wwPDB EM Validation Summary Report (i)

Nov 23, 2022 – 01:32 PM EST

PDB ID	:	7UMS
EMDB ID	:	EMD-26608
Title	:	Structure of the VP5*/VP8* assembly from the human rotavirus strain CDC-9 in complex with antibody 41 - Upright conformation
Authors	:	Jenni, S.; Zongli, L.; Wang, Y.; Bessey, T.; Salgado, E.N.; Schmidt, A.G.; Greenberg, H.B.; Jiang, B.; Harrison, S.C.
Deposited on	:	2022-04-07
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

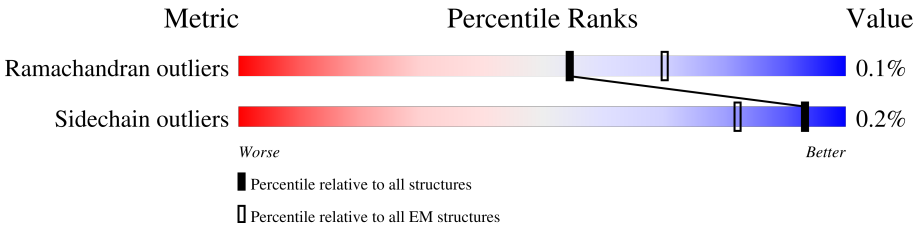
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.50 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% 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.

Mol	Chain	Length	Quality of chain
1	T	230	98%
1	U	230	98%
1	V	230	11% 89%
2	1	529	93% 6%
2	2	529	93% 6%
2	3	529	91% 8%
3	4	236	19% 94%
3	6	236	17% 95%
4	5	217	18% 98%

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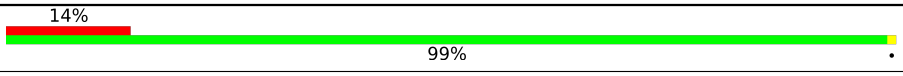
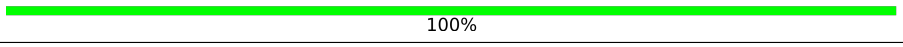
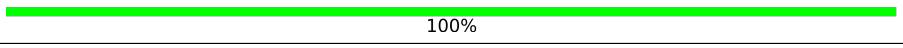
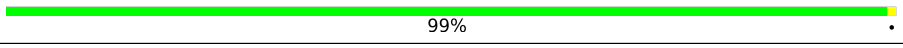
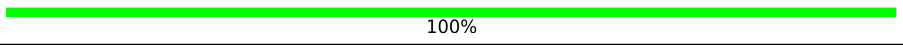
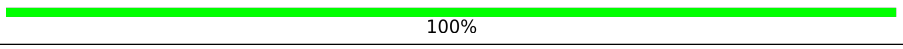
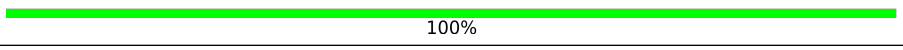
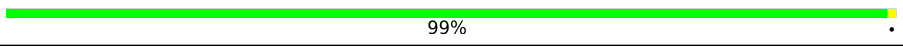
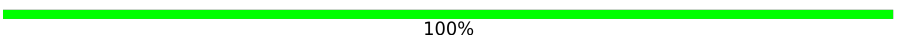
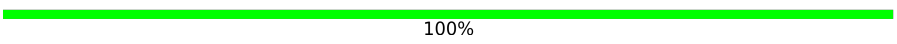
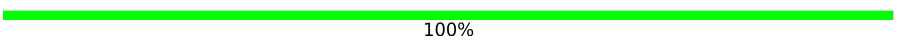
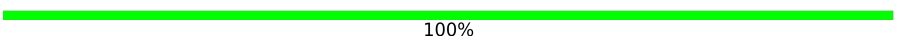
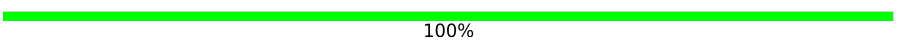
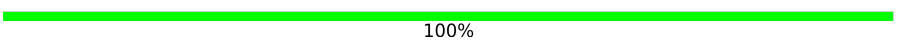
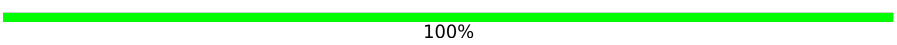
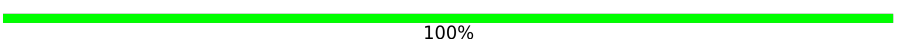
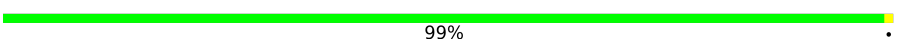
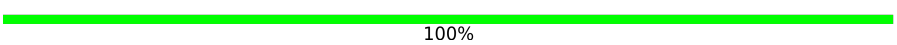
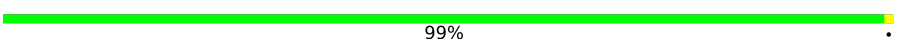
Mol	Chain	Length	Quality of chain
4	7	217	
5	A	397	
5	B	397	
5	C	397	
5	D	397	
5	E	397	
5	F	397	
5	G	397	
5	H	397	
5	I	397	
5	J	397	
5	K	397	
5	L	397	
5	M	397	
5	N	397	
5	O	397	
5	P	397	
5	Q	397	
5	R	397	
6	a	326	
6	b	326	
6	c	326	
6	d	326	
6	e	326	
6	f	326	

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Mol	Chain	Length	Quality of chain
6	g	326	83% 15%
6	h	326	82% 17%
6	i	326	83% 15%
6	j	326	83% 16%
6	k	326	84% 15%
6	l	326	83% 15%
6	m	326	83% 16%
6	n	326	83% 15%
6	o	326	83% 15%
6	p	326	83% 16%
6	q	326	82% 17%
6	r	326	83% 16%
7	S	3	67% 33%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 236285 atoms, of which 116945 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 VP8*.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	T	227	Total	C	H	N	O	S	0	0
			3553	1151	1726	309	364	3		
1	U	227	Total	C	H	N	O	S	0	0
			3553	1151	1726	309	364	3		
1	V	25	Total	C	H	N	O		0	0
			401	130	197	31	43			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	28	GLY	GLU	conflict	UNP X4YMN0
T	51	ASP	GLY	conflict	UNP X4YMN0
U	28	GLY	GLU	conflict	UNP X4YMN0
U	51	ASP	GLY	conflict	UNP X4YMN0
V	28	GLY	GLU	conflict	UNP X4YMN0
V	51	ASP	GLY	conflict	UNP X4YMN0

- Molecule 2 is a protein called Outer capsid protein VP5*.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	499	Total	C	H	N	O	S	0	0
			7914	2514	3951	664	768	17		
2	2	499	Total	C	H	N	O	S	0	0
			7914	2514	3951	664	768	17		
2	3	486	Total	C	H	N	O	S	0	0
			7719	2455	3853	649	745	17		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	250	ASP	ASN	conflict	UNP X4YMN0
1	331	PHE	SER	conflict	UNP X4YMN0
1	364	ILE	MET	conflict	UNP X4YMN0

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Chain	Residue	Modelled	Actual	Comment	Reference
1	378	ARG	LYS	conflict	UNP X4YMN0
1	385	HIS	ASP	conflict	UNP X4YMN0
1	388	LEU	ILE	conflict	UNP X4YMN0
1	499	ASN	ASP	conflict	UNP X4YMN0
1	605	ASN	SER	conflict	UNP X4YMN0
2	250	ASP	ASN	conflict	UNP X4YMN0
2	331	PHE	SER	conflict	UNP X4YMN0
2	364	ILE	MET	conflict	UNP X4YMN0
2	378	ARG	LYS	conflict	UNP X4YMN0
2	385	HIS	ASP	conflict	UNP X4YMN0
2	388	LEU	ILE	conflict	UNP X4YMN0
2	499	ASN	ASP	conflict	UNP X4YMN0
2	605	ASN	SER	conflict	UNP X4YMN0
3	250	ASP	ASN	conflict	UNP X4YMN0
3	331	PHE	SER	conflict	UNP X4YMN0
3	364	ILE	MET	conflict	UNP X4YMN0
3	378	ARG	LYS	conflict	UNP X4YMN0
3	385	HIS	ASP	conflict	UNP X4YMN0
3	388	LEU	ILE	conflict	UNP X4YMN0
3	499	ASN	ASP	conflict	UNP X4YMN0
3	605	ASN	SER	conflict	UNP X4YMN0

- Molecule 3 is a protein called Fab 41 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	230	Total	C	H	N	O	S	0	0
			3396	1094	1667	289	339	7		
3	6	230	Total	C	H	N	O	S	0	0
			3396	1094	1667	289	339	7		

- Molecule 4 is a protein called Fab 41 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	217	Total	C	H	N	O	S	0	0
			3202	1019	1562	276	339	6		
4	7	217	Total	C	H	N	O	S	0	0
			3202	1019	1562	276	339	6		

- Molecule 5 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	B	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	C	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	D	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	E	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	F	397	Total	C	H	N	O	S	0	0
			6296	2012	3128	552	589	15		
5	G	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	H	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	I	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	J	397	Total	C	H	N	O	S	0	0
			6296	2012	3128	552	589	15		
5	K	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	L	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	M	397	Total	C	H	N	O	S	0	0
			6296	2012	3128	552	589	15		
5	N	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	O	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	P	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	Q	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		
5	R	397	Total	C	H	N	O	S	0	0
			6295	2012	3127	552	589	15		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	VAL	ILE	conflict	UNP A0A223GHC7
B	281	VAL	ILE	conflict	UNP A0A223GHC7
C	281	VAL	ILE	conflict	UNP A0A223GHC7
D	281	VAL	ILE	conflict	UNP A0A223GHC7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	281	VAL	ILE	conflict	UNP A0A223GHC7
F	281	VAL	ILE	conflict	UNP A0A223GHC7
G	281	VAL	ILE	conflict	UNP A0A223GHC7
H	281	VAL	ILE	conflict	UNP A0A223GHC7
I	281	VAL	ILE	conflict	UNP A0A223GHC7
J	281	VAL	ILE	conflict	UNP A0A223GHC7
K	281	VAL	ILE	conflict	UNP A0A223GHC7
L	281	VAL	ILE	conflict	UNP A0A223GHC7
M	281	VAL	ILE	conflict	UNP A0A223GHC7
N	281	VAL	ILE	conflict	UNP A0A223GHC7
O	281	VAL	ILE	conflict	UNP A0A223GHC7
P	281	VAL	ILE	conflict	UNP A0A223GHC7
Q	281	VAL	ILE	conflict	UNP A0A223GHC7
R	281	VAL	ILE	conflict	UNP A0A223GHC7

- Molecule 6 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	271	Total	C	H	N	O	S	0	0
			4279	1374	2111	351	426	17		
6	b	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	c	260	Total	C	H	N	O	S	0	0
			4096	1314	2023	333	409	17		
6	d	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	e	261	Total	C	H	N	O	S	0	0
			4103	1316	2026	334	410	17		
6	f	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	g	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	h	271	Total	C	H	N	O	S	0	0
			4279	1374	2111	351	426	17		
6	i	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	j	274	Total	C	H	N	O	S	0	0
			4326	1391	2134	354	430	17		
6	k	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	l	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	m	275	Total	C	H	N	O	S	0	0
			4340	1395	2140	356	432	17		
6	n	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	o	276	Total	C	H	N	O	S	0	0
			4357	1400	2148	358	434	17		
6	p	275	Total	C	H	N	O	S	0	0
			4340	1395	2140	356	432	17		
6	q	271	Total	C	H	N	O	S	0	0
			4279	1374	2111	351	426	17		
6	r	275	Total	C	H	N	O	S	0	0
			4340	1395	2140	356	432	17		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	108	ILE	THR	conflict	UNP B1NP55
a	147	SER	ASN	conflict	UNP B1NP55
b	108	ILE	THR	conflict	UNP B1NP55
b	147	SER	ASN	conflict	UNP B1NP55
c	108	ILE	THR	conflict	UNP B1NP55
c	147	SER	ASN	conflict	UNP B1NP55
d	108	ILE	THR	conflict	UNP B1NP55
d	147	SER	ASN	conflict	UNP B1NP55
e	108	ILE	THR	conflict	UNP B1NP55
e	147	SER	ASN	conflict	UNP B1NP55
f	108	ILE	THR	conflict	UNP B1NP55
f	147	SER	ASN	conflict	UNP B1NP55
g	108	ILE	THR	conflict	UNP B1NP55
g	147	SER	ASN	conflict	UNP B1NP55
h	108	ILE	THR	conflict	UNP B1NP55
h	147	SER	ASN	conflict	UNP B1NP55
i	108	ILE	THR	conflict	UNP B1NP55
i	147	SER	ASN	conflict	UNP B1NP55
j	108	ILE	THR	conflict	UNP B1NP55
j	147	SER	ASN	conflict	UNP B1NP55
k	108	ILE	THR	conflict	UNP B1NP55
k	147	SER	ASN	conflict	UNP B1NP55
l	108	ILE	THR	conflict	UNP B1NP55
l	147	SER	ASN	conflict	UNP B1NP55
m	108	ILE	THR	conflict	UNP B1NP55
m	147	SER	ASN	conflict	UNP B1NP55
n	108	ILE	THR	conflict	UNP B1NP55

