Full wwPDB EM Validation Report

Nov 14, 2022 – 04:36 AM EST

PDB ID	:	6WXF
EMDB ID	:	EMD-21956
Title	:	Cryo-EM reconstruction of VP5*/VP8* assembly from rhesus rotavirus particles - Intermediate conformation
Authors	:	Herrmann, T.; Harrison, S.C.; Jenni, S.
Deposited on	:	2020-05-10
Resolution	:	4.30 Å(reported)
Based on initial models	:	1SLQ, 4V7Q

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

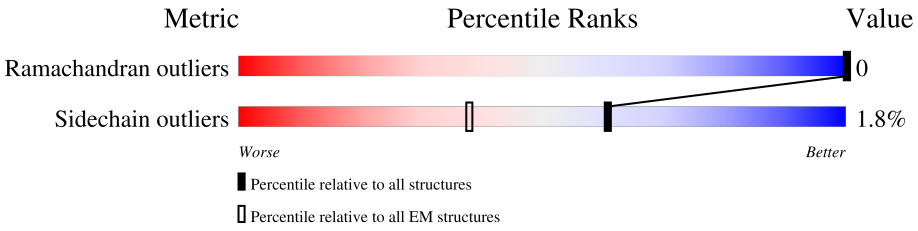
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.30 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% 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	1	776	20% 64% 34%
1	2	776	22% 64% 34%
1	3	776	24% 64% 35%
2	A	397	98%
2	B	397	98%
2	C	397	97%
2	D	397	98%
2	E	397	98%
2	F	397	98%

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Mol	Chain	Length	Quality of chain
2	G	397	99%
2	H	397	97%
2	I	397	99%
2	J	397	99%
2	K	397	99%
2	L	397	98%
2	M	397	98%
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	6% 80% 17%
3	c	326	79% 20%
3	d	326	80% 19%
3	e	326	79% 20%
3	f	326	80% 19%
3	g	326	6% 83% 17%
3	h	326	79% 21%
3	i	326	83% 17%
3	j	326	82% 17%
3	k	326	5% 80% 19%
3	l	326	81% 19%
3	m	326	83% 17%

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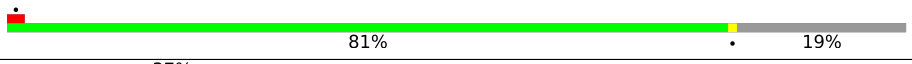
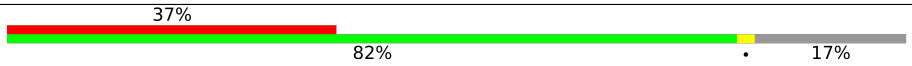
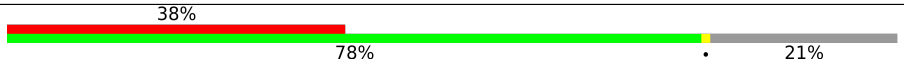
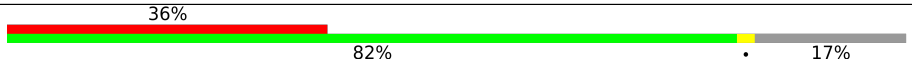
Mol	Chain	Length	Quality of chain
3	n	326	
3	o	326	
3	p	326	
3	q	326	
3	r	326	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 212266 atoms, of which 105044 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	511	Total	C	H	N	O	S	0	0
			8009	2543	3973	688	788	17		
1	2	510	Total	C	H	N	O	S	0	0
			7998	2539	3970	686	785	18		
1	3	507	Total	C	H	N	O	S	0	0
			7944	2524	3943	680	779	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	567	CYS	SER	engineered mutation	UNP G0YZG6
1	590	CYS	ALA	engineered mutation	UNP G0YZG6
2	567	CYS	SER	engineered mutation	UNP G0YZG6
2	590	CYS	ALA	engineered mutation	UNP G0YZG6
3	567	CYS	SER	engineered mutation	UNP G0YZG6
3	590	CYS	ALA	engineered mutation	UNP G0YZG6

- 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
			6275	2004	3112	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
			6275	2004	3112	551	593	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	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
			6276	2004	3113	551	593	15		
2	L	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	M	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	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
			6275	2004	3112	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
			6275	2004	3112	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
			4040	1298	1993	324	409	16		
3	b	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	c	261	Total	C	H	N	O	S	0	0
			4073	1308	2010	327	412	16		
3	d	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	e	260	Total	C	H	N	O	S	0	0
			4049	1302	1997	323	411	16		
3	f	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	g	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	h	259	Total	C	H	N	O	S	0	0
			4040	1298	1993	324	409	16		

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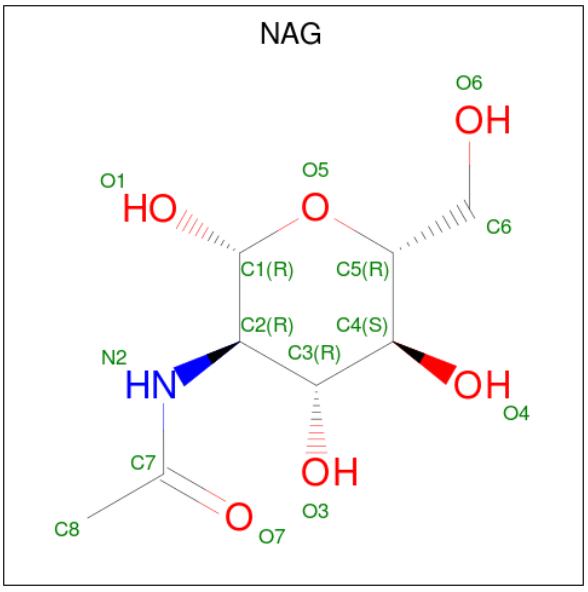
Mol	Chain	Residues	Atoms						AltConf	Trace
3	i	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	j	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	k	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	l	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	m	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	n	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	o	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	p	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	q	259	Total	C	H	N	O	S	0	0
			4040	1298	1993	324	409	16		
3	r	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	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	

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Mol	Chain	Residues	Atoms					AltConf
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	
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	3	Total	Ca	0
			3	3	
5	b	3	Total	Ca	0
			3	3	

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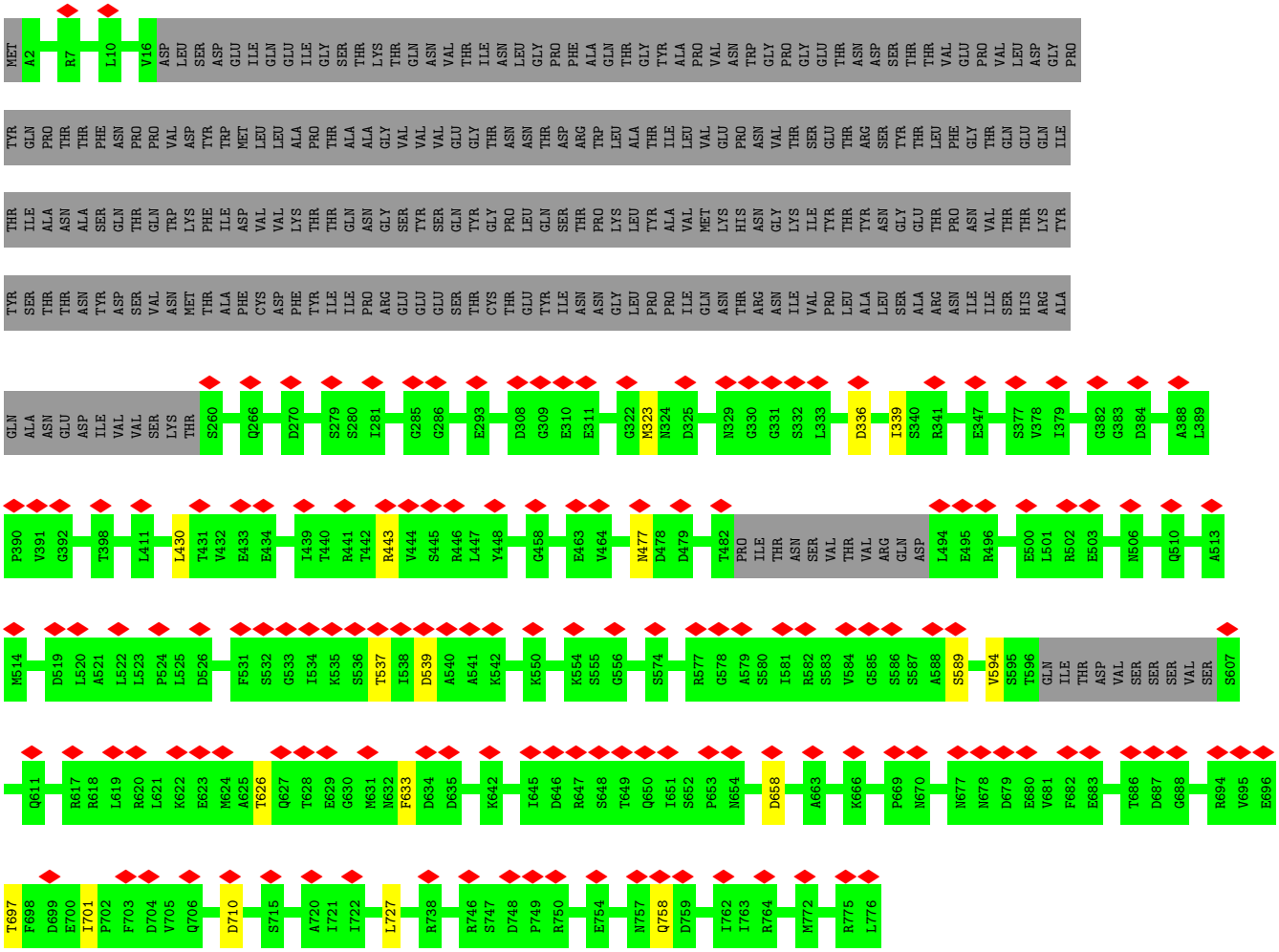
Mol	Chain	Residues	Atoms	AltConf
5	c	3	Total Ca 3 3	0
5	d	3	Total Ca 3 3	0
5	e	3	Total Ca 3 3	0
5	f	3	Total Ca 3 3	0
5	g	3	Total Ca 3 3	0
5	h	3	Total Ca 3 3	0
5	i	3	Total Ca 3 3	0
5	j	3	Total Ca 3 3	0
5	k	3	Total Ca 3 3	0
5	l	3	Total Ca 3 3	0
5	m	3	Total Ca 3 3	0
5	n	3	Total Ca 3 3	0
5	o	3	Total Ca 3 3	0
5	p	3	Total Ca 3 3	0
5	q	3	Total Ca 3 3	0
5	r	3	Total Ca 3 3	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.

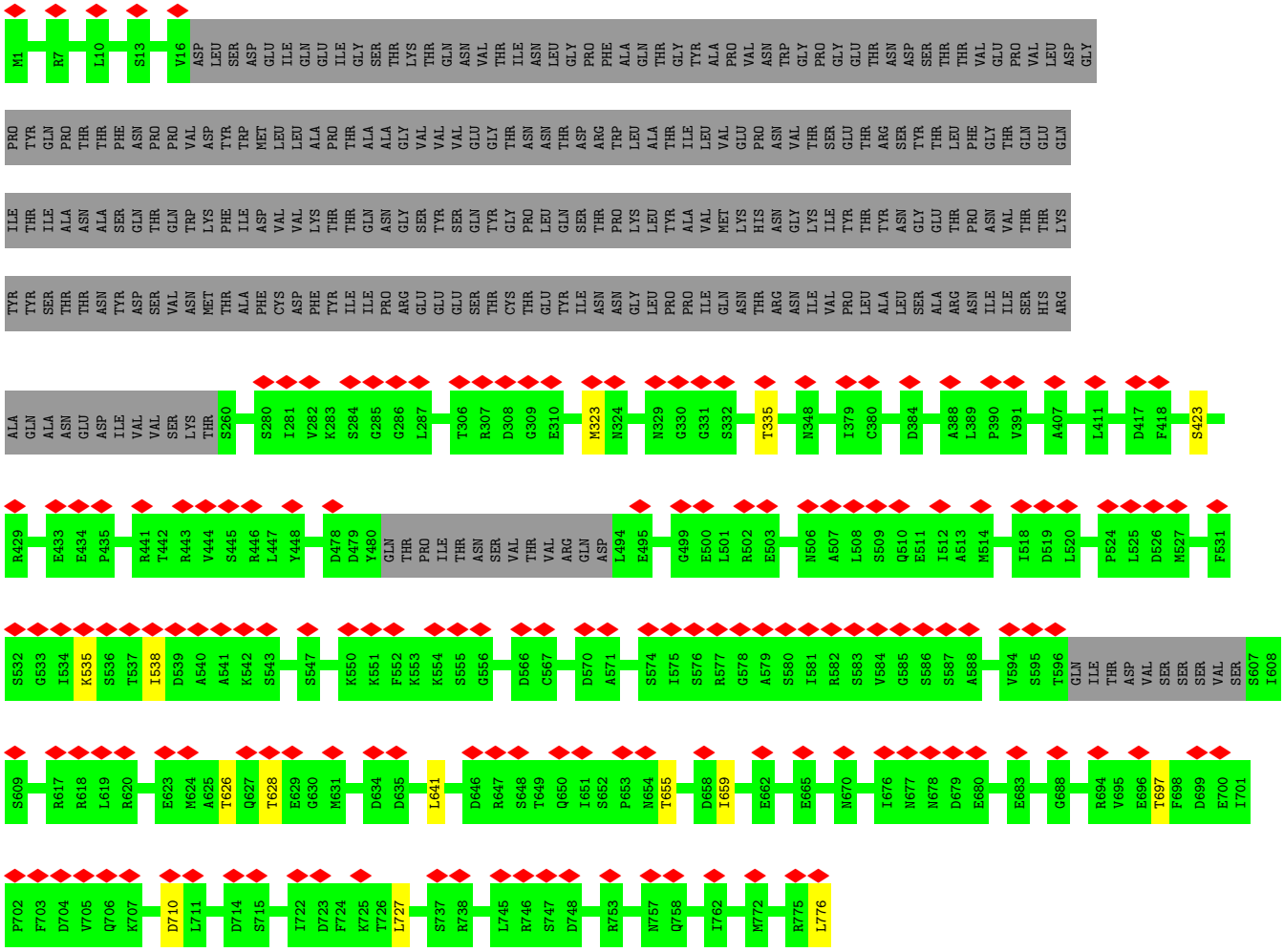
• Molecule 1: Outer capsid protein VP4

Chain 1:



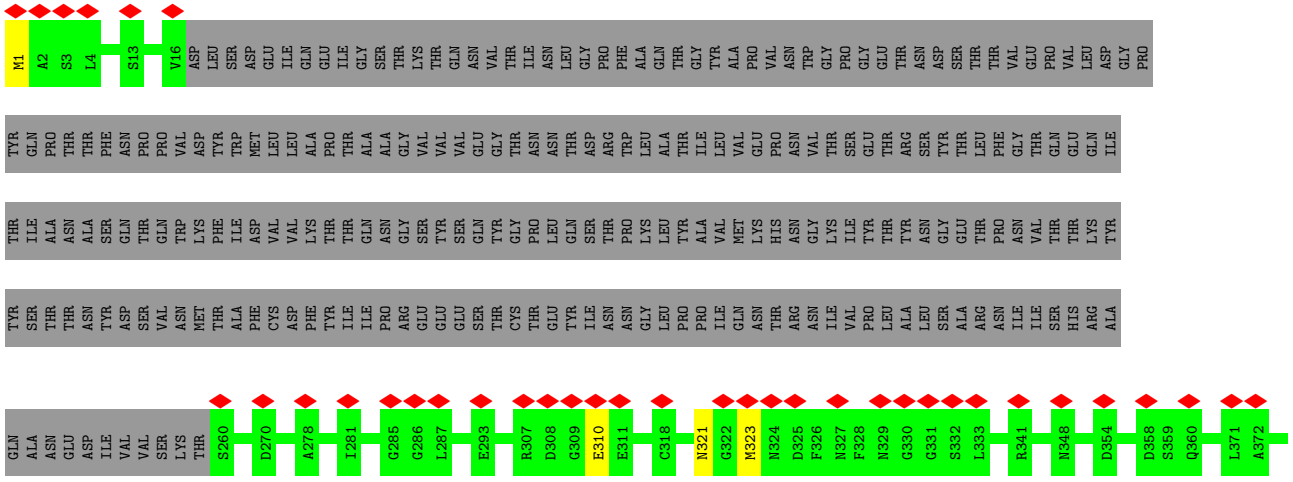
• Molecule 1: Outer capsid protein VP4

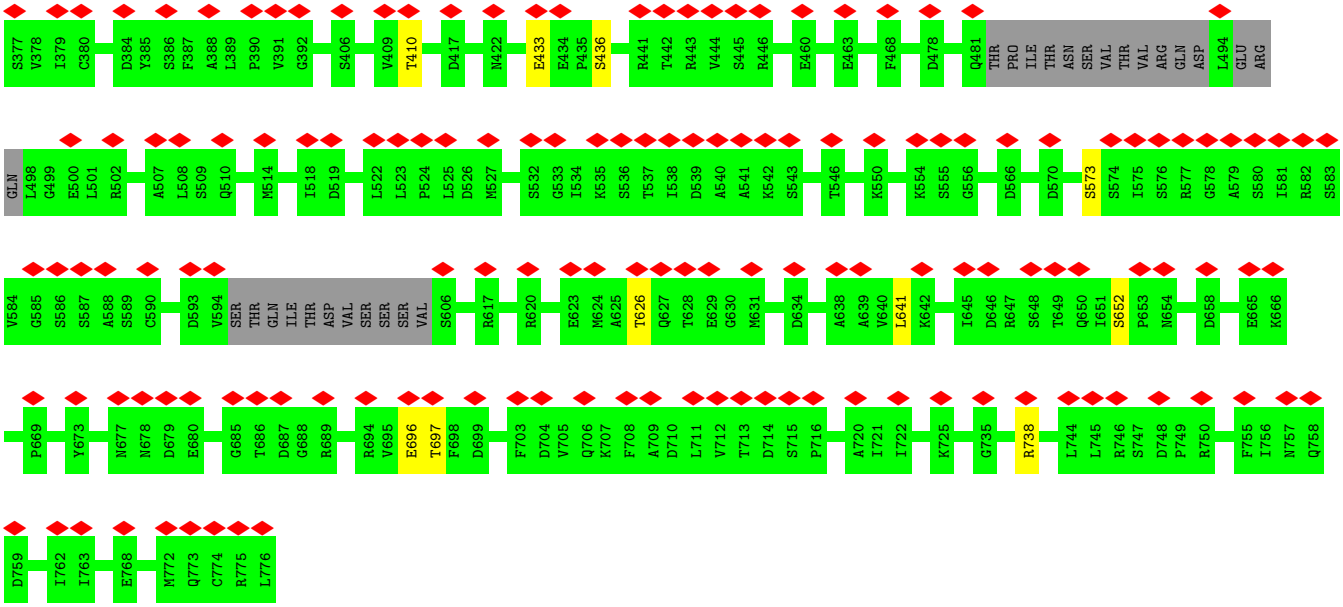
Chain 2:



• Molecule 1: Outer capsid protein VP4

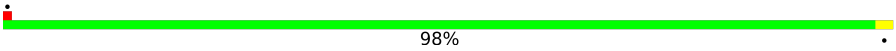
Chain 3:





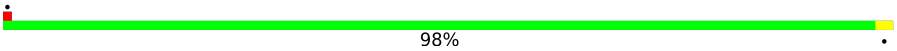
• Molecule 2: Intermediate capsid protein VP6

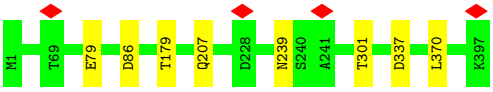
Chain A:



• Molecule 2: Intermediate capsid protein VP6

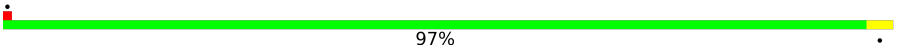
Chain B:

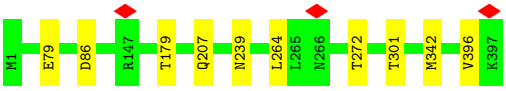




• Molecule 2: Intermediate capsid protein VP6

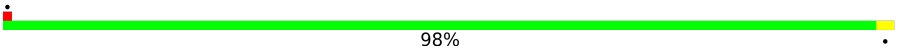
Chain C:

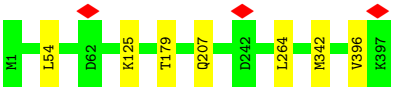




• Molecule 2: Intermediate capsid protein VP6

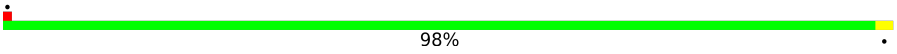
Chain D:

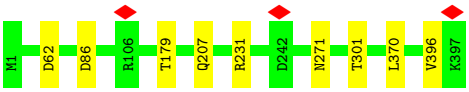




• Molecule 2: Intermediate capsid protein VP6

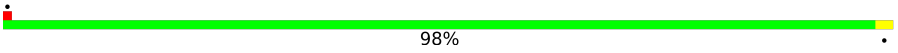
Chain E:





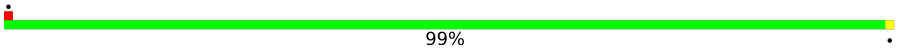
• Molecule 2: Intermediate capsid protein VP6

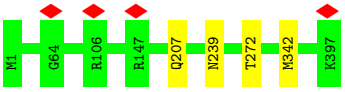
Chain F:



• Molecule 2: Intermediate capsid protein VP6

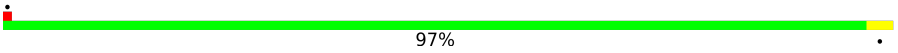
Chain G:

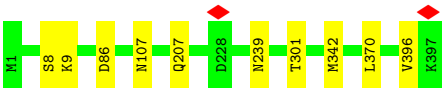




• Molecule 2: Intermediate capsid protein VP6

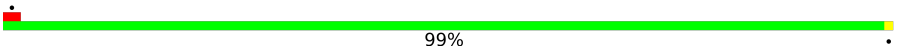
Chain H:

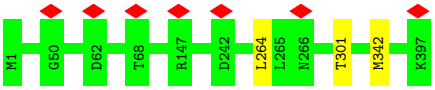




• Molecule 2: Intermediate capsid protein VP6

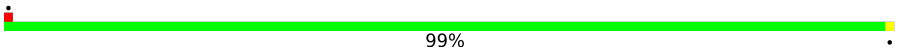
Chain I:

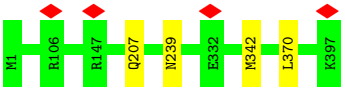




• Molecule 2: Intermediate capsid protein VP6

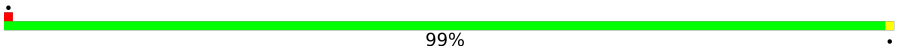
Chain J:

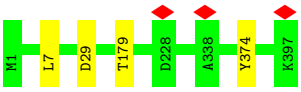




• Molecule 2: Intermediate capsid protein VP6

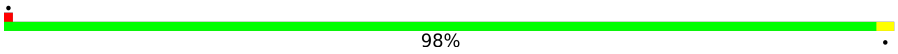
Chain K:

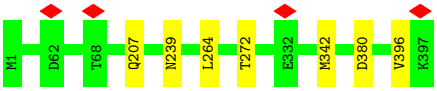




• Molecule 2: Intermediate capsid protein VP6

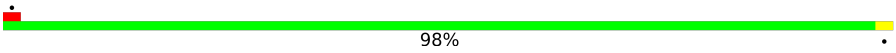
Chain L:

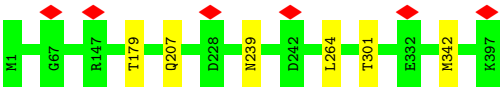




• Molecule 2: Intermediate capsid protein VP6

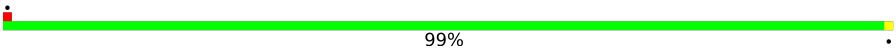
Chain M:

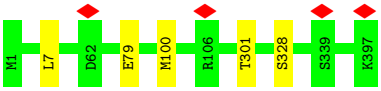




• Molecule 2: Intermediate capsid protein VP6

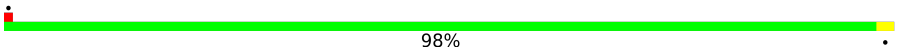
Chain N:

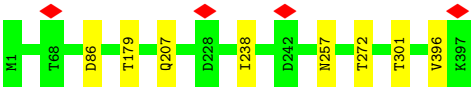




• Molecule 2: Intermediate capsid protein VP6

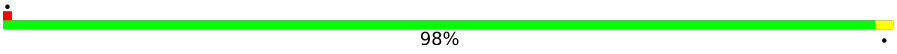
Chain O:





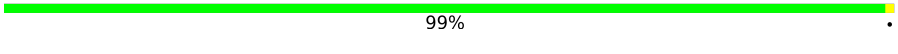
• Molecule 2: Intermediate capsid protein VP6

Chain P:



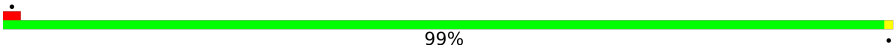
• Molecule 2: Intermediate capsid protein VP6

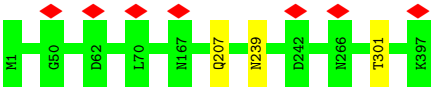
Chain Q:



• Molecule 2: Intermediate capsid protein VP6

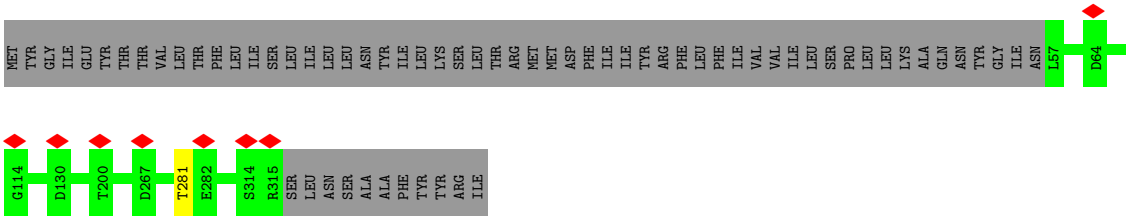
Chain R:





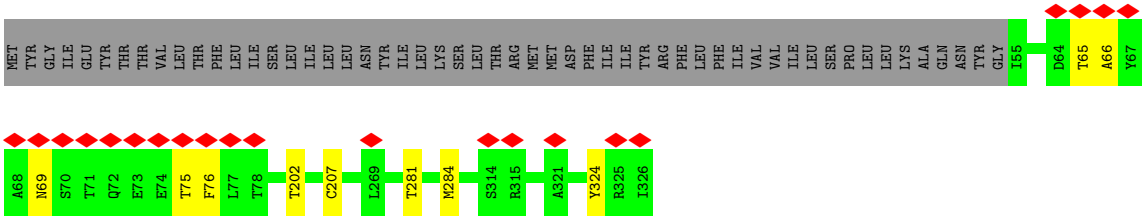
• Molecule 3: Outer capsid glycoprotein VP7

Chain a:



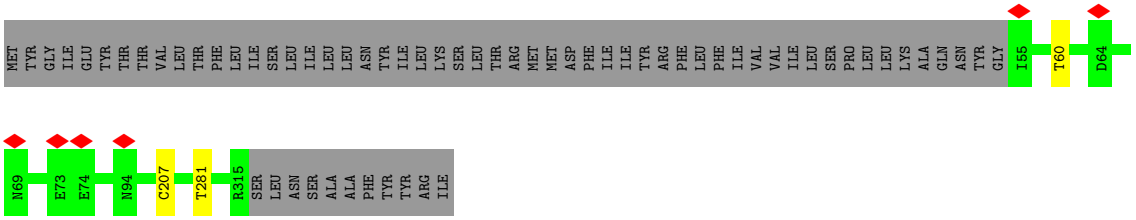
• Molecule 3: Outer capsid glycoprotein VP7

Chain b:



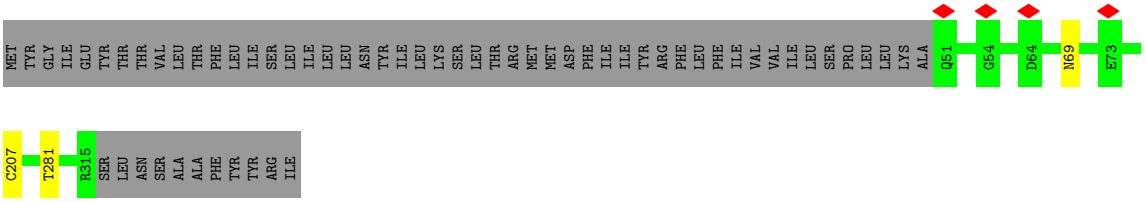
• Molecule 3: Outer capsid glycoprotein VP7

Chain c:



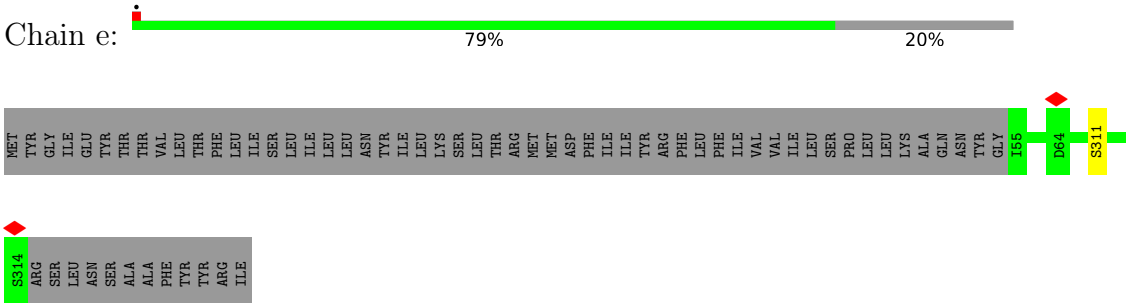
• Molecule 3: Outer capsid glycoprotein VP7

Chain d:



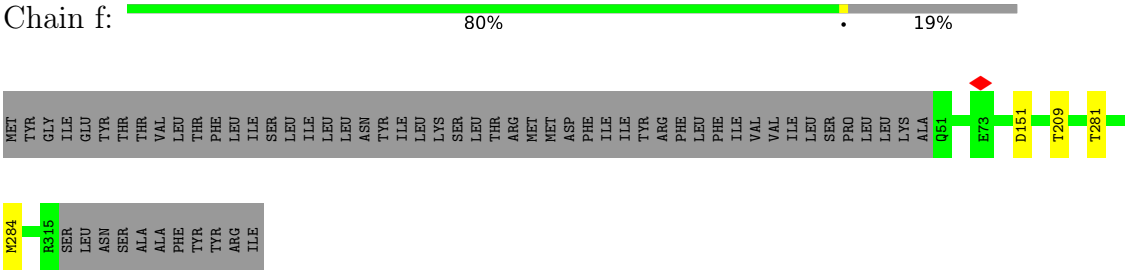
• Molecule 3: Outer capsid glycoprotein VP7

Chain e:



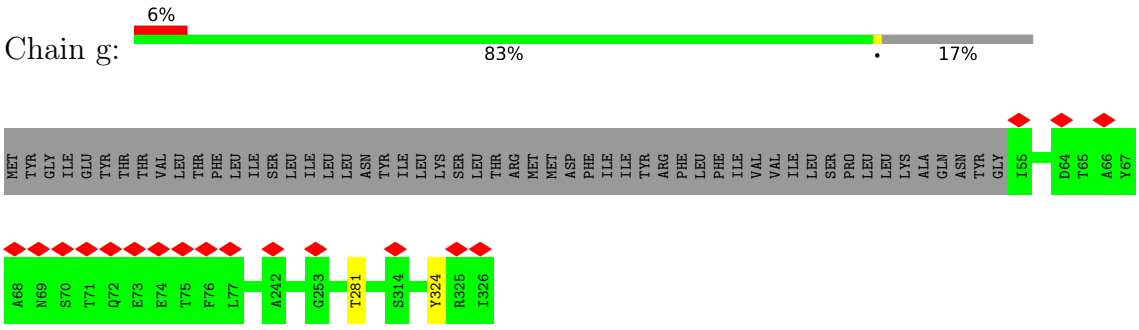
• Molecule 3: Outer capsid glycoprotein VP7

Chain f:



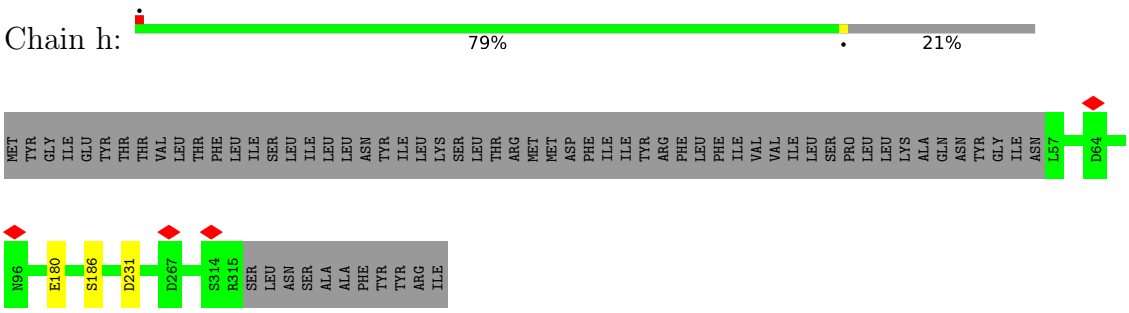
• Molecule 3: Outer capsid glycoprotein VP7

Chain g:



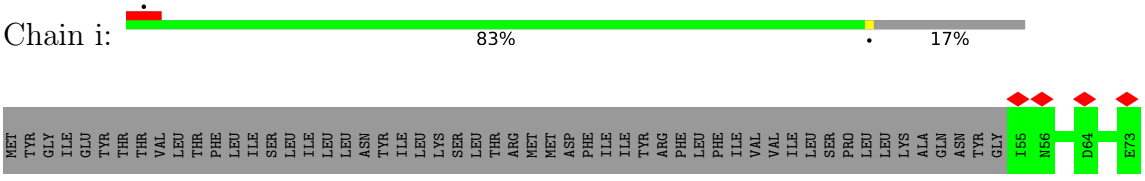
• Molecule 3: Outer capsid glycoprotein VP7

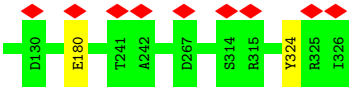
Chain h:



• Molecule 3: Outer capsid glycoprotein VP7

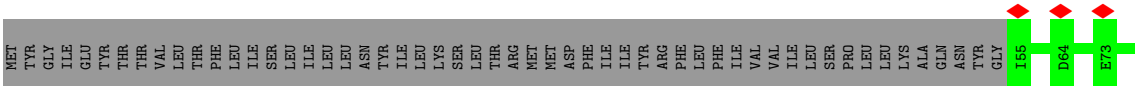
Chain i:

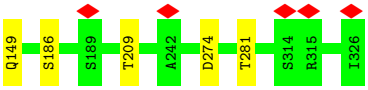




• Molecule 3: Outer capsid glycoprotein VP7

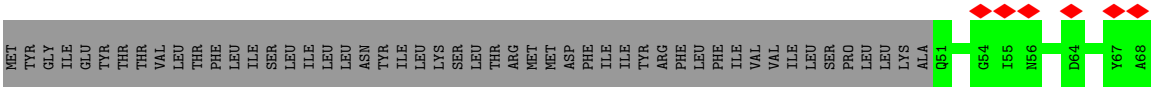
Chain j:

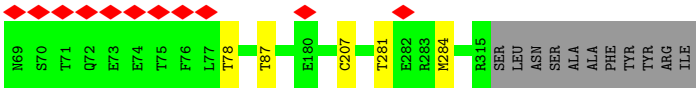




• Molecule 3: Outer capsid glycoprotein VP7

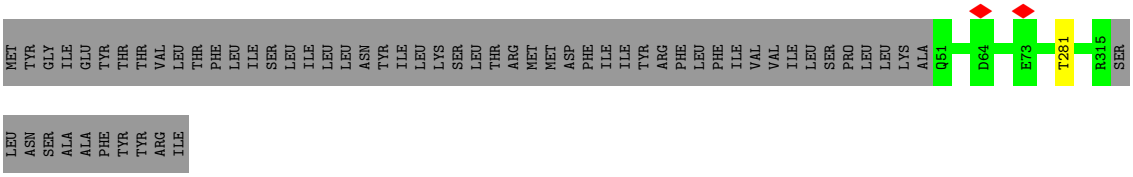
Chain k:





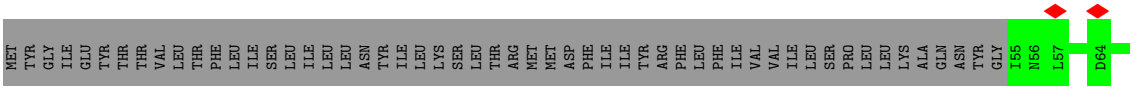
• Molecule 3: Outer capsid glycoprotein VP7

Chain l:



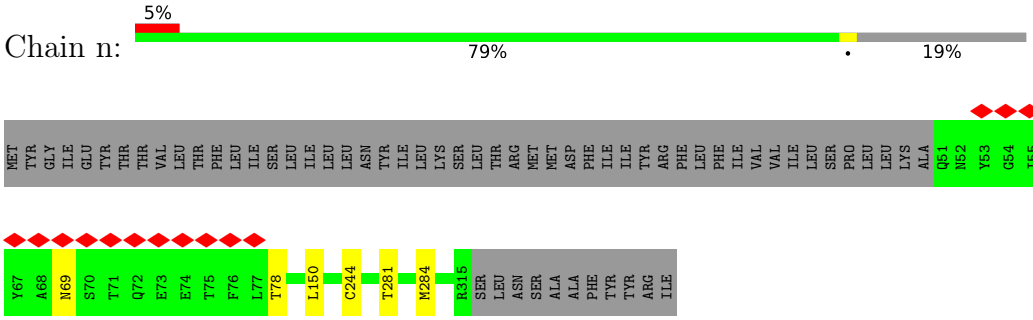
• Molecule 3: Outer capsid glycoprotein VP7

Chain m:



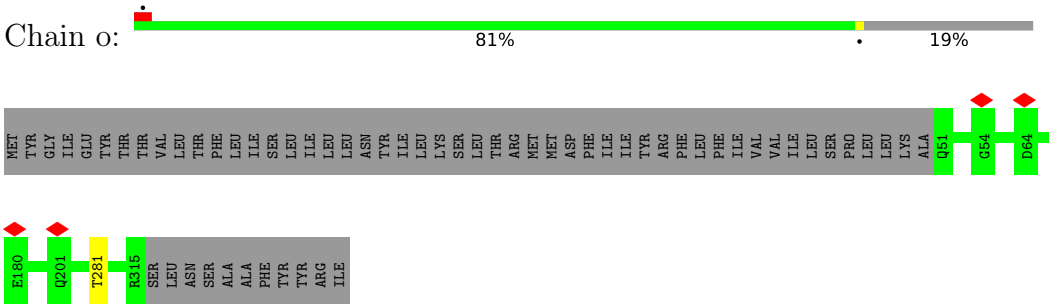
• Molecule 3: Outer capsid glycoprotein VP7

Chain n:



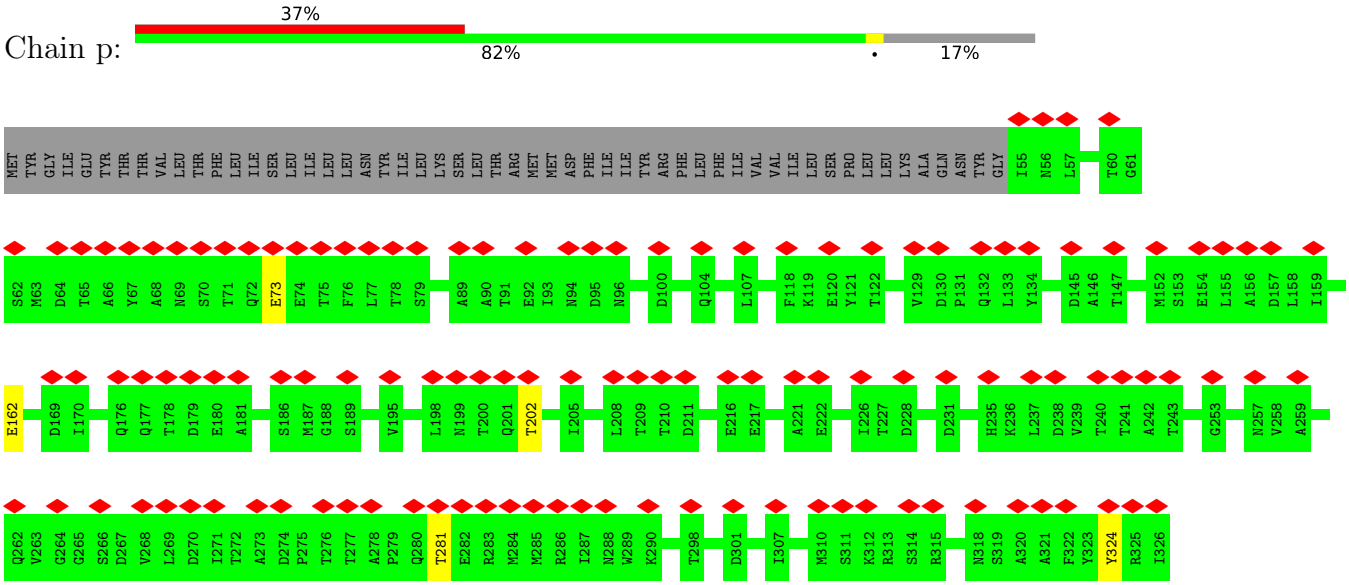
• Molecule 3: Outer capsid glycoprotein VP7

Chain o:



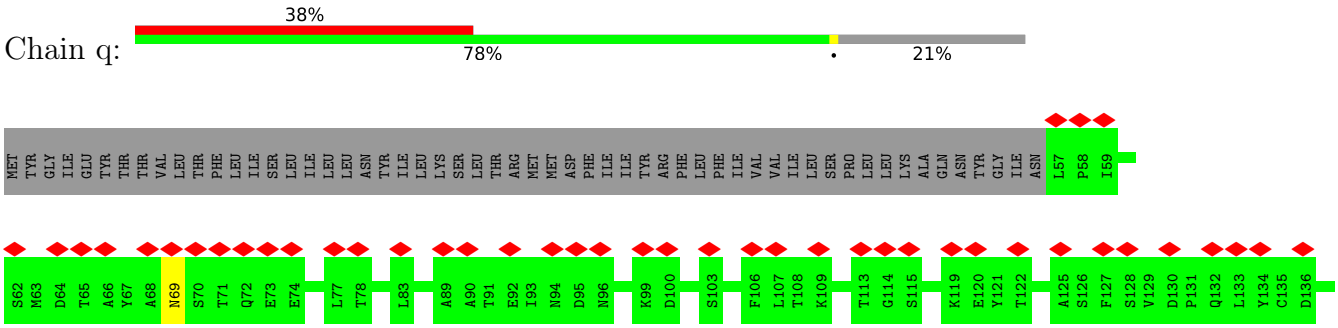
• Molecule 3: Outer capsid glycoprotein VP7

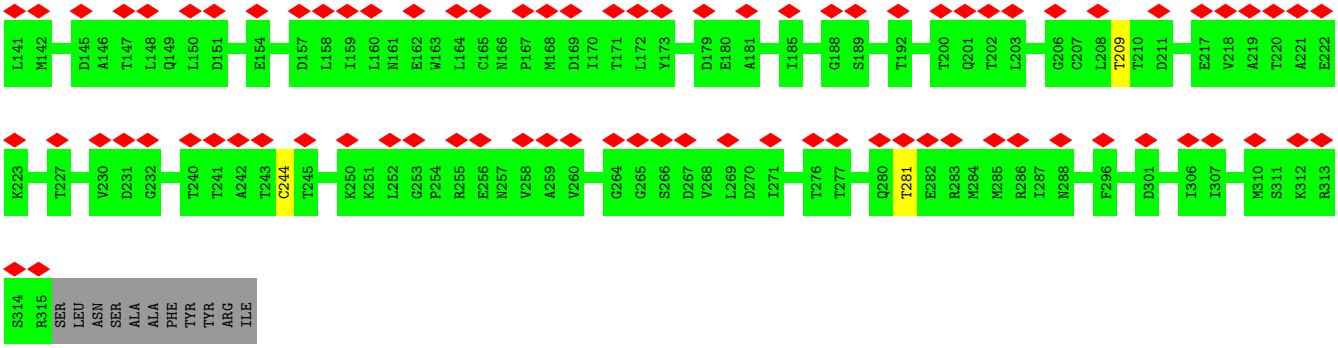
Chain p:



• Molecule 3: Outer capsid glycoprotein VP7

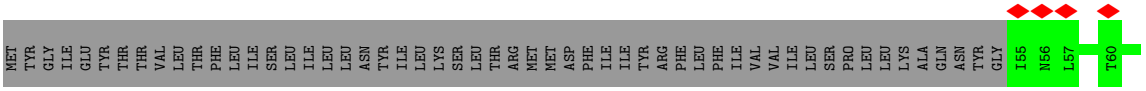
Chain q:

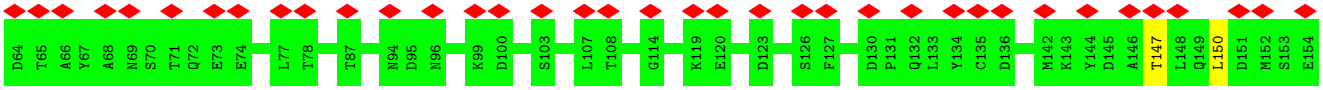


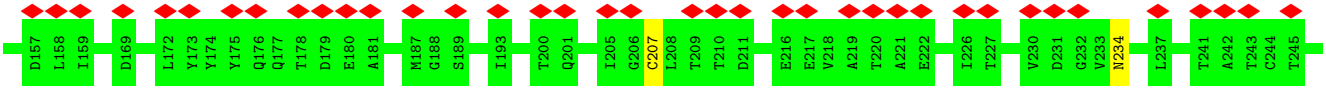


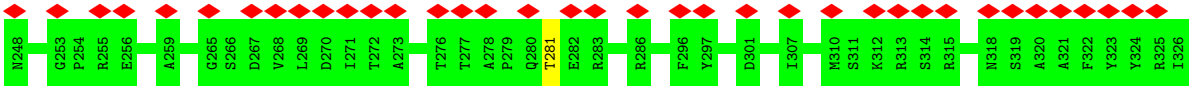
• Molecule 3: Outer capsid glycoprotein VP7

Chain r:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82008	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
Maximum map value	13.304	Depositor
Minimum map value	-6.964	Depositor
Average map value	0.067	Depositor
Map value standard deviation	1.488	Depositor
Recommended contour level	3.5	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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.27	0/4109	0.56	0/5561
1	2	0.27	0/4101	0.57	0/5549
1	3	0.27	0/4073	0.56	0/5510
2	A	0.27	0/3233	0.55	0/4397
2	B	0.27	0/3233	0.55	0/4397
2	C	0.27	0/3233	0.56	0/4397
2	D	0.27	0/3233	0.57	0/4397
2	E	0.26	0/3233	0.56	0/4397
2	F	0.27	0/3233	0.56	0/4397
2	G	0.27	0/3233	0.56	0/4397
2	H	0.28	0/3233	0.56	0/4397
2	I	0.27	0/3233	0.56	0/4397
2	J	0.27	0/3233	0.56	0/4397
2	K	0.27	0/3233	0.56	0/4397
2	L	0.27	0/3233	0.56	0/4397
2	M	0.27	0/3233	0.56	0/4397
2	N	0.27	0/3233	0.56	0/4397
2	O	0.27	0/3233	0.56	0/4397
2	P	0.27	0/3233	0.55	0/4397
2	Q	0.27	0/3233	0.55	0/4397
2	R	0.27	0/3233	0.56	0/4397
3	a	0.26	0/2089	0.51	0/2854
3	b	0.26	0/2200	0.54	0/3005
3	c	0.25	0/2105	0.52	0/2876
3	d	0.25	0/2139	0.51	0/2922
3	e	0.26	0/2094	0.51	0/2862
3	f	0.26	0/2139	0.52	0/2922
3	g	0.26	0/2200	0.53	0/3005
3	h	0.26	0/2089	0.52	0/2854
3	i	0.25	0/2200	0.52	0/3005
3	j	0.25	0/2200	0.51	0/3005
3	k	0.26	0/2139	0.53	0/2922

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	l	0.26	0/2139	0.52	0/2922
3	m	0.25	0/2200	0.51	0/3005
3	n	0.25	0/2139	0.52	0/2922
3	o	0.25	0/2139	0.53	0/2922
3	p	0.26	0/2200	0.52	0/3005
3	q	0.26	0/2089	0.52	0/2854
3	r	0.26	0/2200	0.52	0/3005
All	All	0.26	0/109177	0.55	0/148633

