



## Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 08:37 PM EDT

PDB ID : 9CGM  
EMDB ID : EMD-45583  
Title : The Structure of Spiroplasma Virus 4  
Authors : Mietzsch, M.; McKenna, R.  
Deposited on : 2024-06-30  
Resolution : 2.52 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

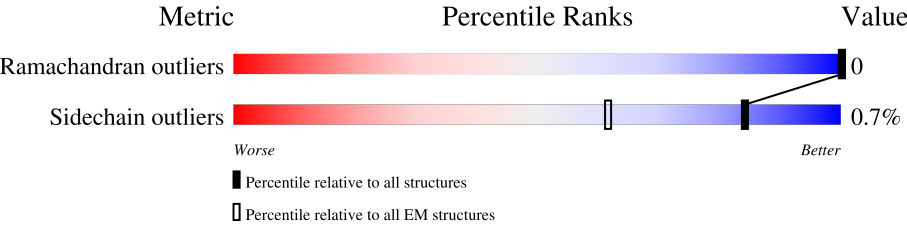
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.52 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.









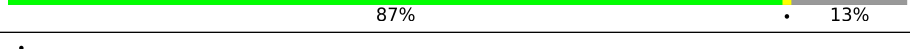
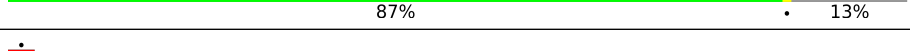
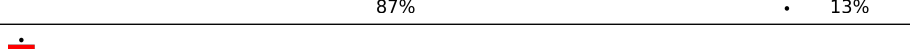
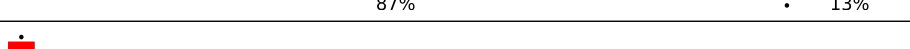
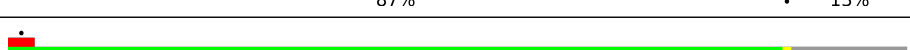

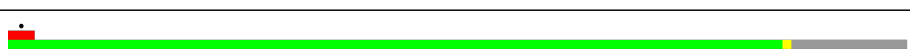

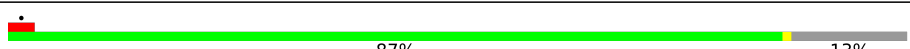





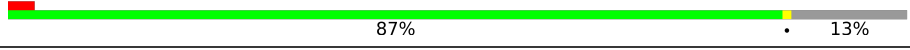
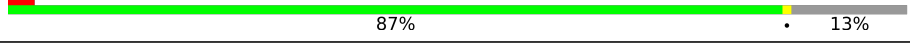



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	2	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	3	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	4	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	5	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	6	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	7	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	8	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>
1	A	553	<div><div></div><div>87%</div><div>•</div><div>13%</div></div>







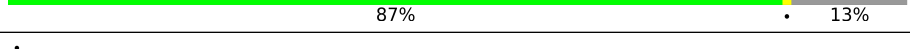
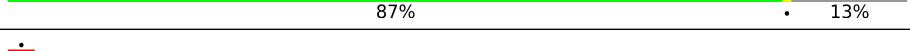
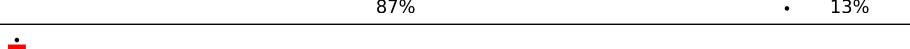
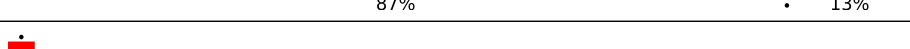
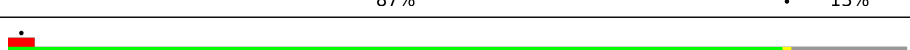

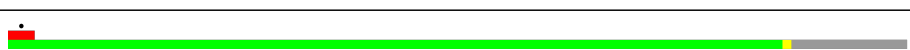

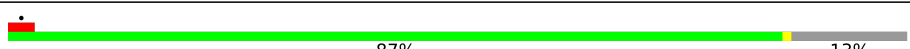





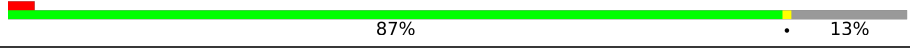
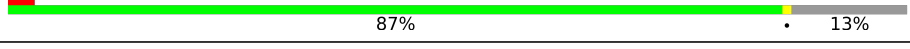



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Mol	Chain	Length	Quality of chain
1	B	553	
1	C	553	
1	D	553	
1	E	553	
1	F	553	
1	G	553	
1	H	553	
1	I	553	
1	J	553	
1	K	553	
1	L	553	
1	M	553	
1	N	553	
1	O	553	
1	P	553	
1	Q	553	
1	R	553	
1	S	553	
1	T	553	
1	U	553	
1	V	553	
1	W	553	
1	X	553	
1	Y	553	
1	Z	553	








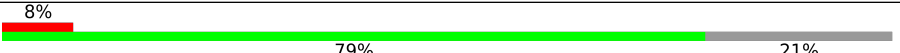
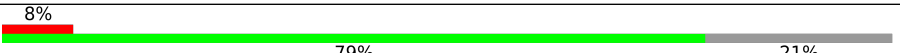
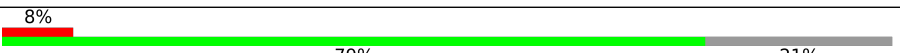
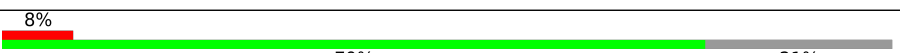
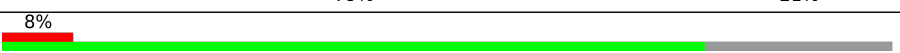

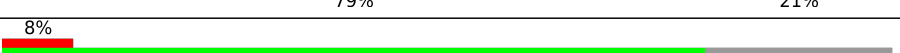
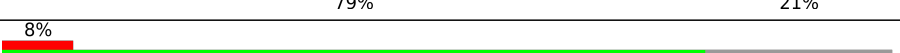

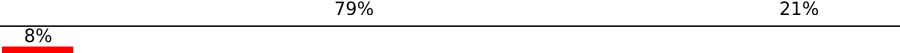
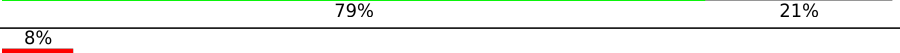





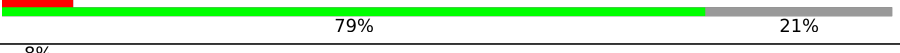
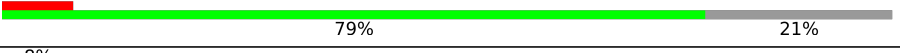
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Mol	Chain	Length	Quality of chain
1	a	553	
1	b	553	
1	c	553	
1	d	553	
1	e	553	
1	f	553	
1	g	553	
1	h	553	
1	i	553	
1	j	553	
1	k	553	
1	l	553	
1	m	553	
1	n	553	
1	o	553	
1	p	553	
1	q	553	
1	r	553	
1	s	553	
1	t	553	
1	u	553	
1	v	553	
1	w	553	
1	x	553	
1	y	553	

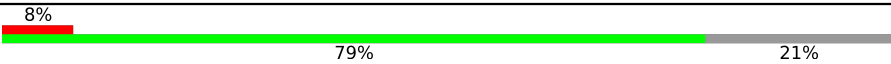

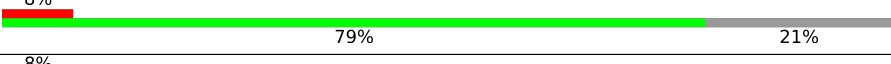
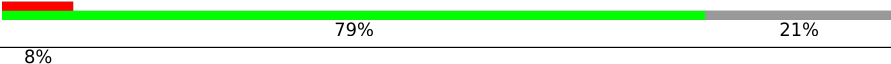
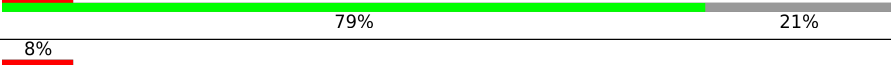
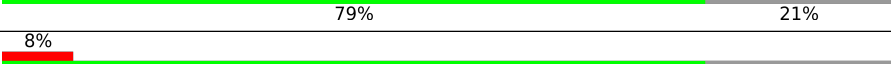
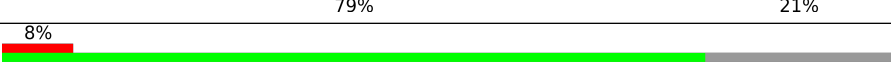
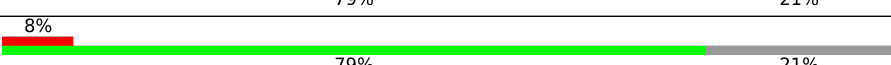
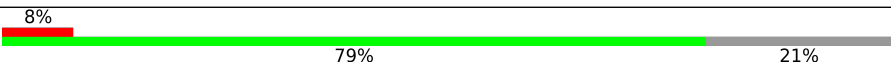

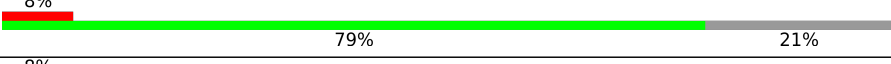




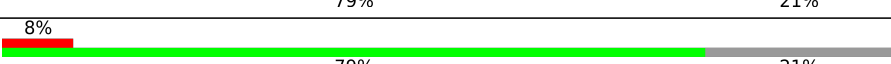
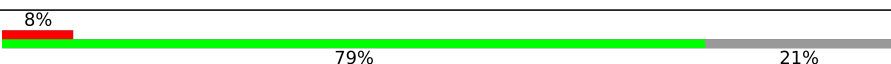
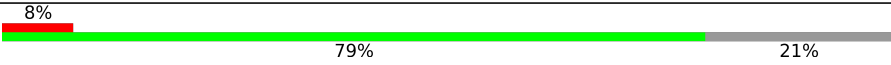


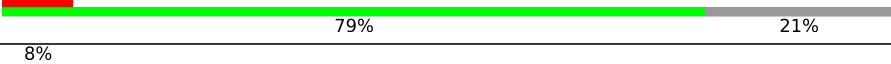

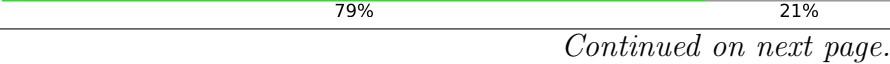


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Mol	Chain	Length	Quality of chain	
1	z	553		
2	0	38		
2	12	38		
2	22	38		
2	32	38		
2	42	38		
2	52	38		
2	62	38		
2	72	38		
2	82	38		
2	9	38		
2	C2	38		
2	D2	38		
2	E2	38		
2	F2	38		
2	G2	38		
2	H2	38		
2	I2	38		
2	J2	38		
2	K2	38		
2	L2	38		
2	M2	38		
2	N2	38		
2	O2	38		
2	P2	38		

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Mol	Chain	Length	Quality of chain		
2	Q2	38		8%	79% 21%
2	R2	38		8%	79% 21%
2	S2	38		8%	79% 21%
2	T2	38		8%	79% 21%
2	U2	38		8%	79% 21%
2	V2	38		8%	79% 21%
2	W2	38		8%	79% 21%
2	X2	38		8%	79% 21%
2	Y2	38		8%	79% 21%
2	Z2	38		8%	79% 21%
2	a2	38		8%	79% 21%
2	b2	38		8%	79% 21%
2	c2	38		8%	79% 21%
2	d2	38		8%	79% 21%
2	e2	38		8%	79% 21%
2	f2	38		8%	79% 21%
2	g2	38		8%	79% 21%
2	h2	38		8%	79% 21%
2	i2	38		8%	79% 21%
2	j2	38		8%	79% 21%
2	k2	38		8%	79% 21%
2	l2	38		8%	79% 21%
2	m2	38		8%	79% 21%
2	n2	38		8%	79% 21%
2	o2	38		8%	79% 21%

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Mol	Chain	Length	Quality of chain		
2	p2	38		8%	79% 21%
2	q2	38		8%	79% 21%
2	r2	38		8%	79% 21%
2	s2	38		8%	79% 21%
2	t2	38		8%	79% 21%
2	u2	38		8%	79% 21%
2	v2	38		8%	79% 21%
2	w2	38		8%	79% 21%
2	x2	38		8%	79% 21%
2	y2	38		8%	79% 21%
2	z2	38		8%	79% 21%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 246420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	B	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	C	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	D	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	E	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	F	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	G	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	H	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	I	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	J	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	K	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	L	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	M	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	N	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	O	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	P	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	Q	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	S	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	T	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	U	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	V	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	W	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	X	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	Y	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	Z	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	a	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	b	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	c	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	d	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	e	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	f	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	g	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	h	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	i	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	j	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	k	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	l	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	n	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	o	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	p	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	q	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	r	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	s	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	t	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	u	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	v	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	w	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	x	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	y	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	z	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	1	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	2	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	3	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	4	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	5	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	6	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		
1	7	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	482	Total	C	N	O	S	0	0
			3853	2458	665	716	14		

- Molecule 2 is a protein called DNA binding protein ORF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	9	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	C2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	D2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	E2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	F2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	G2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	H2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	I2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	J2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	K2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	L2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	M2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	N2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	O2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	P2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	Q2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	R2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	T2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	U2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	V2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	W2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	X2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	Y2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	Z2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	a2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	b2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	c2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	d2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	e2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	f2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	g2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	h2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	i2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	j2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	k2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	l2	30	Total 254	C 155	N 61	O 37	S 1	0	0
2	m2	30	Total 254	C 155	N 61	O 37	S 1	0	0

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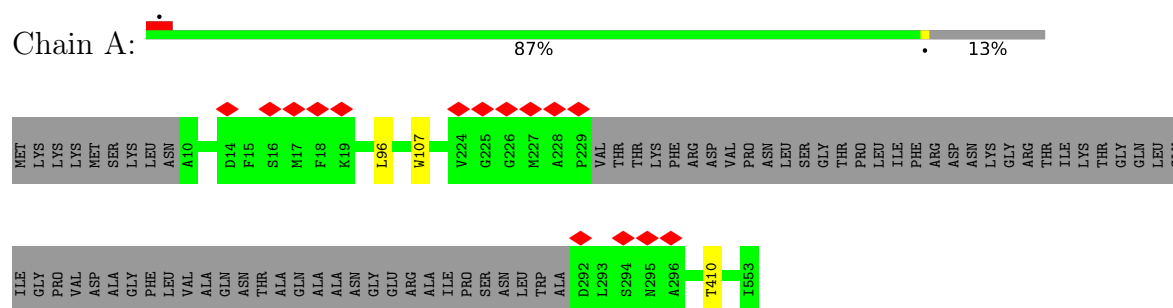
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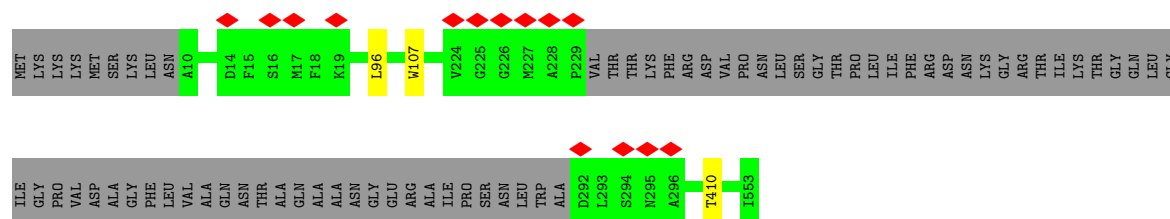
Mol	Chain	Residues	Atoms					AltConf	Trace
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			254	155	61	37	1		
2	o2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	p2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	q2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	r2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	s2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	t2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	u2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	v2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	w2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	x2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	y2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	z2	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	12	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	22	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	32	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	42	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	52	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	62	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	72	30	Total	C	N	O	S	0	0
			254	155	61	37	1		
2	82	30	Total	C	N	O	S	0	0
			254	155	61	37	1		

### 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.

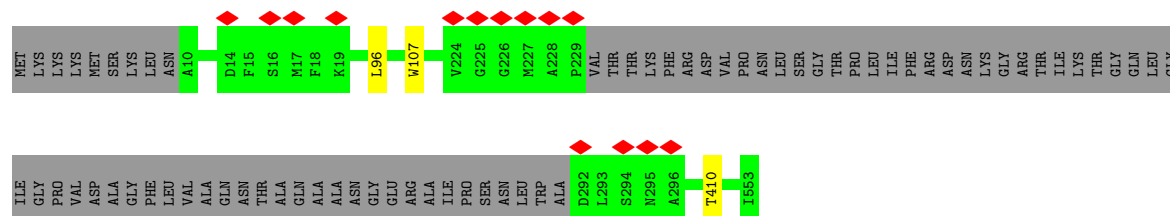
- Molecule 1: Capsid protein VP1





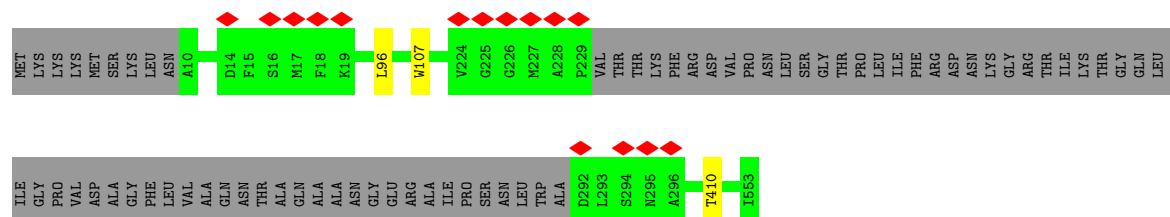
- Molecule 1: Capsid protein VP1

Chain E: 87% 13%



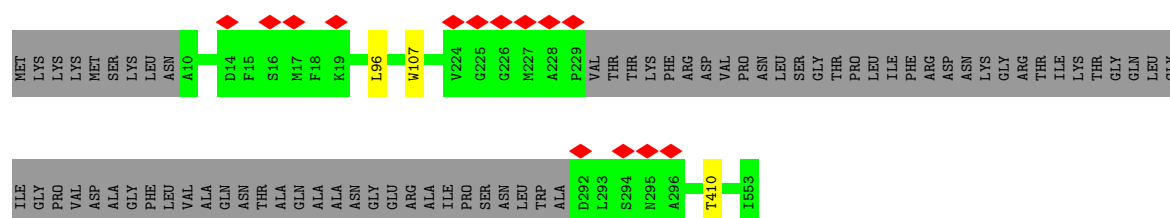
- Molecule 1: Capsid protein VP1

Chain F: 87% 13%



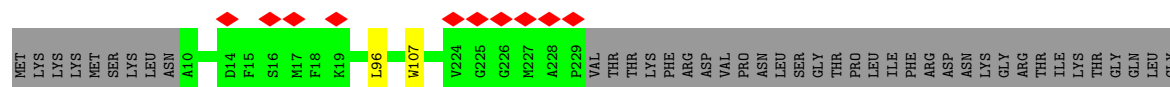
- Molecule 1: Capsid protein VP1

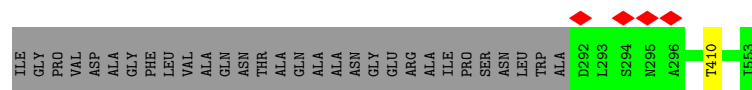
Chain G: 87% 13%



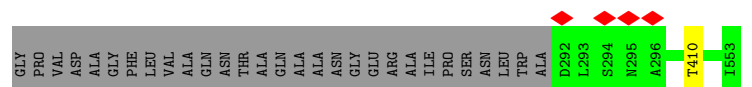
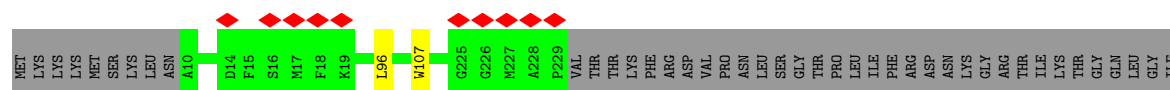
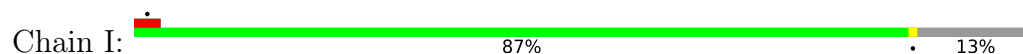
- Molecule 1: Capsid protein VP1