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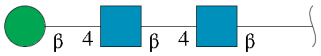
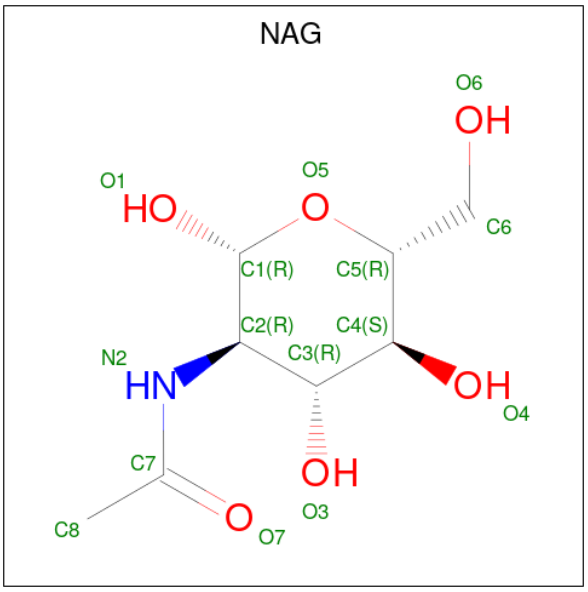
Chain	Residue	Modelled	Actual	Comment	Reference
n	147	SER	ASN	conflict	UNP B1NP55
o	108	ILE	THR	conflict	UNP B1NP55
o	147	SER	ASN	conflict	UNP B1NP55
p	108	ILE	THR	conflict	UNP B1NP55
p	147	SER	ASN	conflict	UNP B1NP55
q	108	ILE	THR	conflict	UNP B1NP55
q	147	SER	ASN	conflict	UNP B1NP55
r	108	ILE	THR	conflict	UNP B1NP55
r	147	SER	ASN	conflict	UNP B1NP55

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
7	S	3	76	22	37	2	15	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
8	a	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	b	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	b	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	c	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	c	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	d	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	d	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	e	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	e	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	f	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	f	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	g	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	g	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	h	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	h	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	i	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	i	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	j	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	j	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	k	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	k	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	l	1	Total	C	H	N	O	0
			56	16	28	2	10	

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Mol	Chain	Residues	Atoms					AltConf
8	l	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	m	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	m	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	n	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	n	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	o	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	o	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	p	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	p	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	q	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	q	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	r	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	r	1	Total	C	H	N	O	0
			56	16	28	2	10	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	a	4	Total	Ca	0
			4	4	
9	b	4	Total	Ca	0
			4	4	
9	c	4	Total	Ca	0
			4	4	
9	d	4	Total	Ca	0
			4	4	
9	e	4	Total	Ca	0
			4	4	
9	f	4	Total	Ca	0
			4	4	

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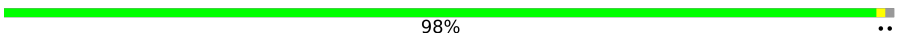
Mol	Chain	Residues	Atoms	AltConf
9	g	4	Total Ca 4 4	0
9	h	4	Total Ca 4 4	0
9	i	4	Total Ca 4 4	0
9	j	4	Total Ca 4 4	0
9	k	4	Total Ca 4 4	0
9	l	4	Total Ca 4 4	0
9	m	4	Total Ca 4 4	0
9	n	4	Total Ca 4 4	0
9	o	4	Total Ca 4 4	0
9	p	4	Total Ca 4 4	0
9	q	4	Total Ca 4 4	0
9	r	4	Total Ca 4 4	0

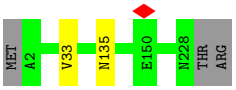
3 Residue-property plots (i)

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.

• Molecule 1: Outer capsid protein VP8*

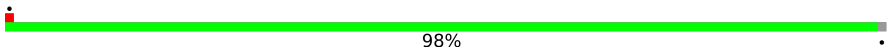
Chain T:

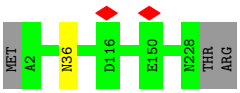




• Molecule 1: Outer capsid protein VP8*

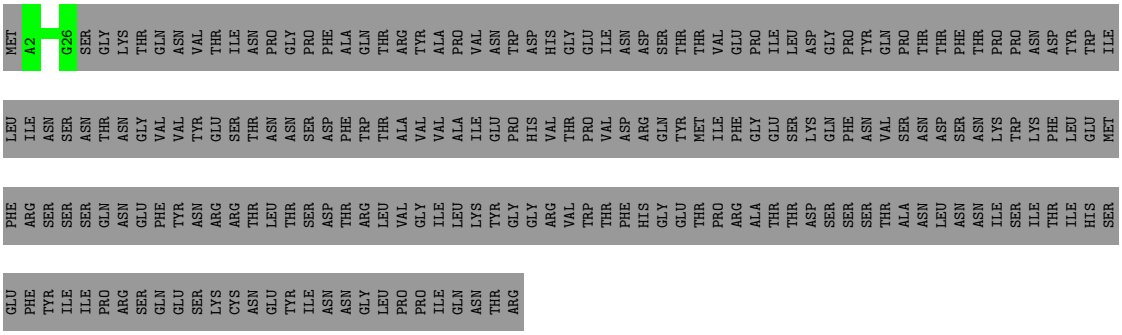
Chain U:





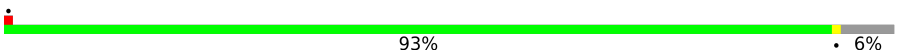
• Molecule 1: Outer capsid protein VP8*

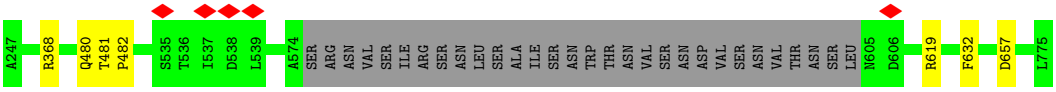
Chain V:



• Molecule 2: Outer capsid protein VP5*

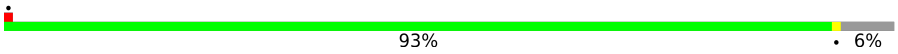
Chain 1:

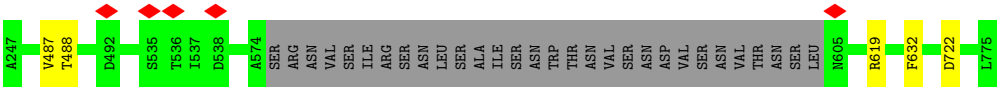




• Molecule 2: Outer capsid protein VP5*

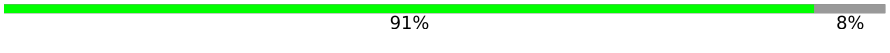
Chain 2:

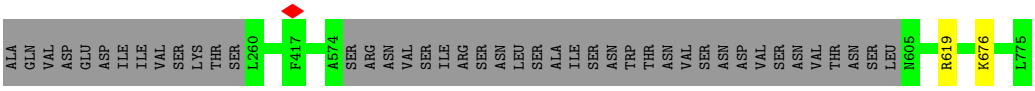




• Molecule 2: Outer capsid protein VP5*

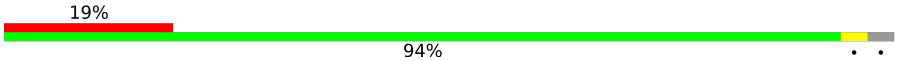
Chain 3:

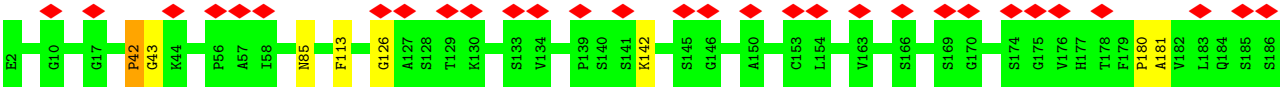


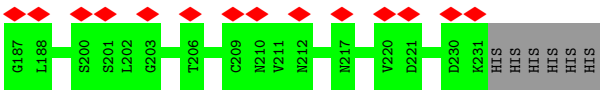


• Molecule 3: Fab 41 heavy chain

Chain 4:

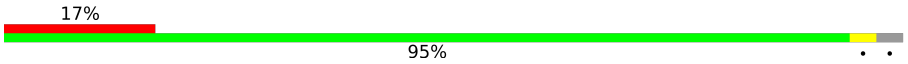


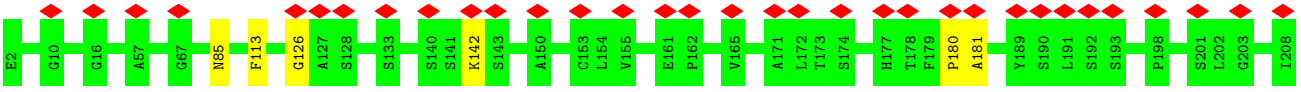


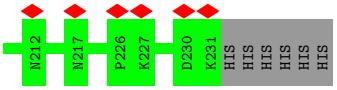


• Molecule 3: Fab 41 heavy chain

Chain 6:

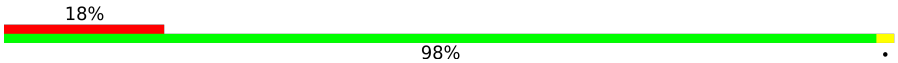


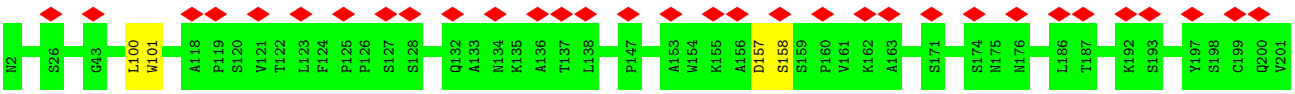


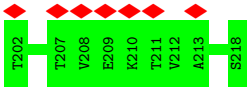


• Molecule 4: Fab 41 light chain

Chain 5:

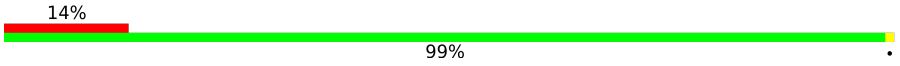


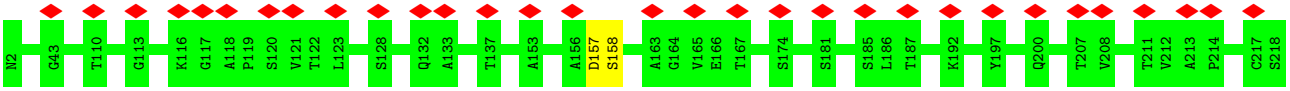




• Molecule 4: Fab 41 light chain

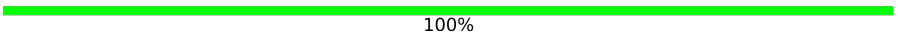
Chain 7:

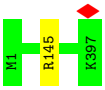




• Molecule 5: Intermediate capsid protein VP6

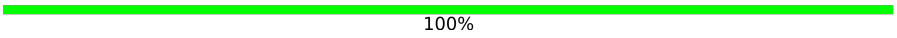
Chain A:

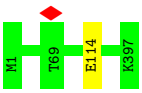




• Molecule 5: Intermediate capsid protein VP6

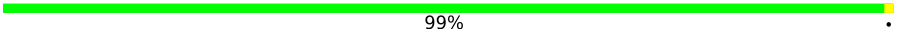
Chain B:





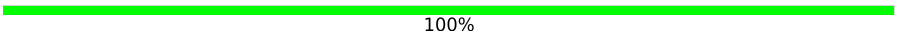
• Molecule 5: Intermediate capsid protein VP6

Chain C:



• Molecule 5: Intermediate capsid protein VP6

Chain D:



There are no outlier residues recorded for this chain.

