



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2024 – 08:48 AM EDT

PDB ID : 7TQS  
EMDB ID : EMD-26068  
Title : Coxsackievirus A21 capsid subdomain in complex with mouse polyclonal antibody pAbC-3  
Authors : Antanasijevic, A.; Ward, A.B.  
Deposited on : 2022-01-26  
Resolution : 3.90 Å(reported)  
Based on initial model : 1Z7S

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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

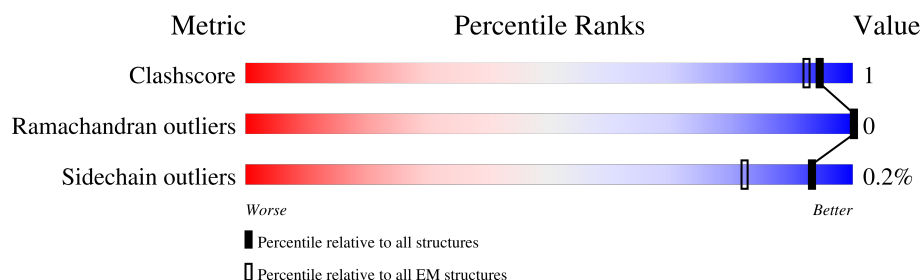
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
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	L	96	<div> <div>95%</div> <div>98%</div> <div>•</div> </div>
2	H	106	<div> <div>66%</div> <div>98%</div> <div>•</div> </div>
3	a	298	<div> <div>67%</div> <div>90%</div> <div>5% 5%</div> </div>
3	e	298	<div> <div>69%</div> <div>89%</div> <div>5% 5%</div> </div>
3	i	298	<div> <div>73%</div> <div>91%</div> <div>• 5%</div> </div>
3	m	298	<div> <div>73%</div> <div>92%</div> <div>• 5%</div> </div>
3	q	298	<div> <div>68%</div> <div>91%</div> <div>• 5%</div> </div>
4	b	272	<div> <div>60%</div> <div>93%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
4	f	272	<div>64%</div> <div>93%</div> <div>• •</div>
4	j	272	<div>76%</div> <div>93%</div> <div>• •</div>
4	n	272	<div>72%</div> <div>92%</div> <div>• 5%</div>
4	r	272	<div>60%</div> <div>92%</div> <div>• 5%</div>
5	c	240	<div>64%</div> <div>97%</div> <div>•</div>
5	g	240	<div>60%</div> <div>96%</div> <div>•</div>
5	k	240	<div>72%</div> <div>95%</div> <div>• •</div>
5	o	240	<div>79%</div> <div>96%</div> <div>•</div>
5	s	240	<div>68%</div> <div>97%</div> <div>•</div>
6	d	69	<div>78%</div> <div>97%</div> <div>• •</div>
6	h	69	<div>78%</div> <div>97%</div> <div>• •</div>
6	l	69	<div>87%</div> <div>97%</div> <div>• •</div>
6	p	69	<div>88%</div> <div>94%</div> <div>• •</div>
6	t	69	<div>83%</div> <div>97%</div> <div>• •</div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 34113 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 pAbC-3 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	L	96	Total	C	N	O	0	0
			480	288	96	96		

- Molecule 2 is a protein called pAbC-3 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	282	Total	C	N	O	S	0	0
			2219	1405	379	425	10		
3	e	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		
3	i	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		
3	m	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		
3	q	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	290	ALA	THR	conflict	UNP Q7T7N6
e	290	ALA	THR	conflict	UNP Q7T7N6
i	290	ALA	THR	conflict	UNP Q7T7N6
m	290	ALA	THR	conflict	UNP Q7T7N6
q	290	ALA	THR	conflict	UNP Q7T7N6

- Molecule 4 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	263	Total	C	N	O	S	0	0
			2044	1301	344	388	11		
4	f	263	Total	C	N	O	S	0	0
			2036	1297	343	384	12		
4	j	261	Total	C	N	O	S	0	0
			2030	1294	342	383	11		
4	n	259	Total	C	N	O	S	0	0
			2013	1282	340	380	11		
4	r	258	Total	C	N	O	S	0	0
			2006	1279	339	377	11		

- Molecule 5 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	240	Total	C	N	O	S	0	0
			1857	1183	309	345	20		
5	g	239	Total	C	N	O	S	0	0
			1848	1178	307	343	20		
5	k	234	Total	C	N	O	S	0	0
			1810	1154	299	337	20		
5	o	239	Total	C	N	O	S	0	0
			1848	1178	307	343	20		
5	s	239	Total	C	N	O	S	0	0
			1848	1178	307	343	20		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	96	HIS	ARG	conflict	UNP Q71LY2
g	96	HIS	ARG	conflict	UNP Q71LY2
k	96	HIS	ARG	conflict	UNP Q71LY2
o	96	HIS	ARG	conflict	UNP Q71LY2
s	96	HIS	ARG	conflict	UNP Q71LY2

- Molecule 6 is a protein called VP4.

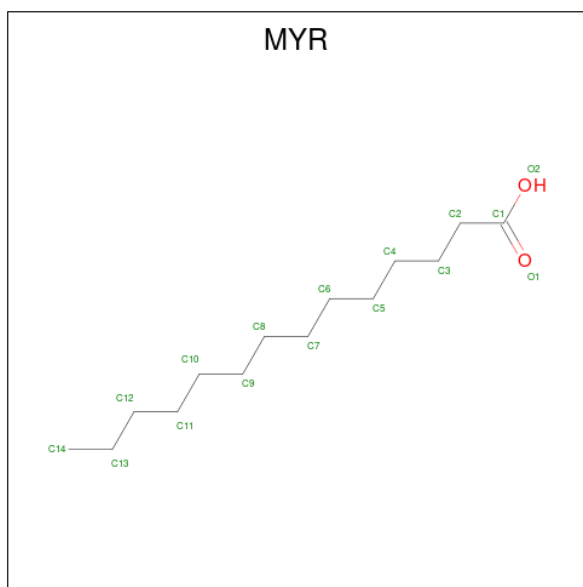
Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	h	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	l	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	p	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	t	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).

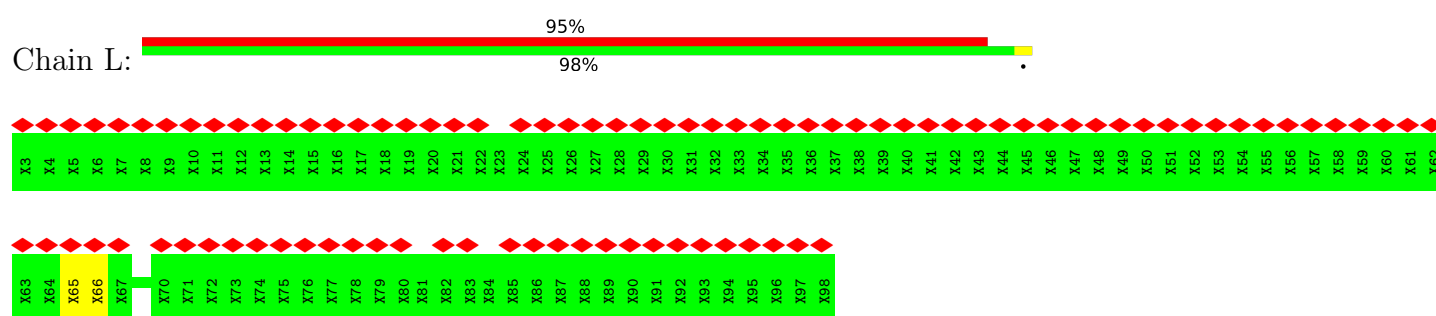


Mol	Chain	Residues	Atoms			AltConf
7	a	1	Total	C	O	0
			16	14	2	
7	e	1	Total	C	O	0
			16	14	2	
7	i	1	Total	C	O	0
			16	14	2	
7	m	1	Total	C	O	0
			16	14	2	
7	q	1	Total	C	O	0
			16	14	2	

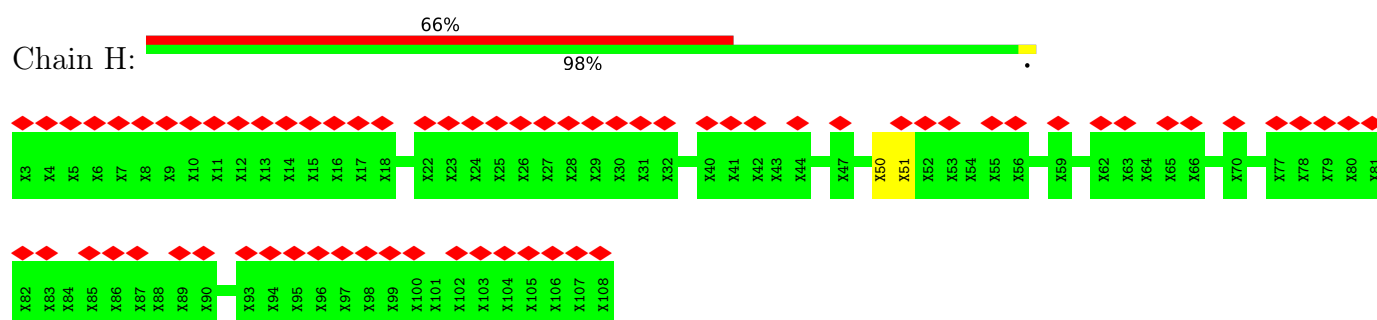
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: pAbC-3 light chain