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	1	0	2
3	b	0	2
3	e	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	537	THR	Peptide
1	1	589	SER	Peptide
3	b	66	ALA	Peptide
3	b	76	PHE	Peptide
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	503/776 (65%)	494 (98%)	9 (2%)	0	100	100
1	2	502/776 (65%)	494 (98%)	8 (2%)	0	100	100
1	3	498/776 (64%)	492 (99%)	6 (1%)	0	100	100
2	A	395/397 (100%)	393 (100%)	2 (0%)	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%)	393 (100%)	2 (0%)	0	100	100
2	F	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	G	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	H	395/397 (100%)	393 (100%)	2 (0%)	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%)	393 (100%)	2 (0%)	0	100	100
2	L	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	M	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	N	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	O	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	P	395/397 (100%)	393 (100%)	2 (0%)	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%)	266 (98%)	4 (2%)	0	100	100
3	c	259/326 (79%)	259 (100%)	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%)	258 (100%)	0	0	100	100
3	f	263/326 (81%)	263 (100%)	0	0	100	100
3	g	270/326 (83%)	270 (100%)	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%)	270 (100%)	0	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%)	270 (100%)	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%)	269 (100%)	1 (0%)	0	100	100
3	q	257/326 (79%)	257 (100%)	0	0	100	100
3	r	270/326 (83%)	270 (100%)	0	0	100	100
All	All	13369/15342 (87%)	13299 (100%)	70 (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	452/689 (66%)	436 (96%)	16 (4%)	36	60
1	2	451/689 (66%)	437 (97%)	14 (3%)	40	63
1	3	448/689 (65%)	434 (97%)	14 (3%)	40	63
2	A	350/350 (100%)	343 (98%)	7 (2%)	55	73
2	B	350/350 (100%)	342 (98%)	8 (2%)	50	70
2	C	350/350 (100%)	340 (97%)	10 (3%)	42	64
2	D	350/350 (100%)	343 (98%)	7 (2%)	55	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	350/350 (100%)	341 (97%)	9 (3%)	46	67
2	F	350/350 (100%)	344 (98%)	6 (2%)	60	78
2	G	350/350 (100%)	346 (99%)	4 (1%)	73	85
2	H	350/350 (100%)	340 (97%)	10 (3%)	42	64
2	I	350/350 (100%)	347 (99%)	3 (1%)	78	88
2	J	350/350 (100%)	346 (99%)	4 (1%)	73	85
2	K	350/350 (100%)	346 (99%)	4 (1%)	73	85
2	L	350/350 (100%)	343 (98%)	7 (2%)	55	73
2	M	350/350 (100%)	344 (98%)	6 (2%)	60	78
2	N	350/350 (100%)	345 (99%)	5 (1%)	67	81
2	O	350/350 (100%)	342 (98%)	8 (2%)	50	70
2	P	350/350 (100%)	344 (98%)	6 (2%)	60	78
2	Q	350/350 (100%)	345 (99%)	5 (1%)	67	81
2	R	350/350 (100%)	347 (99%)	3 (1%)	78	88
3	a	233/295 (79%)	232 (100%)	1 (0%)	91	94
3	b	244/295 (83%)	236 (97%)	8 (3%)	38	62
3	c	235/295 (80%)	232 (99%)	3 (1%)	69	82
3	d	238/295 (81%)	235 (99%)	3 (1%)	69	82
3	e	234/295 (79%)	234 (100%)	0	100	100
3	f	238/295 (81%)	234 (98%)	4 (2%)	60	78
3	g	244/295 (83%)	242 (99%)	2 (1%)	81	89
3	h	233/295 (79%)	230 (99%)	3 (1%)	69	82
3	i	244/295 (83%)	242 (99%)	2 (1%)	81	89
3	j	244/295 (83%)	239 (98%)	5 (2%)	55	73
3	k	238/295 (81%)	233 (98%)	5 (2%)	53	72
3	l	238/295 (81%)	237 (100%)	1 (0%)	91	94
3	m	244/295 (83%)	242 (99%)	2 (1%)	81	89
3	n	238/295 (81%)	232 (98%)	6 (2%)	47	68
3	o	238/295 (81%)	236 (99%)	2 (1%)	81	89
3	p	244/295 (83%)	239 (98%)	5 (2%)	55	73
3	q	233/295 (79%)	229 (98%)	4 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	r	244/295 (83%)	239 (98%)	5 (2%)	55 73
All	All	11955/13677 (87%)	11738 (98%)	217 (2%)	61 77

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	323	MET
1	1	336	ASP
1	1	339	ILE
1	1	430	LEU
1	1	443	ARG
1	1	477	ASN
1	1	539	ASP
1	1	594	VAL
1	1	626	THR
1	1	633	PHE
1	1	658	ASP
1	1	697	THR
1	1	701	ILE
1	1	710	ASP
1	1	727	LEU
1	1	758	GLN
1	2	323	MET
1	2	335	THR
1	2	423	SER
1	2	535	LYS
1	2	538	ILE
1	2	626	THR
1	2	628	THR
1	2	641	LEU
1	2	655	THR
1	2	659	ILE
1	2	697	THR
1	2	710	ASP
1	2	727	LEU
1	2	776	LEU
1	3	1	MET
1	3	310	GLU
1	3	321	ASN
1	3	323	MET
1	3	410	THR
1	3	433	GLU

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Mol	Chain	Res	Type
1	3	436	SER
1	3	573	SER
1	3	626	THR
1	3	641	LEU
1	3	652	SER
1	3	696	GLU
1	3	697	THR
1	3	738	ARG
2	A	54	LEU
2	A	272	THR
2	A	301	THR
2	A	312	GLN
2	A	320	VAL
2	A	342	MET
2	A	370	LEU
2	B	79	GLU
2	B	86	ASP
2	B	179	THR
2	B	207	GLN
2	B	239	ASN
2	B	301	THR
2	B	337	ASP
2	B	370	LEU
2	C	79	GLU
2	C	86	ASP
2	C	179	THR
2	C	207	GLN
2	C	239	ASN
2	C	264	LEU
2	C	272	THR
2	C	301	THR
2	C	342	MET
2	C	396	VAL
2	D	54	LEU
2	D	125	LYS
2	D	179	THR
2	D	207	GLN
2	D	264	LEU
2	D	342	MET
2	D	396	VAL
2	E	62	ASP
2	E	86	ASP

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Mol	Chain	Res	Type
2	E	179	THR
2	E	207	GLN
2	E	231	ARG
2	E	271	ASN
2	E	301	THR
2	E	370	LEU
2	E	396	VAL
2	F	86	ASP
2	F	207	GLN
2	F	239	ASN
2	F	264	LEU
2	F	320	VAL
2	F	342	MET
2	G	207	GLN
2	G	239	ASN
2	G	272	THR
2	G	342	MET
2	H	8	SER
2	H	9	LYS
2	H	86	ASP
2	H	107	ASN
2	H	207	GLN
2	H	239	ASN
2	H	301	THR
2	H	342	MET
2	H	370	LEU
2	H	396	VAL
2	I	264	LEU
2	I	301	THR
2	I	342	MET
2	J	207	GLN
2	J	239	ASN
2	J	342	MET
2	J	370	LEU
2	K	7	LEU
2	K	29	ASP
2	K	179	THR
2	K	374	TYR
2	L	207	GLN
2	L	239	ASN
2	L	264	LEU
2	L	272	THR

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Mol	Chain	Res	Type
2	L	342	MET
2	L	380	ASP
2	L	396	VAL
2	M	179	THR
2	M	207	GLN
2	M	239	ASN
2	M	264	LEU
2	M	301	THR
2	M	342	MET
2	N	7	LEU
2	N	79	GLU
2	N	100	MET
2	N	301	THR
2	N	328	SER
2	O	86	ASP
2	O	179	THR
2	O	207	GLN
2	O	238	ILE
2	O	257	ASN
2	O	272	THR
2	O	301	THR
2	O	396	VAL
2	P	207	GLN
2	P	234	PHE
2	P	239	ASN
2	P	301	THR
2	P	337	ASP
2	P	342	MET
2	Q	54	LEU
2	Q	86	ASP
2	Q	207	GLN
2	Q	239	ASN
2	Q	342	MET
2	R	207	GLN
2	R	239	ASN
2	R	301	THR
3	a	281	THR
3	b	65	THR
3	b	69	ASN
3	b	75	THR
3	b	202	THR
3	b	207	CYS

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Mol	Chain	Res	Type
3	b	281	THR
3	b	284	MET
3	b	324	TYR
3	c	60	THR
3	c	207	CYS
3	c	281	THR
3	d	69	ASN
3	d	207	CYS
3	d	281	THR
3	f	151	ASP
3	f	209	THR
3	f	281	THR
3	f	284	MET
3	g	281	THR
3	g	324	TYR
3	h	180	GLU
3	h	186	SER
3	h	231	ASP
3	i	180	GLU
3	i	324	TYR
3	j	149	GLN
3	j	186	SER
3	j	209	THR
3	j	274	ASP
3	j	281	THR
3	k	78	THR
3	k	87	THR
3	k	207	CYS
3	k	281	THR
3	k	284	MET
3	l	281	THR
3	m	281	THR
3	m	324	TYR
3	n	69	ASN
3	n	78	THR
3	n	150	LEU
3	n	244	CYS
3	n	281	THR
3	n	284	MET
3	o	78	THR
3	o	281	THR
3	p	73	GLU

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Mol	Chain	Res	Type
3	p	162	GLU
3	p	202	THR
3	p	281	THR
3	p	324	TYR
3	q	69	ASN
3	q	209	THR
3	q	244	CYS
3	q	281	THR
3	r	147	THR
3	r	150	LEU
3	r	207	CYS
3	r	234	ASN
3	r	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	300	ASN
2	A	271	ASN
2	H	128	ASN
2	J	383	GLN
2	K	170	GLN
2	L	58	ASN
2	M	310	ASN
2	N	207	GLN
2	N	293	GLN
2	N	383	GLN
2	O	138	ASN
2	P	206	GLN
3	c	149	GLN
3	d	280	GLN
3	e	149	GLN
3	f	104	GLN
3	f	161	ASN
3	h	161	ASN
3	n	248	ASN
3	n	305	GLN
3	o	149	GLN
3	o	305	GLN
3	p	149	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	q	401	3	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	i	503	3	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	n	401	3	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	p	401	3	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	r	503	3	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	a	401	3	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	h	401	3	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	k	401	3	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	m	401	3	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	g	401	3	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	j	401	3	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	e	401	3	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	o	503	3	14,14,15	0.21	0	17,19,21	0.50	0
4	NAG	c	503	3	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	d	401	3	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	l	503	3	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	b	401	3	14,14,15	0.29	0	17,19,21	0.44	0
4	NAG	f	503	3	14,14,15	0.25	0	17,19,21	0.54	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
4	NAG	q	401	3	-	0/6/23/26	0/1/1/1
4	NAG	i	503	3	-	0/6/23/26	0/1/1/1
4	NAG	n	401	3	-	2/6/23/26	0/1/1/1
4	NAG	p	401	3	-	0/6/23/26	0/1/1/1
4	NAG	r	503	3	-	0/6/23/26	0/1/1/1
4	NAG	a	401	3	-	2/6/23/26	0/1/1/1
4	NAG	h	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	m	401	3	-	0/6/23/26	0/1/1/1
4	NAG	g	401	3	-	1/6/23/26	0/1/1/1
4	NAG	j	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	o	503	3	-	0/6/23/26	0/1/1/1
4	NAG	c	503	3	-	0/6/23/26	0/1/1/1
4	NAG	d	401	3	-	0/6/23/26	0/1/1/1
4	NAG	l	503	3	-	0/6/23/26	0/1/1/1
4	NAG	b	401	3	-	2/6/23/26	0/1/1/1
4	NAG	f	503	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	b	401	NAG	O5-C5-C6-O6
4	n	401	NAG	O5-C5-C6-O6
4	b	401	NAG	C4-C5-C6-O6
4	n	401	NAG	C4-C5-C6-O6
4	g	401	NAG	O5-C5-C6-O6
4	a	401	NAG	C4-C5-C6-O6
4	a	401	NAG	O5-C5-C6-O6
4	f	503	NAG	C4-C5-C6-O6
4	f	503	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.

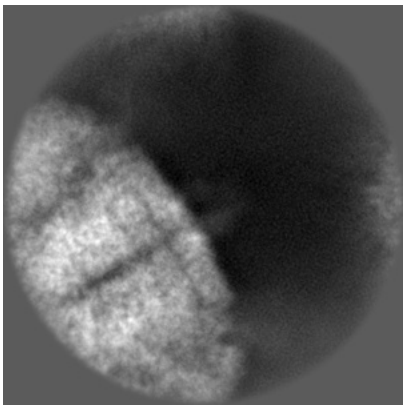
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21956. These allow visual inspection of the internal detail of the map and identification of artifacts.