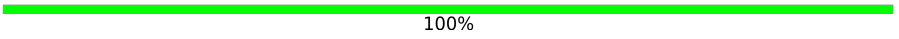
• Molecule 5: Intermediate capsid protein VP6

Chain E:

There are no outlier residues recorded for this chain.

• Molecule 5: Intermediate capsid protein VP6

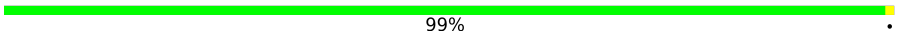
Chain F:



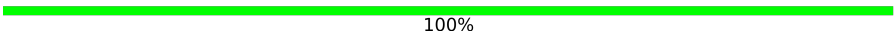
There are no outlier residues recorded for this chain.

• Molecule 5: Intermediate capsid protein VP6

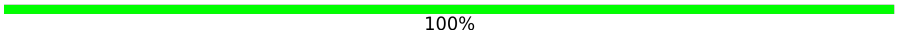
Chain G:



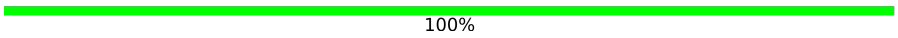
• Molecule 5: Intermediate capsid protein VP6

Chain H: 

• Molecule 5: Intermediate capsid protein VP6

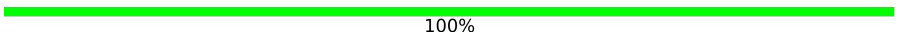
Chain I: 

• Molecule 5: Intermediate capsid protein VP6

Chain J: 

There are no outlier residues recorded for this chain.

• Molecule 5: Intermediate capsid protein VP6

Chain K: 

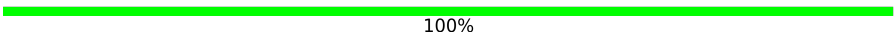
There are no outlier residues recorded for this chain.

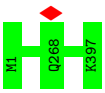
• Molecule 5: Intermediate capsid protein VP6

Chain L: 

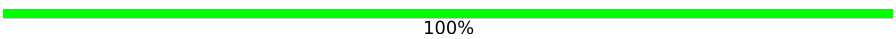
There are no outlier residues recorded for this chain.

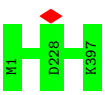
• Molecule 5: Intermediate capsid protein VP6

Chain M: 



• Molecule 5: Intermediate capsid protein VP6

Chain N: 



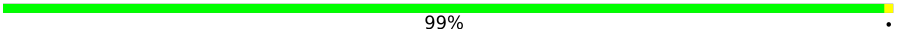
• Molecule 5: Intermediate capsid protein VP6

Chain O:

There are no outlier residues recorded for this chain.

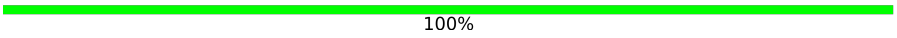
• Molecule 5: Intermediate capsid protein VP6

Chain P:



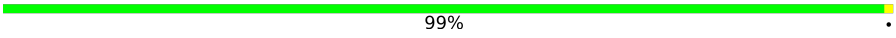
• Molecule 5: Intermediate capsid protein VP6

Chain Q:



• Molecule 5: Intermediate capsid protein VP6

Chain R:

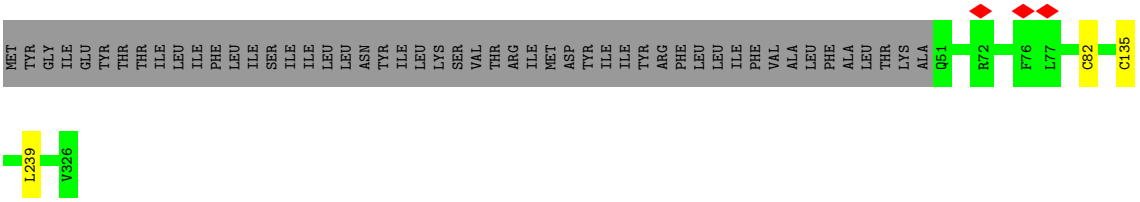


• Molecule 6: Outer capsid glycoprotein VP7

Chain a:

• Molecule 6: Outer capsid glycoprotein VP7

Chain b:

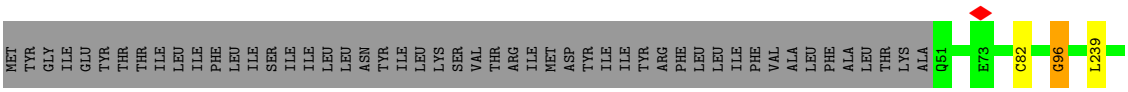


• Molecule 6: Outer capsid glycoprotein VP7

Chain c:

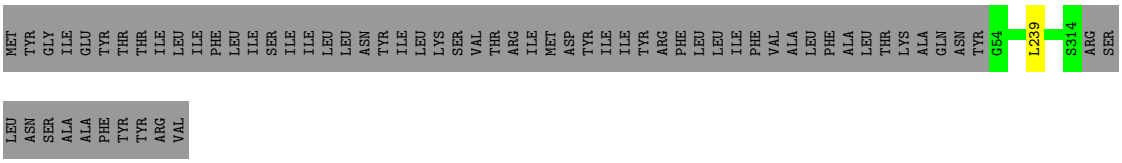
• Molecule 6: Outer capsid glycoprotein VP7

Chain d:



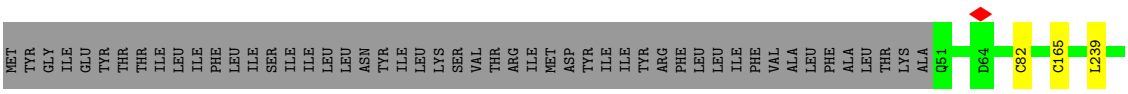
• Molecule 6: Outer capsid glycoprotein VP7

Chain e:



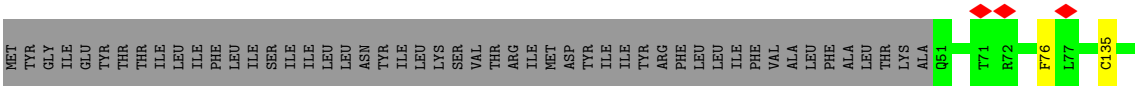
• Molecule 6: Outer capsid glycoprotein VP7

Chain f:



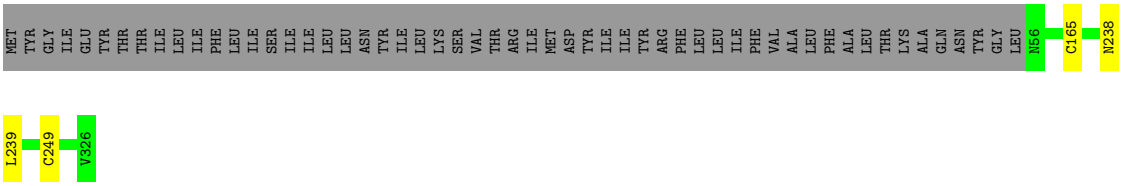
• Molecule 6: Outer capsid glycoprotein VP7

Chain g:



• Molecule 6: Outer capsid glycoprotein VP7

Chain h:

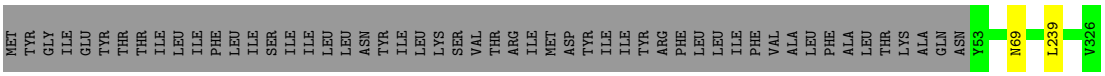


• Molecule 6: Outer capsid glycoprotein VP7

Chain i:

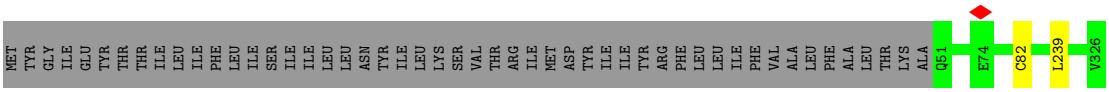
• Molecule 6: Outer capsid glycoprotein VP7

Chain j:



• Molecule 6: Outer capsid glycoprotein VP7

Chain k:

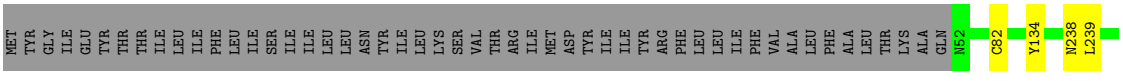


• Molecule 6: Outer capsid glycoprotein VP7

Chain l:

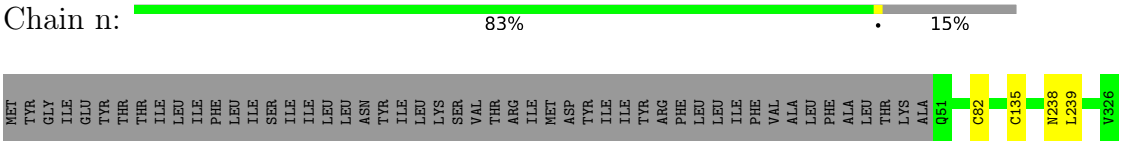
• Molecule 6: Outer capsid glycoprotein VP7

Chain m:



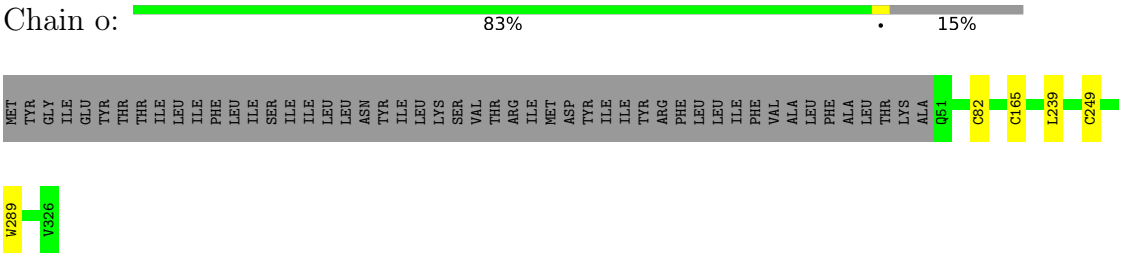
• Molecule 6: Outer capsid glycoprotein VP7

Chain n:



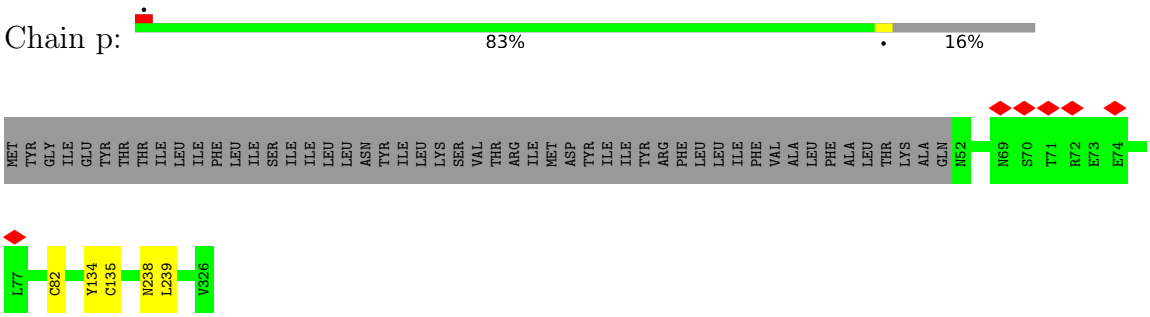
• Molecule 6: Outer capsid glycoprotein VP7

Chain o:



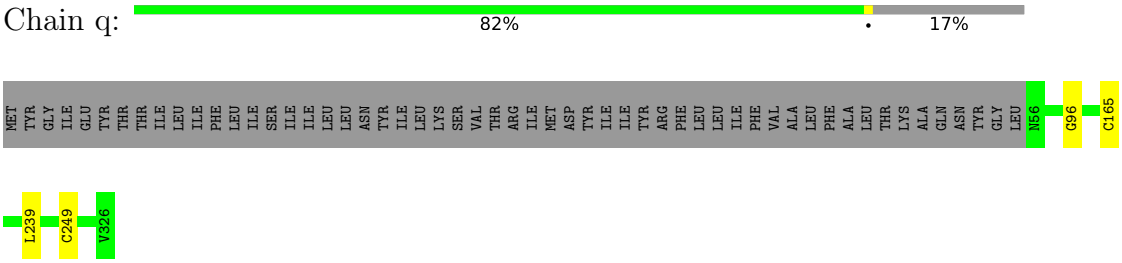
• Molecule 6: Outer capsid glycoprotein VP7

Chain p:



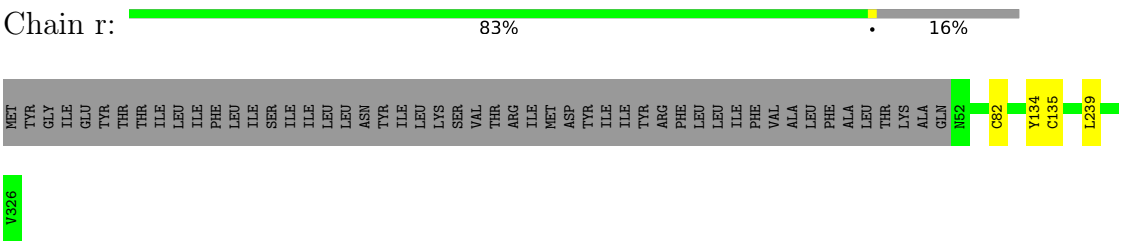
• Molecule 6: Outer capsid glycoprotein VP7

Chain q:



• Molecule 6: Outer capsid glycoprotein VP7

Chain r:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	422920	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	393.91998, 393.91998, 393.91998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.231, 1.231, 1.231	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, 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	T	0.30	0/1876	0.54	0/2565
1	U	0.30	0/1876	0.54	0/2565
1	V	0.32	0/206	0.55	0/279
2	1	0.31	0/4035	0.53	1/5459 (0.0%)
2	2	0.31	0/4035	0.52	0/5459
2	3	0.33	0/3938	0.55	0/5327
3	4	0.33	0/1777	0.65	0/2425
3	6	0.34	0/1777	0.66	0/2425
4	5	0.36	1/1681 (0.1%)	0.66	1/2295 (0.0%)
4	7	0.35	1/1681 (0.1%)	0.66	0/2295
5	A	0.34	0/3238	0.54	0/4404
5	B	0.35	0/3238	0.54	0/4404
5	C	0.34	0/3238	0.55	0/4404
5	D	0.34	0/3238	0.52	0/4404
5	E	0.33	0/3238	0.53	0/4404
5	F	0.34	0/3238	0.52	0/4404
5	G	0.34	0/3238	0.56	0/4404
5	H	0.33	0/3238	0.53	0/4404
5	I	0.33	0/3238	0.55	0/4404
5	J	0.33	0/3238	0.53	0/4404
5	K	0.33	0/3238	0.53	0/4404
5	L	0.34	0/3238	0.53	0/4404
5	M	0.33	0/3238	0.53	0/4404
5	N	0.34	0/3238	0.55	0/4404
5	O	0.32	0/3238	0.53	0/4404
5	P	0.32	0/3238	0.53	0/4404
5	Q	0.34	0/3238	0.54	0/4404
5	R	0.33	0/3238	0.54	0/4404
6	a	0.35	0/2213	0.50	0/3013
6	b	0.42	2/2255 (0.1%)	0.54	0/3070
6	c	0.35	1/2115 (0.0%)	0.52	0/2882
6	d	0.37	1/2255 (0.0%)	0.53	0/3070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	e	0.32	0/2119	0.50	0/2887
6	f	0.40	3/2255 (0.1%)	0.55	1/3070 (0.0%)
6	g	0.34	1/2255 (0.0%)	0.53	0/3070
6	h	0.38	2/2213 (0.1%)	0.54	1/3013 (0.0%)
6	i	0.41	2/2255 (0.1%)	0.53	0/3070
6	j	0.34	0/2238	0.52	0/3047
6	k	0.35	1/2255 (0.0%)	0.52	0/3070
6	l	0.39	3/2255 (0.1%)	0.57	1/3070 (0.0%)
6	m	0.37	1/2246 (0.0%)	0.52	0/3058
6	n	0.37	2/2255 (0.1%)	0.52	1/3070 (0.0%)
6	o	0.41	3/2255 (0.1%)	0.57	2/3070 (0.1%)
6	p	0.41	2/2246 (0.1%)	0.56	0/3058
6	q	0.38	2/2213 (0.1%)	0.54	1/3013 (0.0%)
6	r	0.37	2/2246 (0.1%)	0.53	0/3058
All	All	0.35	30/121310 (0.0%)	0.54	9/165025 (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	T	0	1
1	U	0	1
2	1	0	3
2	2	0	1
3	4	0	4
3	6	0	3
4	5	0	1
5	A	0	1
5	C	0	1
5	P	0	1
5	Q	0	1
6	a	0	1
6	b	0	1
6	c	0	1
6	d	0	2
6	e	0	1
6	f	0	1
6	g	0	2
6	h	0	1
6	i	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	j	0	1
6	k	0	1
6	l	0	2
6	m	0	2
6	n	0	1
6	o	0	2
6	p	0	2
6	q	0	2
6	r	0	2
All	All	0	45

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	82	CYS	CB-SG	-8.95	1.67	1.82
6	i	82	CYS	CB-SG	-8.57	1.67	1.82
6	p	82	CYS	CB-SG	-8.22	1.68	1.82
6	b	135	CYS	CB-SG	-7.23	1.70	1.82
6	p	135	CYS	CB-SG	-6.93	1.70	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	165	CYS	CA-CB-SG	10.78	133.40	114.00
6	o	165	CYS	CA-CB-SG	10.64	133.15	114.00
6	f	165	CYS	CA-CB-SG	10.57	133.02	114.00
6	q	165	CYS	CA-CB-SG	10.03	132.05	114.00
6	h	165	CYS	CA-CB-SG	9.84	131.72	114.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	480	GLN	Peptide
2	1	481	THR	Peptide
2	1	482	PRO	Peptide
1	T	33	VAL	Peptide
1	U	36	ASN	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	225/230 (98%)	202 (90%)	23 (10%)	0	100	100
1	U	225/230 (98%)	200 (89%)	25 (11%)	0	100	100
1	V	23/230 (10%)	23 (100%)	0	0	100	100
2	1	495/529 (94%)	444 (90%)	50 (10%)	1 (0%)	47	81
2	2	495/529 (94%)	452 (91%)	40 (8%)	3 (1%)	25	64
2	3	482/529 (91%)	438 (91%)	44 (9%)	0	100	100
3	4	228/236 (97%)	204 (90%)	20 (9%)	4 (2%)	8	41
3	6	228/236 (97%)	204 (90%)	22 (10%)	2 (1%)	17	56
4	5	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	29	68
4	7	215/217 (99%)	193 (90%)	21 (10%)	1 (0%)	29	68
5	A	395/397 (100%)	370 (94%)	25 (6%)	0	100	100
5	B	395/397 (100%)	365 (92%)	29 (7%)	1 (0%)	41	75
5	C	395/397 (100%)	373 (94%)	21 (5%)	1 (0%)	41	75
5	D	395/397 (100%)	374 (95%)	21 (5%)	0	100	100
5	E	395/397 (100%)	364 (92%)	31 (8%)	0	100	100
5	F	395/397 (100%)	366 (93%)	29 (7%)	0	100	100
5	G	395/397 (100%)	372 (94%)	22 (6%)	1 (0%)	41	75
5	H	395/397 (100%)	374 (95%)	21 (5%)	0	100	100
5	I	395/397 (100%)	372 (94%)	23 (6%)	0	100	100
5	J	395/397 (100%)	372 (94%)	23 (6%)	0	100	100
5	K	395/397 (100%)	369 (93%)	26 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	395/397 (100%)	376 (95%)	19 (5%)	0	100	100
5	M	395/397 (100%)	367 (93%)	28 (7%)	0	100	100
5	N	395/397 (100%)	369 (93%)	26 (7%)	0	100	100
5	O	395/397 (100%)	372 (94%)	23 (6%)	0	100	100
5	P	395/397 (100%)	366 (93%)	29 (7%)	0	100	100
5	Q	395/397 (100%)	372 (94%)	23 (6%)	0	100	100
5	R	395/397 (100%)	364 (92%)	31 (8%)	0	100	100
6	a	269/326 (82%)	254 (94%)	15 (6%)	0	100	100
6	b	274/326 (84%)	248 (90%)	26 (10%)	0	100	100
6	c	258/326 (79%)	239 (93%)	19 (7%)	0	100	100
6	d	274/326 (84%)	254 (93%)	19 (7%)	1 (0%)	34	72
6	e	259/326 (79%)	243 (94%)	16 (6%)	0	100	100
6	f	274/326 (84%)	253 (92%)	21 (8%)	0	100	100
6	g	274/326 (84%)	257 (94%)	17 (6%)	0	100	100
6	h	269/326 (82%)	255 (95%)	14 (5%)	0	100	100
6	i	274/326 (84%)	250 (91%)	24 (9%)	0	100	100
6	j	272/326 (83%)	253 (93%)	19 (7%)	0	100	100
6	k	274/326 (84%)	256 (93%)	18 (7%)	0	100	100
6	l	274/326 (84%)	255 (93%)	19 (7%)	0	100	100
6	m	273/326 (84%)	256 (94%)	17 (6%)	0	100	100
6	n	274/326 (84%)	250 (91%)	24 (9%)	0	100	100
6	o	274/326 (84%)	252 (92%)	22 (8%)	0	100	100
6	p	273/326 (84%)	249 (91%)	24 (9%)	0	100	100
6	q	269/326 (82%)	248 (92%)	21 (8%)	0	100	100
6	r	273/326 (84%)	241 (88%)	32 (12%)	0	100	100
All	All	14822/16197 (92%)	13726 (93%)	1080 (7%)	16 (0%)	54	84

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	181	ALA
3	6	181	ALA
4	7	157	ASP

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Mol	Chain	Res	Type
2	1	632	PHE
3	4	180	PRO

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	T	208/211 (99%)	207 (100%)	1 (0%)	88 94
1	U	208/211 (99%)	208 (100%)	0	100 100
1	V	23/211 (11%)	23 (100%)	0	100 100
2	1	448/477 (94%)	446 (100%)	2 (0%)	91 96
2	2	448/477 (94%)	447 (100%)	1 (0%)	93 98
2	3	436/477 (91%)	434 (100%)	2 (0%)	88 94
3	4	193/199 (97%)	192 (100%)	1 (0%)	88 94
3	6	193/199 (97%)	192 (100%)	1 (0%)	88 94
4	5	187/187 (100%)	187 (100%)	0	100 100
4	7	187/187 (100%)	187 (100%)	0	100 100
5	A	348/348 (100%)	348 (100%)	0	100 100
5	B	348/348 (100%)	348 (100%)	0	100 100
5	C	348/348 (100%)	348 (100%)	0	100 100
5	D	348/348 (100%)	348 (100%)	0	100 100
5	E	348/348 (100%)	348 (100%)	0	100 100
5	F	348/348 (100%)	348 (100%)	0	100 100
5	G	348/348 (100%)	347 (100%)	1 (0%)	92 97
5	H	348/348 (100%)	347 (100%)	1 (0%)	92 97
5	I	348/348 (100%)	347 (100%)	1 (0%)	92 97
5	J	348/348 (100%)	348 (100%)	0	100 100
5	K	348/348 (100%)	348 (100%)	0	100 100
5	L	348/348 (100%)	348 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	348/348 (100%)	348 (100%)	0	100	100
5	N	348/348 (100%)	348 (100%)	0	100	100
5	O	348/348 (100%)	348 (100%)	0	100	100
5	P	348/348 (100%)	346 (99%)	2 (1%)	86	94
5	Q	348/348 (100%)	348 (100%)	0	100	100
5	R	348/348 (100%)	346 (99%)	2 (1%)	86	94
6	a	250/300 (83%)	250 (100%)	0	100	100
6	b	254/300 (85%)	254 (100%)	0	100	100
6	c	241/300 (80%)	240 (100%)	1 (0%)	91	96
6	d	254/300 (85%)	253 (100%)	1 (0%)	91	96
6	e	241/300 (80%)	241 (100%)	0	100	100
6	f	254/300 (85%)	254 (100%)	0	100	100
6	g	254/300 (85%)	253 (100%)	1 (0%)	91	96
6	h	250/300 (83%)	249 (100%)	1 (0%)	91	96
6	i	254/300 (85%)	253 (100%)	1 (0%)	91	96
6	j	252/300 (84%)	251 (100%)	1 (0%)	91	96
6	k	254/300 (85%)	254 (100%)	0	100	100
6	l	254/300 (85%)	253 (100%)	1 (0%)	91	96
6	m	253/300 (84%)	252 (100%)	1 (0%)	91	96
6	n	254/300 (85%)	253 (100%)	1 (0%)	91	96
6	o	254/300 (85%)	254 (100%)	0	100	100
6	p	253/300 (84%)	252 (100%)	1 (0%)	91	96
6	q	250/300 (83%)	250 (100%)	0	100	100
6	r	253/300 (84%)	253 (100%)	0	100	100
All	All	13324/14500 (92%)	13299 (100%)	25 (0%)	93	98

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	305	ASN
6	g	238	ASN
6	p	238	ASN
6	d	315	ARG
6	h	238	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
6	k	51	GLN
6	n	51	GLN
6	p	257	ASN
5	H	72	ASN
5	H	317	HIS

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)

3 monosaccharides 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	$\#\|Z\| > 2$
7	NAG	S	1	7,6	14,14,15	0.58	0	17,19,21	1.11	1 (5%)
7	NAG	S	2	7	14,14,15	0.25	0	17,19,21	0.37	0
7	BMA	S	3	7	11,11,12	0.66	0	15,15,17	0.71	0

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
7	NAG	S	1	7,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	S	2	7	-	3/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	1	NAG	C1-O5-C5	3.62	117.09	112.19

There are no chirality outliers.