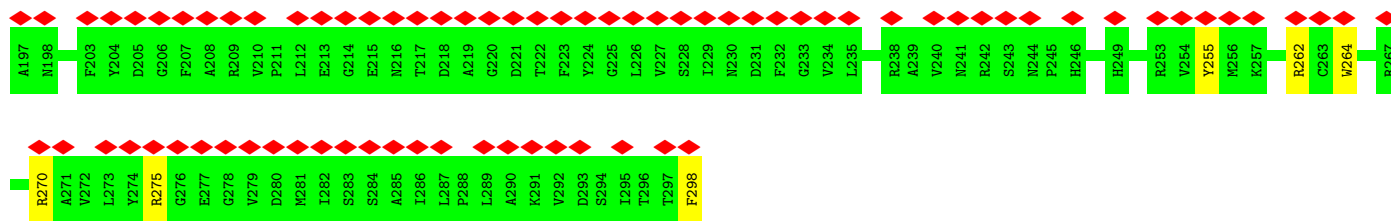


#### • Molecule 2: pAbC-3 heavy chain

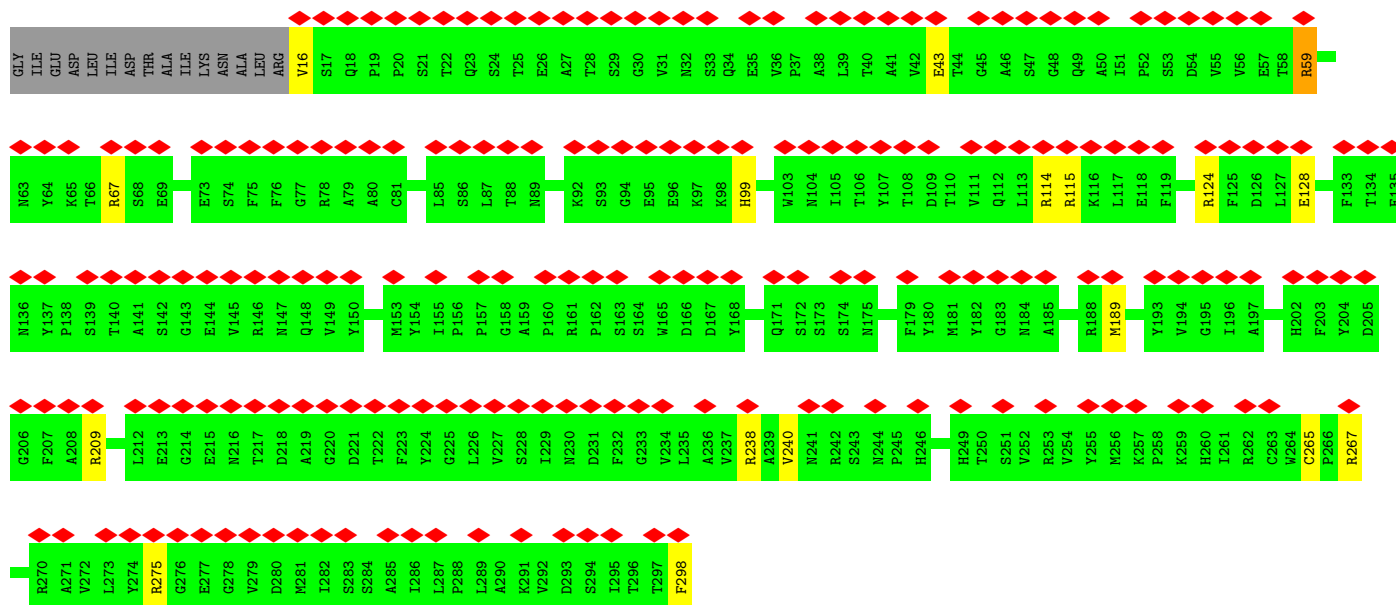
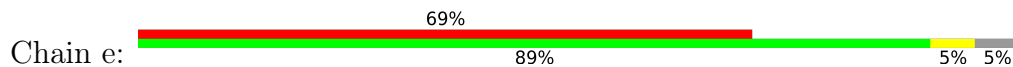