Chain H: 87% 13%

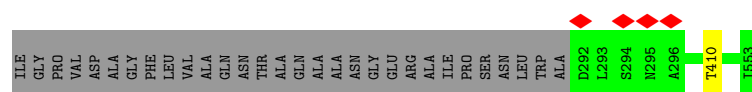
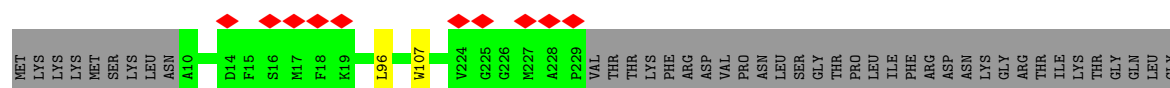
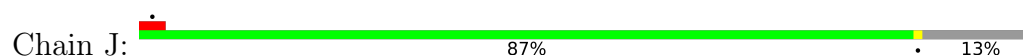




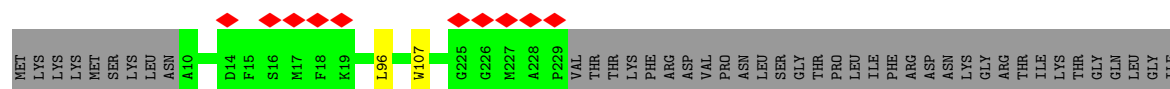
• Molecule 1: Capsid protein VP1



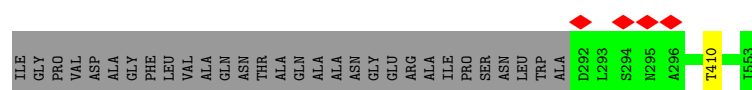
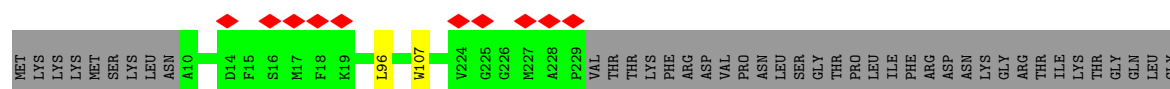
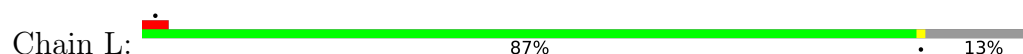
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1




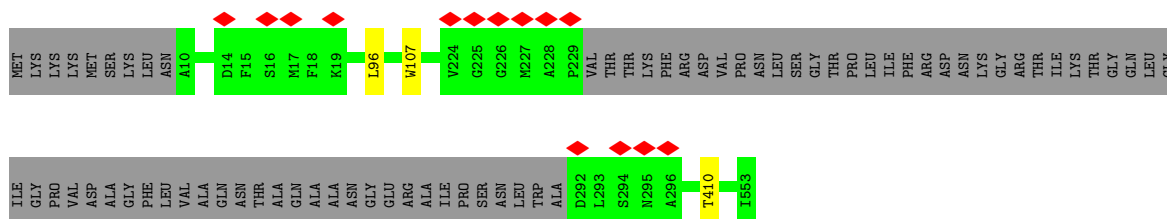
• Molecule 1: Capsid protein VP1




• Molecule 1: Capsid protein VP1

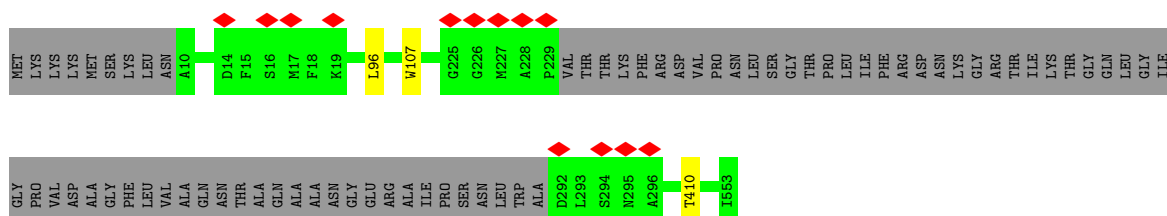


Chain M: 




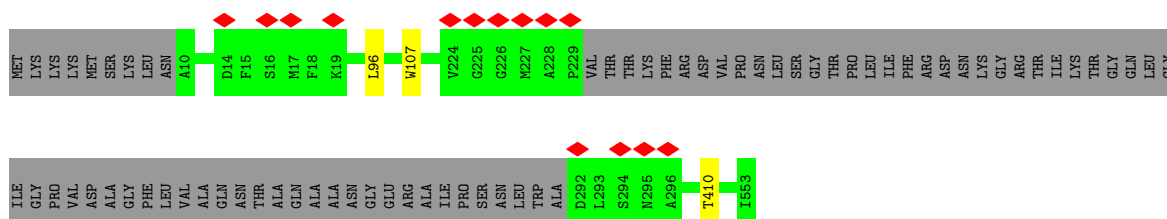
• Molecule 1: Capsid protein VP1

Chain N: 




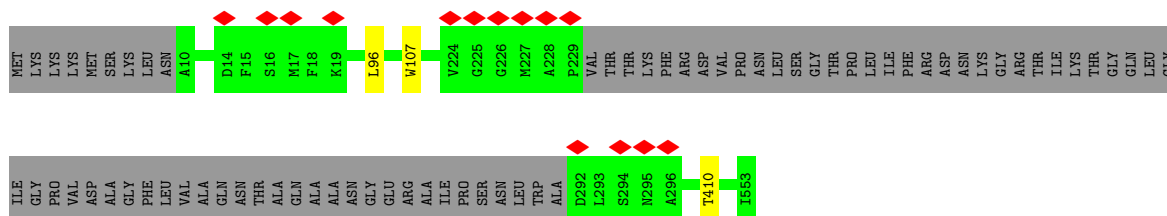
• Molecule 1: Capsid protein VP1

Chain O: 




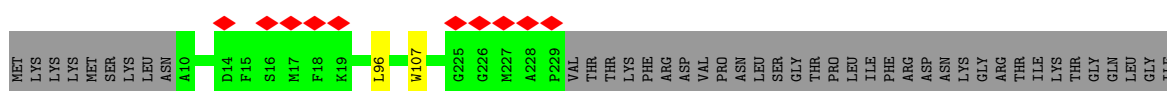
• Molecule 1: Capsid protein VP1

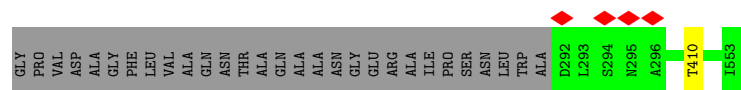
Chain P: 



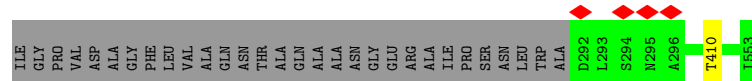
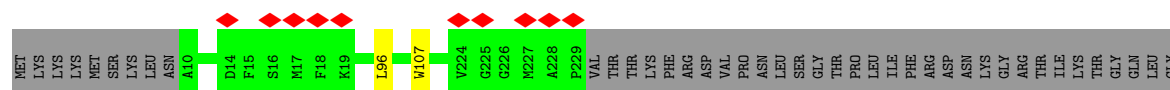
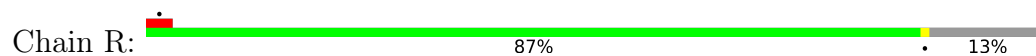
• Molecule 1: Capsid protein VP1

Chain Q: 

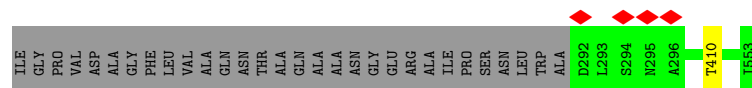
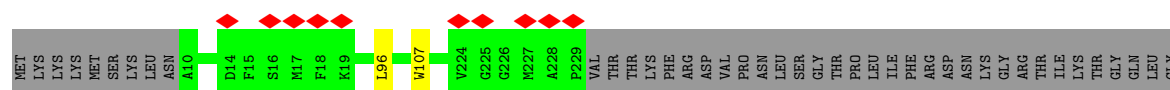
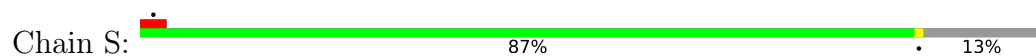




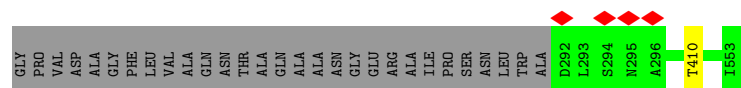
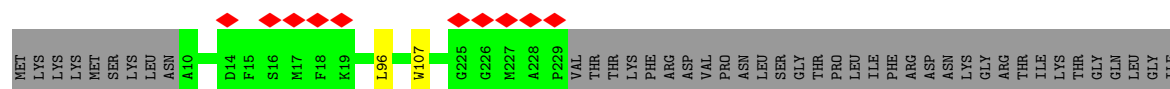
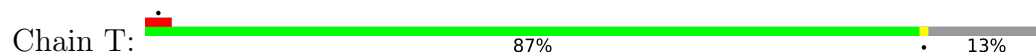
• Molecule 1: Capsid protein VP1



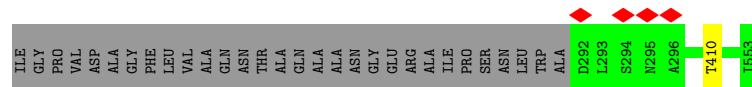
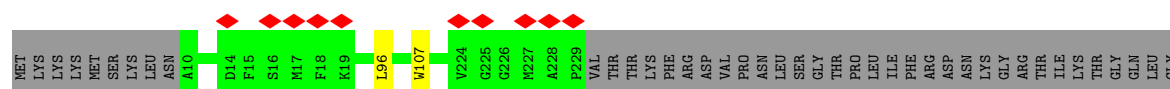
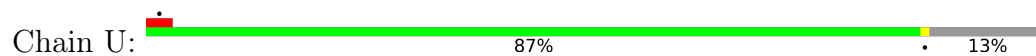
• Molecule 1: Capsid protein VP1




• Molecule 1: Capsid protein VP1

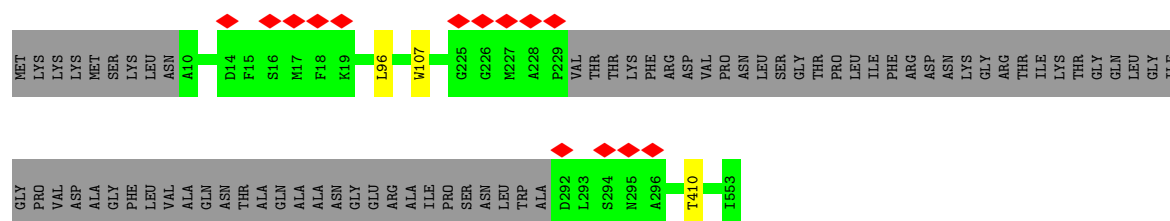


• Molecule 1: Capsid protein VP1




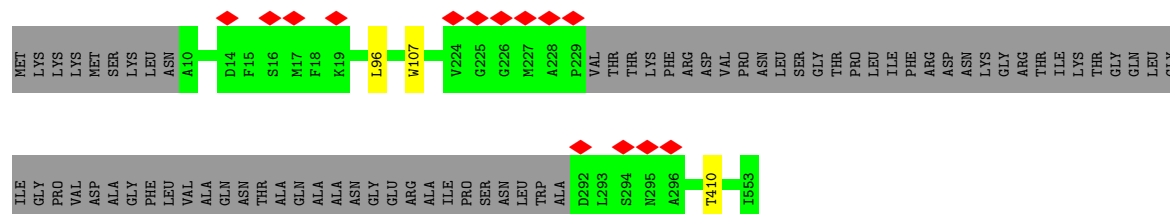
• Molecule 1: Capsid protein VP1

Chain V: 




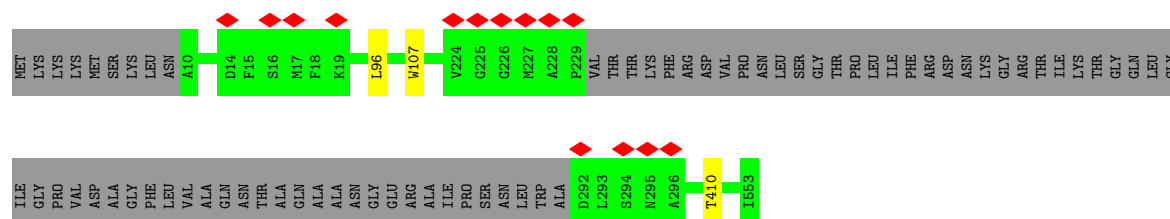
• Molecule 1: Capsid protein VP1

Chain W: 




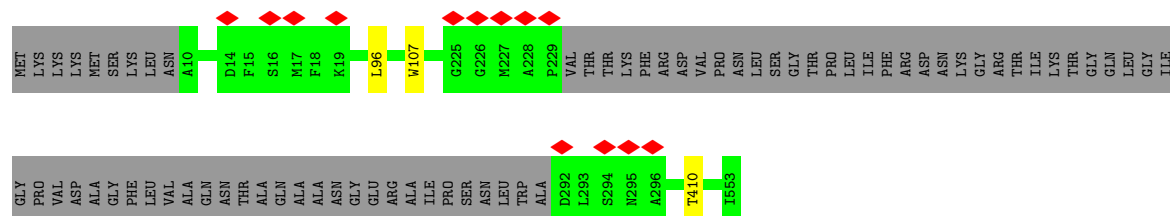
• Molecule 1: Capsid protein VP1

Chain X: 




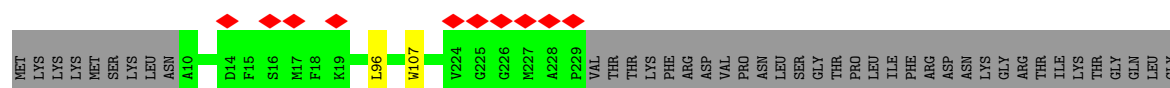
• Molecule 1: Capsid protein VP1

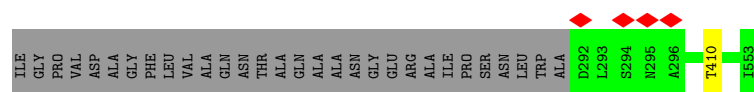
Chain Y: 



• Molecule 1: Capsid protein VP1

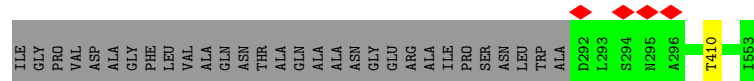
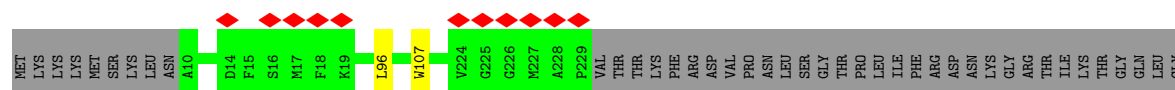
Chain Z: 





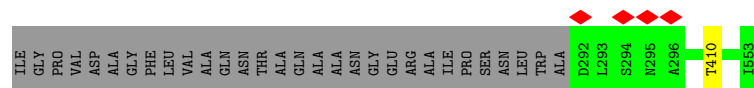
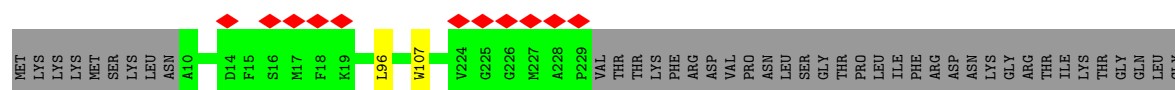
• Molecule 1: Capsid protein VP1

Chain a:   
87% 13%



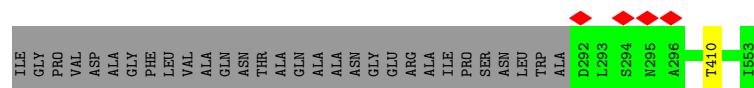
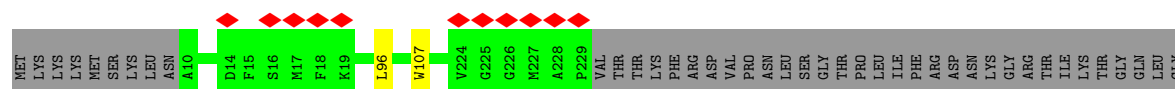
• Molecule 1: Capsid protein VP1

Chain b:   
87% 13%



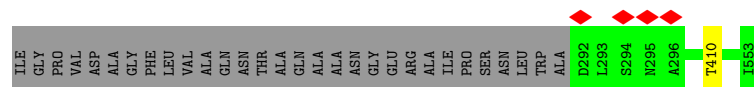
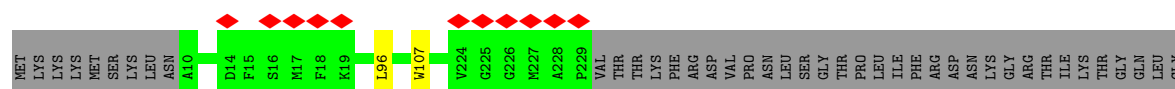
• Molecule 1: Capsid protein VP1

Chain c:   
87% 13%



• Molecule 1: Capsid protein VP1

Chain d:   
87% 13%

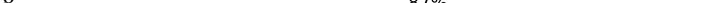


• Molecule 1: Capsid protein VP1

Amino Acid	Information Content (bits)
ILE	0.00
GLY	0.00
PRO	0.00
VAL	0.38
ASP	0.15
ALA	0.00
GLY	0.00
PHE	0.00
LEU	0.00
VAL	0.38
ALA	0.00
GLN	0.12
ASN	0.18
THR	0.00
ALA	0.00
GLN	0.12
ALA	0.00
ASN	0.18
GLY	0.00
GLU	0.00
ARG	0.00
ALA	0.00
ILE	0.00
PRO	0.00
SER	0.00
ASN	0.18
LEU	0.00
TRP	0.00
ALA	0.00
D292	0.00
L293	0.00
S294	0.00
N295	0.00
A296	0.00
T410	0.00
I553	0.00

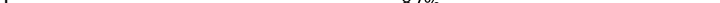
Chain f:  87% 13%

Two bar charts showing the distribution of amino acids in the protein. The top chart shows the distribution of amino acids in the protein, with the y-axis representing the number of amino acids (0 to 20) and the x-axis representing the amino acid (MET, LYS, PRO, VAL, ASP, ALA, PHE, LEU, ASN, ARG, THR, PRO, LEU, SER, GLY, THR, PRO, LEU, ILE, PHE, ARG, ASP, ASN, LYS, GLY, ARG, THR, ILE, LYS, THR, GLY, GLN, LEU). The bottom chart shows the distribution of amino acids in the protein, with the y-axis representing the number of amino acids (0 to 20) and the x-axis representing the amino acid (ILE, GLY, PRO, VAL, ASP, ALA, PHE, LEU, VAL, ALA, GLN, ASN, THR, GLN, ALA, ALA, ASN, GLY, ARG, ALA, ILE, PRO, SER, ASN, LEU, TRP, ALA, D292, L293, S294, N295, A296, T410, I553).