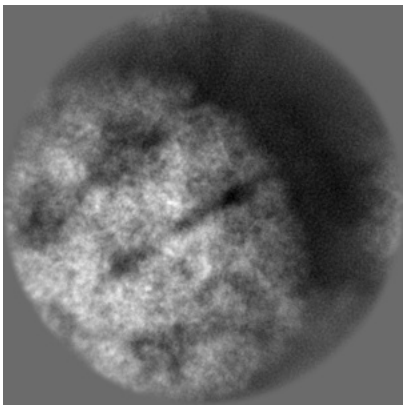
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

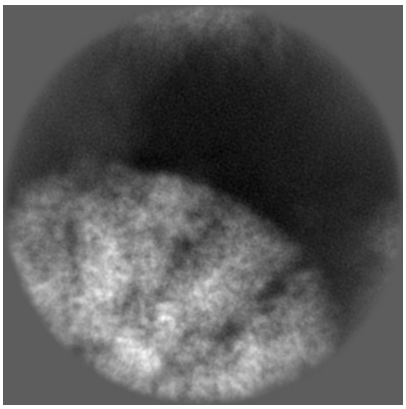
6.1.1 Primary map



X

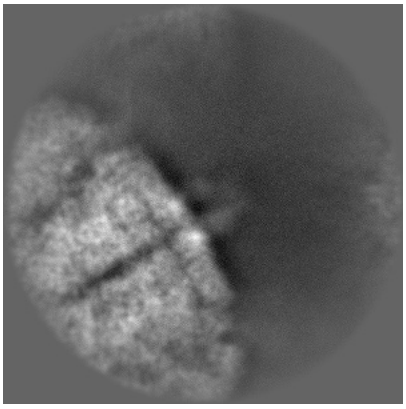


Y

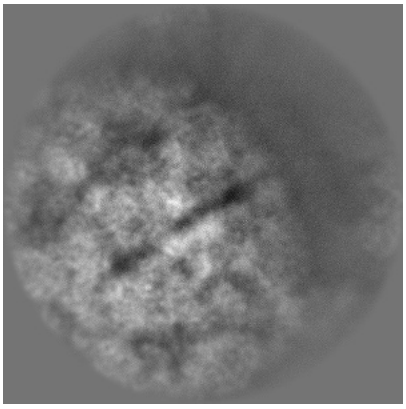


Z

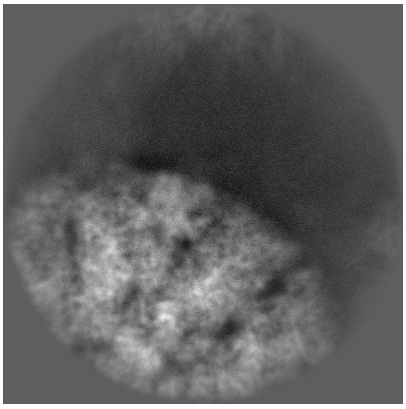
6.1.2 Raw map



X



Y

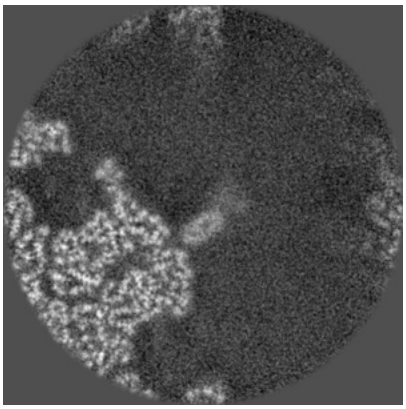


Z

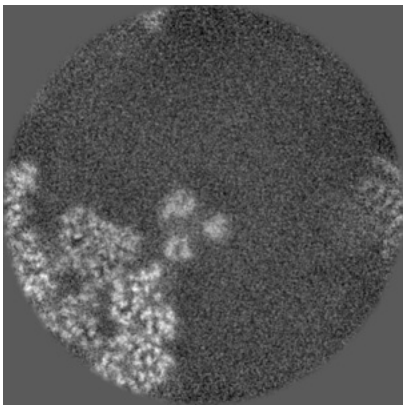
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

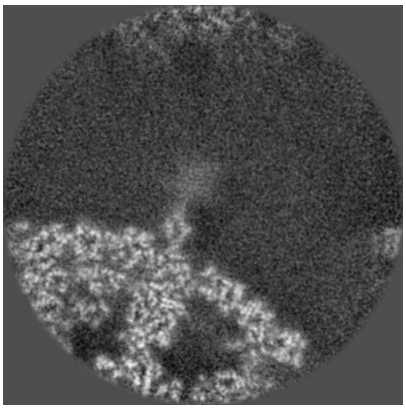
6.2.1 Primary map



X Index: 160

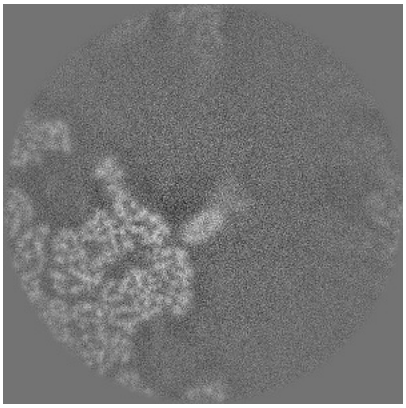


Y Index: 160

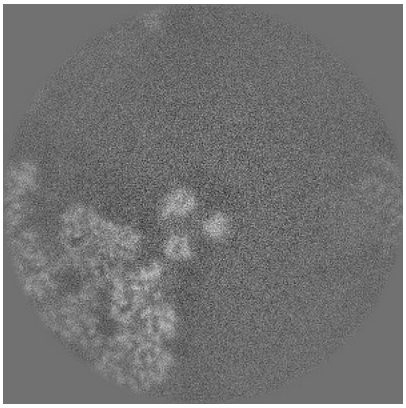


Z Index: 160

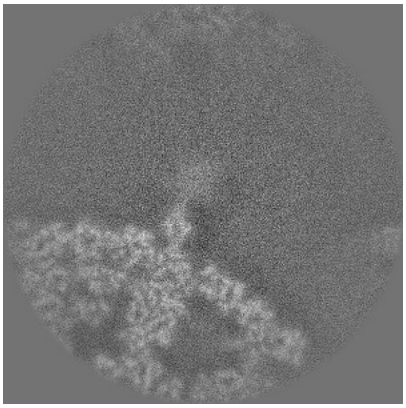
6.2.2 Raw map



X Index: 160



Y Index: 160

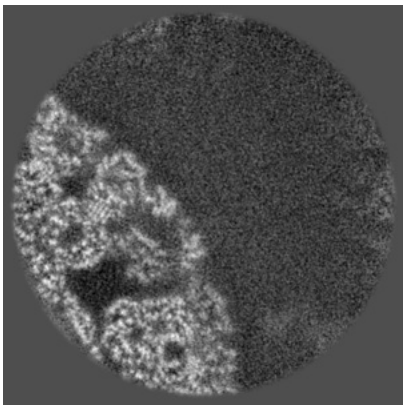


Z Index: 160

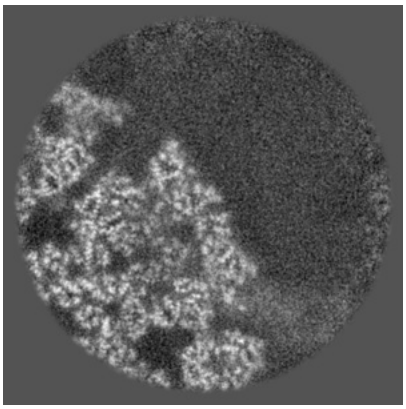
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

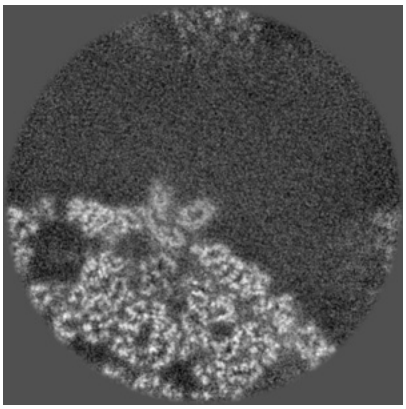
6.3.1 Primary map



X Index: 112

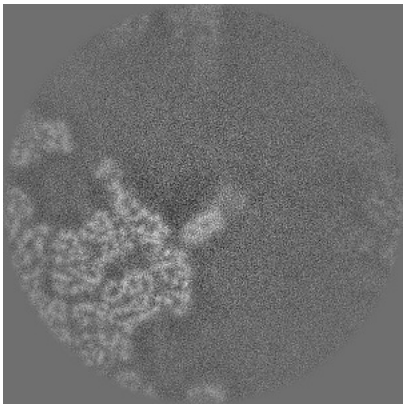


Y Index: 103

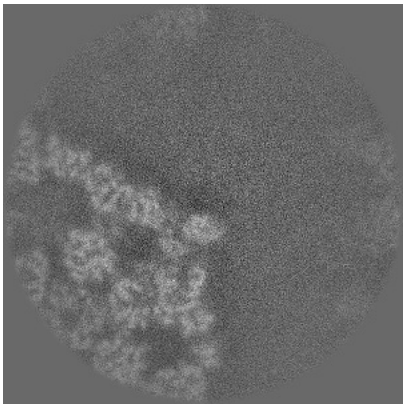


Z Index: 134

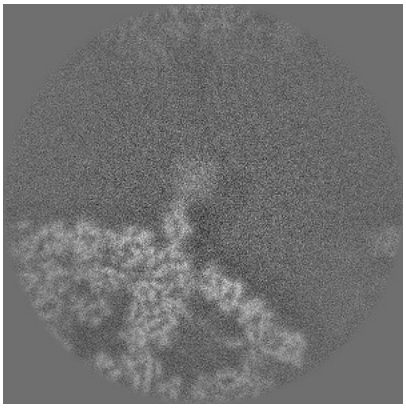
6.3.2 Raw map



X Index: 161



Y Index: 140

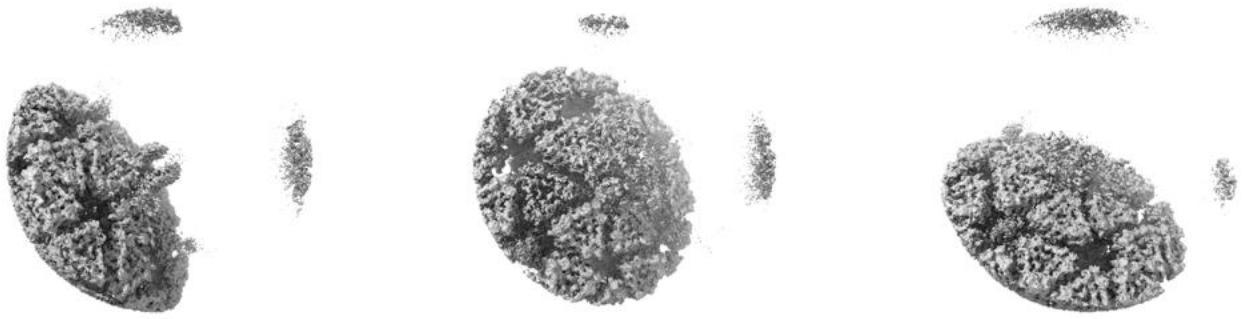


Z Index: 161

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

6.4 Orthogonal surface views (i)

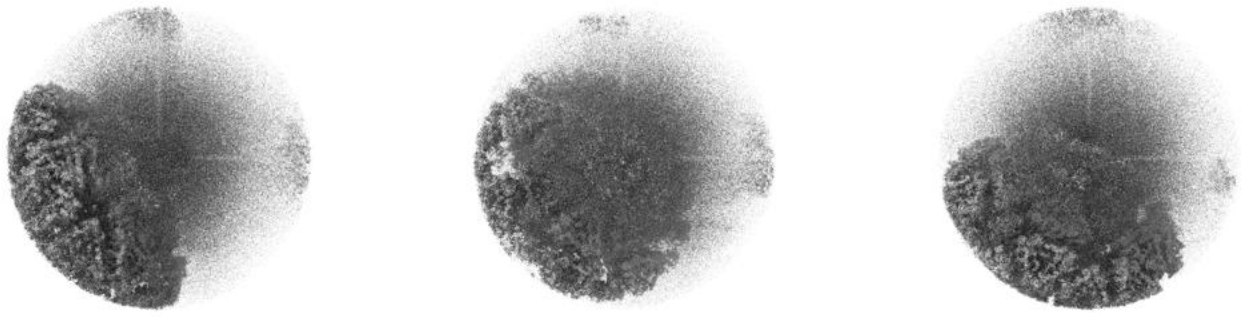
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

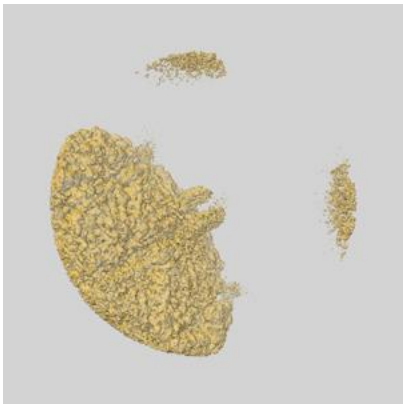
6.5 Mask visualisation (i)

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

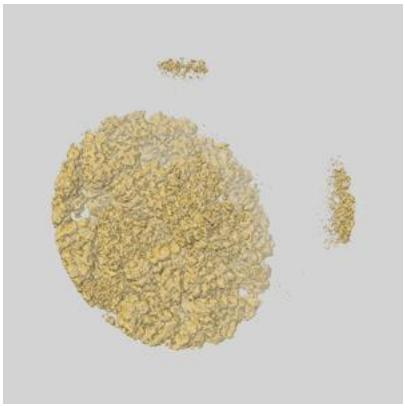
A mask typically either:

- 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_21956_msk_1.map (i)



X



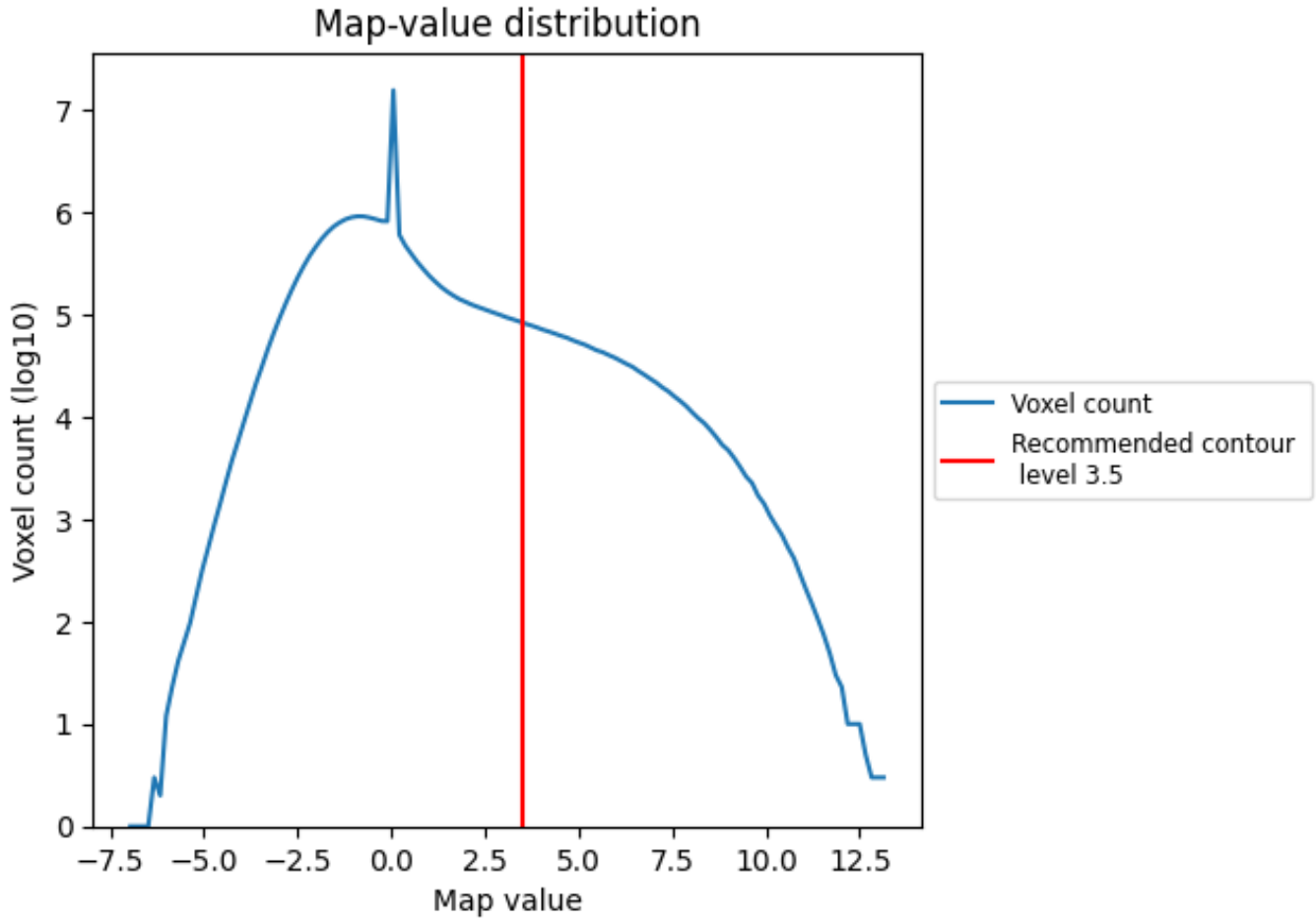
Y

Z

7 Map analysis

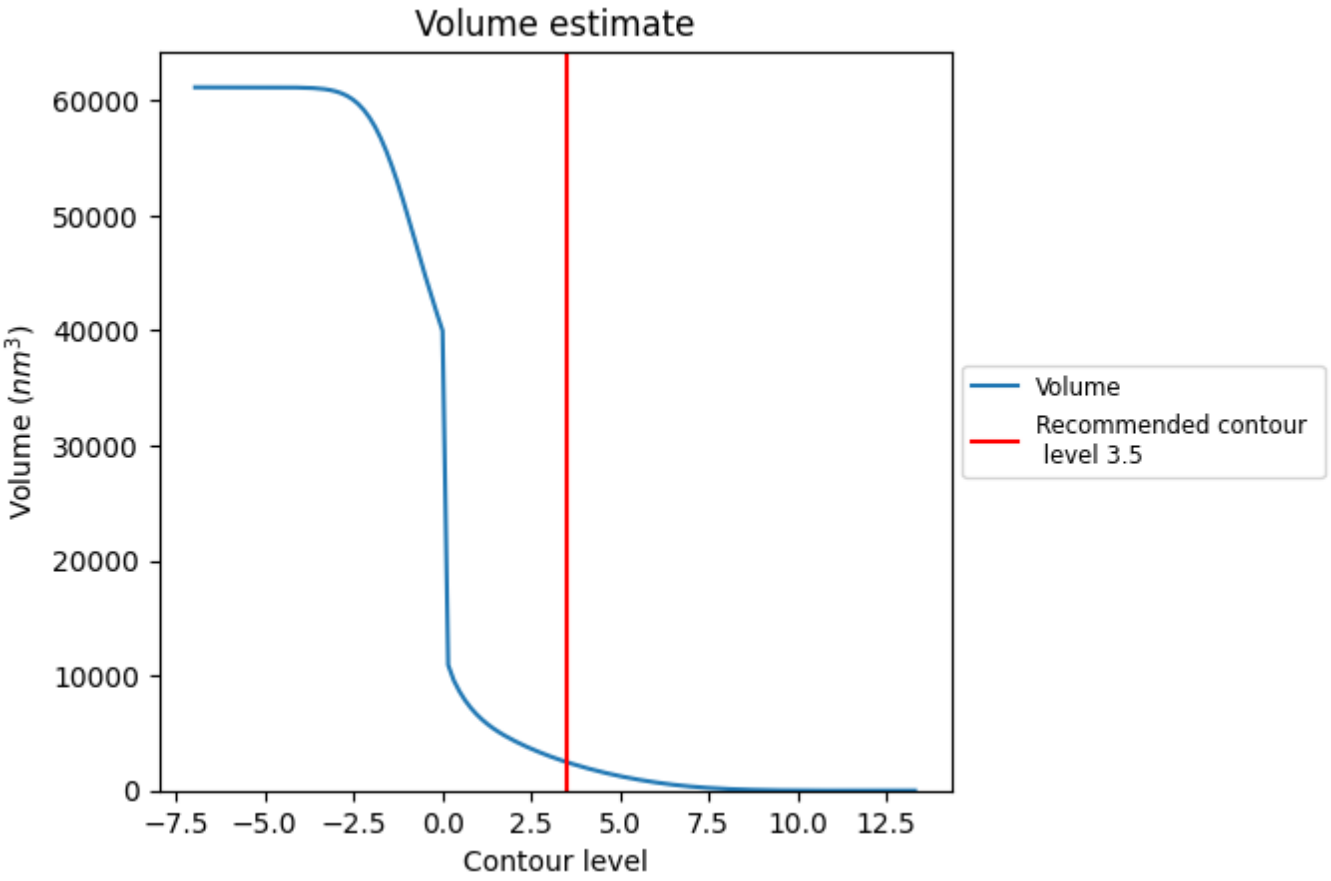
This section contains the results of statistical analysis of the map.

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.

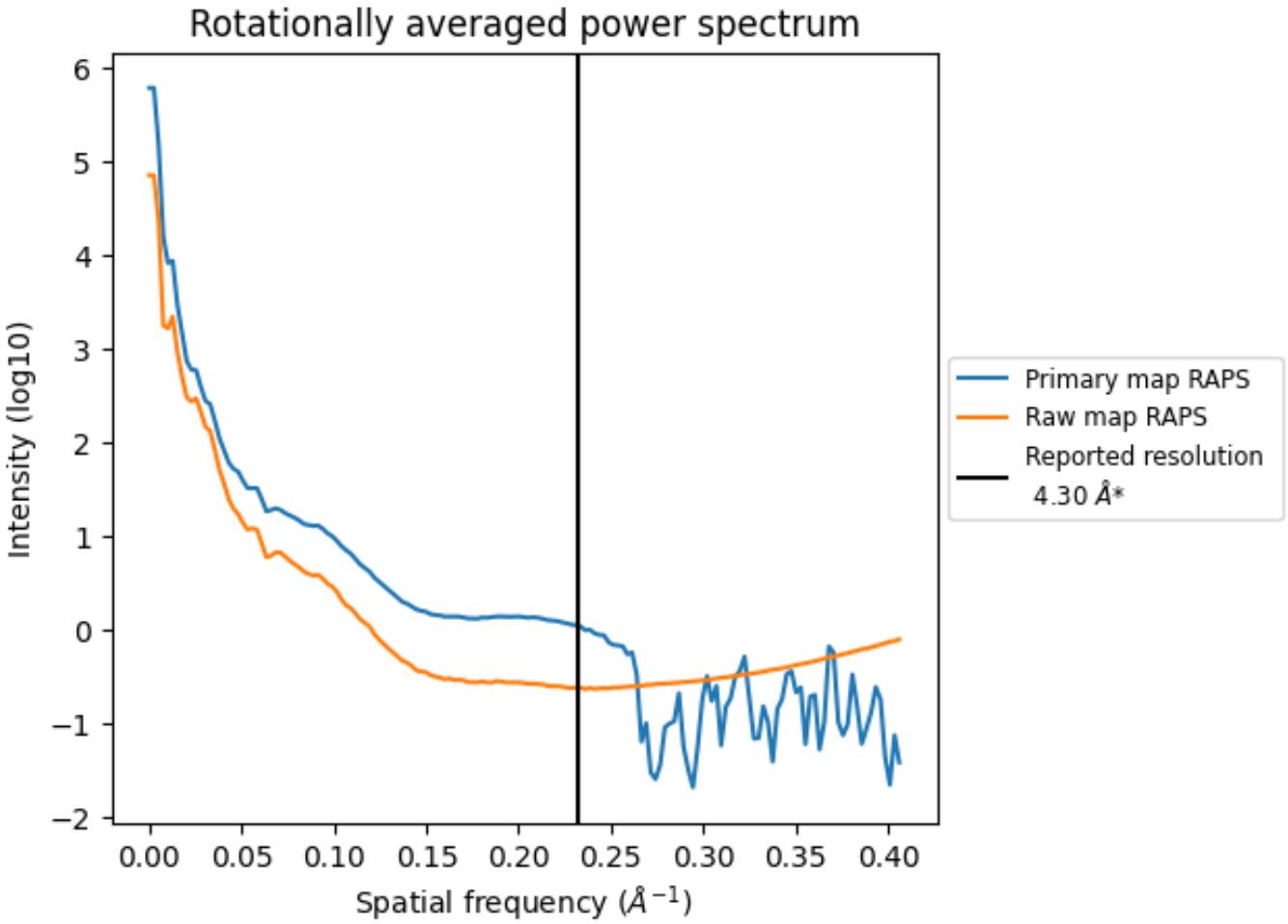
7.2 Volume estimate



The volume at the recommended contour level is 2472 nm^3; this corresponds to an approximate mass of 2233 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)