#### • Molecule 3: VP1

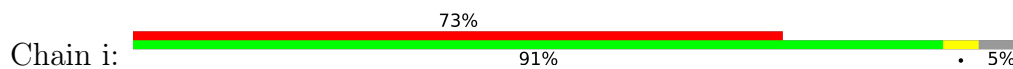




• Molecule 3: VP1

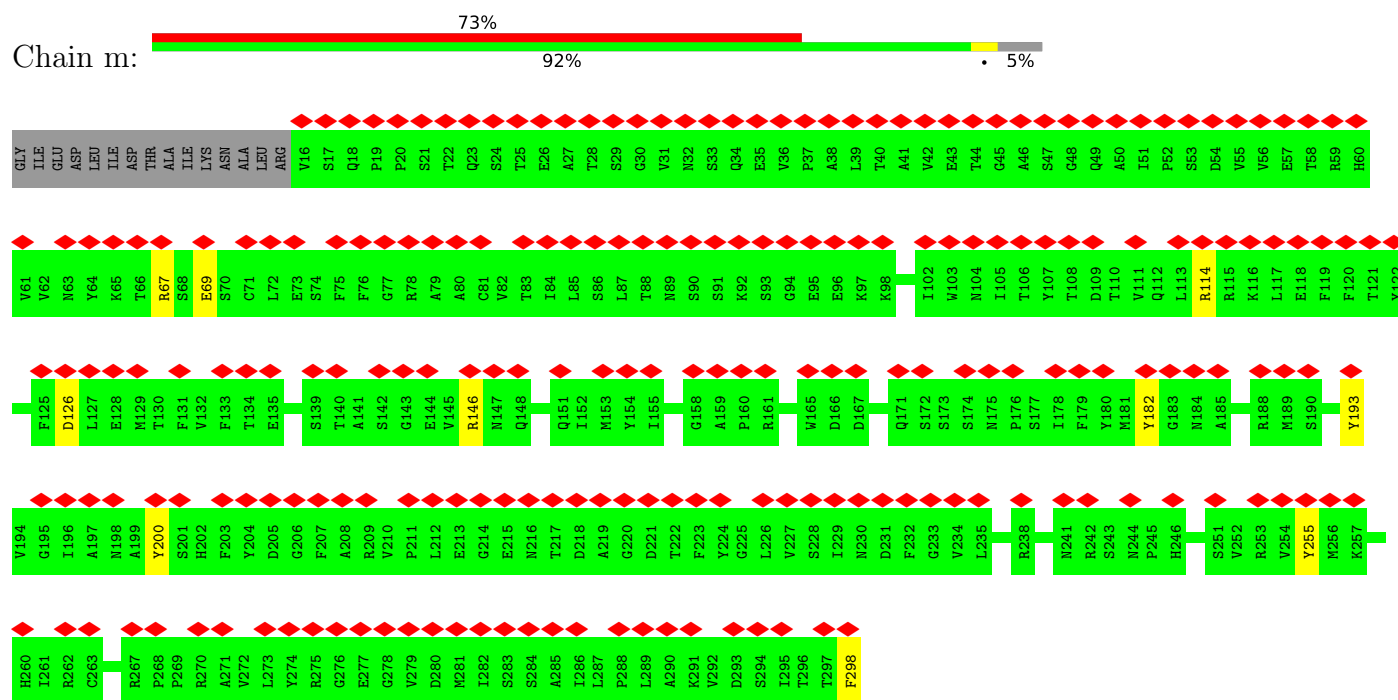


• Molecule 3: VP1

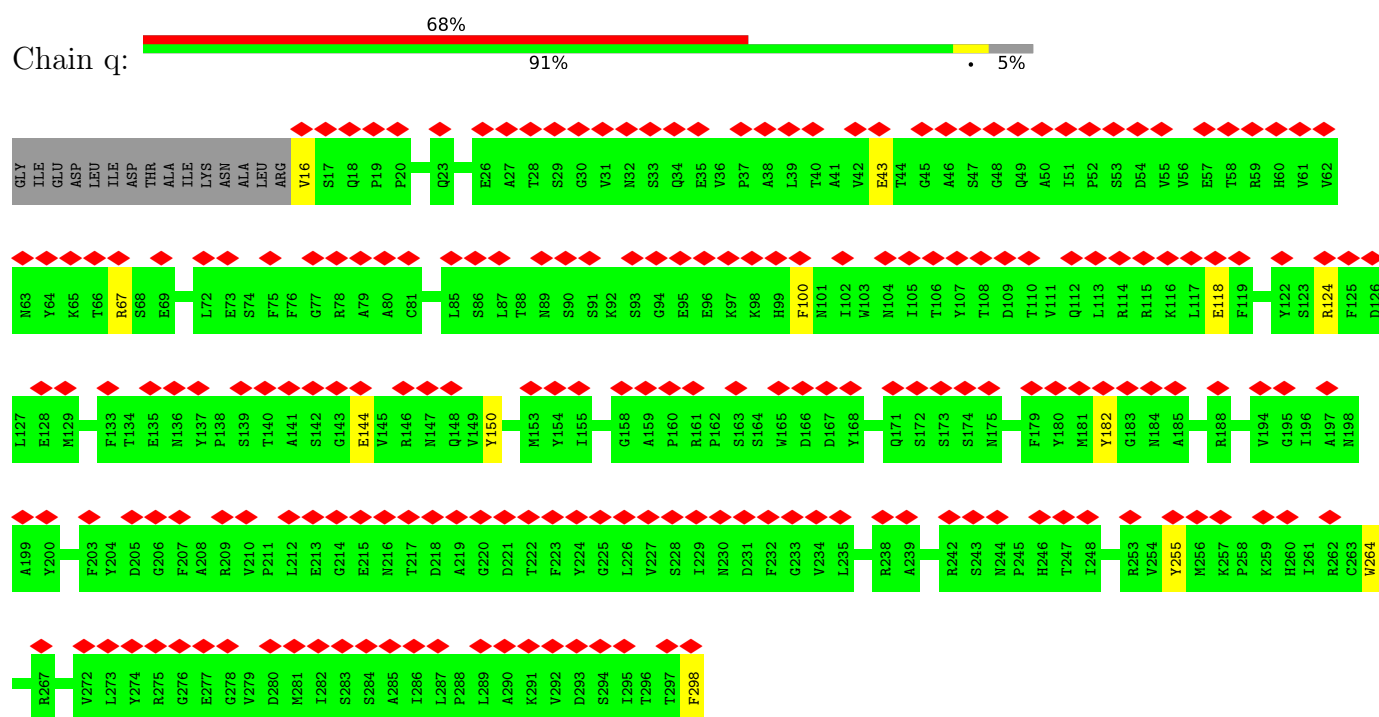




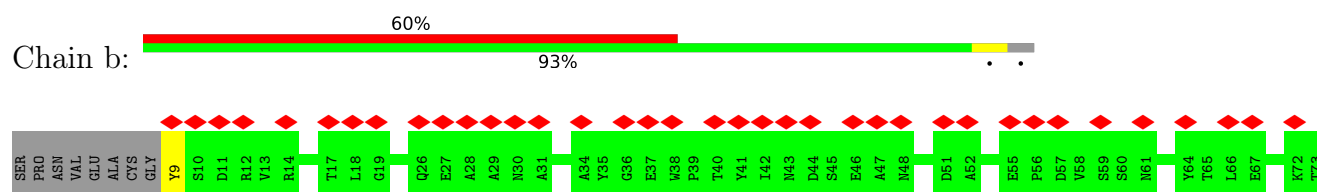
## • Molecule 3: VP1

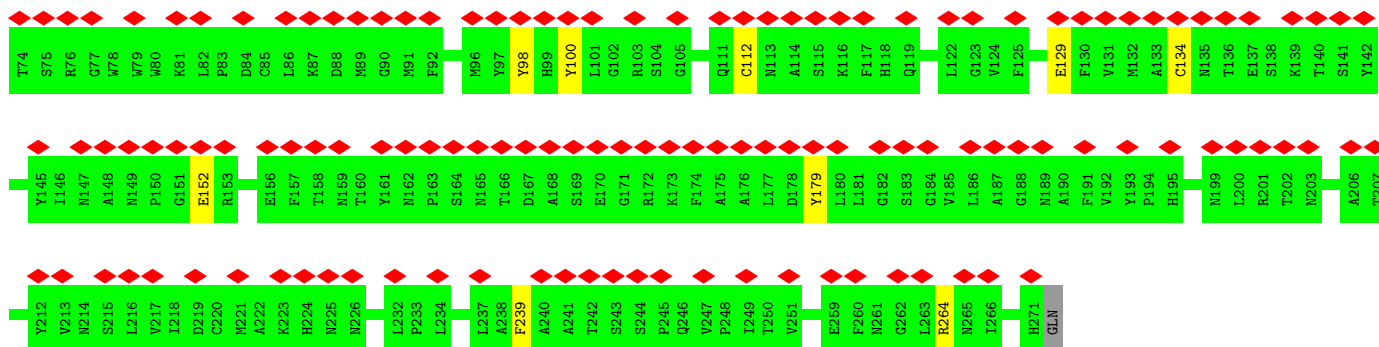


## • Molecule 3: VP1

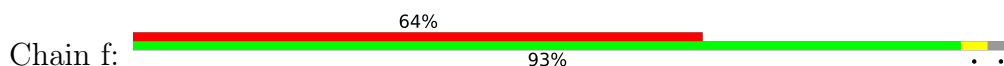


## • Molecule 4: VP2

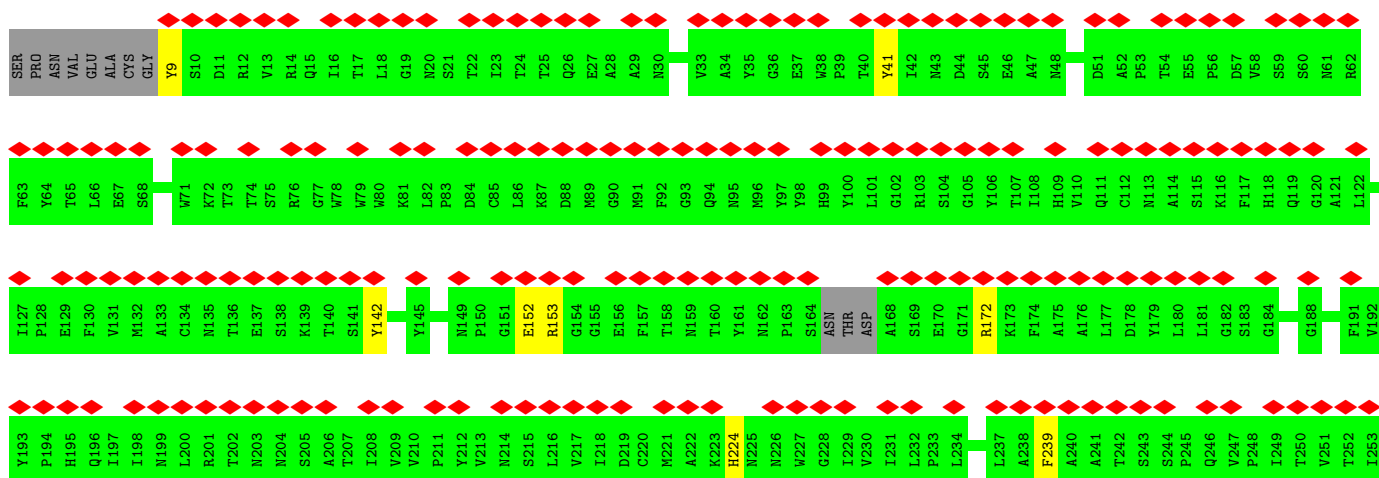
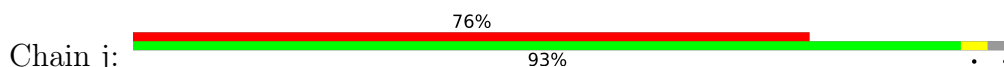