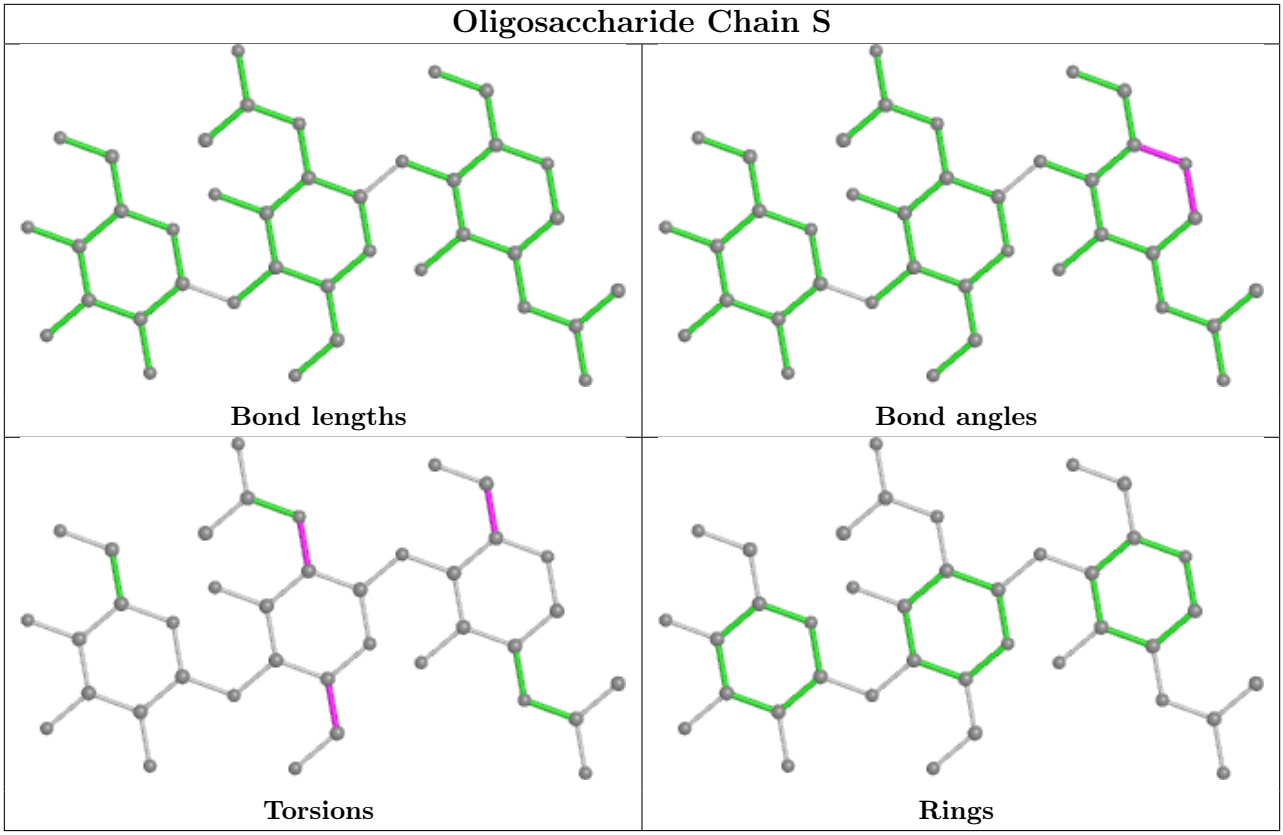
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	1	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	S	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 107 ligands modelled in this entry, 72 are monoatomic - leaving 35 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	$\#\|Z\| > 2$
8	NAG	a	401	6	14,14,15	0.24	0	17,19,21	0.53	0
8	NAG	r	504	6	14,14,15	0.35	0	17,19,21	0.43	0
8	NAG	n	402	6	14,14,15	0.20	0	17,19,21	0.37	0
8	NAG	m	402	6	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	r	503	6	14,14,15	0.27	0	17,19,21	0.38	0
8	NAG	h	402	6	14,14,15	0.22	0	17,19,21	0.39	0
8	NAG	f	504	6	14,14,15	0.51	0	17,19,21	0.51	0
8	NAG	q	402	6	14,14,15	0.31	0	17,19,21	0.39	0
8	NAG	m	401	6	14,14,15	0.22	0	17,19,21	0.39	0
8	NAG	i	503	6	14,14,15	0.20	0	17,19,21	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	k	401	6	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
8	NAG	q	401	6	14,14,15	0.20	0	17,19,21	0.42	0
8	NAG	o	503	6	14,14,15	0.39	0	17,19,21	0.55	0
8	NAG	c	503	6	14,14,15	0.18	0	17,19,21	0.47	0
8	NAG	d	402	6	14,14,15	0.49	0	17,19,21	0.49	0
8	NAG	i	504	6	14,14,15	0.26	0	17,19,21	0.37	0
8	NAG	h	401	6	14,14,15	0.23	0	17,19,21	0.43	0
8	NAG	b	402	6	14,14,15	0.26	0	17,19,21	0.40	0
8	NAG	f	503	6	14,14,15	0.26	0	17,19,21	0.44	0
8	NAG	g	401	6	14,14,15	0.29	0	17,19,21	1.48	2 (11%)
8	NAG	e	401	6	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	b	401	6	14,14,15	0.36	0	17,19,21	0.40	0
8	NAG	l	504	6	14,14,15	0.36	0	17,19,21	0.37	0
8	NAG	n	401	6	14,14,15	0.35	0	17,19,21	0.51	0
8	NAG	k	402	6	14,14,15	0.40	0	17,19,21	0.56	0
8	NAG	d	401	6	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	p	401	6	14,14,15	0.58	1 (7%)	17,19,21	0.49	0
8	NAG	g	402	6	14,14,15	0.29	0	17,19,21	0.37	0
8	NAG	j	402	6	14,14,15	0.41	0	17,19,21	0.41	0
8	NAG	e	402	6	14,14,15	0.34	0	17,19,21	0.37	0
8	NAG	l	503	6	14,14,15	0.28	0	17,19,21	0.45	0
8	NAG	o	504	6	14,14,15	0.39	0	17,19,21	0.59	0
8	NAG	c	504	6	14,14,15	0.30	0	17,19,21	0.35	0
8	NAG	p	402	6	14,14,15	0.32	0	17,19,21	0.41	0
8	NAG	j	401	6	14,14,15	0.28	0	17,19,21	0.50	0

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
8	NAG	a	401	6	-	0/6/23/26	0/1/1/1
8	NAG	r	504	6	-	2/6/23/26	0/1/1/1
8	NAG	n	402	6	-	0/6/23/26	0/1/1/1
8	NAG	m	402	6	-	1/6/23/26	0/1/1/1
8	NAG	r	503	6	-	2/6/23/26	0/1/1/1
8	NAG	h	402	6	-	2/6/23/26	0/1/1/1
8	NAG	f	504	6	-	2/6/23/26	0/1/1/1
8	NAG	q	402	6	-	0/6/23/26	0/1/1/1
8	NAG	m	401	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	i	503	6	-	1/6/23/26	0/1/1/1
8	NAG	k	401	6	-	2/6/23/26	0/1/1/1
8	NAG	q	401	6	-	2/6/23/26	0/1/1/1
8	NAG	o	503	6	-	3/6/23/26	0/1/1/1
8	NAG	c	503	6	-	2/6/23/26	0/1/1/1
8	NAG	d	402	6	-	0/6/23/26	0/1/1/1
8	NAG	i	504	6	-	1/6/23/26	0/1/1/1
8	NAG	h	401	6	-	2/6/23/26	0/1/1/1
8	NAG	b	402	6	-	0/6/23/26	0/1/1/1
8	NAG	f	503	6	-	2/6/23/26	0/1/1/1
8	NAG	g	401	6	-	5/6/23/26	0/1/1/1
8	NAG	e	401	6	-	2/6/23/26	0/1/1/1
8	NAG	b	401	6	-	3/6/23/26	0/1/1/1
8	NAG	l	504	6	-	0/6/23/26	0/1/1/1
8	NAG	n	401	6	-	2/6/23/26	0/1/1/1
8	NAG	k	402	6	-	0/6/23/26	0/1/1/1
8	NAG	d	401	6	-	2/6/23/26	0/1/1/1
8	NAG	p	401	6	-	4/6/23/26	0/1/1/1
8	NAG	g	402	6	-	2/6/23/26	0/1/1/1
8	NAG	j	402	6	-	2/6/23/26	0/1/1/1
8	NAG	e	402	6	-	2/6/23/26	0/1/1/1
8	NAG	l	503	6	-	2/6/23/26	0/1/1/1
8	NAG	o	504	6	-	2/6/23/26	0/1/1/1
8	NAG	c	504	6	-	1/6/23/26	0/1/1/1
8	NAG	p	402	6	-	2/6/23/26	0/1/1/1
8	NAG	j	401	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	401	NAG	C1-C2	2.03	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	g	401	NAG	C2-N2-C7	4.65	129.52	122.90
8	g	401	NAG	C1-C2-N2	3.00	115.61	110.49
8	k	401	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	b	401	NAG	C1-C2-N2-C7
8	j	401	NAG	C4-C5-C6-O6
8	e	401	NAG	O5-C5-C6-O6
8	m	401	NAG	O5-C5-C6-O6
8	h	402	NAG	O5-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.

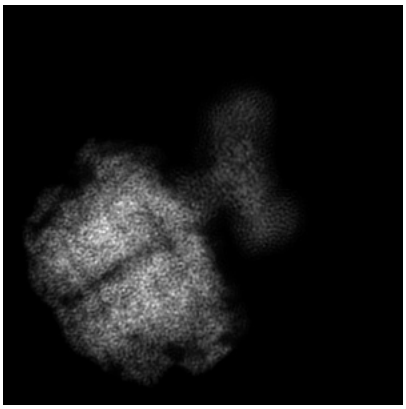
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26608. These allow visual inspection of the internal detail of the map and identification of artifacts.