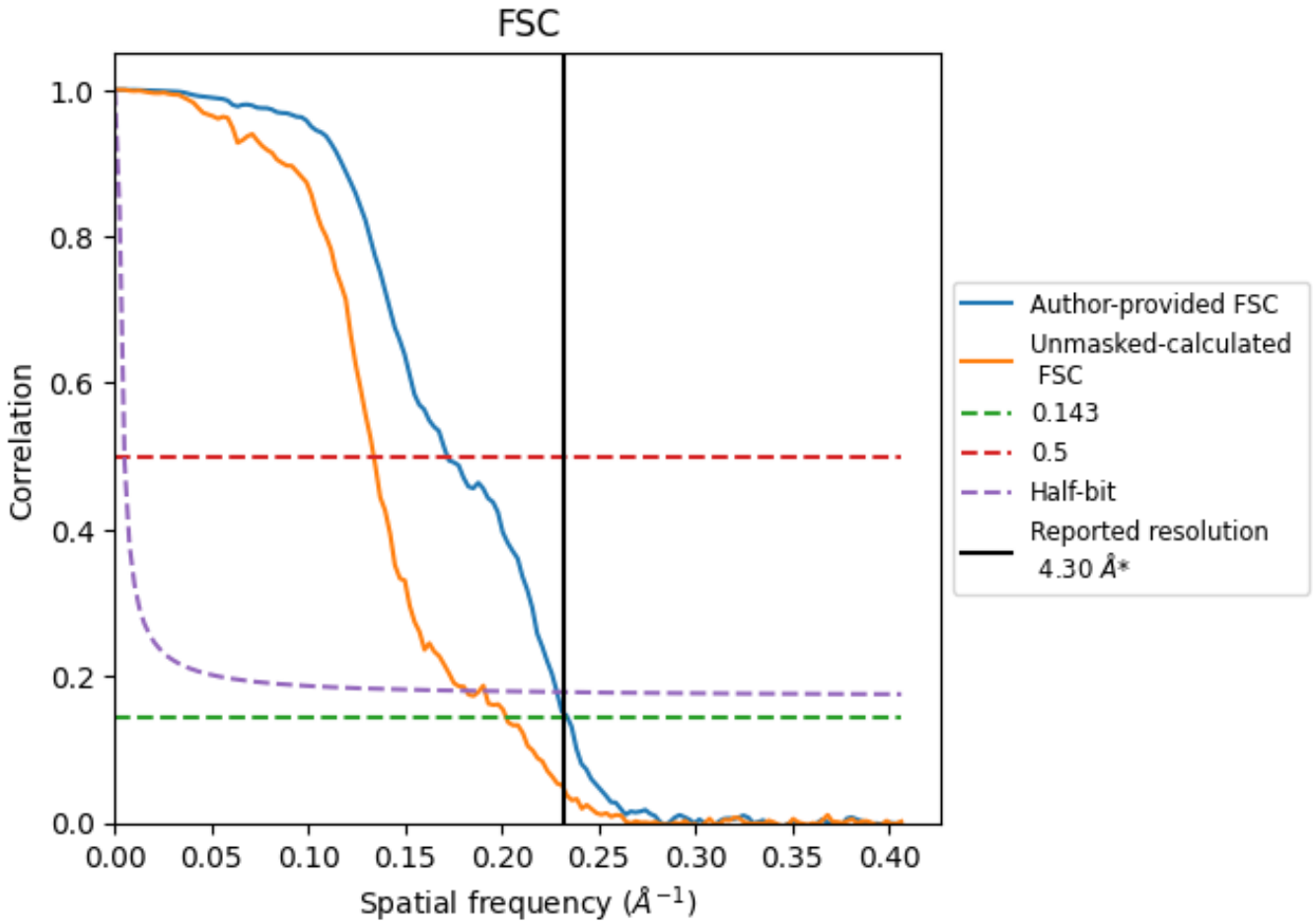


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

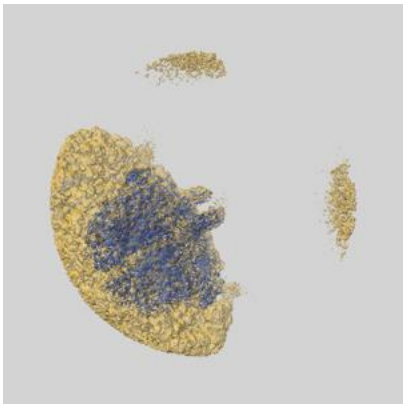
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	5.82	4.38
Unmasked-calculated*	4.94	7.47	5.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.94 differs from the reported value 4.3 by more than 10 %

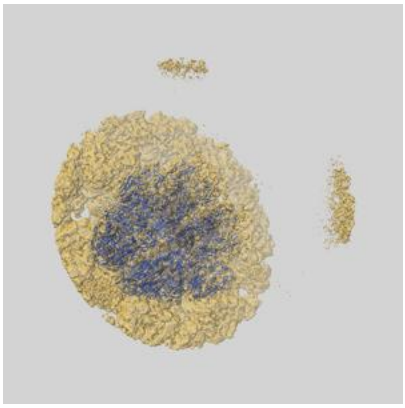
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21956 and PDB model 6WXF. Per-residue inclusion information can be found in section 3 on page 10.

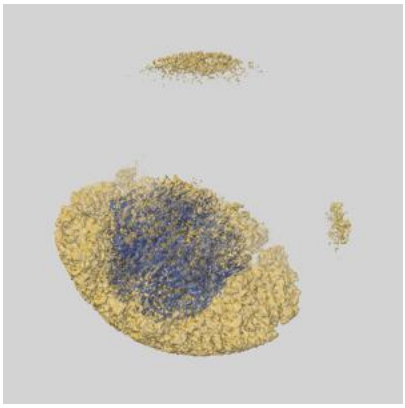
9.1 Map-model overlay



X



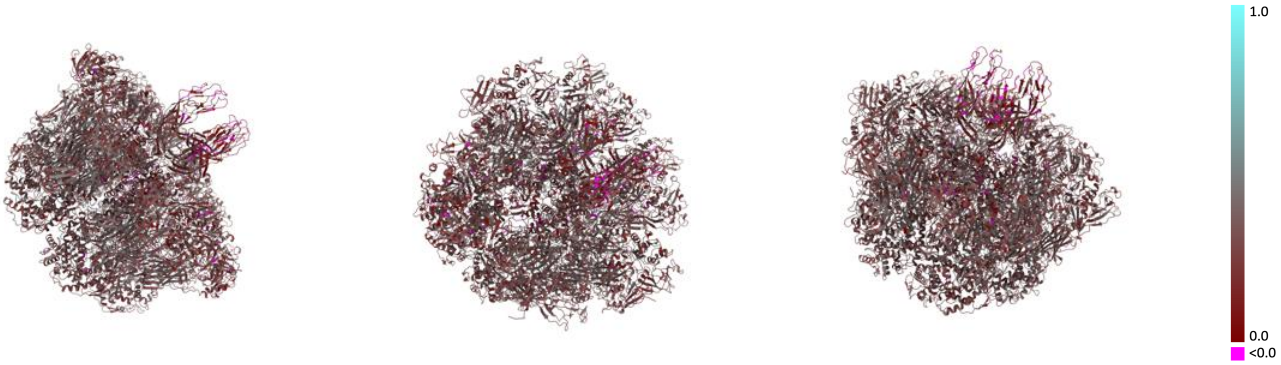
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

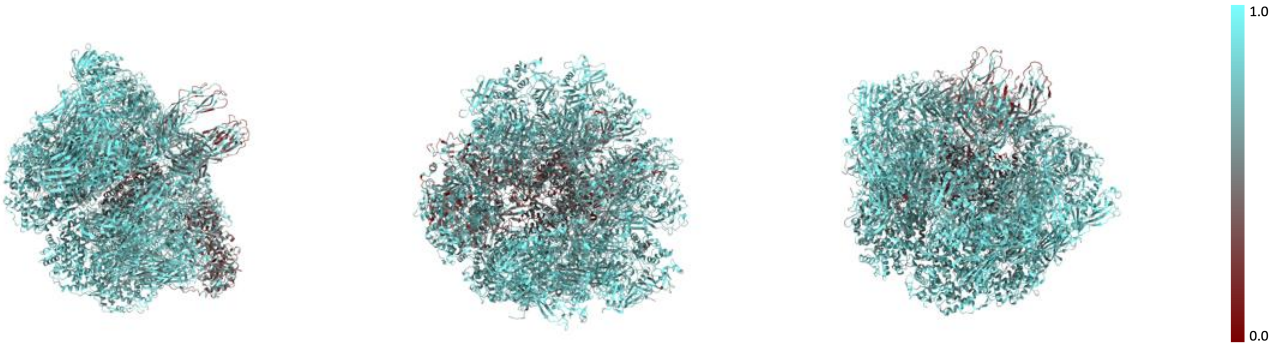
9.2 Q-score mapped to coordinate model (i)



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.

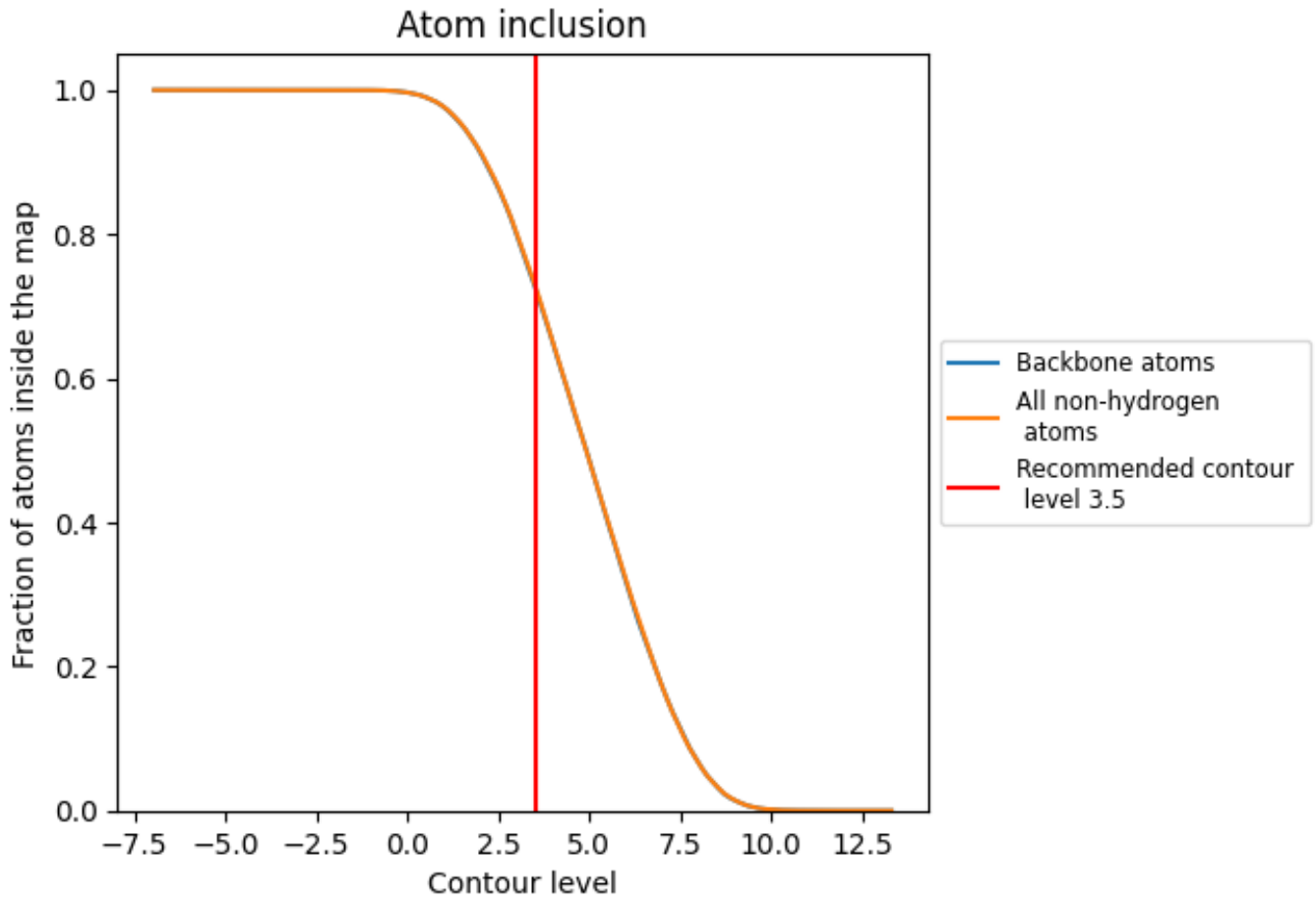
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7298	0.3060
1	0.5303	0.2350
2	0.5184	0.2330
3	0.4916	0.2340
A	0.8069	0.3500
B	0.8240	0.3380
C	0.8201	0.3380
D	0.7914	0.3360
E	0.8163	0.3420
F	0.8034	0.3380
G	0.7959	0.3350
H	0.8198	0.3360
I	0.8059	0.3380
J	0.7808	0.3370
K	0.7956	0.3430
L	0.7798	0.3370
M	0.7782	0.3450
N	0.7782	0.3290
O	0.7953	0.3360
P	0.8079	0.3300
Q	0.8160	0.3320
R	0.8001	0.3160
a	0.7530	0.2790
b	0.7186	0.2780
c	0.7510	0.2780
d	0.8010	0.3080
e	0.8254	0.3090
f	0.8279	0.3070
g	0.7453	0.2700
h	0.7908	0.2800
i	0.7753	0.2960
j	0.7832	0.2790
k	0.7716	0.2940
l	0.7918	0.3000
m	0.7959	0.2980

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Chain	Atom inclusion	Q-score
n	0.7740	0.2930
o	0.7990	0.3050
p	0.4185	0.2470
q	0.4222	0.2500
r	0.4457	0.2470