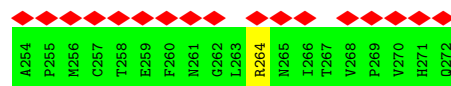


• Molecule 4: VP2

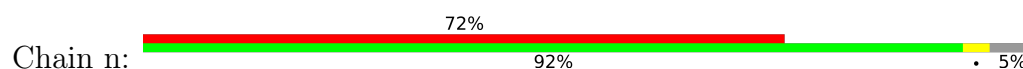


• Molecule 4: VP2

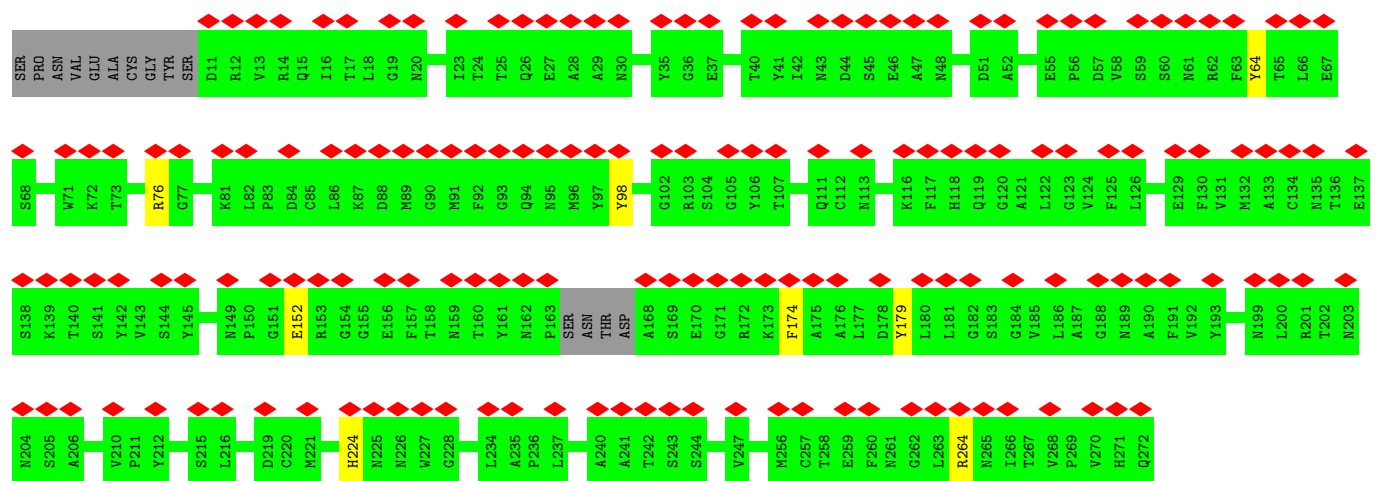




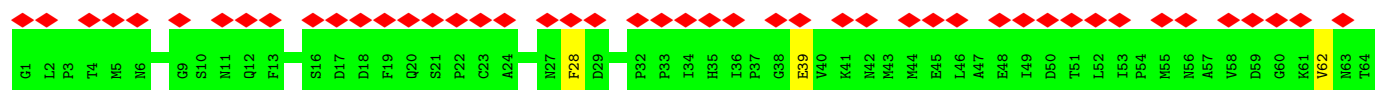
• Molecule 4: VP2

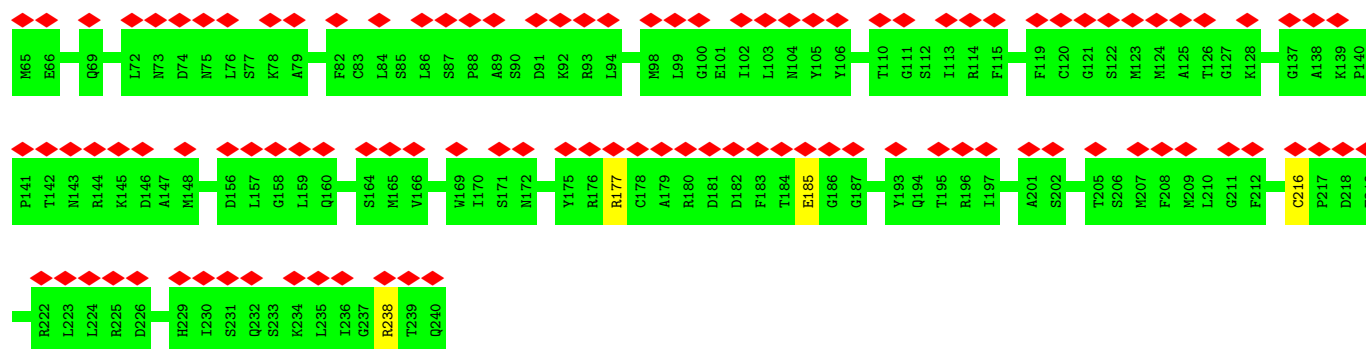


• Molecule 4: VP2

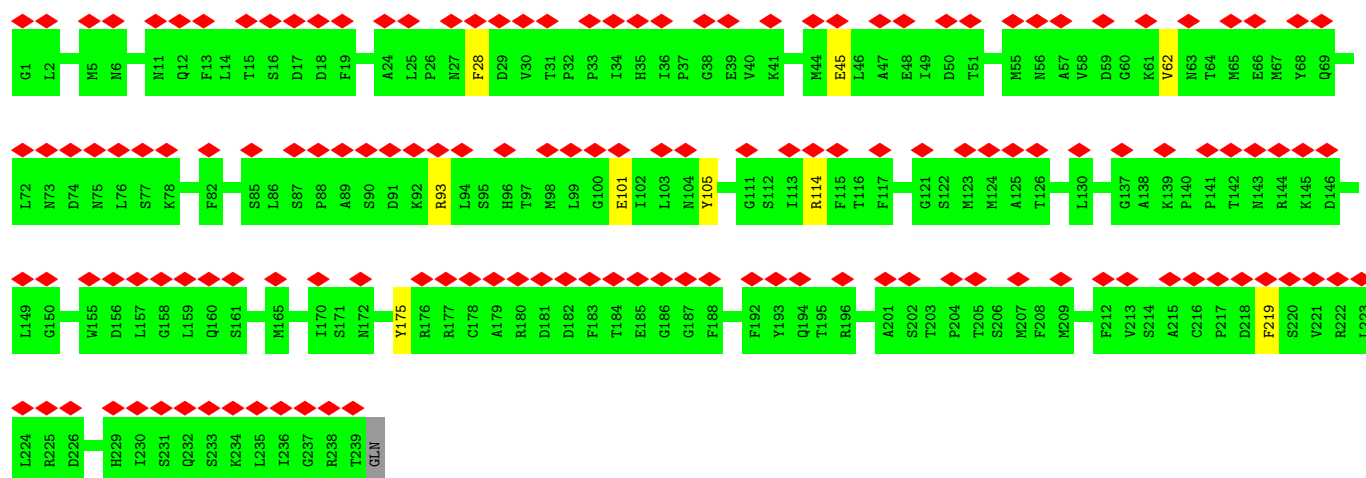


• Molecule 5: VP3

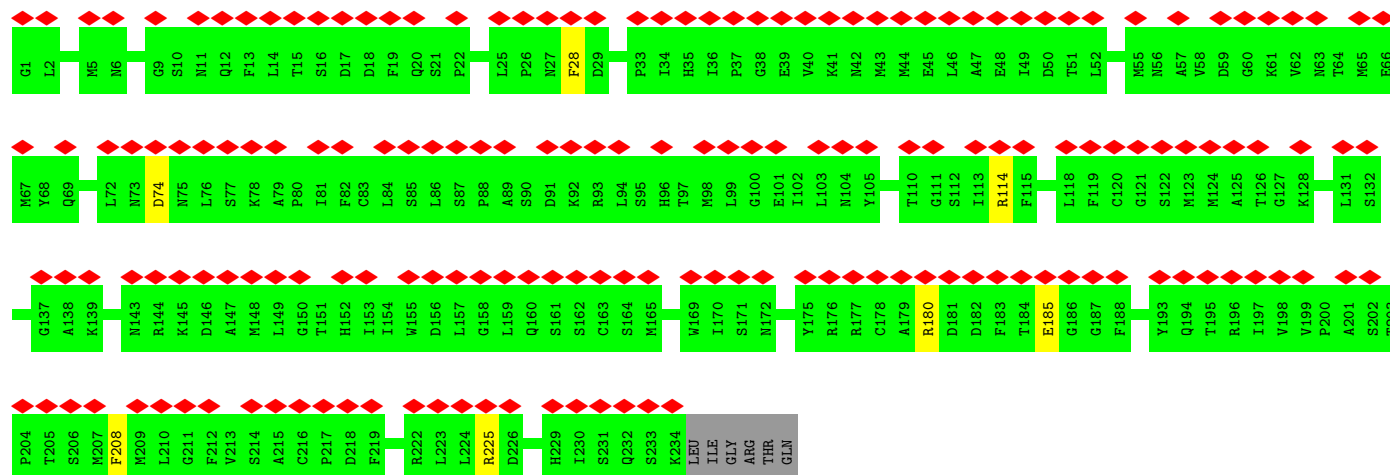




• Molecule 5: VP3



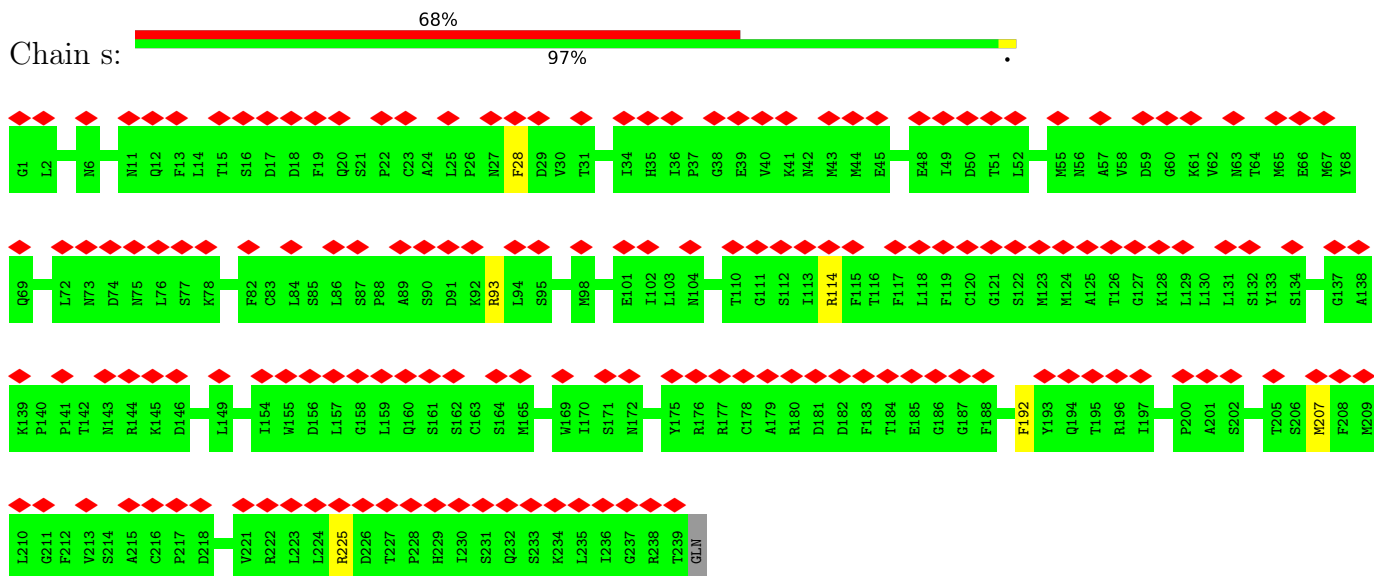
• Molecule 5: VP3



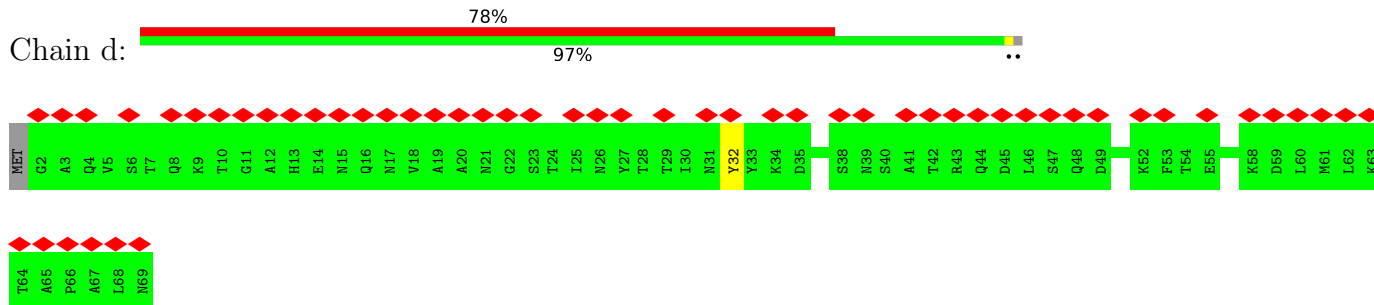
• Molecule 5: VP3



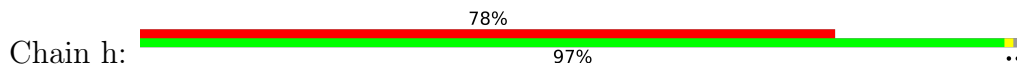
- Molecule 5: VP3

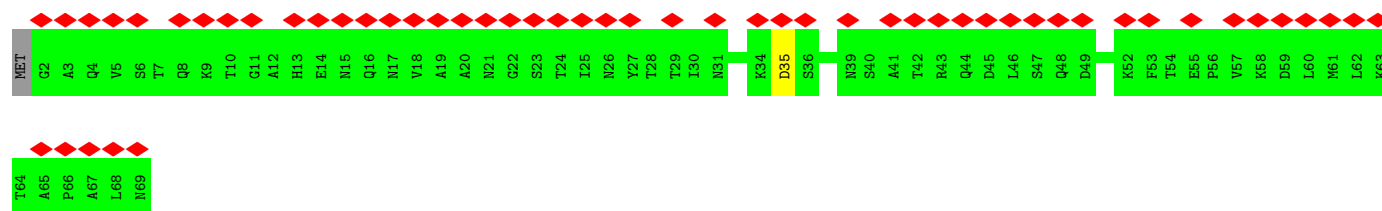


- Molecule 6: VP4

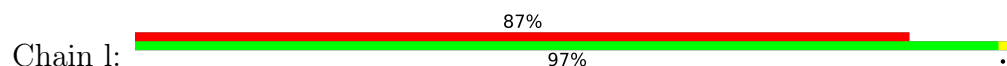


- Molecule 6: VP4

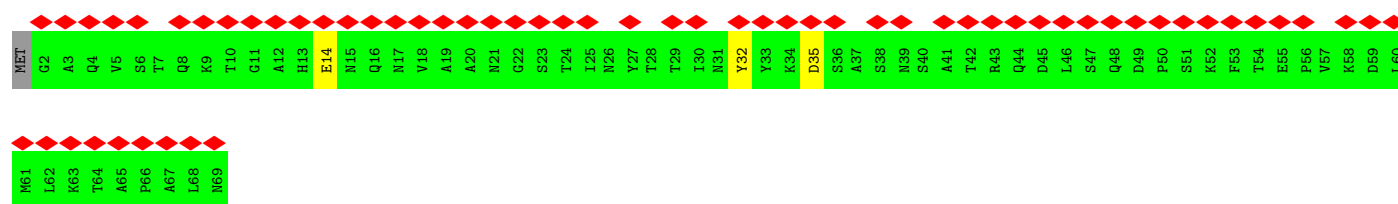
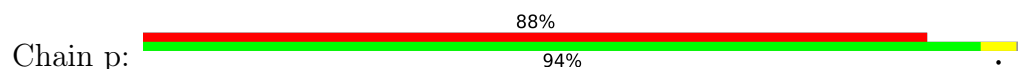




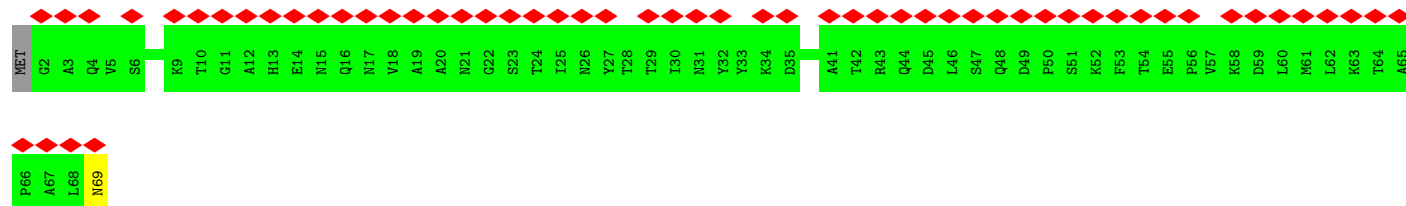
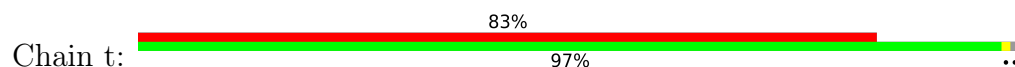
• Molecule 6: VP4