Chain g:  87% 13%


The figure displays two sequence logos. The top logo, labeled 'Protein', shows high conservation across the entire sequence, with a prominent peak at position 100 (G225). The bottom logo, labeled 'Protein (residues 1-100)', shows a similar pattern of conservation, with a peak at position 100 (G225) and a smaller peak at position 101 (L293).

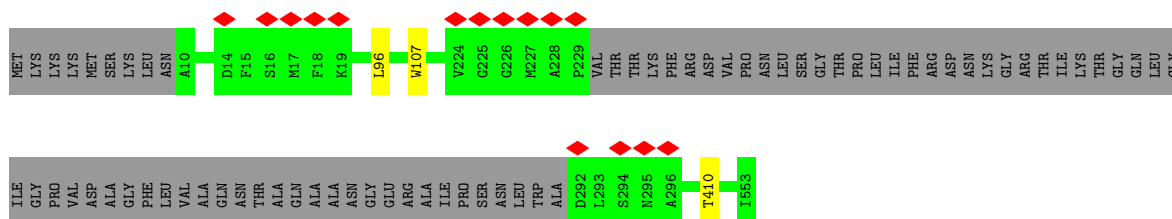
Chain h:  87% 13%

Chain i:  87% 13%


MET	LYS	LYS	LYS	MET	SER	LYS	LEU	ASN	A10	D14	F15	S16	M17	F18	K19	L96	W107	V224	G225	G226	M227	A228	P229	VAL	THR	THR	THR	LYS	PHE	ARG	ASP	ASP	VAL	PRO	ASN	ASN	LEU	SER	GLY	THR	PRO	THR	LEU	ILE	PHE	ASP	ASP	ASN	LYS	GLY	ARG	THR	THR	ILE	THR	THR	GLN	GLY	LEU	LEU
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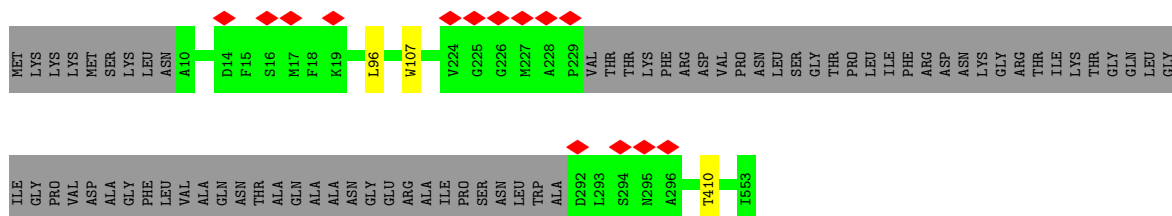


Chain n:  87% 13%




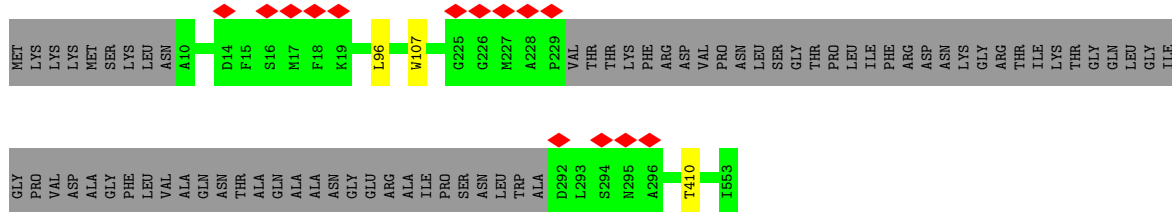
• Molecule 1: Capsid protein VP1

Chain o:  87% 13%




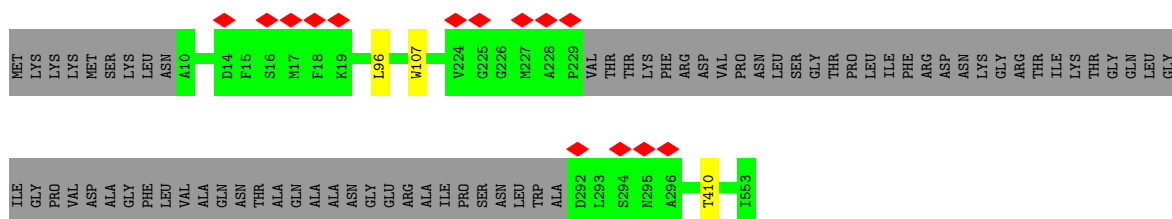
• Molecule 1: Capsid protein VP1

Chain p:  87% 13%




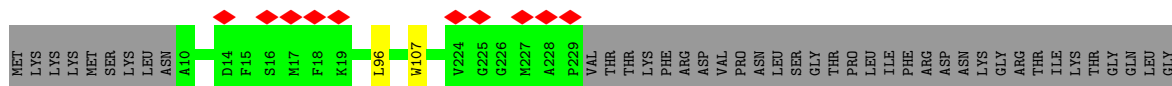
• Molecule 1: Capsid protein VP1

Chain q:  87% 13%




• Molecule 1: Capsid protein VP1

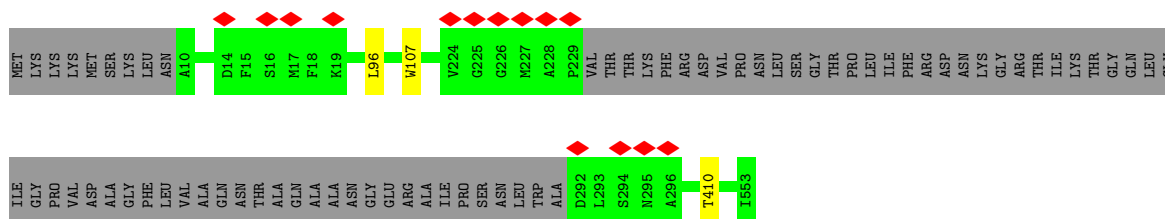
Chain r:  87% 13%






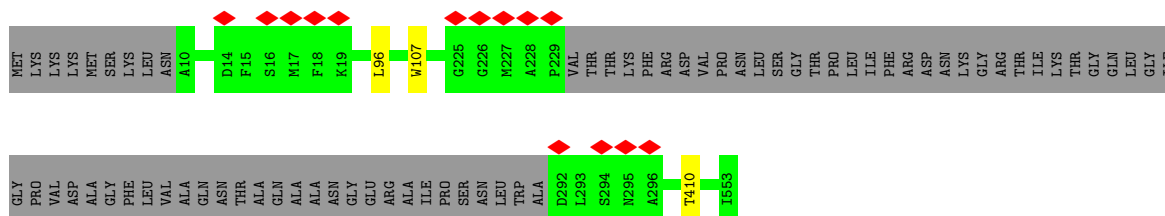


Chain w:  87% 13%




• Molecule 1: Capsid protein VP1

Chain x:  87% 13%




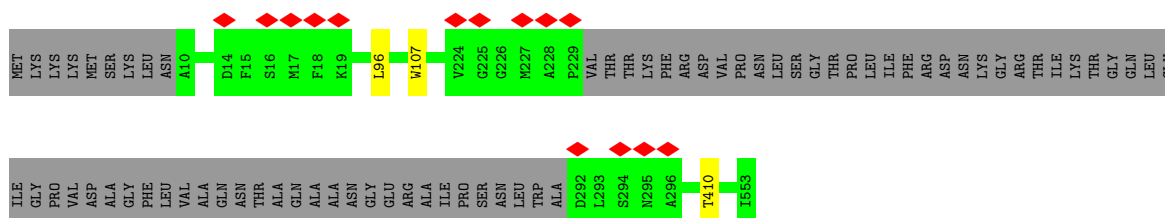
• Molecule 1: Capsid protein VP1

Chain y:  87% 13%




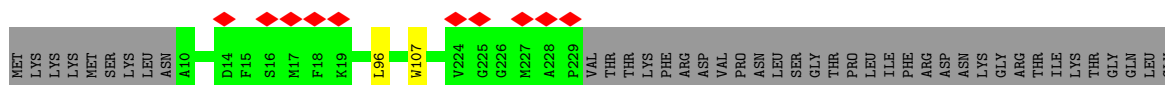
• Molecule 1: Capsid protein VP1

Chain z:  87% 13%

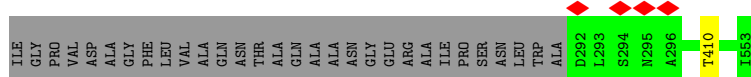
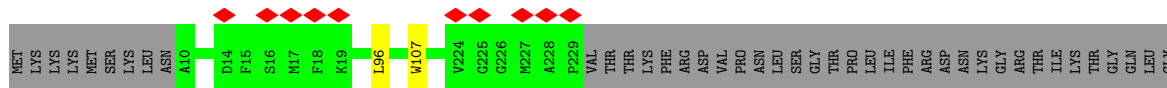
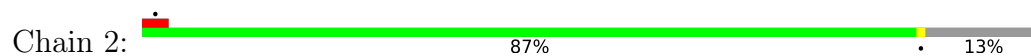


• Molecule 1: Capsid protein VP1

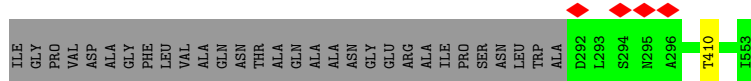
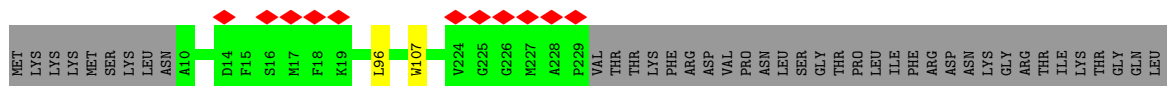
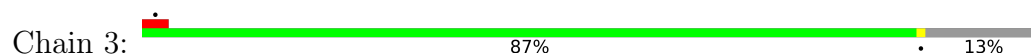
Chain 1:  87% 13%



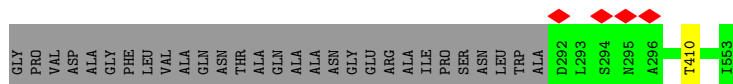
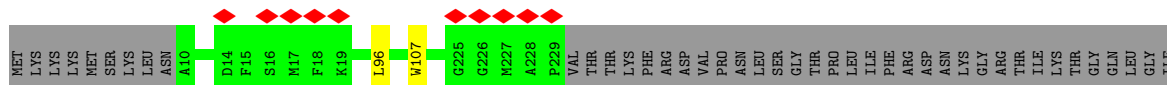
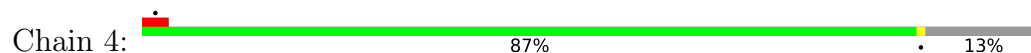
- Molecule 1: Capsid protein VP1



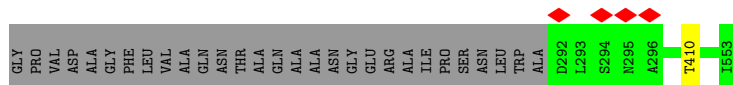
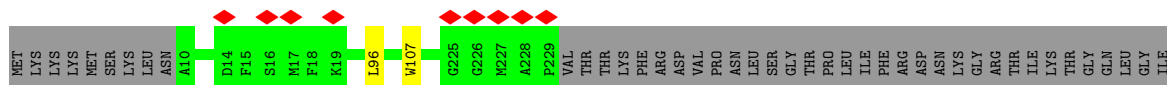
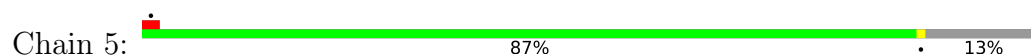
- Molecule 1: Capsid protein VP1




- Molecule 1: Capsid protein VP1

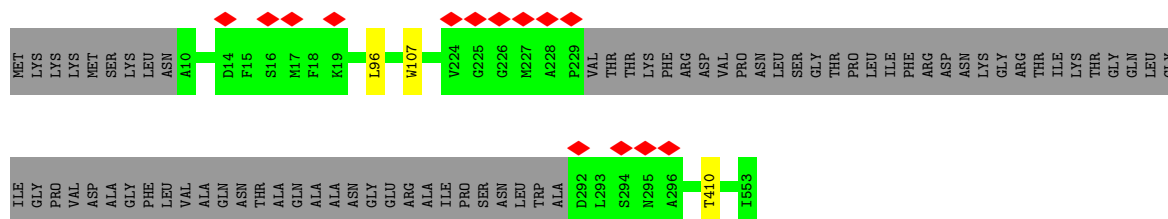


- Molecule 1: Capsid protein VP1




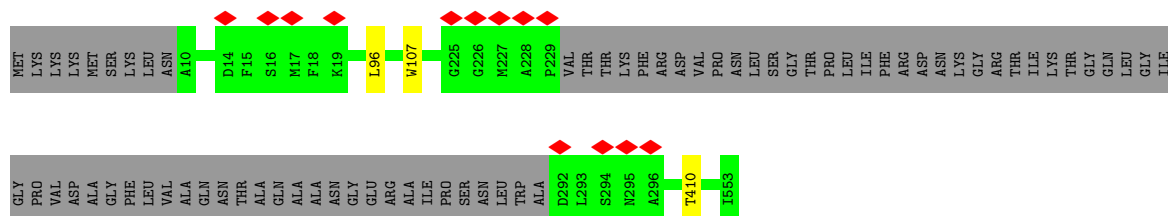
- Molecule 1: Capsid protein VP1

Chain 6:  87% 13%




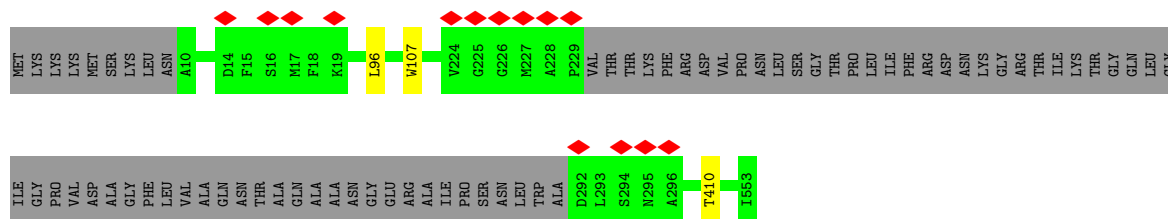
• Molecule 1: Capsid protein VP1

Chain 7:  87% 13%




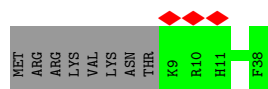
• Molecule 1: Capsid protein VP1

Chain 8:  87% 13%




• Molecule 2: DNA binding protein ORF8

Chain 0:  8% 79% 21%




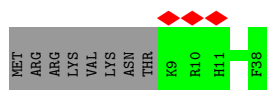
• Molecule 2: DNA binding protein ORF8

Chain 9:  8% 79% 21%

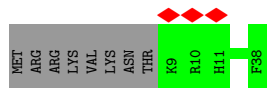
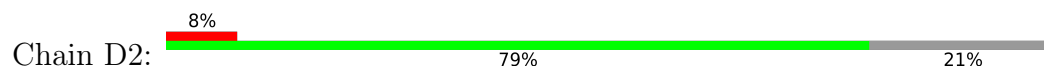


• Molecule 2: DNA binding protein ORF8

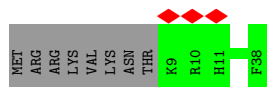
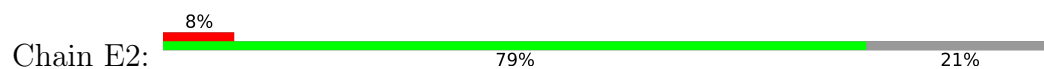
Chain C2:  8% 79% 21%



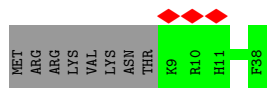
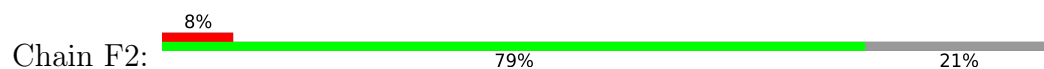
- Molecule 2: DNA binding protein ORF8