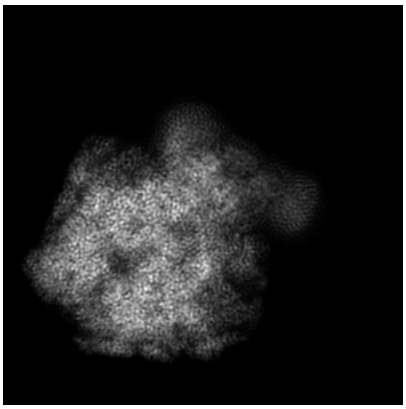
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

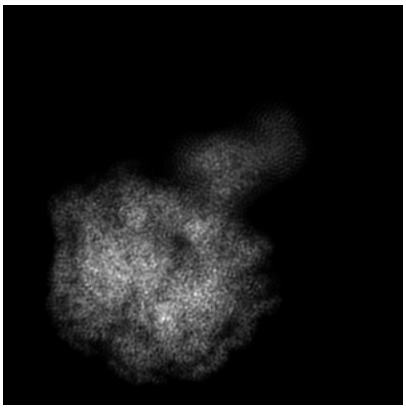
6.1.1 Primary map



X

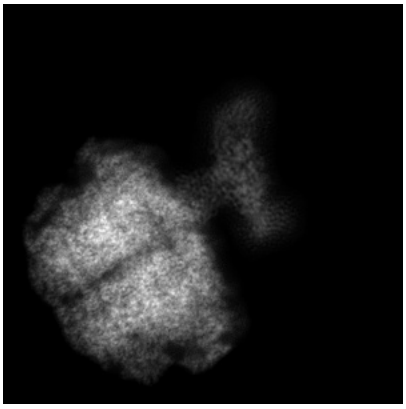


Y

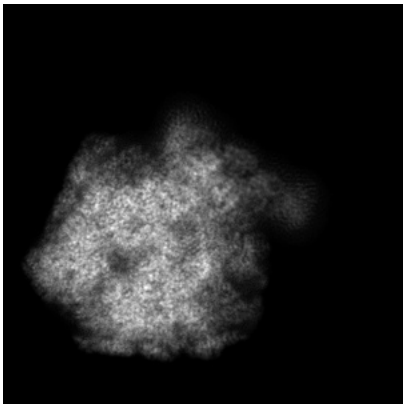


Z

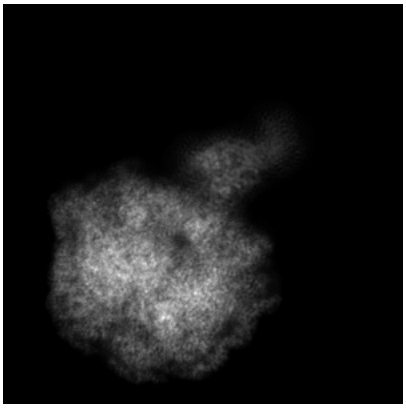
6.1.2 Raw map



X



Y



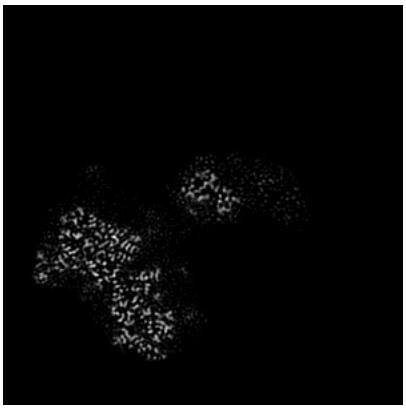
Z

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

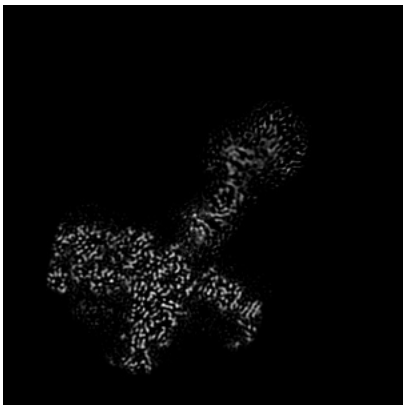
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160

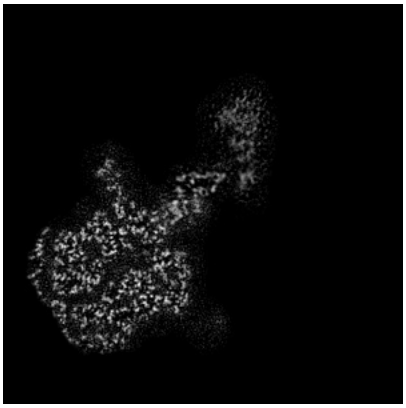


Y Index: 160

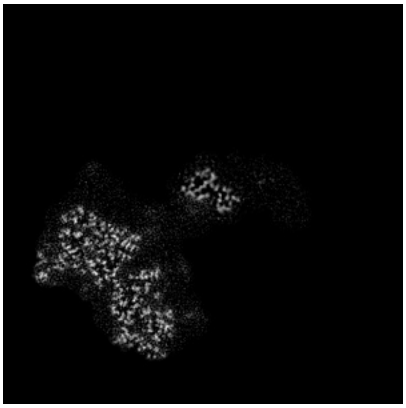


Z Index: 160

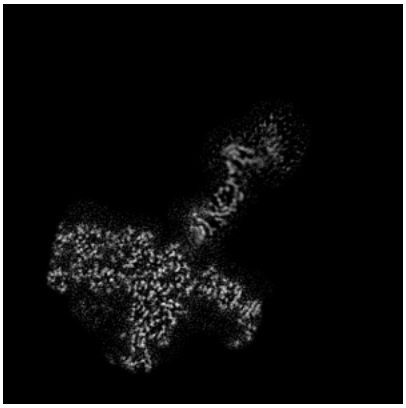
6.2.2 Raw map



X Index: 160



Y Index: 160

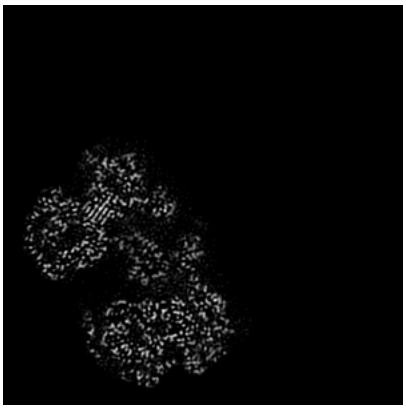


Z Index: 160

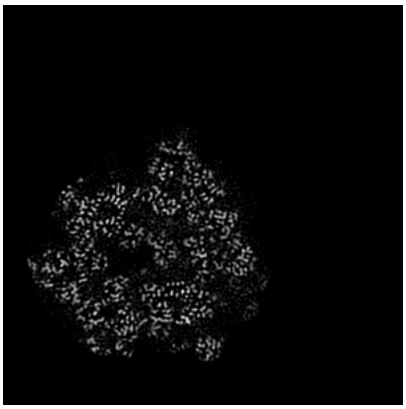
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

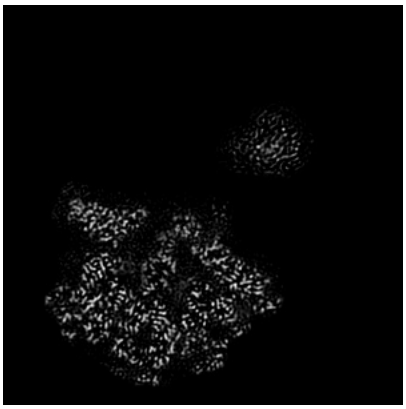
6.3.1 Primary map



X Index: 111

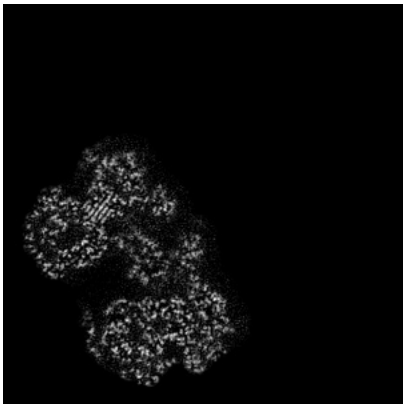


Y Index: 96

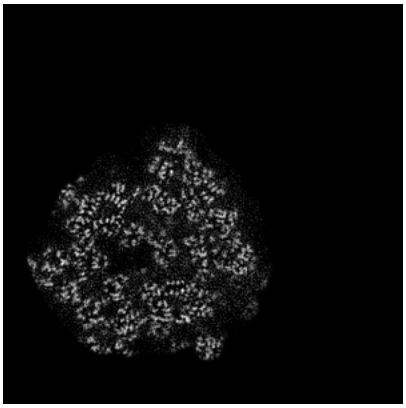


Z Index: 134

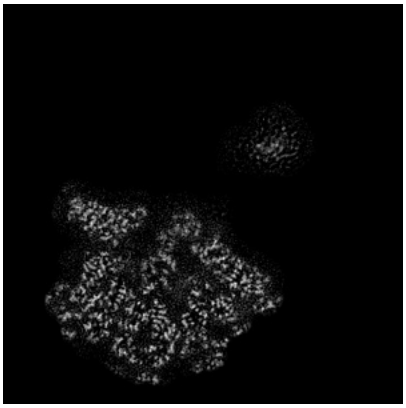
6.3.2 Raw map



X Index: 111



Y Index: 96

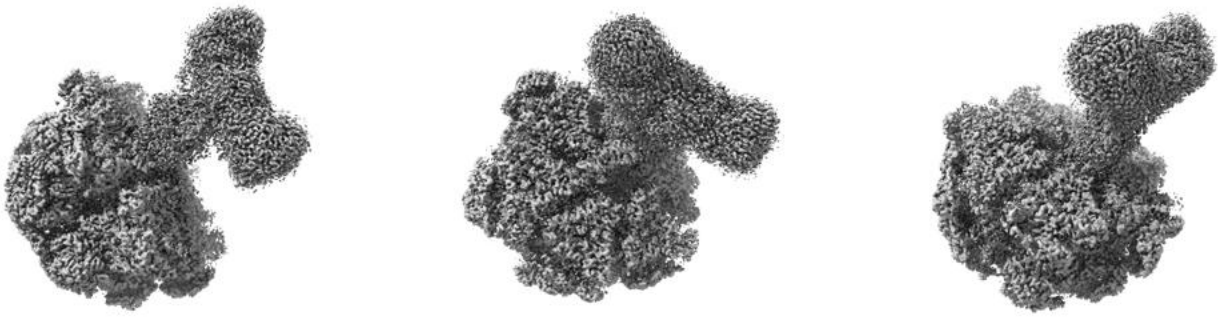


Z Index: 134

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

6.4 Orthogonal surface views (i)

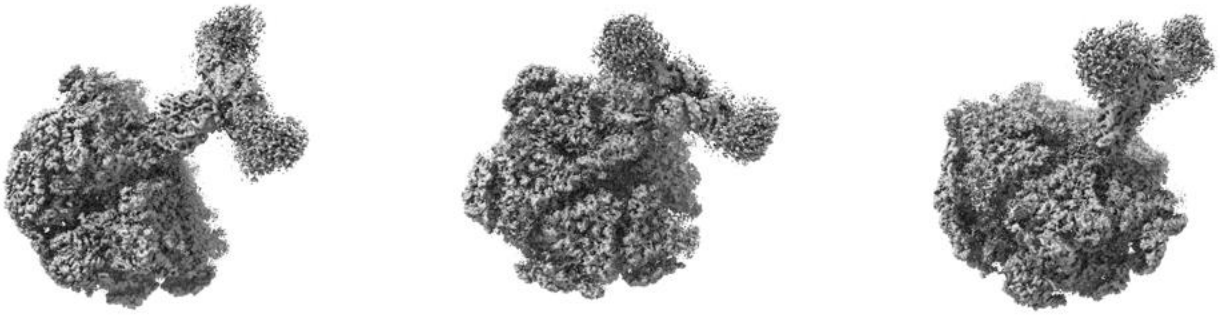
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

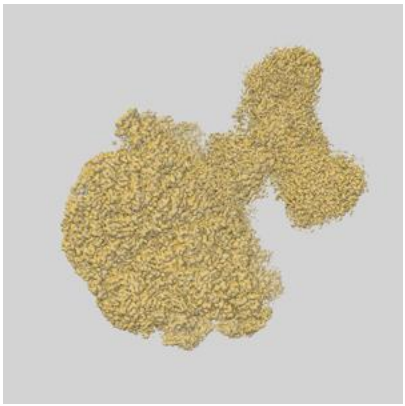
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

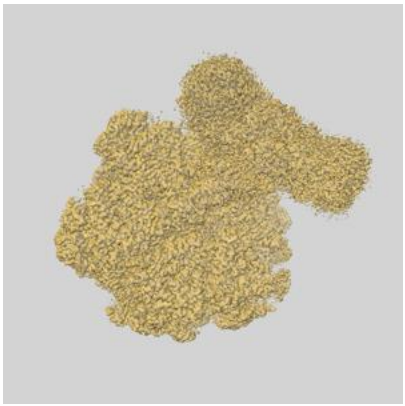
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

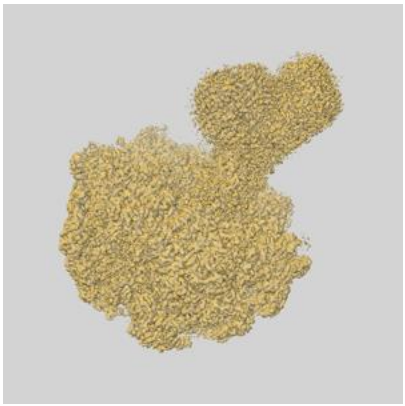
6.5.1 emd_26608_msk_1.map (i)