• Molecule 6: VP4



• Molecule 6: VP4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	292.59998, 292.59998, 292.59998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.045, 1.045, 1.045	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 5$
3	a	1.20	9/2281 (0.4%)	1.00	9/3111 (0.3%)
3	e	1.20	8/2288 (0.3%)	1.00	11/3121 (0.4%)
3	i	1.22	9/2288 (0.4%)	0.99	9/3121 (0.3%)
3	m	1.17	5/2288 (0.2%)	0.95	6/3121 (0.2%)
3	q	1.23	13/2288 (0.6%)	0.96	4/3121 (0.1%)
4	b	1.22	12/2101 (0.6%)	0.92	2/2876 (0.1%)
4	f	1.15	7/2092 (0.3%)	0.91	2/2861 (0.1%)
4	j	1.16	9/2086 (0.4%)	0.92	3/2852 (0.1%)
4	n	1.15	7/2068 (0.3%)	0.92	2/2827 (0.1%)
4	r	1.16	5/2061 (0.2%)	0.92	4/2818 (0.1%)
5	c	1.10	5/1906 (0.3%)	0.93	2/2594 (0.1%)
5	g	1.12	6/1897 (0.3%)	0.94	4/2582 (0.2%)
5	k	1.10	3/1859 (0.2%)	0.98	5/2531 (0.2%)
5	o	1.15	9/1897 (0.5%)	0.94	2/2582 (0.1%)
5	s	1.06	3/1897 (0.2%)	0.96	4/2582 (0.2%)
6	d	1.03	0/519	0.84	1/705 (0.1%)
6	h	1.06	0/519	0.94	2/705 (0.3%)
6	l	1.02	1/519 (0.2%)	0.80	0/705
6	p	1.04	2/519 (0.4%)	0.95	3/705 (0.4%)
6	t	1.04	1/519 (0.2%)	0.84	0/705
All	All	1.15	114/33892 (0.3%)	0.95	75/46225 (0.2%)

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	i	100	PHE	CB-CG	-10.20	1.34	1.51
3	q	100	PHE	CB-CG	-9.94	1.34	1.51
4	r	179	TYR	CB-CG	-9.93	1.36	1.51
4	n	129	GLU	CG-CD	-8.81	1.38	1.51
4	b	179	TYR	CB-CG	-8.32	1.39	1.51
3	m	298	PHE	CG-CD1	8.25	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	9	TYR	CE2-CZ	7.98	1.49	1.38
4	j	9	TYR	CG-CD1	7.91	1.49	1.39
4	b	9	TYR	CG-CD1	7.84	1.49	1.39
4	j	9	TYR	CE2-CZ	7.83	1.48	1.38
3	i	69	GLU	CD-OE2	-7.71	1.17	1.25
4	n	129	GLU	CD-OE2	-7.67	1.17	1.25
4	j	9	TYR	CG-CD2	7.58	1.49	1.39
3	e	298	PHE	CG-CD2	7.36	1.49	1.38
4	b	9	TYR	CG-CD2	7.32	1.48	1.39
3	q	264	TRP	CB-CG	-7.18	1.37	1.50
3	q	298	PHE	CG-CD1	7.12	1.49	1.38
3	a	264	TRP	CB-CG	-7.10	1.37	1.50
4	b	134	CYS	CB-SG	-7.08	1.70	1.82
4	n	129	GLU	CB-CG	-7.08	1.38	1.52
4	f	210	VAL	CB-CG2	-7.04	1.38	1.52
6	l	14	GLU	CD-OE2	-7.04	1.18	1.25
3	i	298	PHE	CG-CD2	7.01	1.49	1.38
3	q	298	PHE	CG-CD2	7.01	1.49	1.38
3	a	298	PHE	CG-CD2	6.92	1.49	1.38
3	e	298	PHE	CG-CD1	6.78	1.49	1.38
3	i	298	PHE	CG-CD1	6.77	1.49	1.38
5	o	28	PHE	CB-CG	-6.77	1.39	1.51
4	b	129	GLU	CG-CD	-6.73	1.41	1.51
5	o	105	TYR	CG-CD1	-6.72	1.30	1.39
5	c	62	VAL	CB-CG2	-6.71	1.38	1.52
5	k	28	PHE	CB-CG	-6.65	1.40	1.51
4	n	174	PHE	CB-CG	-6.59	1.40	1.51
5	g	62	VAL	CB-CG2	-6.51	1.39	1.52
5	g	28	PHE	CB-CG	-6.51	1.40	1.51
4	j	224	HIS	CB-CG	-6.46	1.38	1.50
4	b	9	TYR	CE1-CZ	6.34	1.46	1.38
5	o	222	ARG	CG-CD	-6.32	1.36	1.51
3	e	265	CYS	CB-SG	-6.28	1.71	1.82
3	a	298	PHE	CG-CD1	6.25	1.48	1.38
3	q	43	GLU	CG-CD	-6.20	1.42	1.51
4	j	9	TYR	CE1-CZ	6.18	1.46	1.38
3	q	182	TYR	CB-CG	-6.16	1.42	1.51
4	f	129	GLU	CD-OE2	-6.00	1.19	1.25
5	o	62	VAL	CB-CG2	-5.99	1.40	1.52
4	b	239	PHE	CB-CG	-5.93	1.41	1.51
3	q	118	GLU	CD-OE1	-5.93	1.19	1.25
5	g	45	GLU	CD-OE1	-5.81	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	s	28	PHE	CB-CG	-5.76	1.41	1.51
5	s	207	MET	CG-SD	-5.76	1.66	1.81
6	p	14	GLU	CG-CD	-5.70	1.43	1.51
5	o	105	TYR	CB-CG	-5.68	1.43	1.51
3	q	144	GLU	CD-OE2	-5.66	1.19	1.25
4	r	224	HIS	CB-CG	-5.61	1.40	1.50
5	k	185	GLU	CG-CD	-5.59	1.43	1.51
3	i	69	GLU	CG-CD	-5.58	1.43	1.51
3	a	128	GLU	CD-OE1	-5.56	1.19	1.25
3	e	128	GLU	CD-OE1	-5.55	1.19	1.25
5	o	105	TYR	CD1-CE1	-5.52	1.31	1.39
4	j	9	TYR	CD2-CE2	5.52	1.47	1.39
3	q	255	TYR	CB-CG	-5.50	1.43	1.51
3	i	298	PHE	CE1-CZ	5.50	1.47	1.37
4	n	272	GLN	CG-CD	5.49	1.63	1.51
4	n	210	VAL	CB-CG1	-5.47	1.41	1.52
3	a	69	GLU	CG-CD	-5.47	1.43	1.51
4	f	98	TYR	CG-CD2	-5.46	1.32	1.39
4	r	174	PHE	CB-CG	-5.44	1.42	1.51
3	q	298	PHE	CE1-CZ	5.42	1.47	1.37
4	f	129	GLU	CG-CD	-5.39	1.43	1.51
5	c	28	PHE	CB-CG	-5.37	1.42	1.51
3	m	298	PHE	CB-CG	5.37	1.60	1.51
3	i	255	TYR	CB-CG	-5.36	1.43	1.51
5	k	208	PHE	CB-CG	-5.36	1.42	1.51
3	m	69	GLU	CD-OE1	-5.36	1.19	1.25
5	g	105	TYR	CB-CG	-5.36	1.43	1.51
3	i	43	GLU	CD-OE1	-5.35	1.19	1.25
3	a	255	TYR	CB-CG	-5.34	1.43	1.51
3	m	193	TYR	CE2-CZ	-5.34	1.31	1.38
4	b	152	GLU	CD-OE2	-5.33	1.19	1.25
4	f	224	HIS	CB-CG	-5.32	1.40	1.50
3	e	16	VAL	CB-CG1	5.32	1.64	1.52
5	c	216	CYS	CB-SG	-5.30	1.73	1.81
4	r	179	TYR	CD1-CE1	-5.30	1.31	1.39
3	q	150	TYR	CB-CG	-5.26	1.43	1.51
4	j	142	TYR	CB-CG	-5.26	1.43	1.51
5	g	101	GLU	CD-OE1	-5.25	1.19	1.25
3	m	255	TYR	CB-CG	-5.25	1.43	1.51
3	a	193	TYR	CE2-CZ	-5.24	1.31	1.38
4	j	239	PHE	CB-CG	-5.24	1.42	1.51
5	o	192	PHE	CB-CG	-5.23	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	112	CYS	CB-SG	-5.20	1.73	1.81
4	j	152	GLU	CD-OE2	-5.19	1.20	1.25
3	a	43	GLU	CD-OE2	-5.16	1.20	1.25
6	t	69	ASN	CB-CG	5.15	1.62	1.51
4	r	152	GLU	CD-OE1	-5.14	1.20	1.25
3	e	298	PHE	CE1-CZ	5.13	1.47	1.37
5	g	175	TYR	CB-CG	-5.13	1.44	1.51
4	f	112	CYS	CB-SG	-5.12	1.73	1.81
5	o	163	CYS	CB-SG	-5.12	1.73	1.81
3	e	43	GLU	CD-OE2	-5.11	1.20	1.25
3	q	43	GLU	CD-OE2	-5.11	1.20	1.25
4	b	9	TYR	CD2-CE2	5.11	1.47	1.39
3	e	240	VAL	CB-CG2	-5.11	1.42	1.52
5	o	185	GLU	CD-OE2	-5.10	1.20	1.25
3	a	270	ARG	CG-CD	-5.09	1.39	1.51
5	c	39	GLU	CG-CD	-5.07	1.44	1.51
4	b	129	GLU	CD-OE2	-5.07	1.20	1.25
4	f	239	PHE	CB-CG	-5.05	1.42	1.51
5	s	192	PHE	CB-CG	-5.04	1.42	1.51
5	c	185	GLU	CD-OE2	-5.04	1.20	1.25
6	p	14	GLU	CD-OE2	-5.04	1.20	1.25
4	n	103	ARG	CG-CD	-5.03	1.39	1.51
3	i	16	VAL	CB-CG1	5.02	1.63	1.52
3	q	16	VAL	CB-CG1	5.01	1.63	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	114	ARG	NE-CZ-NH2	-9.48	115.56	120.30
3	e	59	ARG	NE-CZ-NH2	-9.10	115.75	120.30
5	k	225	ARG	NE-CZ-NH2	-8.99	115.80	120.30
5	s	93	ARG	NE-CZ-NH1	8.98	124.79	120.30
3	q	67	ARG	NE-CZ-NH1	8.37	124.49	120.30
5	k	225	ARG	NE-CZ-NH1	8.36	124.48	120.30
3	i	67	ARG	NE-CZ-NH1	8.05	124.32	120.30
5	c	238	ARG	NE-CZ-NH1	8.01	124.30	120.30
5	g	93	ARG	NE-CZ-NH1	7.95	124.27	120.30
3	i	275	ARG	NE-CZ-NH2	-7.67	116.47	120.30
3	a	275	ARG	NE-CZ-NH1	7.59	124.10	120.30
6	h	35	ASP	CB-CG-OD1	7.45	125.01	118.30
6	p	35	ASP	CB-CG-OD1	7.42	124.98	118.30
5	o	177	ARG	NE-CZ-NH2	-7.37	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	o	105	TYR	CB-CG-CD1	-7.36	116.58	121.00
3	m	146	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	e	275	ARG	NE-CZ-NH2	-7.13	116.73	120.30
4	j	153	ARG	NE-CZ-NH2	-7.09	116.75	120.30
5	c	177	ARG	NE-CZ-NH1	7.07	123.83	120.30
3	a	146	ARG	NE-CZ-NH2	-7.01	116.79	120.30
4	r	76	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	e	67	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	i	126	ASP	CB-CG-OD1	6.86	124.47	118.30
3	e	114	ARG	NE-CZ-NH2	-6.79	116.90	120.30
3	m	67	ARG	NE-CZ-NH1	6.67	123.64	120.30
5	s	114	ARG	NE-CZ-NH2	-6.56	117.02	120.30
3	a	107	TYR	CB-CG-CD2	-6.53	117.08	121.00
4	b	100	TYR	CB-CG-CD2	-6.48	117.11	121.00
3	i	200	TYR	CB-CG-CD2	-6.32	117.21	121.00
5	s	93	ARG	NE-CZ-NH2	-6.25	117.18	120.30
3	a	67	ARG	NE-CZ-NH1	6.23	123.42	120.30
5	k	114	ARG	NE-CZ-NH2	-6.20	117.20	120.30
3	e	238	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	i	100	PHE	CB-CG-CD2	-6.07	116.55	120.80
3	e	267	ARG	NE-CZ-NH2	-6.06	117.27	120.30
3	a	188	ARG	NE-CZ-NH2	-6.05	117.27	120.30
3	i	115	ARG	NE-CZ-NH2	-6.05	117.27	120.30
5	g	114	ARG	NE-CZ-NH2	-6.03	117.28	120.30
6	h	35	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	q	100	PHE	CB-CG-CD2	-6.00	116.60	120.80
5	k	180	ARG	NE-CZ-NH2	-5.99	117.31	120.30
3	e	67	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	a	262	ARG	NE-CZ-NH2	-5.90	117.35	120.30
3	m	200	TYR	CB-CG-CD2	-5.83	117.50	121.00
4	f	172	ARG	NE-CZ-NH2	-5.69	117.46	120.30
5	g	93	ARG	NE-CZ-NH2	-5.62	117.49	120.30
5	k	74	ASP	CB-CG-OD1	5.62	123.36	118.30
3	a	262	ARG	NE-CZ-NH1	5.56	123.08	120.30
4	j	172	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	e	124	ARG	NE-CZ-NH1	5.51	123.06	120.30
4	r	98	TYR	CB-CG-CD1	-5.47	117.72	121.00
5	s	225	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	e	115	ARG	NE-CZ-NH2	-5.40	117.60	120.30
4	r	64	TYR	CB-CG-CD2	-5.39	117.76	121.00
3	a	275	ARG	NE-CZ-NH2	-5.38	117.61	120.30
4	n	41	TYR	CB-CG-CD1	-5.36	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	124	ARG	NE-CZ-NH1	5.36	122.98	120.30
4	n	57	ASP	CB-CG-OD2	-5.33	113.50	118.30
4	f	41	TYR	CB-CG-CD1	-5.30	117.82	121.00
6	p	32	TYR	CB-CG-CD2	-5.30	117.82	121.00
4	b	98	TYR	CB-CG-CD1	-5.26	117.84	121.00
3	e	209	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	e	99	HIS	CA-CB-CG	5.22	122.48	113.60
6	d	32	TYR	CB-CG-CD2	-5.19	117.89	121.00
3	m	126	ASP	CB-CG-OD2	5.18	122.96	118.30
6	p	35	ASP	CB-CG-OD2	-5.16	113.66	118.30
3	i	262	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	i	67	ARG	NE-CZ-NH2	-5.10	117.75	120.30
5	g	219	PHE	CB-CG-CD1	5.09	124.36	120.80
4	r	76	ARG	NE-CZ-NH2	-5.07	117.77	120.30
3	m	182	TYR	CB-CG-CD1	-5.06	117.97	121.00
4	j	41	TYR	CB-CG-CD1	-5.04	117.98	121.00
3	i	124	ARG	NE-CZ-NH2	5.03	122.82	120.30
3	m	114	ARG	NE-CZ-NH2	-5.02	117.79	120.30
3	q	100	PHE	N-CA-CB	-5.02	101.56	110.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	480	0	125	1	0
2	H	530	0	135	1	0
3	a	2219	0	2137	0	0
3	e	2226	0	2146	0	0
3	i	2226	0	2146	0	0
3	m	2226	0	2146	0	0
3	q	2226	0	2146	0	0
4	b	2044	0	1967	0	0
4	f	2036	0	1962	0	0
4	j	2030	0	1957	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	n	2013	0	1943	0	0
4	r	2006	0	1938	0	0
5	c	1857	0	1844	0	0
5	g	1848	0	1836	0	0
5	k	1810	0	1791	0	0
5	o	1848	0	1836	0	0
5	s	1848	0	1836	0	0
6	d	512	0	493	0	0
6	h	512	0	493	0	0
6	l	512	0	493	0	0
6	p	512	0	493	0	0
6	t	512	0	493	0	0
7	a	16	0	27	0	0
7	e	16	0	27	0	0
7	i	16	0	27	0	0
7	m	16	0	27	0	0
7	q	16	0	27	0	0
All	All	34113	0	32491	2	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:UNK:O	1:L:66:UNK:C	2.57	0.52
2:H:50:UNK:O	2:H:51:UNK:C	2.64	0.46