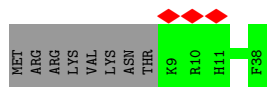
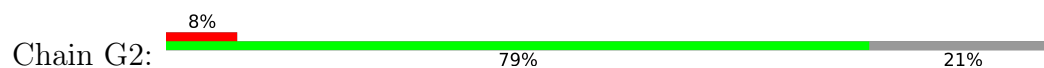
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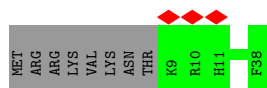
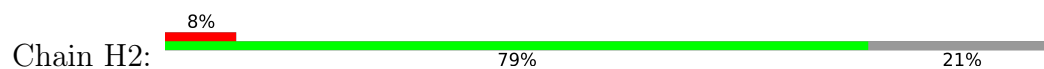
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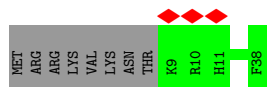
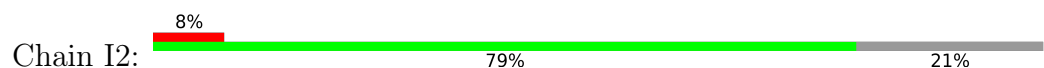
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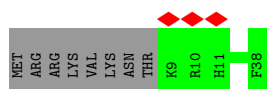
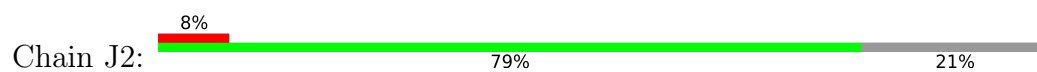
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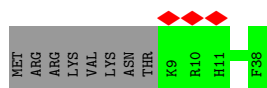
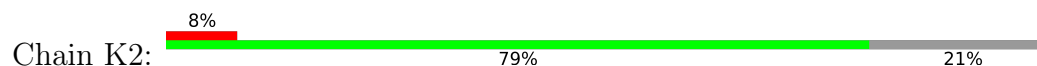
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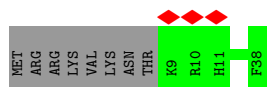
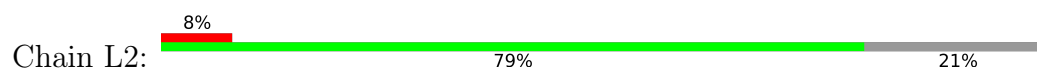
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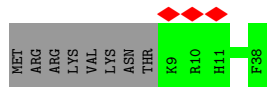
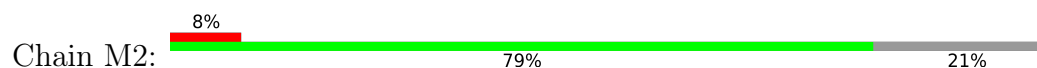
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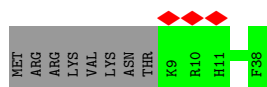
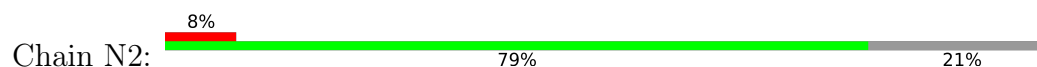
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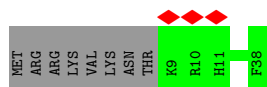
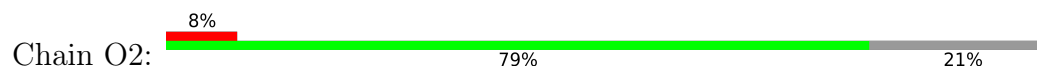
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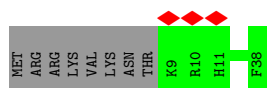
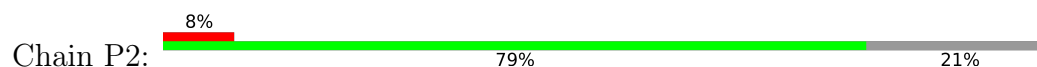
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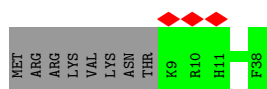
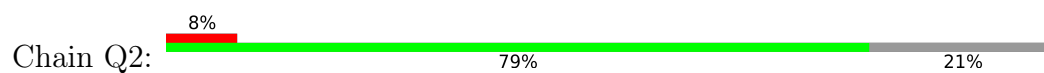
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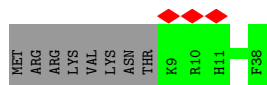
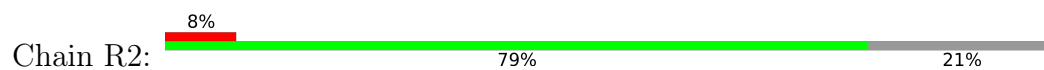
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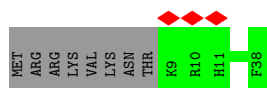
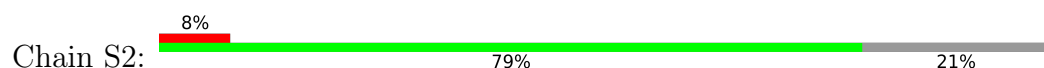
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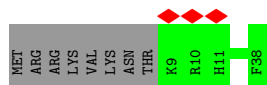
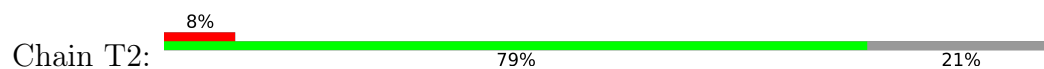
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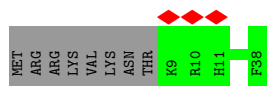
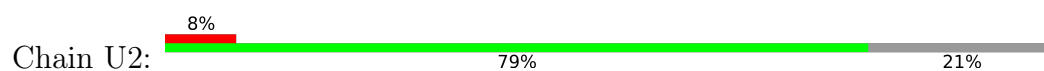
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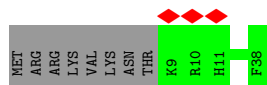
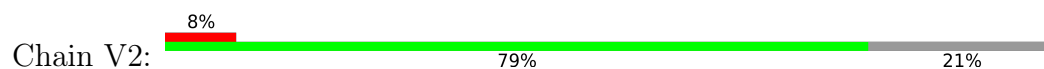
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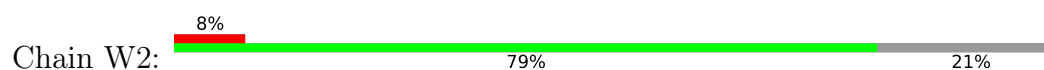
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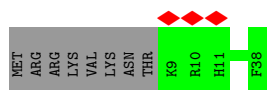


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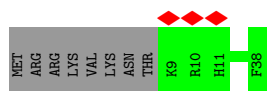
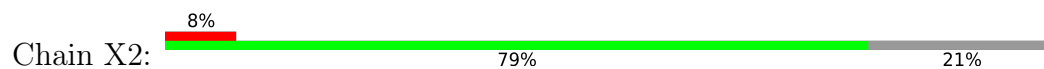


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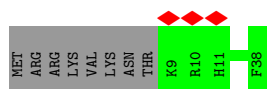
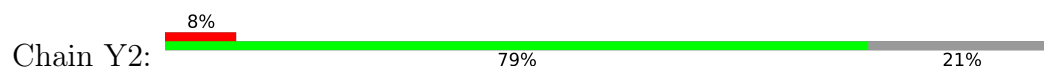




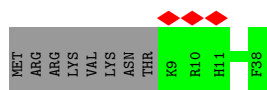
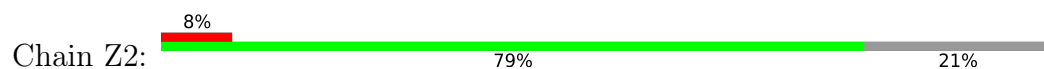
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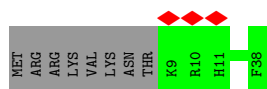
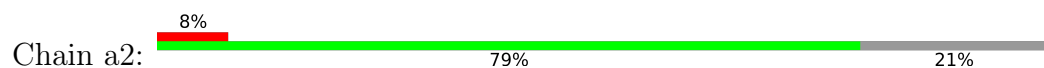
- Molecule 2: DNA binding protein ORF8



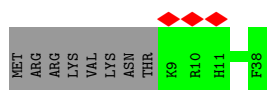
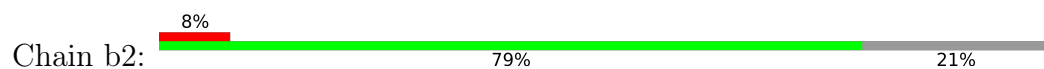
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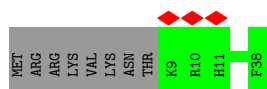
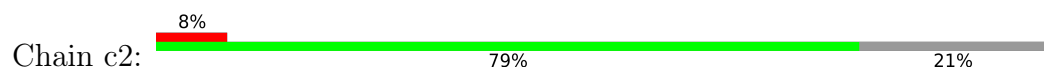
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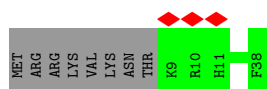
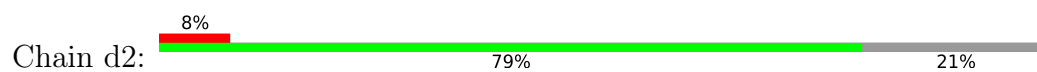
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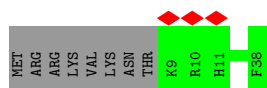
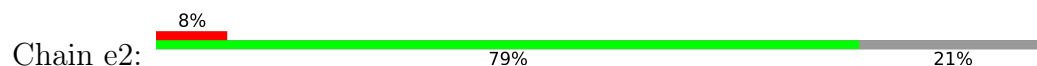
- Molecule 2: DNA binding protein ORF8



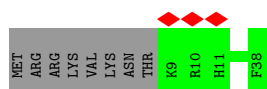
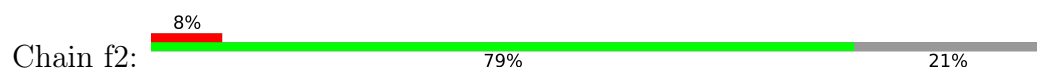
- Molecule 2: DNA binding protein ORF8



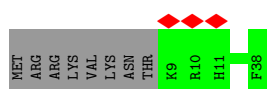
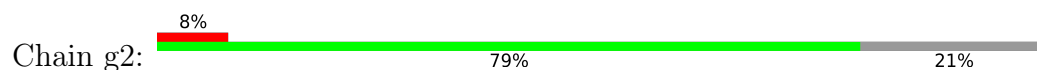
- Molecule 2: DNA binding protein ORF8



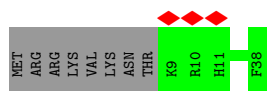
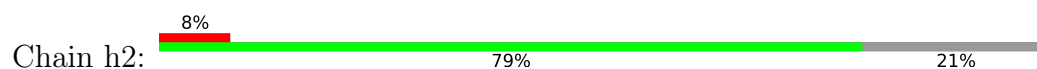
- Molecule 2: DNA binding protein ORF8



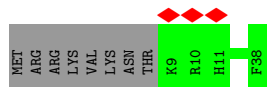
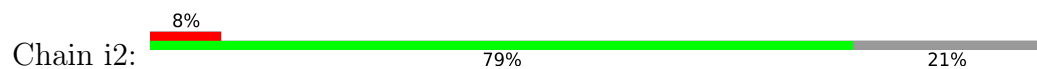
- Molecule 2: DNA binding protein ORF8



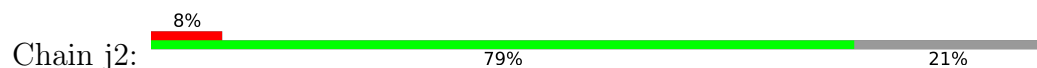
- Molecule 2: DNA binding protein ORF8



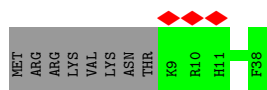
- Molecule 2: DNA binding protein ORF8



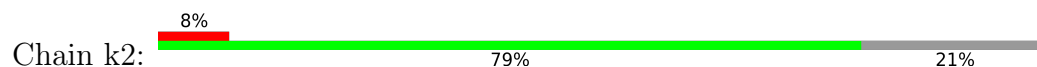
- Molecule 2: DNA binding protein ORF8



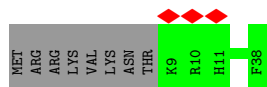
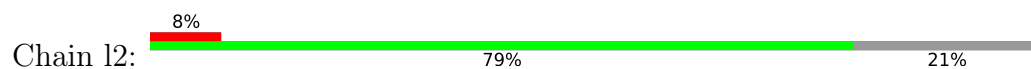




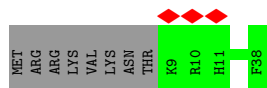
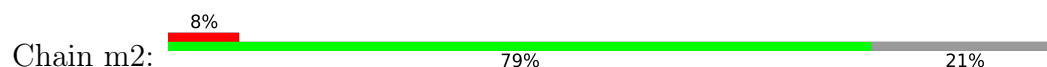
- Molecule 2: DNA binding protein ORF8



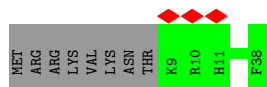
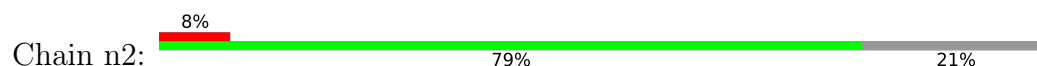
- Molecule 2: DNA binding protein ORF8



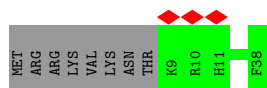
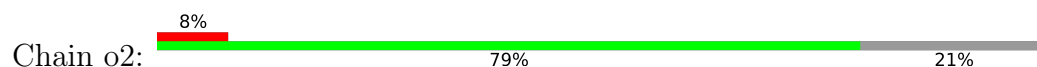
- Molecule 2: DNA binding protein ORF8



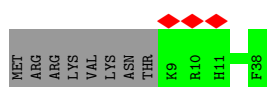
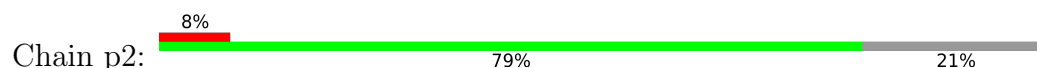
- Molecule 2: DNA binding protein ORF8



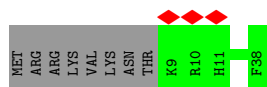
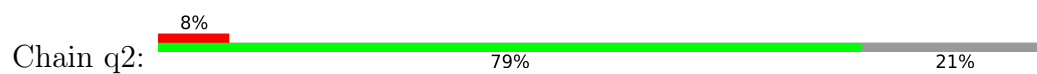
- Molecule 2: DNA binding protein ORF8



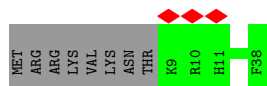
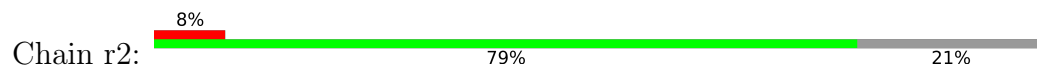
- Molecule 2: DNA binding protein ORF8



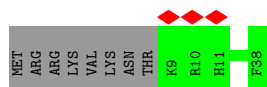
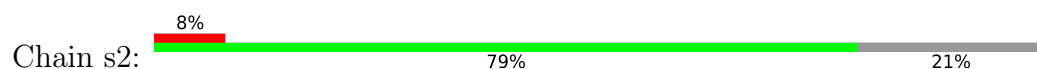
- Molecule 2: DNA binding protein ORF8



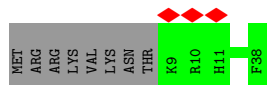
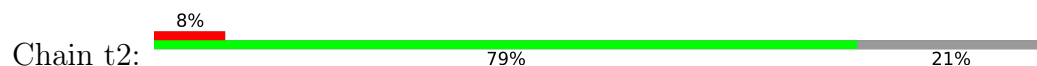
- Molecule 2: DNA binding protein ORF8



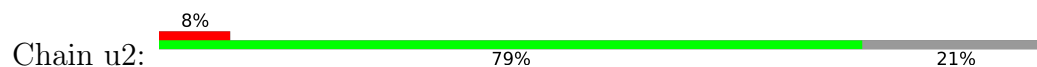
- Molecule 2: DNA binding protein ORF8



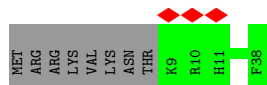
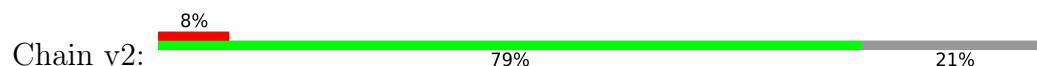
- Molecule 2: DNA binding protein ORF8



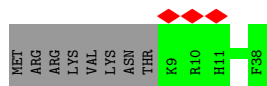
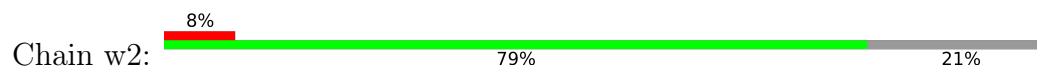
- Molecule 2: DNA binding protein ORF8



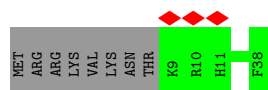
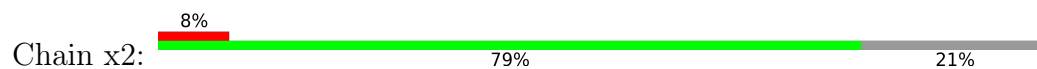
- Molecule 2: DNA binding protein ORF8



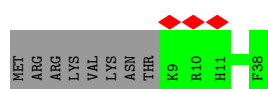
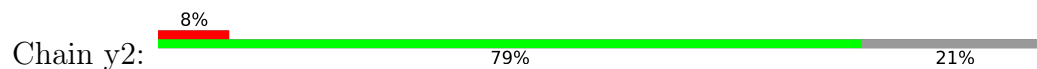
- Molecule 2: DNA binding protein ORF8



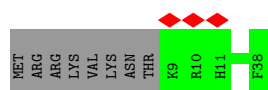
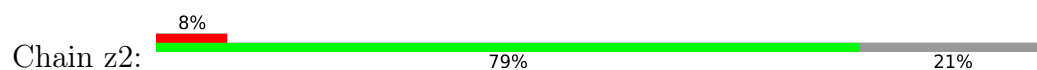
- Molecule 2: DNA binding protein ORF8



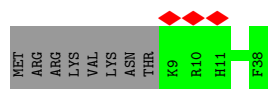
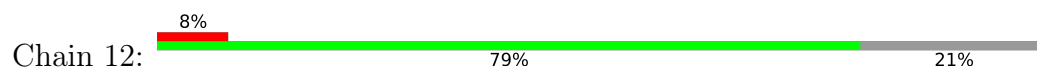
- Molecule 2: DNA binding protein ORF8



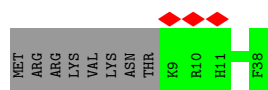
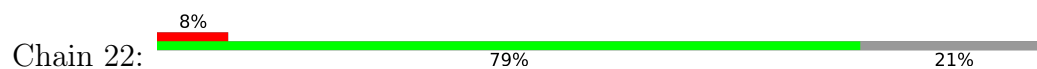
- Molecule 2: DNA binding protein ORF8