X



Y

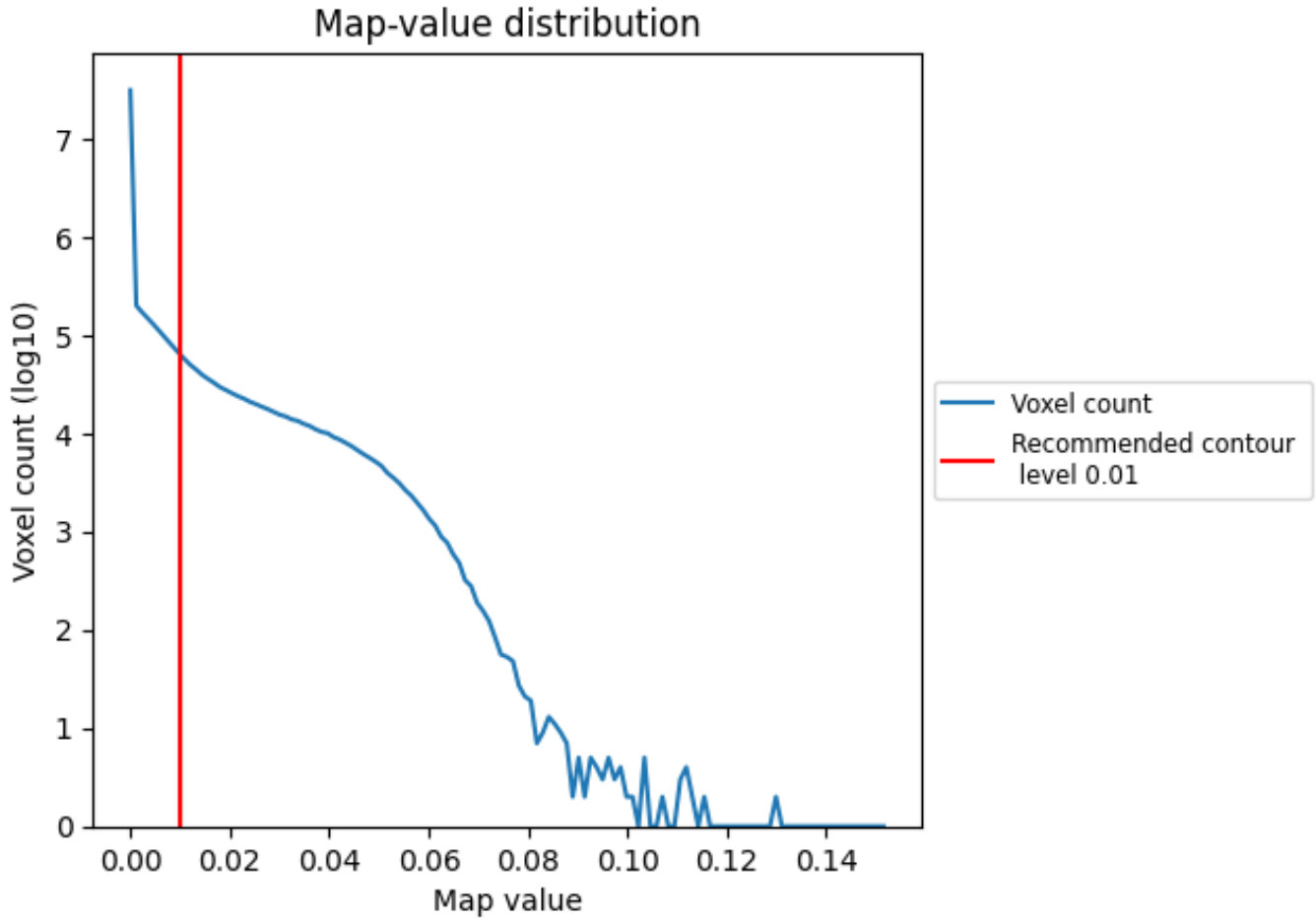


Z

7 Map analysis

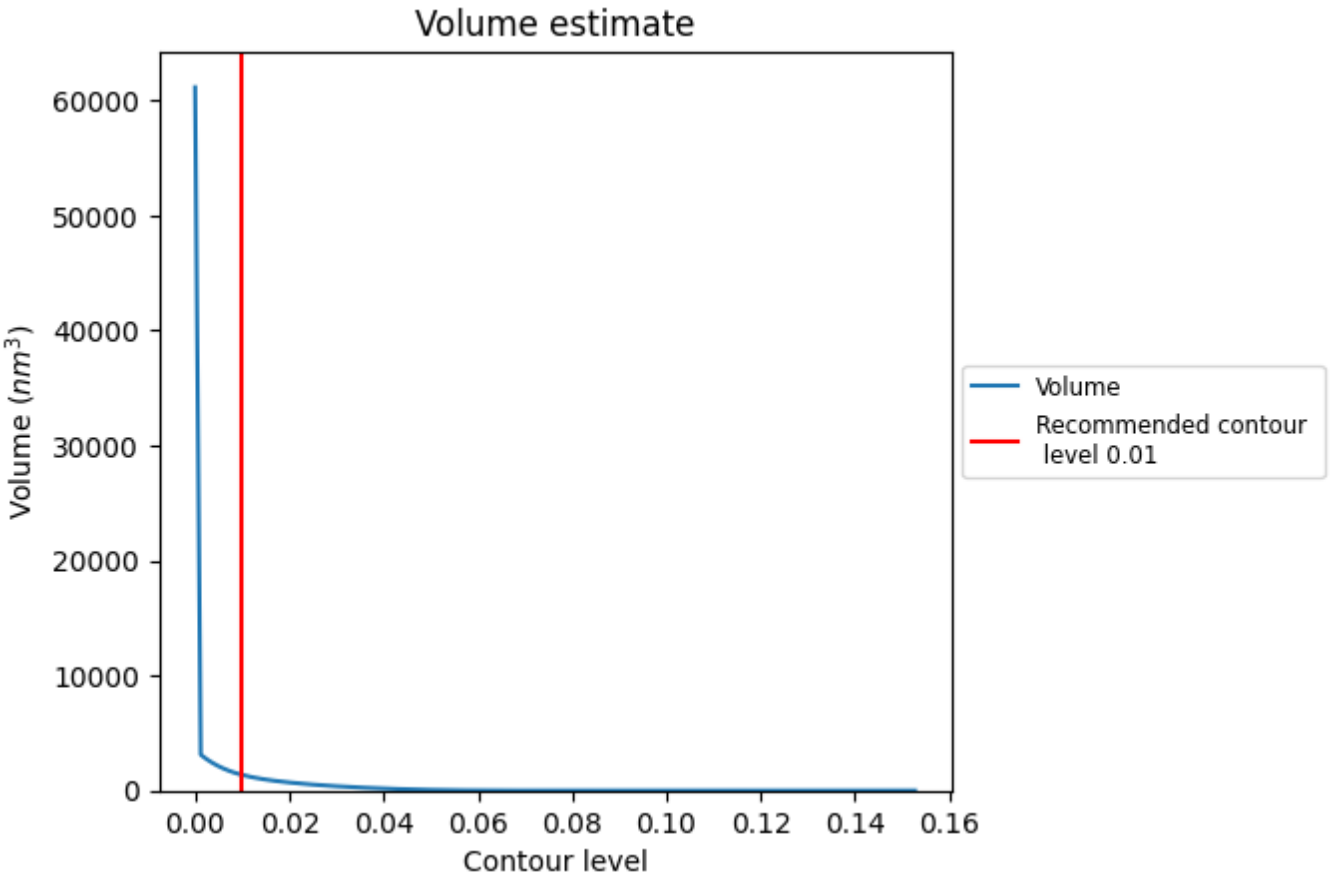
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

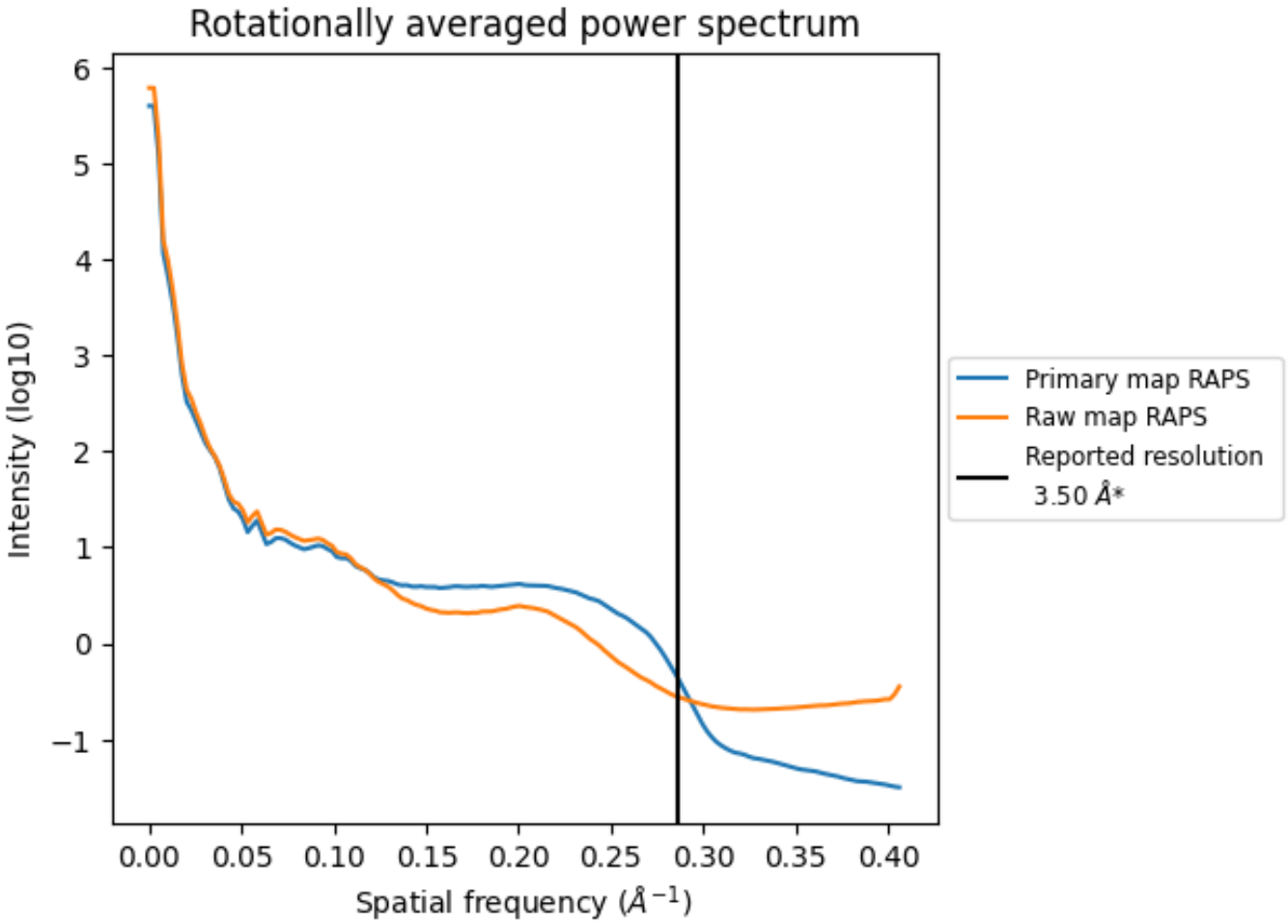
7.2 Volume estimate (i)



The volume at the recommended contour level is 1360 nm^3; this corresponds to an approximate mass of 1229 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)