There are no symmetry-related clashes.

## 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	
3	a	280/298 (94%)	277 (99%)	3 (1%)	0	100	100
3	e	281/298 (94%)	275 (98%)	6 (2%)	0	100	100
3	i	281/298 (94%)	277 (99%)	4 (1%)	0	100	100
3	m	281/298 (94%)	276 (98%)	5 (2%)	0	100	100
3	q	281/298 (94%)	278 (99%)	3 (1%)	0	100	100
4	b	261/272 (96%)	254 (97%)	7 (3%)	0	100	100
4	f	259/272 (95%)	255 (98%)	4 (2%)	0	100	100
4	j	257/272 (94%)	252 (98%)	5 (2%)	0	100	100
4	n	255/272 (94%)	248 (97%)	7 (3%)	0	100	100
4	r	254/272 (93%)	250 (98%)	4 (2%)	0	100	100
5	c	238/240 (99%)	234 (98%)	4 (2%)	0	100	100
5	g	237/240 (99%)	233 (98%)	4 (2%)	0	100	100
5	k	232/240 (97%)	229 (99%)	3 (1%)	0	100	100
5	o	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
5	s	237/240 (99%)	234 (99%)	3 (1%)	0	100	100
6	d	66/69 (96%)	66 (100%)	0	0	100	100
6	h	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	l	66/69 (96%)	63 (96%)	3 (4%)	0	100	100
6	p	66/69 (96%)	63 (96%)	3 (4%)	0	100	100
6	t	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
All	All	4201/4395 (96%)	4128 (98%)	73 (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	
3	a	247/260 (95%)	247 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	248/260 (95%)	246 (99%)	2 (1%)	81	89
3	i	248/260 (95%)	248 (100%)	0	100	100
3	m	248/260 (95%)	248 (100%)	0	100	100
3	q	248/260 (95%)	248 (100%)	0	100	100
4	b	223/230 (97%)	222 (100%)	1 (0%)	91	94
4	f	221/230 (96%)	220 (100%)	1 (0%)	88	93
4	j	221/230 (96%)	220 (100%)	1 (0%)	88	93
4	n	220/230 (96%)	219 (100%)	1 (0%)	88	93
4	r	218/230 (95%)	217 (100%)	1 (0%)	88	93
5	c	213/213 (100%)	213 (100%)	0	100	100
5	g	212/213 (100%)	212 (100%)	0	100	100
5	k	208/213 (98%)	208 (100%)	0	100	100
5	o	212/213 (100%)	212 (100%)	0	100	100
5	s	212/213 (100%)	212 (100%)	0	100	100
6	d	57/58 (98%)	57 (100%)	0	100	100
6	h	57/58 (98%)	57 (100%)	0	100	100
6	l	57/58 (98%)	57 (100%)	0	100	100
6	p	57/58 (98%)	57 (100%)	0	100	100
6	t	57/58 (98%)	57 (100%)	0	100	100
All	All	3684/3805 (97%)	3677 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	b	264	ARG
3	e	59	ARG
3	e	189	MET
4	f	264	ARG
4	j	264	ARG
4	n	264	ARG
4	r	264	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
3	i	18	GLN
6	l	17	ASN
6	l	21	ASN
3	m	112	GLN
4	n	261	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	MYR	i	300	-	15,15,15	1.45	2 (13%)	15,15,15	1.23	2 (13%)
7	MYR	m	300	-	15,15,15	1.47	2 (13%)	15,15,15	1.08	2 (13%)
7	MYR	a	300	-	15,15,15	1.36	2 (13%)	15,15,15	0.85	1 (6%)
7	MYR	q	300	-	15,15,15	1.36	2 (13%)	15,15,15	1.07	2 (13%)
7	MYR	e	300	-	15,15,15	0.90	0	15,15,15	0.99	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	i	300	-	-	2/13/13/13	-
7	MYR	m	300	-	-	5/13/13/13	-
7	MYR	a	300	-	-	3/13/13/13	-
7	MYR	q	300	-	-	2/13/13/13	-
7	MYR	e	300	-	-	7/13/13/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	m	300	MYR	O1-C1	3.22	1.32	1.22
7	m	300	MYR	O2-C1	-3.14	1.20	1.30
7	q	300	MYR	O2-C1	-3.13	1.20	1.30
7	i	300	MYR	O2-C1	-3.07	1.20	1.30
7	i	300	MYR	O1-C1	3.06	1.32	1.22
7	q	300	MYR	O1-C1	3.04	1.32	1.22
7	a	300	MYR	O1-C1	3.04	1.32	1.22
7	a	300	MYR	O2-C1	-2.87	1.21	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	300	MYR	O2-C1-O1	-3.39	114.84	123.30
7	i	300	MYR	O2-C1-C2	3.14	124.13	114.03
7	e	300	MYR	O2-C1-O1	-2.81	116.29	123.30
7	m	300	MYR	O2-C1-O1	-2.81	116.30	123.30
7	m	300	MYR	O2-C1-C2	2.78	122.96	114.03
7	q	300	MYR	O2-C1-C2	2.77	122.92	114.03
7	q	300	MYR	O2-C1-O1	-2.75	116.44	123.30
7	e	300	MYR	O2-C1-C2	2.42	121.81	114.03
7	a	300	MYR	O2-C1-O1	-2.42	117.27	123.30