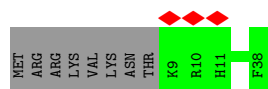
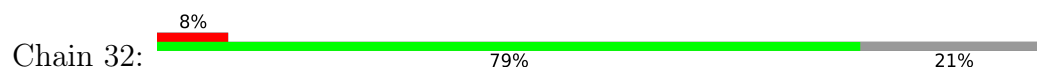
- Molecule 2: DNA binding protein ORF8



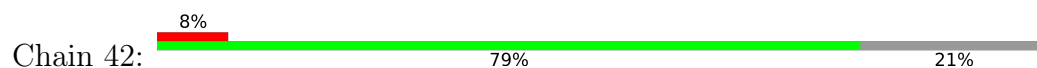
- Molecule 2: DNA binding protein ORF8

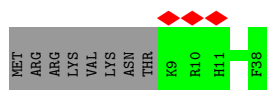


- Molecule 2: DNA binding protein ORF8

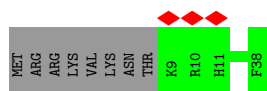
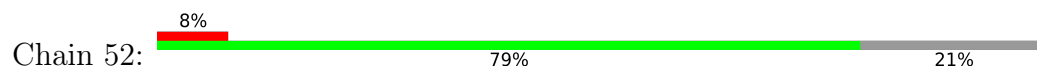


- Molecule 2: DNA binding protein ORF8

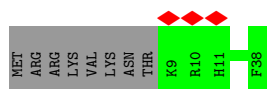
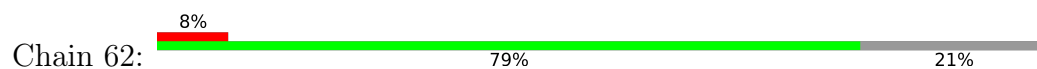




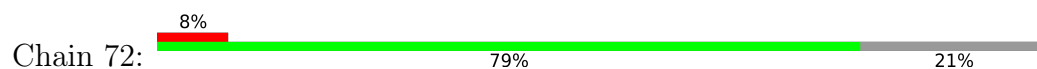
- Molecule 2: DNA binding protein ORF8



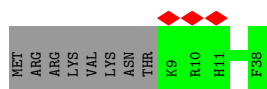
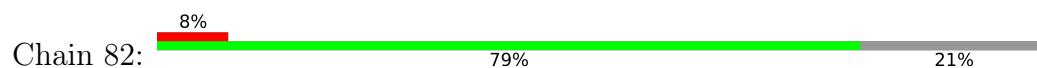
- Molecule 2: DNA binding protein ORF8



- Molecule 2: DNA binding protein ORF8



- Molecule 2: DNA binding protein ORF8



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	77204	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.707	Depositor
Minimum map value	-14.782	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	583.55, 583.55, 583.55	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.46	0/3961	0.54	0/5385
1	2	0.46	0/3961	0.54	0/5385
1	3	0.46	0/3961	0.54	0/5385
1	4	0.46	0/3961	0.54	0/5385
1	5	0.46	0/3961	0.54	0/5385
1	6	0.46	0/3961	0.54	0/5385
1	7	0.46	0/3961	0.54	0/5385
1	8	0.46	0/3961	0.54	0/5385
1	A	0.46	0/3961	0.54	0/5385
1	B	0.46	0/3961	0.54	0/5385
1	C	0.46	0/3961	0.54	0/5385
1	D	0.46	0/3961	0.54	0/5385
1	E	0.46	0/3961	0.54	0/5385
1	F	0.46	0/3961	0.54	0/5385
1	G	0.46	0/3961	0.54	0/5385
1	H	0.46	0/3961	0.54	0/5385
1	I	0.45	0/3961	0.54	0/5385
1	J	0.46	0/3961	0.54	0/5385
1	K	0.46	0/3961	0.54	0/5385
1	L	0.46	0/3961	0.54	0/5385
1	M	0.46	0/3961	0.54	0/5385
1	N	0.46	0/3961	0.54	0/5385
1	O	0.46	0/3961	0.54	0/5385
1	P	0.46	0/3961	0.54	0/5385
1	Q	0.46	0/3961	0.54	0/5385
1	R	0.46	0/3961	0.54	0/5385
1	S	0.46	0/3961	0.54	0/5385
1	T	0.46	0/3961	0.54	0/5385
1	U	0.46	0/3961	0.54	0/5385
1	V	0.46	0/3961	0.54	0/5385
1	W	0.46	0/3961	0.54	0/5385
1	X	0.46	0/3961	0.54	0/5385
1	Y	0.46	0/3961	0.54	0/5385
1	Z	0.46	0/3961	0.54	0/5385

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.46	0/3961	0.54	0/5385
1	b	0.46	0/3961	0.54	0/5385
1	c	0.46	0/3961	0.54	0/5385
1	d	0.46	0/3961	0.54	0/5385
1	e	0.46	0/3961	0.54	0/5385
1	f	0.46	0/3961	0.54	0/5385
1	g	0.46	0/3961	0.54	0/5385
1	h	0.46	0/3961	0.54	0/5385
1	i	0.46	0/3961	0.54	0/5385
1	j	0.46	0/3961	0.54	0/5385
1	k	0.46	0/3961	0.54	0/5385
1	l	0.46	0/3961	0.54	0/5385
1	m	0.46	0/3961	0.54	0/5385
1	n	0.46	0/3961	0.54	0/5385
1	o	0.46	0/3961	0.54	0/5385
1	p	0.46	0/3961	0.54	0/5385
1	q	0.46	0/3961	0.54	0/5385
1	r	0.46	0/3961	0.54	0/5385
1	s	0.46	0/3961	0.54	0/5385
1	t	0.46	0/3961	0.54	0/5385
1	u	0.46	0/3961	0.54	0/5385
1	v	0.46	0/3961	0.54	0/5385
1	w	0.46	0/3961	0.54	0/5385
1	x	0.46	0/3961	0.54	0/5385
1	y	0.46	0/3961	0.54	0/5385
1	z	0.46	0/3961	0.54	0/5385
2	0	0.38	0/260	0.57	0/345
2	12	0.38	0/260	0.57	0/345
2	22	0.38	0/260	0.57	0/345
2	32	0.38	0/260	0.58	0/345
2	42	0.38	0/260	0.57	0/345
2	52	0.38	0/260	0.58	0/345
2	62	0.38	0/260	0.57	0/345
2	72	0.38	0/260	0.57	0/345
2	82	0.37	0/260	0.58	0/345
2	9	0.38	0/260	0.57	0/345
2	C2	0.38	0/260	0.57	0/345
2	D2	0.38	0/260	0.57	0/345
2	E2	0.38	0/260	0.57	0/345
2	F2	0.38	0/260	0.57	0/345
2	G2	0.38	0/260	0.57	0/345
2	H2	0.38	0/260	0.58	0/345
2	I2	0.38	0/260	0.57	0/345

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	J2	0.38	0/260	0.57	0/345
2	K2	0.38	0/260	0.57	0/345
2	L2	0.38	0/260	0.57	0/345
2	M2	0.38	0/260	0.57	0/345
2	N2	0.38	0/260	0.57	0/345
2	O2	0.38	0/260	0.57	0/345
2	P2	0.38	0/260	0.58	0/345
2	Q2	0.38	0/260	0.57	0/345
2	R2	0.38	0/260	0.57	0/345
2	S2	0.38	0/260	0.57	0/345
2	T2	0.38	0/260	0.57	0/345
2	U2	0.37	0/260	0.57	0/345
2	V2	0.38	0/260	0.57	0/345
2	W2	0.38	0/260	0.58	0/345
2	X2	0.38	0/260	0.57	0/345
2	Y2	0.38	0/260	0.57	0/345
2	Z2	0.38	0/260	0.57	0/345
2	a2	0.38	0/260	0.57	0/345
2	b2	0.38	0/260	0.58	0/345
2	c2	0.38	0/260	0.58	0/345
2	d2	0.38	0/260	0.57	0/345
2	e2	0.38	0/260	0.57	0/345
2	f2	0.38	0/260	0.58	0/345
2	g2	0.38	0/260	0.57	0/345
2	h2	0.38	0/260	0.57	0/345
2	i2	0.38	0/260	0.57	0/345
2	j2	0.38	0/260	0.58	0/345
2	k2	0.38	0/260	0.57	0/345
2	l2	0.38	0/260	0.57	0/345
2	m2	0.38	0/260	0.57	0/345
2	n2	0.38	0/260	0.57	0/345
2	o2	0.38	0/260	0.57	0/345
2	p2	0.38	0/260	0.57	0/345
2	q2	0.38	0/260	0.57	0/345
2	r2	0.38	0/260	0.57	0/345
2	s2	0.38	0/260	0.57	0/345
2	t2	0.38	0/260	0.57	0/345
2	u2	0.38	0/260	0.57	0/345
2	v2	0.38	0/260	0.57	0/345
2	w2	0.38	0/260	0.57	0/345
2	x2	0.38	0/260	0.57	0/345
2	y2	0.38	0/260	0.57	0/345
2	z2	0.37	0/260	0.58	0/345



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.45	0/253260	0.54	0/343800

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	2	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	3	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	4	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	5	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	6	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	7	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	8	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	A	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	B	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	C	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	D	478/553 (86%)	467 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	F	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	G	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	H	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	I	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	J	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	K	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	L	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	M	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	N	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	O	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	P	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Q	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	R	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	S	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	T	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	U	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	V	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	W	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	X	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Y	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Z	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	a	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	b	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	c	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	d	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	e	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	f	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	g	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	h	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	i	478/553 (86%)	467 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	k	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	l	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	m	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	n	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	o	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	p	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	q	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	r	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	s	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	t	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	u	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	v	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	w	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	x	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	y	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	z	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
2	0	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	12	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	22	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	32	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	42	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	52	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	62	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	72	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	82	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	9	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	C2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	D2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	E2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	F2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	H2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	I2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	J2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	K2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	L2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	M2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	N2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	O2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	P2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Q2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	R2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	S2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	T2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	U2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	V2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	W2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	X2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Y2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Z2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	a2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	b2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	c2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	d2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	e2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	f2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	g2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	h2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	i2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	j2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	k2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	m2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	n2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	o2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	p2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	q2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	r2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	s2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	t2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	u2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	v2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	w2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	x2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	y2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	z2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
All	All	30360/35460 (86%)	29620 (98%)	740 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	2	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	3	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	4	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	5	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	6	420/478 (88%)	417 (99%)	3 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	8	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	A	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	B	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	C	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	D	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	E	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	F	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	G	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	H	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	I	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	J	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	K	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	L	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	M	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	N	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	O	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	P	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Q	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	R	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	S	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	T	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	U	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	V	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	W	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	X	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Y	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Z	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	a	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	b	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	c	420/478 (88%)	417 (99%)	3 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	e	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	f	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	g	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	h	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	i	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	j	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	k	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	l	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	m	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	n	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	o	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	p	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	q	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	r	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	s	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	t	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	u	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	v	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	w	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	x	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	y	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	z	420/478 (88%)	417 (99%)	3 (1%)	84	93
2	0	26/34 (76%)	26 (100%)	0	100	100
2	12	26/34 (76%)	26 (100%)	0	100	100
2	22	26/34 (76%)	26 (100%)	0	100	100
2	32	26/34 (76%)	26 (100%)	0	100	100
2	42	26/34 (76%)	26 (100%)	0	100	100
2	52	26/34 (76%)	26 (100%)	0	100	100
2	62	26/34 (76%)	26 (100%)	0	100	100
2	72	26/34 (76%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	82	26/34 (76%)	26 (100%)	0	100	100
2	9	26/34 (76%)	26 (100%)	0	100	100
2	C2	26/34 (76%)	26 (100%)	0	100	100
2	D2	26/34 (76%)	26 (100%)	0	100	100
2	E2	26/34 (76%)	26 (100%)	0	100	100
2	F2	26/34 (76%)	26 (100%)	0	100	100
2	G2	26/34 (76%)	26 (100%)	0	100	100
2	H2	26/34 (76%)	26 (100%)	0	100	100
2	I2	26/34 (76%)	26 (100%)	0	100	100
2	J2	26/34 (76%)	26 (100%)	0	100	100
2	K2	26/34 (76%)	26 (100%)	0	100	100
2	L2	26/34 (76%)	26 (100%)	0	100	100
2	M2	26/34 (76%)	26 (100%)	0	100	100
2	N2	26/34 (76%)	26 (100%)	0	100	100
2	O2	26/34 (76%)	26 (100%)	0	100	100
2	P2	26/34 (76%)	26 (100%)	0	100	100
2	Q2	26/34 (76%)	26 (100%)	0	100	100
2	R2	26/34 (76%)	26 (100%)	0	100	100
2	S2	26/34 (76%)	26 (100%)	0	100	100
2	T2	26/34 (76%)	26 (100%)	0	100	100
2	U2	26/34 (76%)	26 (100%)	0	100	100
2	V2	26/34 (76%)	26 (100%)	0	100	100
2	W2	26/34 (76%)	26 (100%)	0	100	100
2	X2	26/34 (76%)	26 (100%)	0	100	100
2	Y2	26/34 (76%)	26 (100%)	0	100	100
2	Z2	26/34 (76%)	26 (100%)	0	100	100
2	a2	26/34 (76%)	26 (100%)	0	100	100
2	b2	26/34 (76%)	26 (100%)	0	100	100
2	c2	26/34 (76%)	26 (100%)	0	100	100
2	d2	26/34 (76%)	26 (100%)	0	100	100
2	e2	26/34 (76%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f2	26/34 (76%)	26 (100%)	0	100	100
2	g2	26/34 (76%)	26 (100%)	0	100	100
2	h2	26/34 (76%)	26 (100%)	0	100	100
2	i2	26/34 (76%)	26 (100%)	0	100	100
2	j2	26/34 (76%)	26 (100%)	0	100	100
2	k2	26/34 (76%)	26 (100%)	0	100	100
2	l2	26/34 (76%)	26 (100%)	0	100	100
2	m2	26/34 (76%)	26 (100%)	0	100	100
2	n2	26/34 (76%)	26 (100%)	0	100	100
2	o2	26/34 (76%)	26 (100%)	0	100	100
2	p2	26/34 (76%)	26 (100%)	0	100	100
2	q2	26/34 (76%)	26 (100%)	0	100	100
2	r2	26/34 (76%)	26 (100%)	0	100	100
2	s2	26/34 (76%)	26 (100%)	0	100	100
2	t2	26/34 (76%)	26 (100%)	0	100	100
2	u2	26/34 (76%)	26 (100%)	0	100	100
2	v2	26/34 (76%)	26 (100%)	0	100	100
2	w2	26/34 (76%)	26 (100%)	0	100	100
2	x2	26/34 (76%)	26 (100%)	0	100	100
2	y2	26/34 (76%)	26 (100%)	0	100	100
2	z2	26/34 (76%)	26 (100%)	0	100	100
All	All	26760/30720 (87%)	26580 (99%)	180 (1%)	84	93

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	107	TRP
1	A	410	THR
1	B	96	LEU
1	B	107	TRP
1	B	410	THR
1	C	96	LEU
1	C	107	TRP
1	C	410	THR

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Mol	Chain	Res	Type
1	D	96	LEU
1	D	107	TRP
1	D	410	THR
1	E	96	LEU
1	E	107	TRP
1	E	410	THR
1	F	96	LEU
1	F	107	TRP
1	F	410	THR
1	G	96	LEU
1	G	107	TRP
1	G	410	THR
1	H	96	LEU
1	H	107	TRP
1	H	410	THR
1	I	96	LEU
1	I	107	TRP
1	I	410	THR
1	J	96	LEU
1	J	107	TRP
1	J	410	THR
1	K	96	LEU
1	K	107	TRP
1	K	410	THR
1	L	96	LEU
1	L	107	TRP
1	L	410	THR
1	M	96	LEU
1	M	107	TRP
1	M	410	THR
1	N	96	LEU
1	N	107	TRP
1	N	410	THR
1	O	96	LEU
1	O	107	TRP
1	O	410	THR
1	P	96	LEU
1	P	107	TRP
1	P	410	THR
1	Q	96	LEU
1	Q	107	TRP
1	Q	410	THR

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Mol	Chain	Res	Type
1	R	96	LEU
1	R	107	TRP
1	R	410	THR
1	S	96	LEU
1	S	107	TRP
1	S	410	THR
1	T	96	LEU
1	T	107	TRP
1	T	410	THR
1	U	96	LEU
1	U	107	TRP
1	U	410	THR
1	V	96	LEU
1	V	107	TRP
1	V	410	THR
1	W	96	LEU
1	W	107	TRP
1	W	410	THR
1	X	96	LEU
1	X	107	TRP
1	X	410	THR
1	Y	96	LEU
1	Y	107	TRP
1	Y	410	THR
1	Z	96	LEU
1	Z	107	TRP
1	Z	410	THR
1	a	96	LEU
1	a	107	TRP
1	a	410	THR
1	b	96	LEU
1	b	107	TRP
1	b	410	THR
1	c	96	LEU
1	c	107	TRP
1	c	410	THR
1	d	96	LEU
1	d	107	TRP
1	d	410	THR
1	e	96	LEU
1	e	107	TRP
1	e	410	THR

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Mol	Chain	Res	Type
1	f	96	LEU
1	f	107	TRP
1	f	410	THR
1	g	96	LEU
1	g	107	TRP
1	g	410	THR
1	h	96	LEU
1	h	107	TRP
1	h	410	THR
1	i	96	LEU
1	i	107	TRP
1	i	410	THR
1	j	96	LEU
1	j	107	TRP
1	j	410	THR
1	k	96	LEU
1	k	107	TRP
1	k	410	THR
1	l	96	LEU
1	l	107	TRP
1	l	410	THR
1	m	96	LEU
1	m	107	TRP
1	m	410	THR
1	n	96	LEU
1	n	107	TRP
1	n	410	THR
1	o	96	LEU
1	o	107	TRP
1	o	410	THR
1	p	96	LEU
1	p	107	TRP
1	p	410	THR
1	q	96	LEU
1	q	107	TRP
1	q	410	THR
1	r	96	LEU
1	r	107	TRP
1	r	410	THR
1	s	96	LEU
1	s	107	TRP
1	s	410	THR