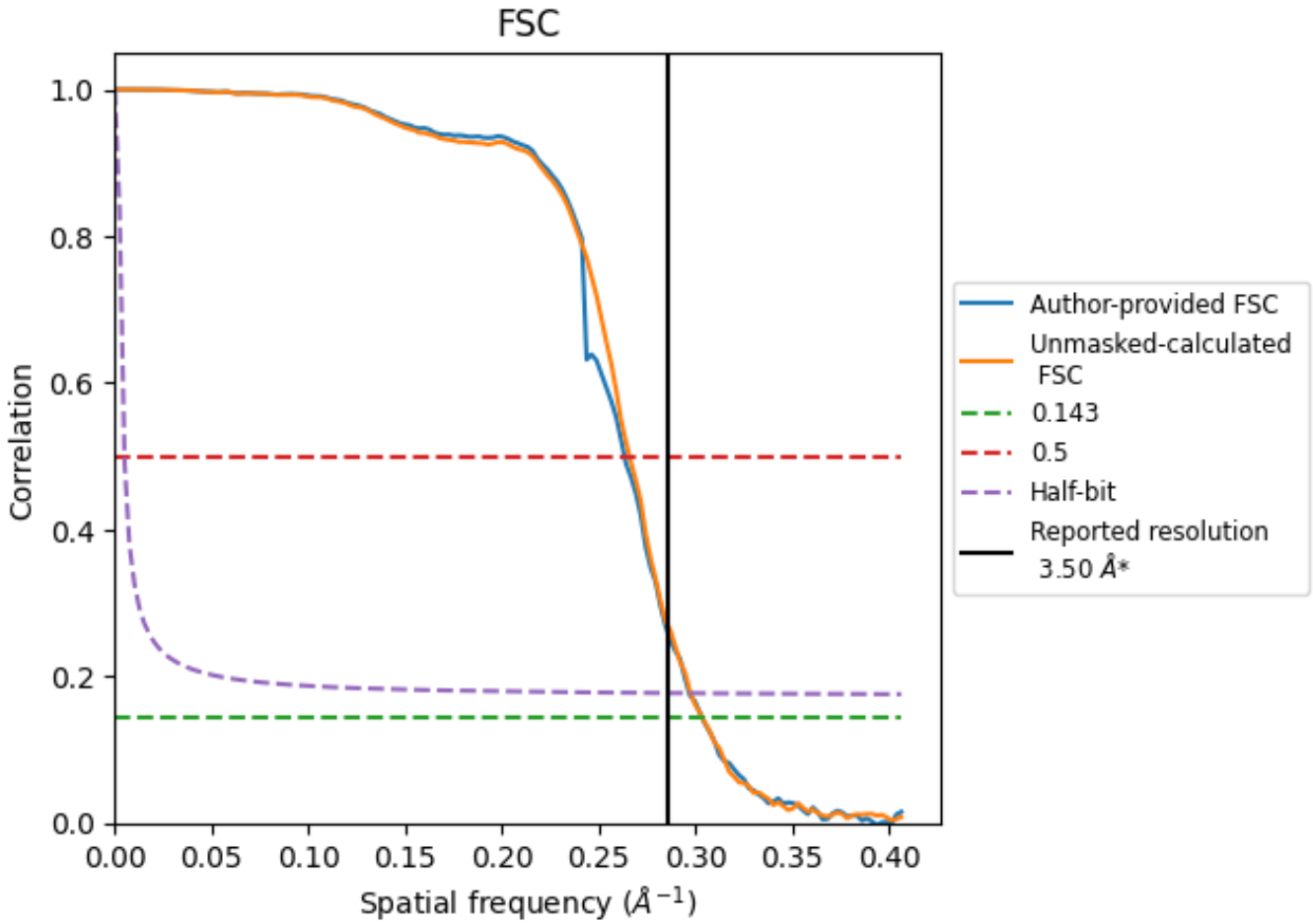


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

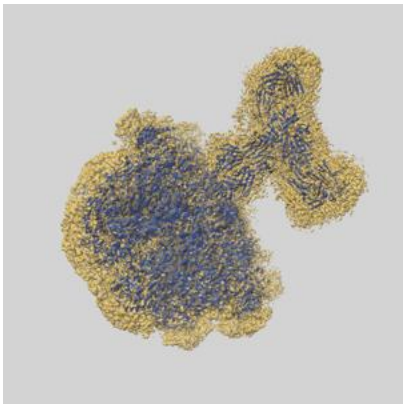
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.30	3.80	3.37
Unmasked-calculated*	3.29	3.76	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

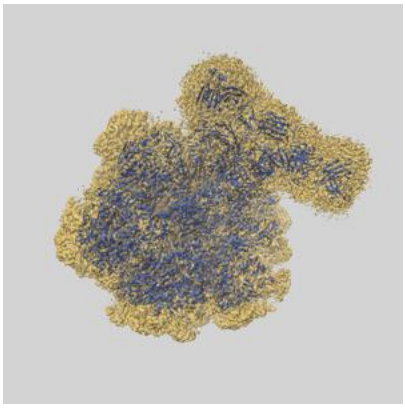
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26608 and PDB model 7UMS. Per-residue inclusion information can be found in section 3 on page 14.

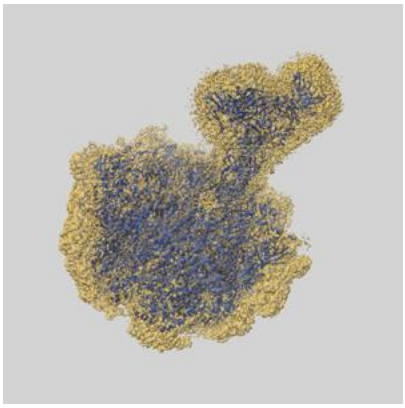
9.1 Map-model overlay



X



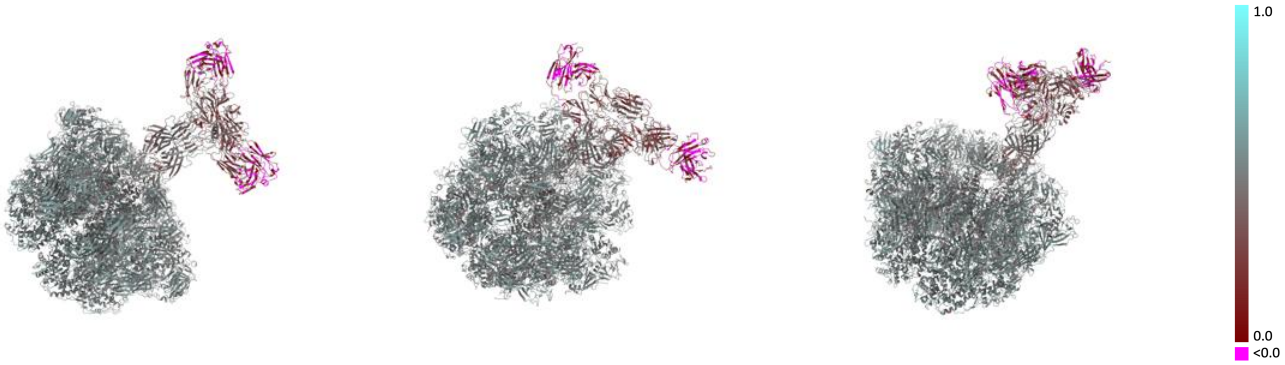
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

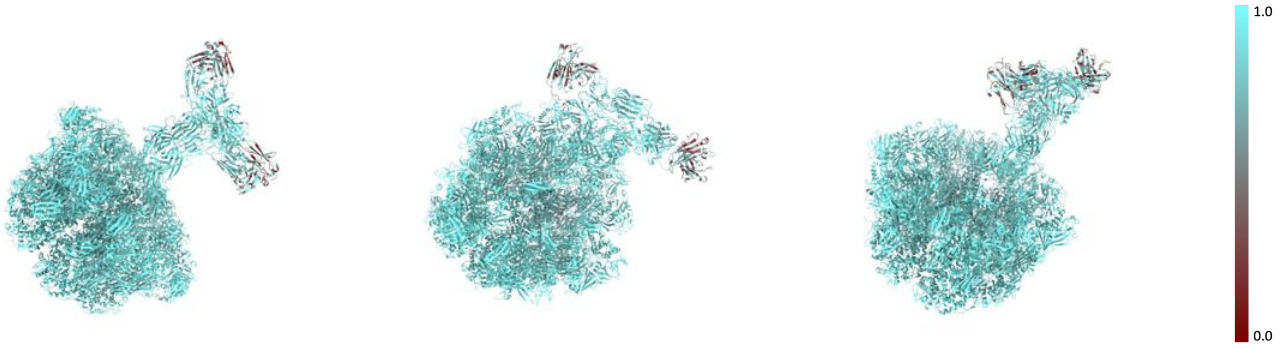
9.2 Q-score mapped to coordinate model



X Y Z

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.

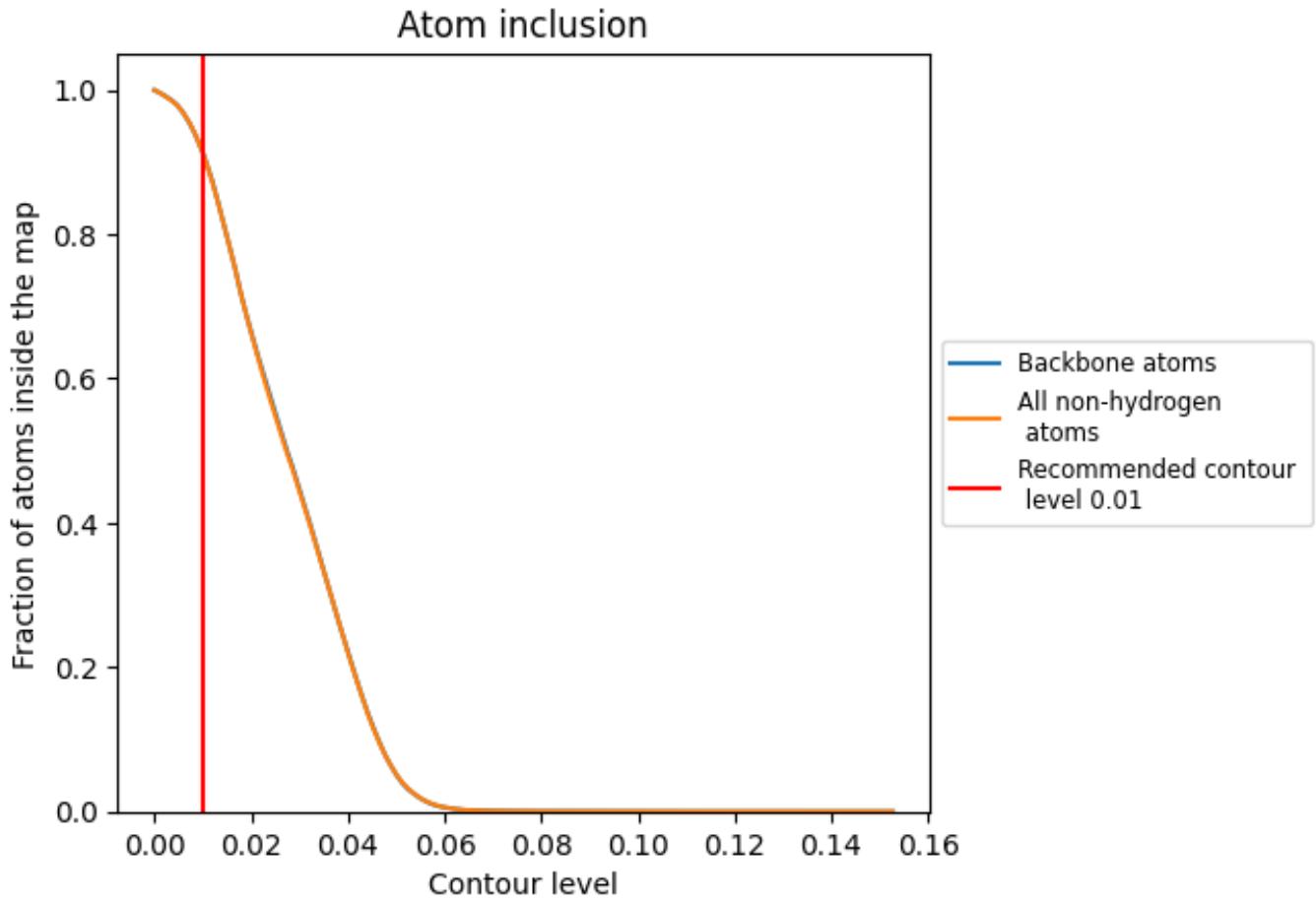
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9127	0.4930
1	0.8623	0.4540
2	0.8639	0.4520
3	0.8923	0.4830
4	0.6794	0.1990
5	0.6727	0.1990
6	0.6924	0.2080
7	0.6906	0.2010
A	0.9349	0.5300
B	0.9465	0.5270
C	0.9407	0.5250
D	0.9365	0.5330
E	0.9430	0.5310
F	0.9452	0.5360
G	0.9346	0.5260
H	0.9394	0.5270
I	0.9391	0.5300
J	0.9355	0.5280
K	0.9391	0.5280
L	0.9320	0.5230
M	0.9343	0.5230
N	0.9346	0.5250
O	0.9372	0.5240
P	0.9433	0.5260
Q	0.9365	0.5240
R	0.9401	0.5240
S	0.7692	0.4220
T	0.8626	0.3750
U	0.8704	0.3810
V	0.8894	0.4790
a	0.9390	0.5200
b	0.9332	0.5100
c	0.9377	0.5160
d	0.9400	0.5170
e	0.9388	0.5180

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Chain	Atom inclusion	Q-score
f	0.9368	0.5120
g	0.9277	0.5090
h	0.9352	0.5120
i	0.9382	0.5160
j	0.9354	0.5130
k	0.9332	0.5070
l	0.9318	0.5170
m	0.9361	0.5190
n	0.9468	0.5160
o	0.9327	0.5120
p	0.9293	0.5100
q	0.9403	0.5090
r	0.9329	0.5050