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	i	300	MYR	C3-C4-C5-C6
7	e	300	MYR	C7-C8-C9-C10
7	q	300	MYR	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	m	300	MYR	C1-C2-C3-C4
7	e	300	MYR	C1-C2-C3-C4
7	m	300	MYR	C4-C5-C6-C7
7	m	300	MYR	C10-C11-C12-C13
7	e	300	MYR	C2-C3-C4-C5
7	e	300	MYR	C3-C4-C5-C6
7	q	300	MYR	C6-C7-C8-C9
7	e	300	MYR	O1-C1-C2-C3
7	e	300	MYR	O2-C1-C2-C3
7	a	300	MYR	C4-C5-C6-C7
7	e	300	MYR	C4-C5-C6-C7
7	a	300	MYR	O2-C1-C2-C3
7	a	300	MYR	O1-C1-C2-C3
7	i	300	MYR	C7-C8-C9-C10
7	m	300	MYR	O2-C1-C2-C3
7	m	300	MYR	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

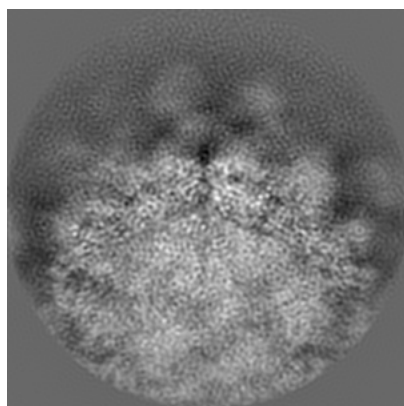
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26068. These allow visual inspection of the internal detail of the map and identification of artifacts.

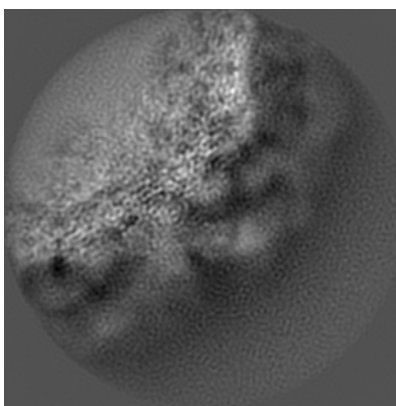
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

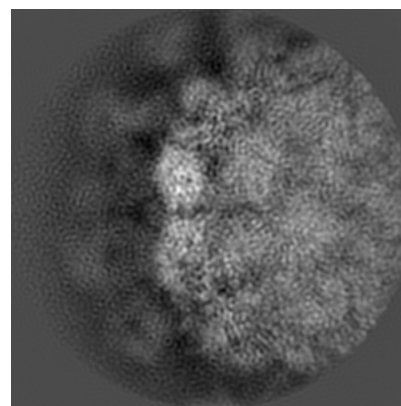
#### 6.1.1 Primary map



X

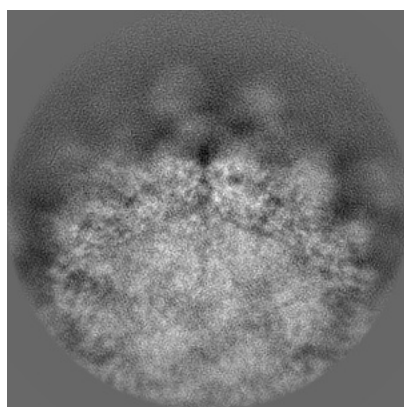


Y

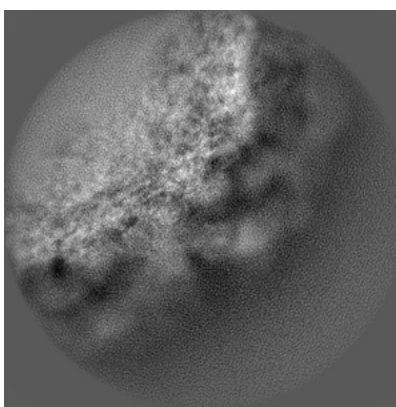


Z

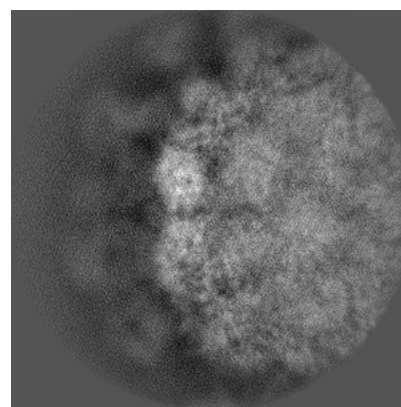
#### 6.1.2 Raw map



X



Y

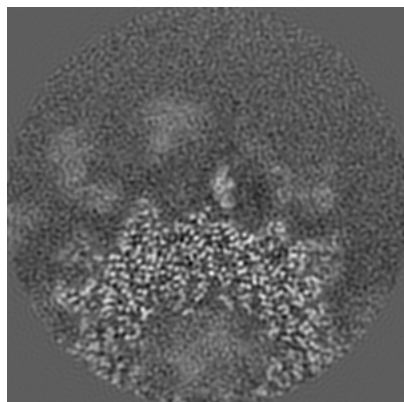


Z

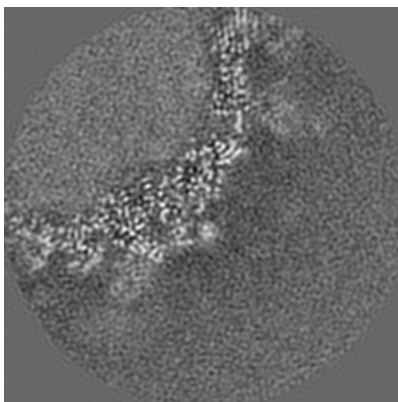
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