*Continued on next page...*

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Mol	Chain	Res	Type
1	t	96	LEU
1	t	107	TRP
1	t	410	THR
1	u	96	LEU
1	u	107	TRP
1	u	410	THR
1	v	96	LEU
1	v	107	TRP
1	v	410	THR
1	w	96	LEU
1	w	107	TRP
1	w	410	THR
1	x	96	LEU
1	x	107	TRP
1	x	410	THR
1	y	96	LEU
1	y	107	TRP
1	y	410	THR
1	z	96	LEU
1	z	107	TRP
1	z	410	THR
1	1	96	LEU
1	1	107	TRP
1	1	410	THR
1	2	96	LEU
1	2	107	TRP
1	2	410	THR
1	3	96	LEU
1	3	107	TRP
1	3	410	THR
1	4	96	LEU
1	4	107	TRP
1	4	410	THR
1	5	96	LEU
1	5	107	TRP
1	5	410	THR
1	6	96	LEU
1	6	107	TRP
1	6	410	THR
1	7	96	LEU
1	7	107	TRP
1	7	410	THR

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Mol	Chain	Res	Type
1	8	96	LEU
1	8	107	TRP
1	8	410	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (368) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	56	HIS
1	A	342	GLN
1	A	396	HIS
1	A	412	GLN
2	0	17	HIS
1	B	29	HIS
1	B	56	HIS
1	B	342	GLN
1	B	396	HIS
1	B	412	GLN
1	C	29	HIS
1	C	56	HIS
1	C	342	GLN
1	C	396	HIS
1	C	412	GLN
1	D	29	HIS
1	D	56	HIS
1	D	342	GLN
1	D	396	HIS
1	D	412	GLN
1	E	29	HIS
1	E	56	HIS
1	E	342	GLN
1	E	396	HIS
1	E	412	GLN
1	F	29	HIS
1	F	56	HIS
1	F	342	GLN
1	F	396	HIS
1	F	412	GLN
1	G	29	HIS
1	G	56	HIS
1	G	342	GLN
1	G	396	HIS

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Mol	Chain	Res	Type
1	H	29	HIS
1	H	56	HIS
1	H	342	GLN
1	H	396	HIS
1	H	412	GLN
1	I	29	HIS
1	I	56	HIS
1	I	342	GLN
1	I	396	HIS
1	I	412	GLN
1	J	29	HIS
1	J	56	HIS
1	J	342	GLN
1	J	396	HIS
1	J	412	GLN
1	K	29	HIS
1	K	56	HIS
1	K	164	GLN
1	K	342	GLN
1	K	396	HIS
1	K	412	GLN
1	L	29	HIS
1	L	56	HIS
1	L	342	GLN
1	L	396	HIS
1	L	412	GLN
1	M	29	HIS
1	M	56	HIS
1	M	342	GLN
1	M	396	HIS
1	M	412	GLN
1	N	29	HIS
1	N	56	HIS
1	N	342	GLN
1	N	396	HIS
1	N	412	GLN
1	O	29	HIS
1	O	56	HIS
1	O	342	GLN
1	O	396	HIS
1	O	412	GLN
1	P	29	HIS

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Mol	Chain	Res	Type
1	P	56	HIS
1	P	342	GLN
1	P	396	HIS
1	P	412	GLN
1	Q	29	HIS
1	Q	56	HIS
1	Q	342	GLN
1	Q	396	HIS
1	Q	412	GLN
1	R	29	HIS
1	R	56	HIS
1	R	164	GLN
1	R	342	GLN
1	R	396	HIS
1	R	412	GLN
1	S	29	HIS
1	S	56	HIS
1	S	164	GLN
1	S	342	GLN
1	S	396	HIS
1	T	29	HIS
1	T	56	HIS
1	T	164	GLN
1	T	342	GLN
1	T	396	HIS
1	T	412	GLN
1	U	29	HIS
1	U	56	HIS
1	U	342	GLN
1	U	396	HIS
1	U	412	GLN
1	V	29	HIS
1	V	56	HIS
1	V	164	GLN
1	V	342	GLN
1	V	396	HIS
1	V	412	GLN
1	W	29	HIS
1	W	56	HIS
1	W	342	GLN
1	W	396	HIS
1	W	412	GLN

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Mol	Chain	Res	Type
1	X	29	HIS
1	X	56	HIS
1	X	342	GLN
1	X	396	HIS
1	X	412	GLN
1	Y	29	HIS
1	Y	56	HIS
1	Y	342	GLN
1	Y	396	HIS
1	Y	412	GLN
1	Z	29	HIS
1	Z	56	HIS
1	Z	164	GLN
1	Z	342	GLN
1	Z	396	HIS
1	Z	412	GLN
1	a	29	HIS
1	a	56	HIS
1	a	342	GLN
1	a	396	HIS
1	a	412	GLN
1	b	29	HIS
1	b	56	HIS
1	b	342	GLN
1	b	396	HIS
1	b	412	GLN
1	c	29	HIS
1	c	56	HIS
1	c	342	GLN
1	c	396	HIS
1	c	412	GLN
1	d	29	HIS
1	d	56	HIS
1	d	342	GLN
1	d	396	HIS
1	d	412	GLN
1	e	29	HIS
1	e	56	HIS
1	e	342	GLN
1	e	396	HIS
1	e	412	GLN
1	f	29	HIS

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Mol	Chain	Res	Type
1	f	56	HIS
1	f	342	GLN
1	f	396	HIS
1	f	412	GLN
1	g	29	HIS
1	g	56	HIS
1	g	342	GLN
1	g	396	HIS
1	g	412	GLN
1	h	29	HIS
1	h	56	HIS
1	h	342	GLN
1	h	396	HIS
1	h	412	GLN
1	i	29	HIS
1	i	56	HIS
1	i	164	GLN
1	i	342	GLN
1	i	396	HIS
1	i	412	GLN
1	j	29	HIS
1	j	56	HIS
1	j	342	GLN
1	j	396	HIS
1	j	412	GLN
1	k	29	HIS
1	k	56	HIS
1	k	342	GLN
1	k	396	HIS
1	k	412	GLN
1	l	29	HIS
1	l	56	HIS
1	l	342	GLN
1	l	396	HIS
1	l	412	GLN
1	m	29	HIS
1	m	56	HIS
1	m	164	GLN
1	m	342	GLN
1	m	396	HIS
1	m	412	GLN
1	n	29	HIS

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Mol	Chain	Res	Type
1	n	56	HIS
1	n	342	GLN
1	n	396	HIS
1	n	412	GLN
1	o	29	HIS
1	o	56	HIS
1	o	342	GLN
1	o	396	HIS
1	o	412	GLN
1	p	29	HIS
1	p	56	HIS
1	p	164	GLN
1	p	342	GLN
1	p	396	HIS
1	p	412	GLN
1	q	29	HIS
1	q	56	HIS
1	q	342	GLN
1	q	396	HIS
1	q	412	GLN
1	r	29	HIS
1	r	56	HIS
1	r	164	GLN
1	r	342	GLN
1	r	396	HIS
1	s	29	HIS
1	s	56	HIS
1	s	342	GLN
1	s	396	HIS
1	s	412	GLN
1	t	29	HIS
1	t	56	HIS
1	t	342	GLN
1	t	396	HIS
1	u	29	HIS
1	u	56	HIS
1	u	342	GLN
1	u	396	HIS
1	u	412	GLN
1	v	29	HIS
1	v	56	HIS
1	v	342	GLN

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Mol	Chain	Res	Type
1	v	396	HIS
1	v	412	GLN
1	v	449	GLN
1	w	29	HIS
1	w	56	HIS
1	w	342	GLN
1	w	396	HIS
1	w	412	GLN
1	x	29	HIS
1	x	56	HIS
1	x	342	GLN
1	x	396	HIS
1	x	412	GLN
1	y	29	HIS
1	y	56	HIS
1	y	342	GLN
1	y	396	HIS
1	y	412	GLN
1	z	29	HIS
1	z	56	HIS
1	z	342	GLN
1	z	396	HIS
1	z	412	GLN
1	1	29	HIS
1	1	56	HIS
1	1	342	GLN
1	1	396	HIS
1	1	412	GLN
1	2	29	HIS
1	2	56	HIS
1	2	342	GLN
1	2	396	HIS
1	2	412	GLN
1	3	29	HIS
1	3	56	HIS
1	3	342	GLN
1	3	396	HIS
1	3	412	GLN
1	4	29	HIS
1	4	56	HIS
1	4	342	GLN
1	4	396	HIS

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Mol	Chain	Res	Type
1	4	412	GLN
1	5	29	HIS
1	5	56	HIS
1	5	164	GLN
1	5	342	GLN
1	5	396	HIS
1	5	412	GLN
1	6	29	HIS
1	6	56	HIS
1	6	342	GLN
1	6	396	HIS
1	6	412	GLN
1	7	29	HIS
1	7	56	HIS
1	7	342	GLN
1	7	396	HIS
1	7	412	GLN
1	8	29	HIS
1	8	56	HIS
1	8	164	GLN
1	8	342	GLN
1	8	396	HIS
2	9	17	HIS
2	C2	17	HIS
2	D2	17	HIS
2	E2	17	HIS
2	F2	17	HIS
2	G2	17	HIS
2	H2	17	HIS
2	I2	17	HIS
2	J2	17	HIS
2	K2	17	HIS
2	L2	17	HIS
2	M2	17	HIS
2	N2	17	HIS
2	O2	17	HIS
2	P2	17	HIS
2	Q2	17	HIS
2	R2	17	HIS
2	S2	17	HIS
2	T2	17	HIS
2	U2	17	HIS

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Mol	Chain	Res	Type
2	V2	17	HIS
2	W2	17	HIS
2	X2	17	HIS
2	Y2	17	HIS
2	Z2	17	HIS
2	a2	17	HIS
2	b2	17	HIS
2	c2	17	HIS
2	d2	17	HIS
2	e2	17	HIS
2	f2	17	HIS
2	g2	17	HIS
2	h2	17	HIS
2	i2	17	HIS
2	j2	17	HIS
2	k2	17	HIS
2	l2	17	HIS
2	m2	17	HIS
2	n2	17	HIS
2	o2	17	HIS
2	p2	17	HIS
2	q2	17	HIS
2	r2	17	HIS
2	s2	17	HIS
2	t2	17	HIS
2	u2	17	HIS
2	v2	17	HIS
2	w2	17	HIS
2	x2	17	HIS
2	y2	17	HIS
2	z2	17	HIS
2	12	17	HIS
2	22	17	HIS
2	32	17	HIS
2	42	17	HIS
2	52	17	HIS
2	62	17	HIS
2	72	17	HIS
2	82	17	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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

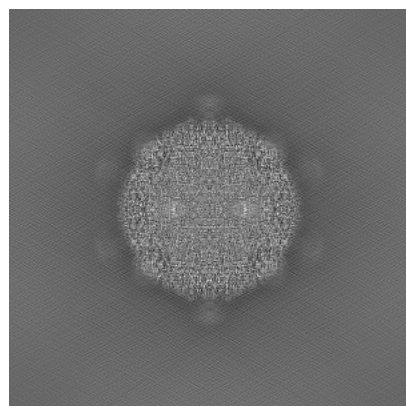
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45583. These allow visual inspection of the internal detail of the map and identification of artifacts.

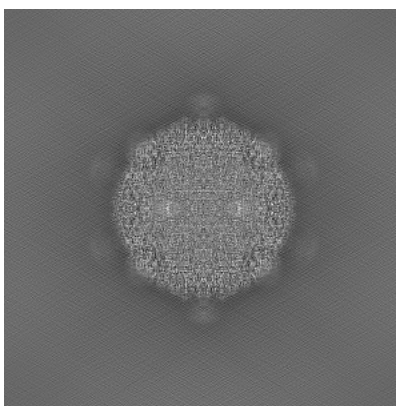
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

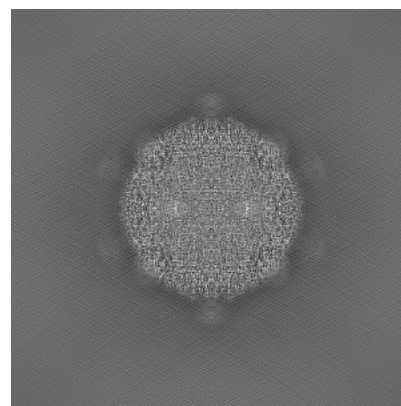
#### 6.1.1 Primary map



X

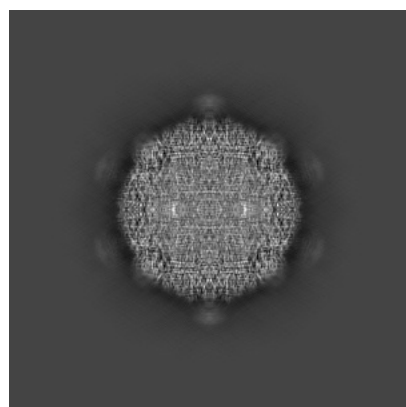


Y

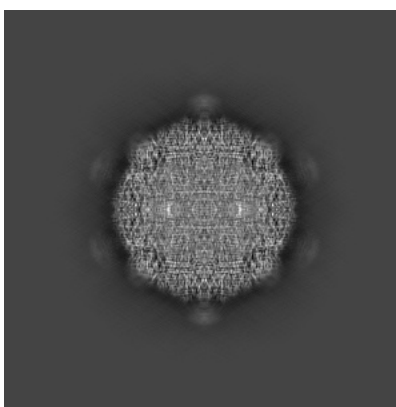


Z

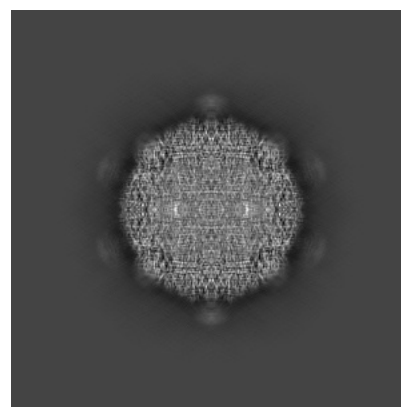
#### 6.1.2 Raw map



X



Y



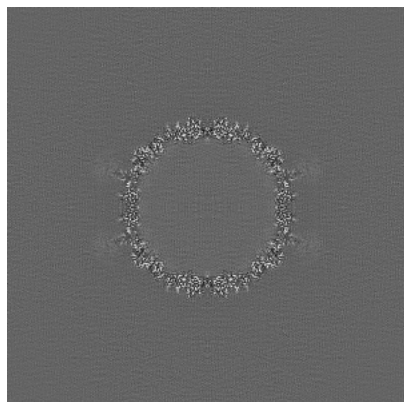
Z

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

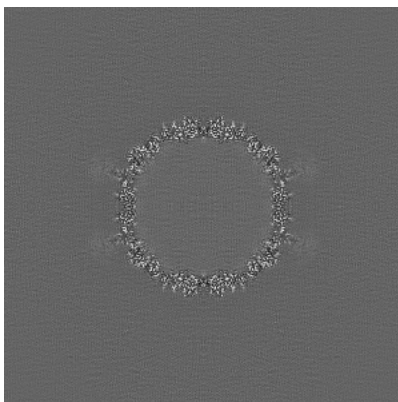


## 6.2 Central slices [i](#)

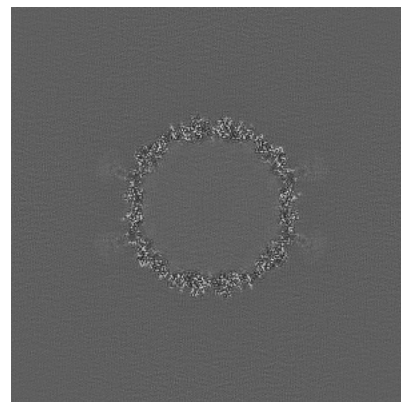
### 6.2.1 Primary map



X Index: 275

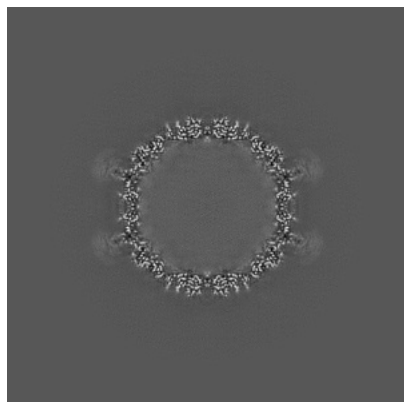


Y Index: 275

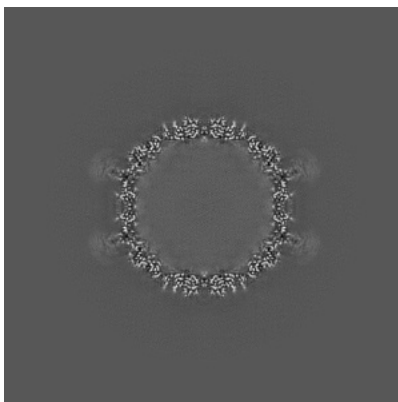


Z Index: 275

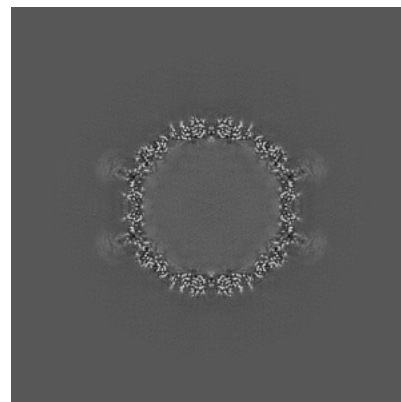
### 6.2.2 Raw map



X Index: 275



Y Index: 275

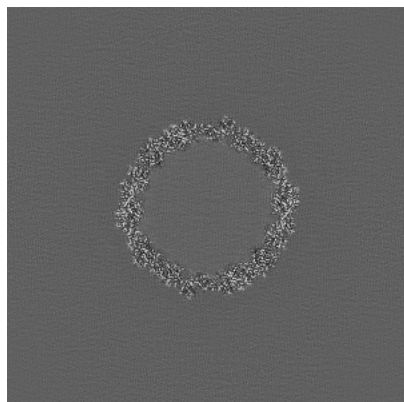


Z Index: 275

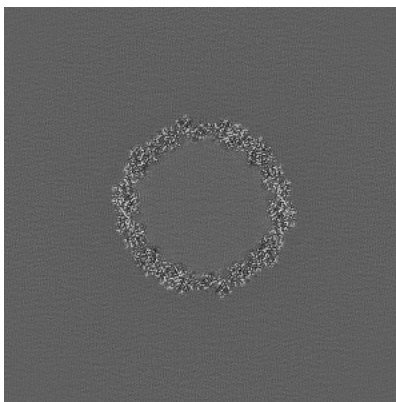
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

