-C5-C6-O6
4	p	401	NAG	C4-C5-C6-O6

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-21957. 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 surface views

This section was not generated.

6.5 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.