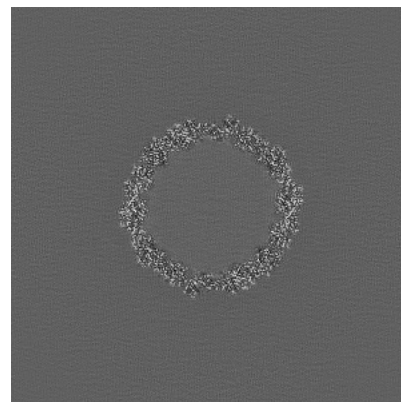
### 6.3.1 Primary map



X Index: 251

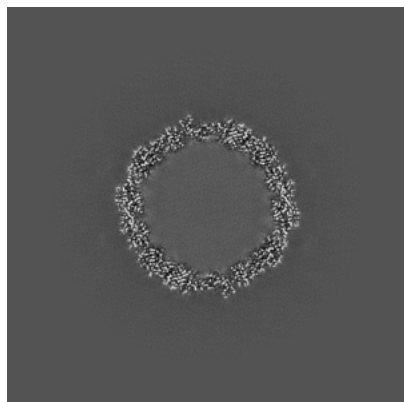


Y Index: 299

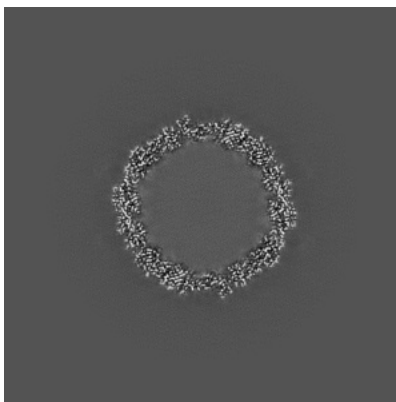


Z Index: 250

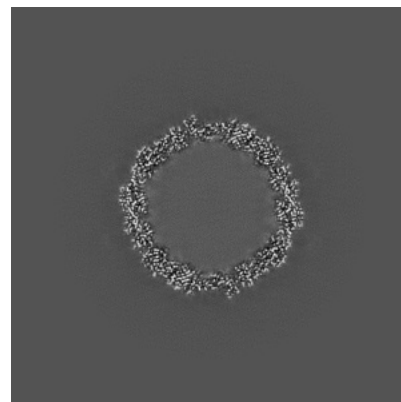
### 6.3.2 Raw map



X Index: 251



Y Index: 251

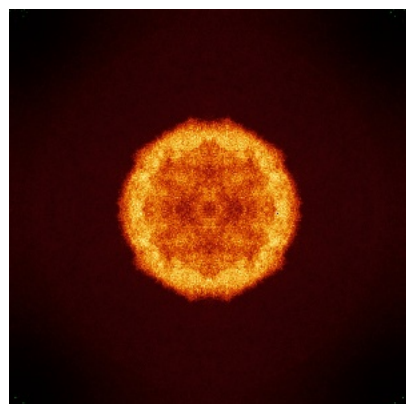


Z Index: 251

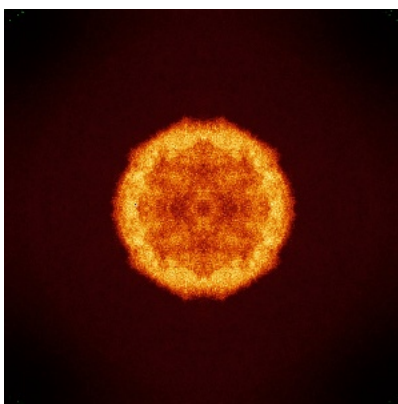
The images above show the largest variance slices of the map in three orthogonal directions.

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

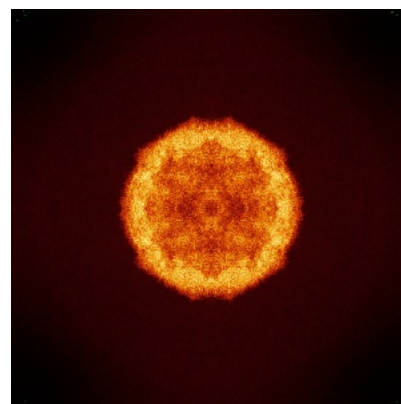
### 6.4.1 Primary map



X

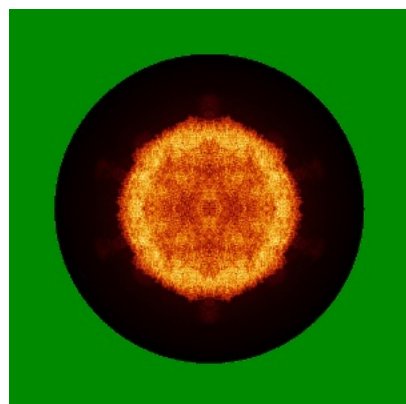


Y

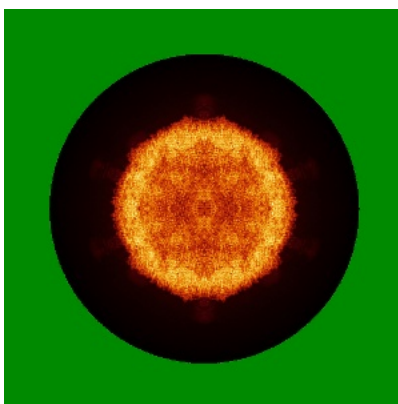


Z

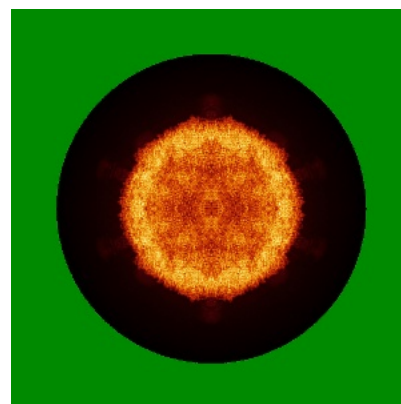
### 6.4.2 Raw map



X



Y

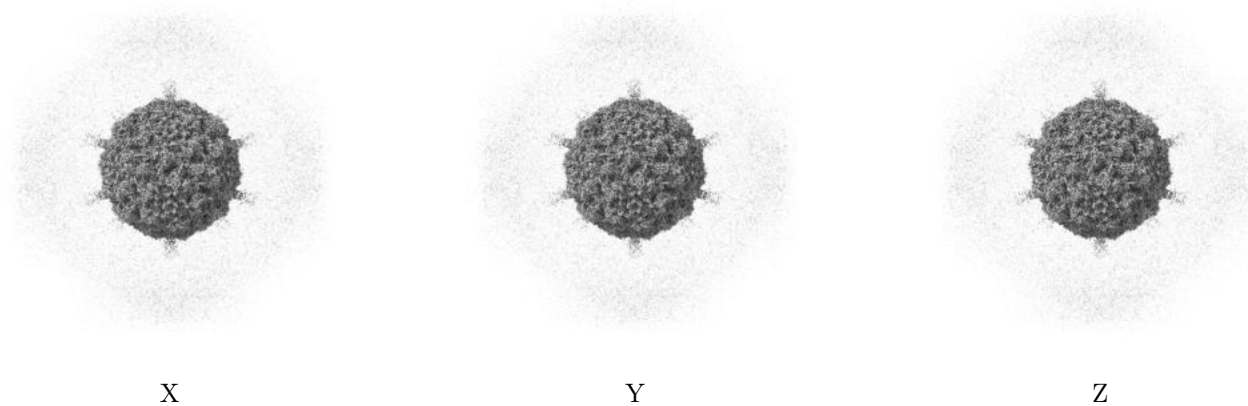


Z

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

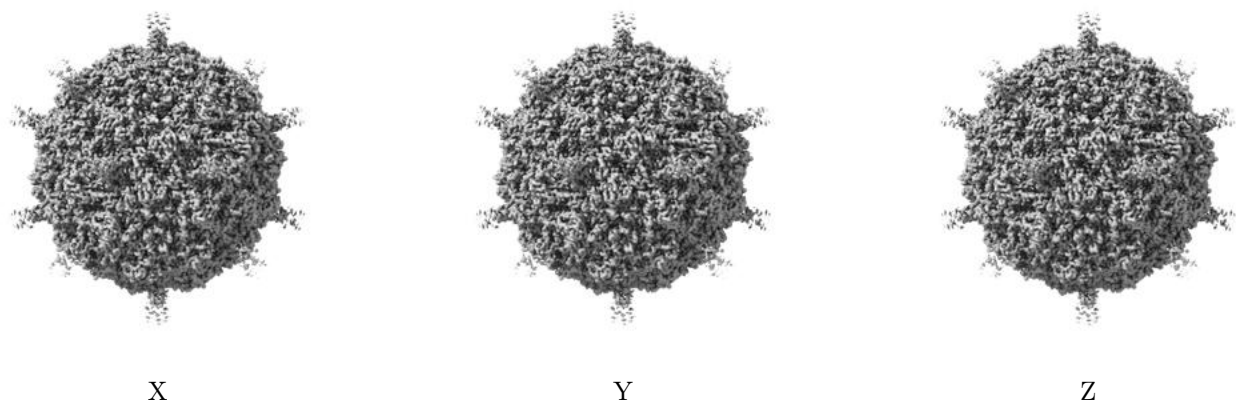
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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.

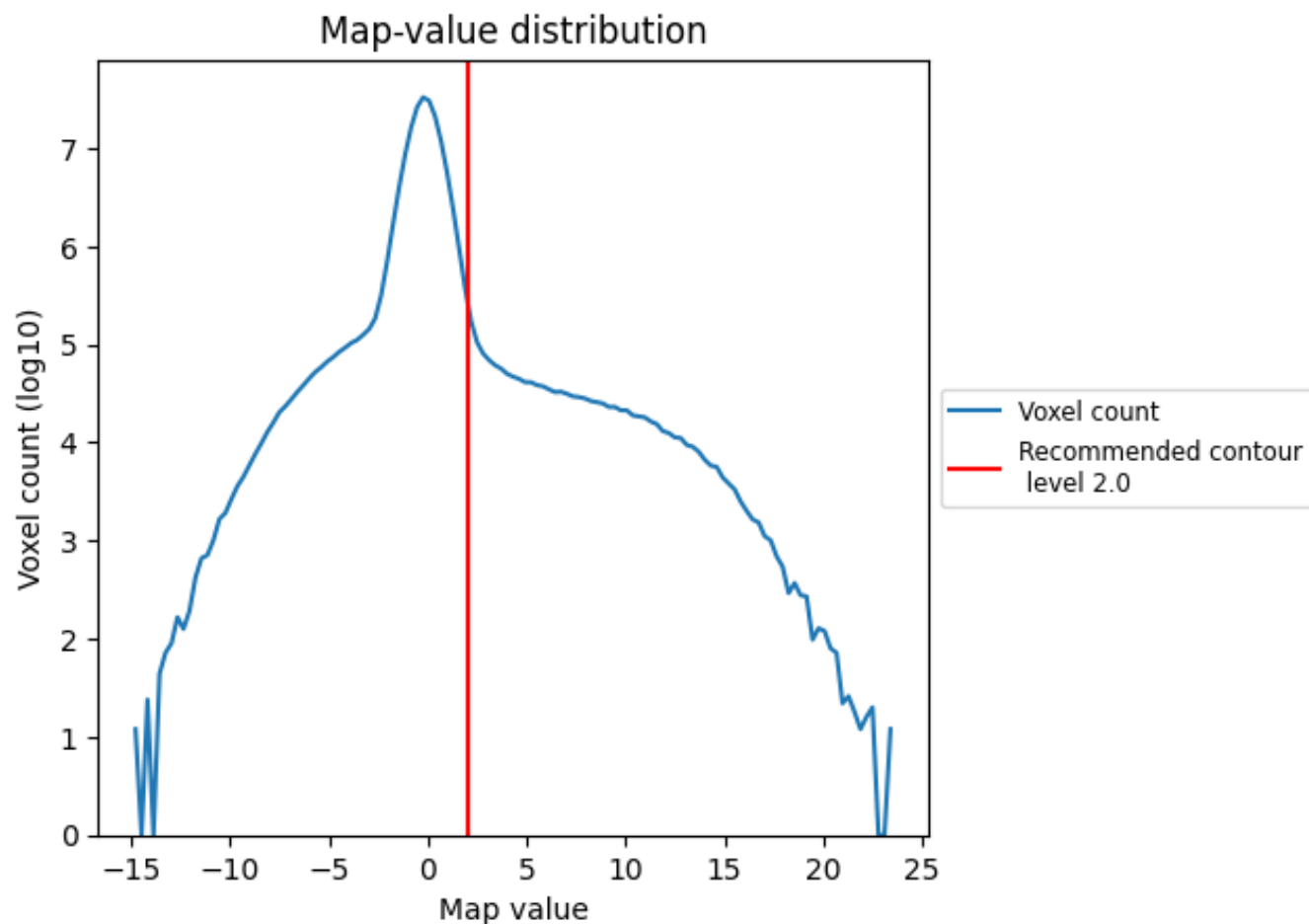
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

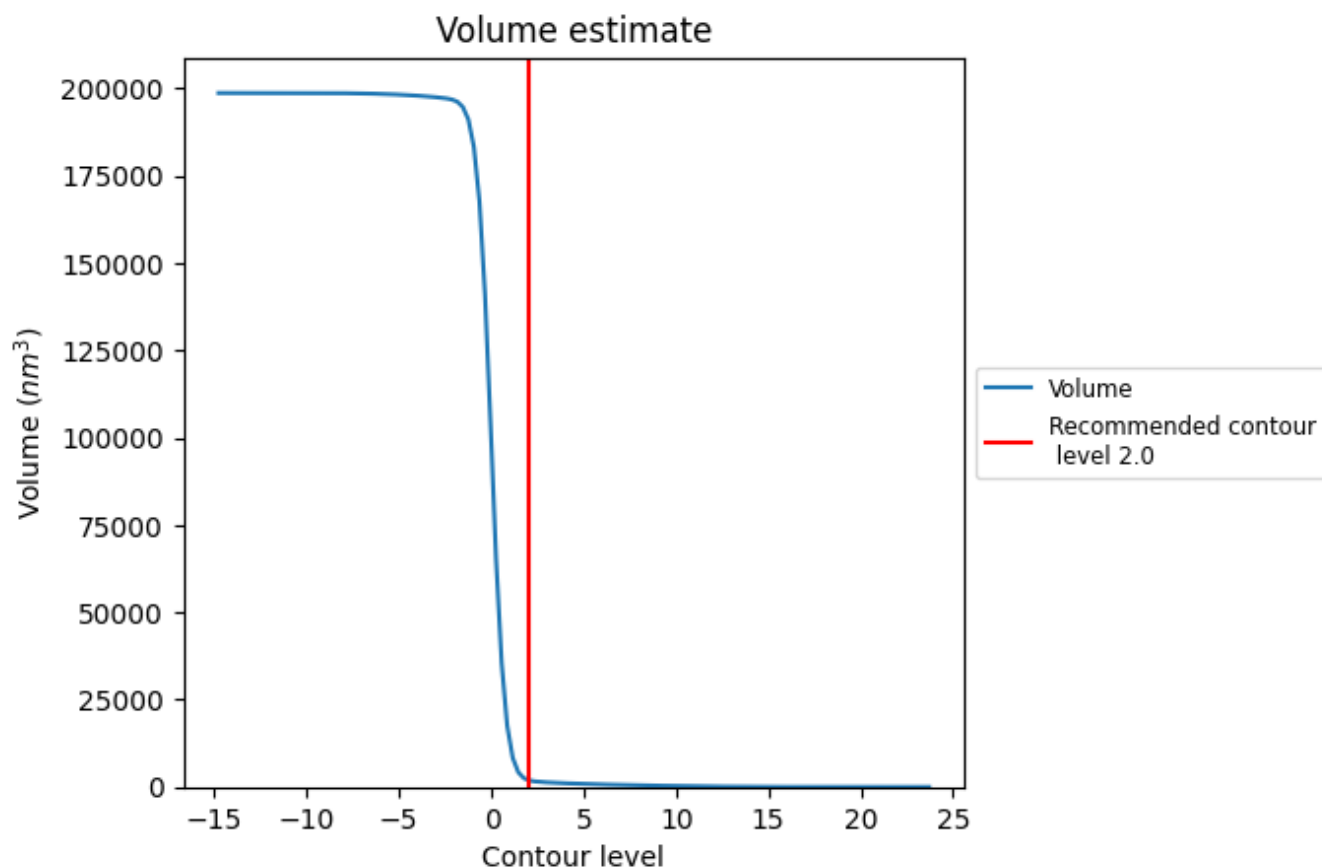
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

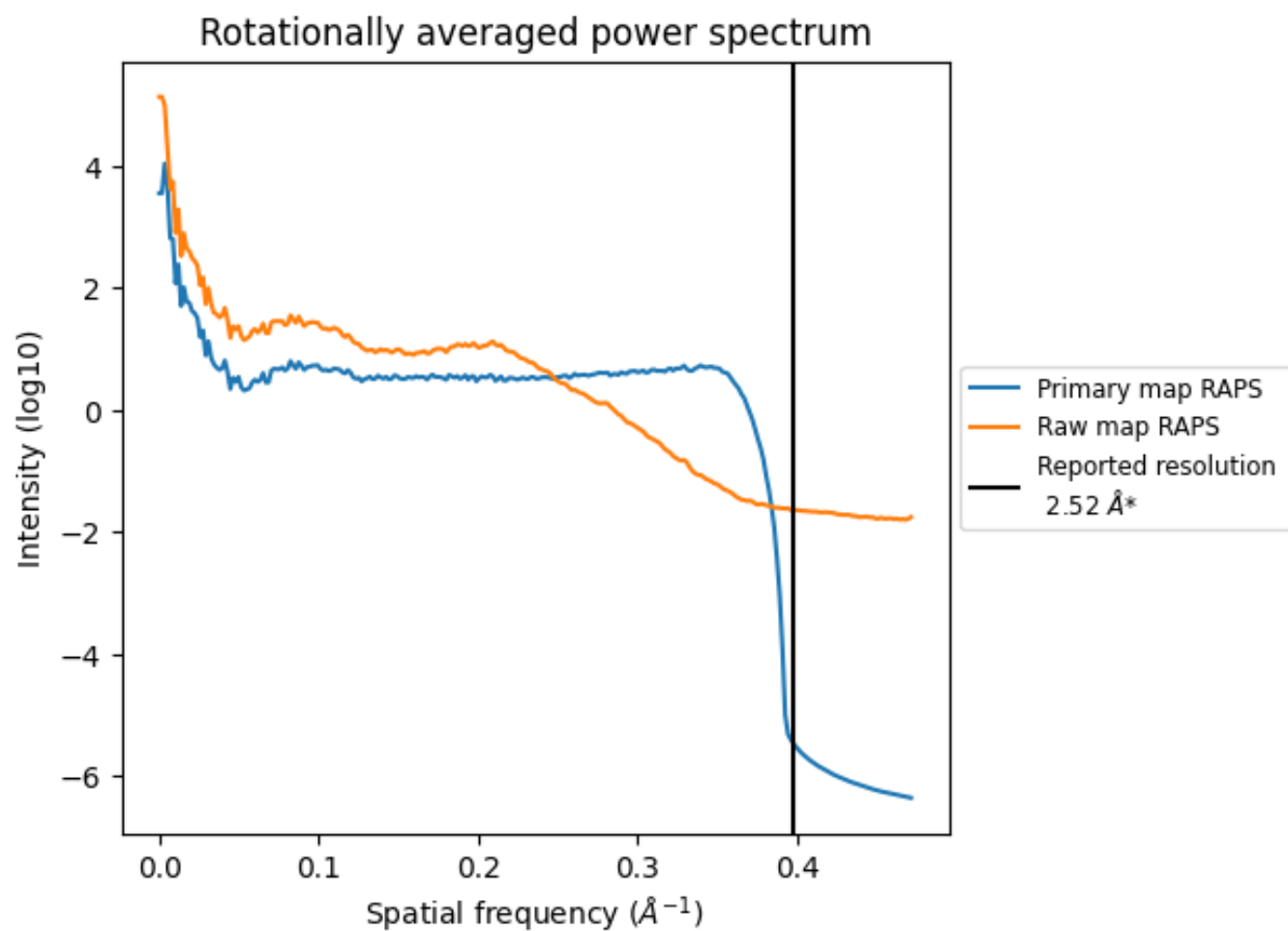
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1990  $\text{nm}^3$ ; this corresponds to an approximate mass of 1798 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 ⓘ



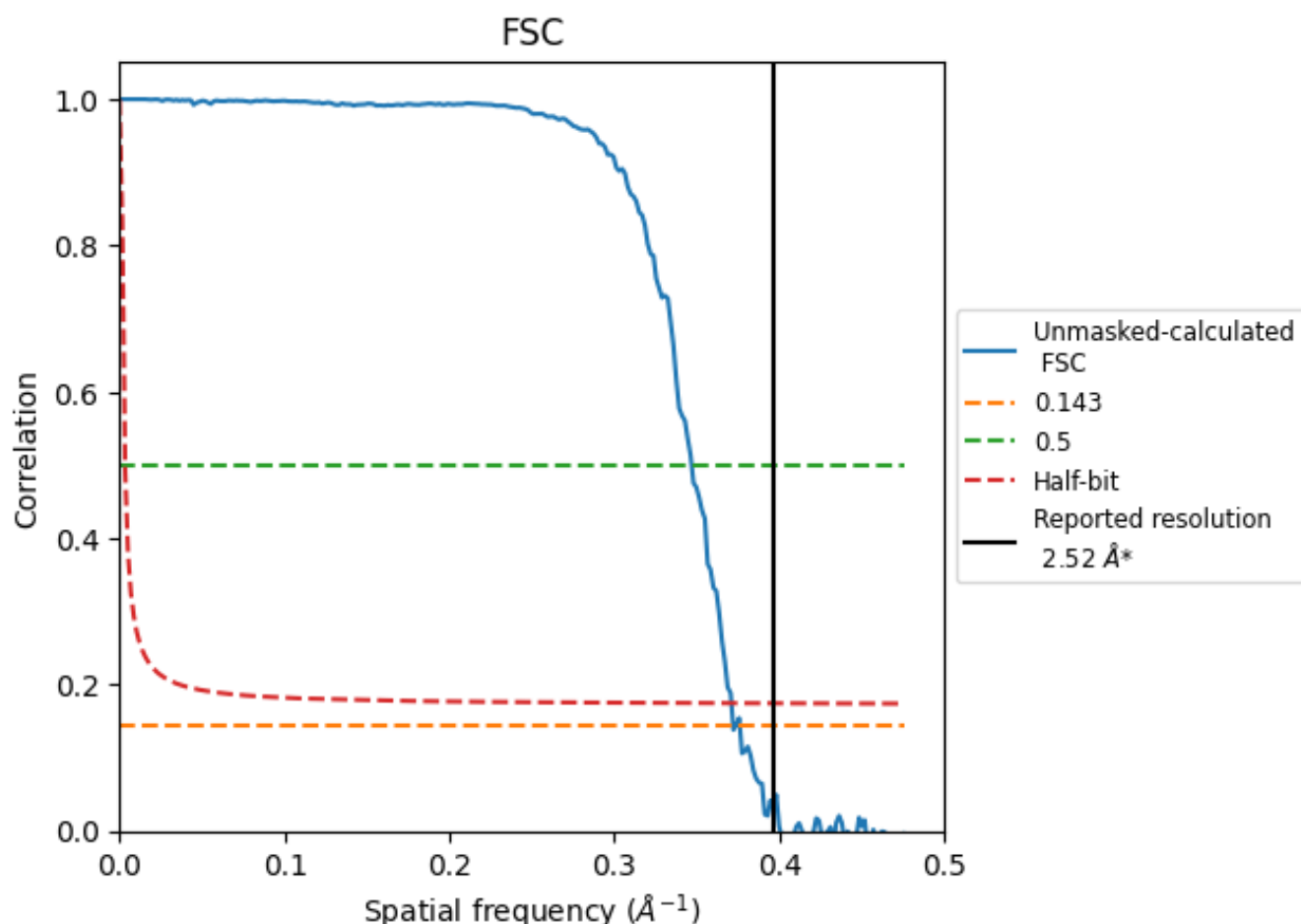
\*Reported resolution corresponds to spatial frequency of 0.397 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.397  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

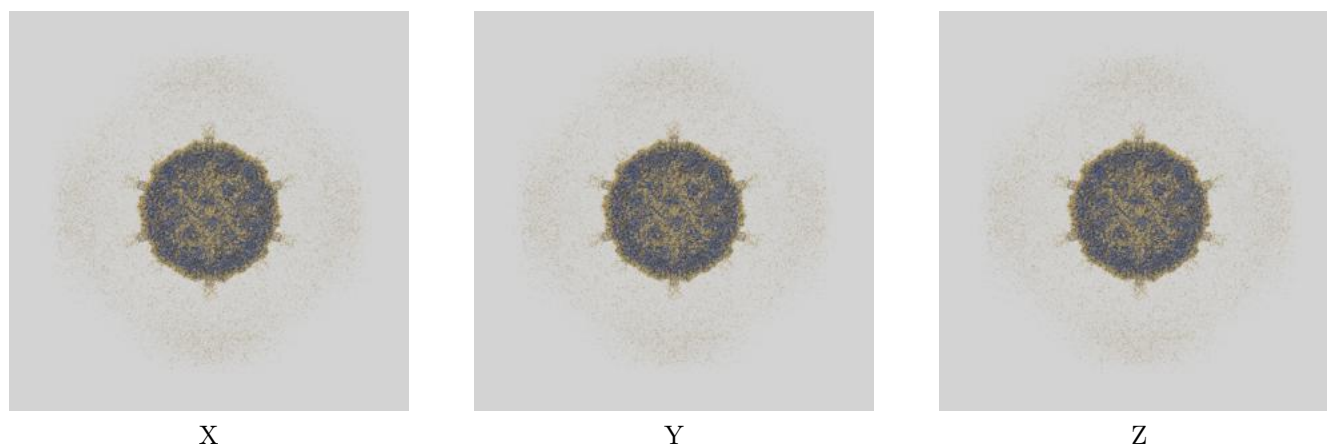
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	2.88	2.70

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

## 9 Map-model fit [i](#)

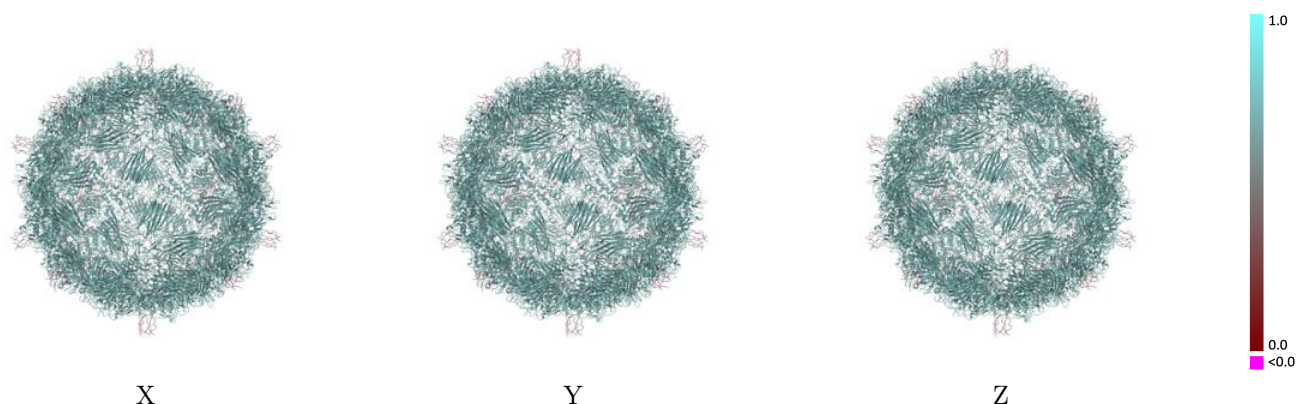
This section contains information regarding the fit between EMDB map EMD-45583 and PDB model 9CGM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



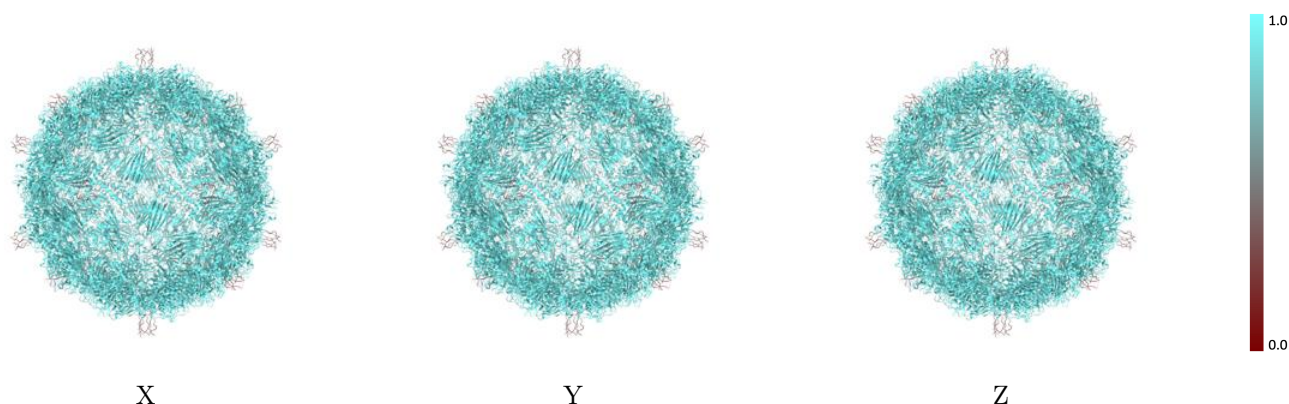
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



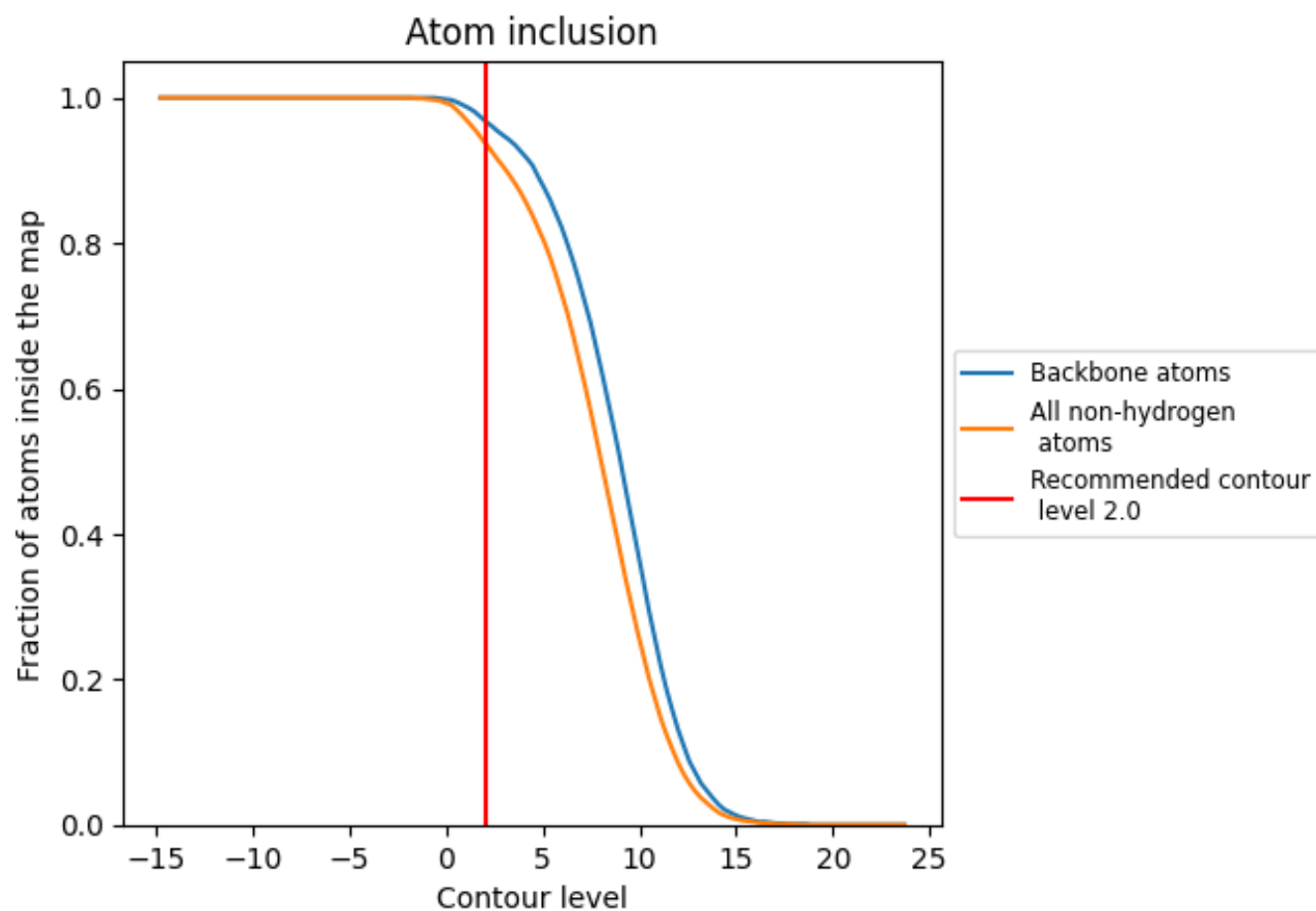
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9380	 0.6470
0	 0.8160	 0.5870
1	 0.9460	 0.6510
12	 0.8120	 0.5890
2	 0.9460	 0.6530
22	 0.8120	 0.5880
3	 0.9450	 0.6510
32	 0.8030	 0.5900
4	 0.9470	 0.6510
42	 0.8070	 0.5860
5	 0.9480	 0.6510
52	 0.8070	 0.5880
6	 0.9470	 0.6510
62	 0.8070	 0.5920
7	 0.9470	 0.6510
72	 0.8070	 0.5900
8	 0.9490	 0.6520
82	 0.7990	 0.5820
9	 0.8120	 0.5850
A	 0.9450	 0.6510
B	 0.9460	 0.6510
C	 0.9470	 0.6510
C2	 0.8070	 0.5850
D	 0.9470	 0.6520
D2	 0.8070	 0.5880
E	 0.9490	 0.6510
E2	 0.7990	 0.5840
F	 0.9450	 0.6510
F2	 0.8030	 0.5860
G	 0.9490	 0.6510
G2	 0.7990	 0.5800
H	 0.9470	 0.6510
H2	 0.8070	 0.5840
I	 0.9470	 0.6500
I2	 0.8070	 0.5810























































































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Chain	Atom inclusion	Q-score
J	 0.9460	 0.6510
J2	 0.8120	 0.5850
K	 0.9470	 0.6520
K2	 0.8070	 0.5840
L	 0.9460	 0.6520
L2	 0.8120	 0.5840
M	 0.9490	 0.6520
M2	 0.7990	 0.5760
N	 0.9470	 0.6510
N2	 0.8070	 0.5870
O	 0.9490	 0.6520
O2	 0.7990	 0.5820
P	 0.9470	 0.6510
P2	 0.8070	 0.5890
Q	 0.9470	 0.6520
Q2	 0.8070	 0.5830
R	 0.9460	 0.6520
R2	 0.8120	 0.5890
S	 0.9460	 0.6510
S2	 0.8120	 0.5860
T	 0.9470	 0.6520
T2	 0.8070	 0.5870
U	 0.9460	 0.6520
U2	 0.8120	 0.5840
V	 0.9470	 0.6510
V2	 0.8070	 0.5880
W	 0.9470	 0.6510
W2	 0.8070	 0.5880
X	 0.9490	 0.6520
X2	 0.7990	 0.5830
Y	 0.9470	 0.6510
Y2	 0.8070	 0.5900
Z	 0.9490	 0.6520
Z2	 0.7990	 0.5820
a	 0.9450	 0.6520
a2	 0.8030	 0.5900
b	 0.9450	 0.6520
b2	 0.8030	 0.5910
c	 0.9450	 0.6510
c2	 0.8030	 0.5900
d	 0.9450	 0.6520
d2	 0.8030	 0.5860




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Chain	Atom inclusion	Q-score
e	 0.9450	 0.6520
e2	 0.8030	 0.5900
f	 0.9450	 0.6520
f2	 0.8030	 0.5920
g	 0.9470	 0.6510
g2	 0.8070	 0.5820
h	 0.9490	 0.6510
h2	 0.7950	 0.5770
i	 0.9470	 0.6520
i2	 0.8070	 0.5870
j	 0.9480	 0.6510
j2	 0.8070	 0.5880
k	 0.9470	 0.6510
k2	 0.8070	 0.5880
l	 0.9490	 0.6520
l2	 0.7990	 0.5820
m	 0.9470	 0.6520
m2	 0.8070	 0.5860
n	 0.9450	 0.6530
n2	 0.8030	 0.5890
o	 0.9490	 0.6510
o2	 0.7990	 0.5800
p	 0.9470	 0.6520
p2	 0.8070	 0.5860
q	 0.9460	 0.6510
q2	 0.8120	 0.5860
r	 0.9460	 0.6500
r2	 0.8120	 0.5880
s	 0.9460	 0.6510
s2	 0.8120	 0.5840
t	 0.9490	 0.6520
t2	 0.7990	 0.5830
u	 0.9470	 0.6510
u2	 0.8070	 0.5840
v	 0.9450	 0.6510
v2	 0.8070	 0.5860
w	 0.9490	 0.6510
w2	 0.7990	 0.5810
x	 0.9470	 0.6500
x2	 0.8070	 0.5840
y	 0.9450	 0.6500
y2	 0.8070	 0.5890

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Chain	Atom inclusion	Q-score
z	 0.9460	 0.6520
z2	 0.8120	 0.5830