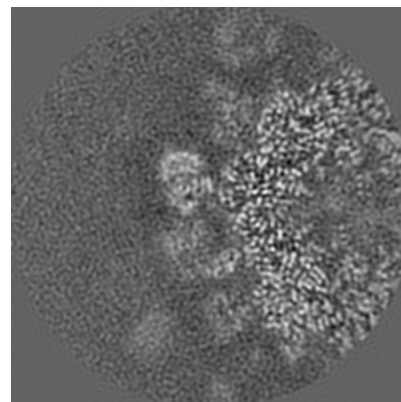
### 6.2.1 Primary map



X Index: 140

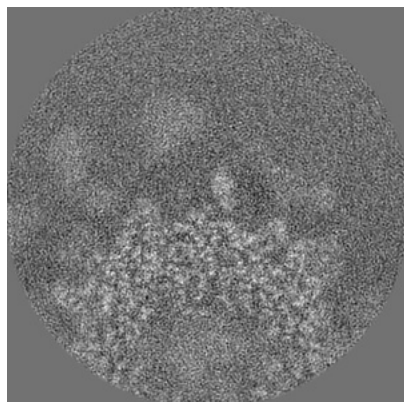


Y Index: 140

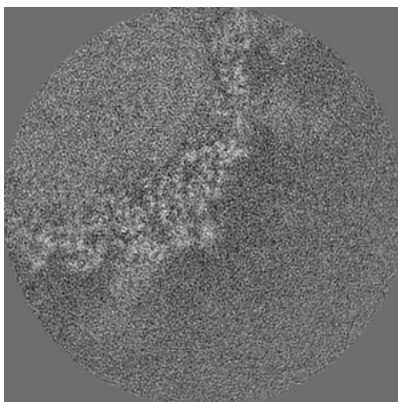


Z Index: 140

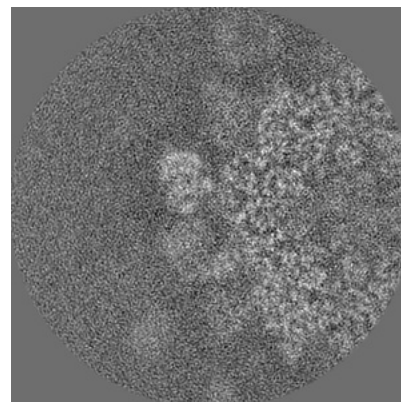
### 6.2.2 Raw map



X Index: 140



Y Index: 140



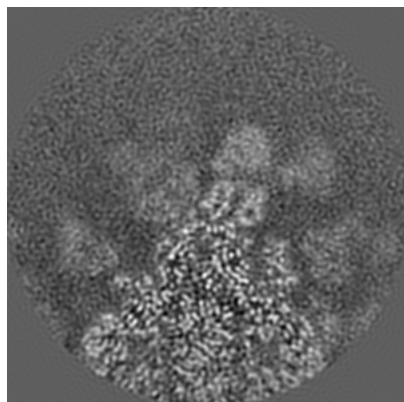
Z Index: 140

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

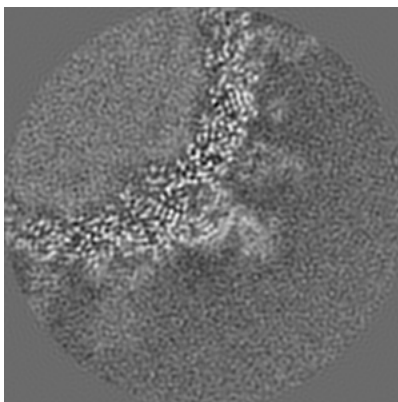


## 6.3 Largest variance slices [i](#)

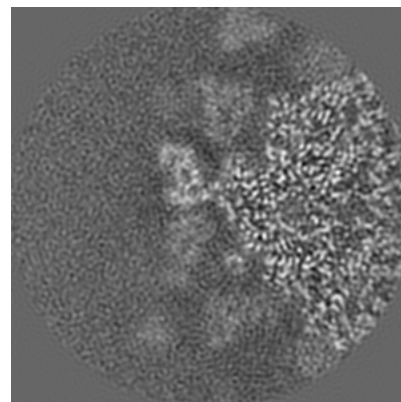
### 6.3.1 Primary map



X Index: 124

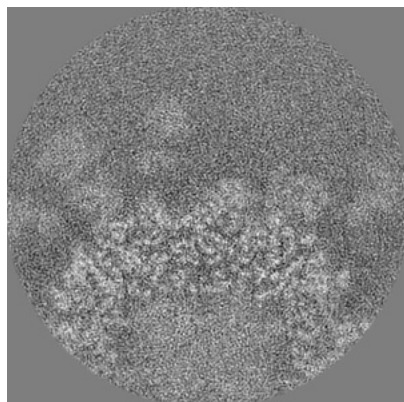


Y Index: 153

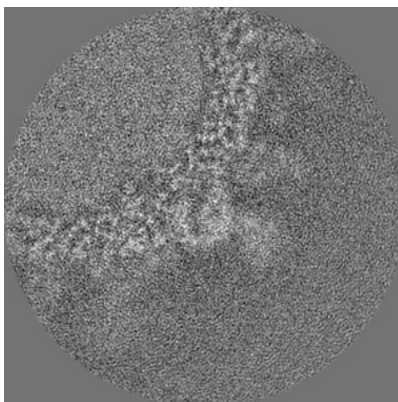


Z Index: 148

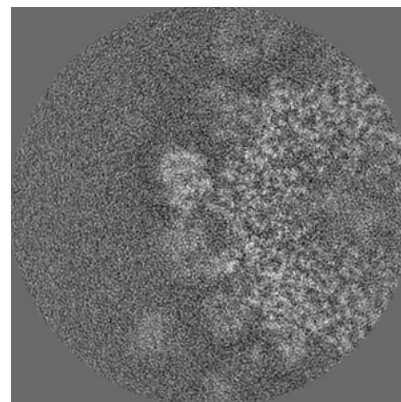
### 6.3.2 Raw map



X Index: 149



Y Index: 155

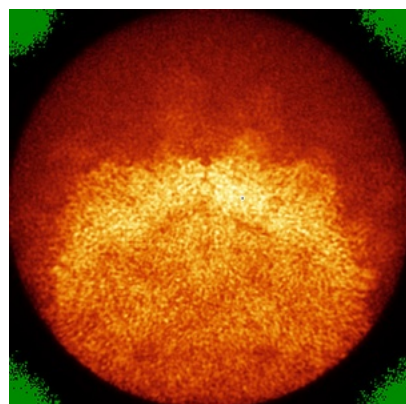


Z Index: 139

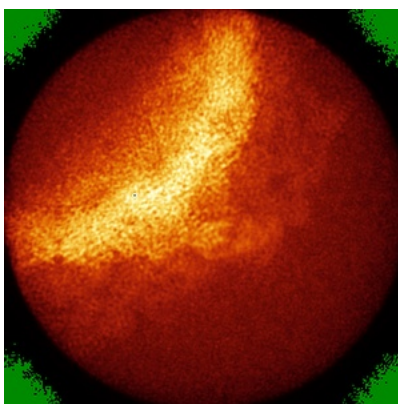
The images above show the largest variance slices of the map in three orthogonal directions.

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

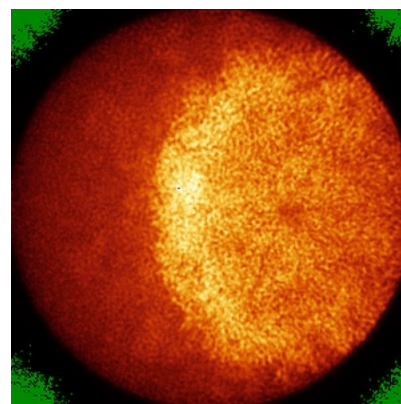
### 6.4.1 Primary map



X

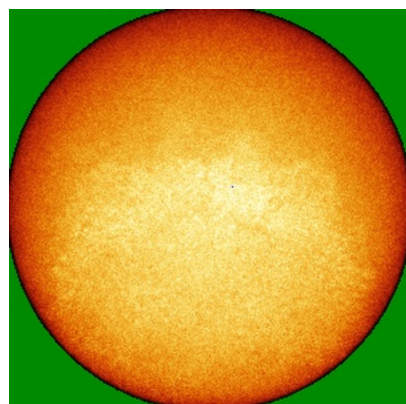


Y

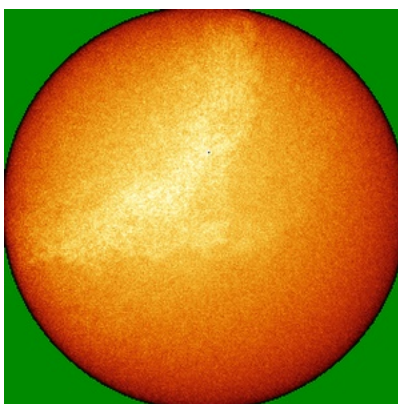


Z

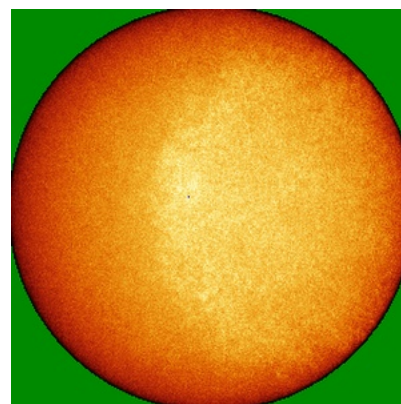
### 6.4.2 Raw map



X



Y

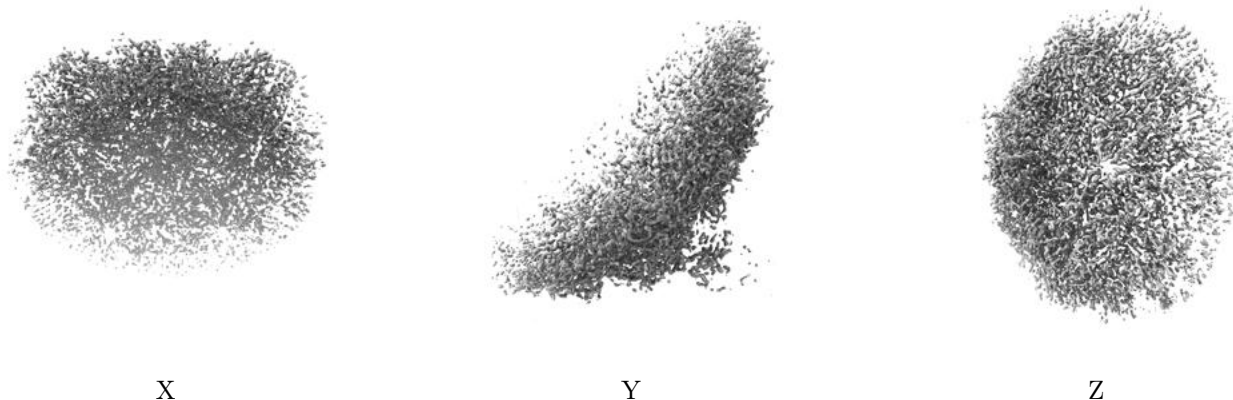


Z

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.

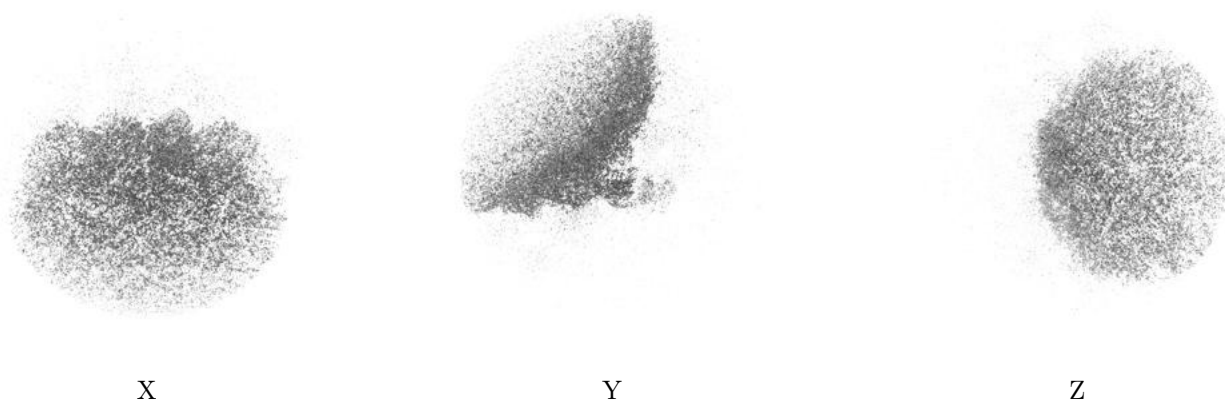
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



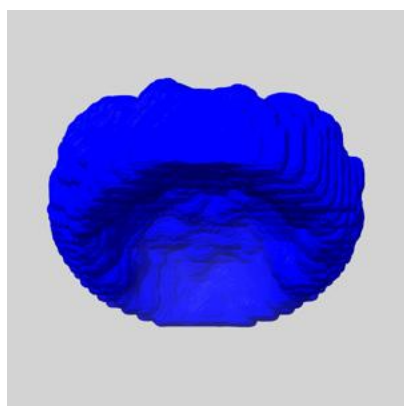
## 6.6 Mask visualisation [i](#)

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

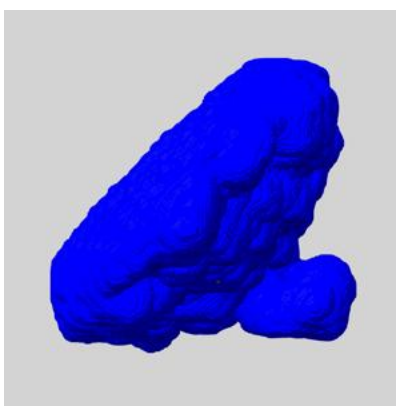
A mask typically either:

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

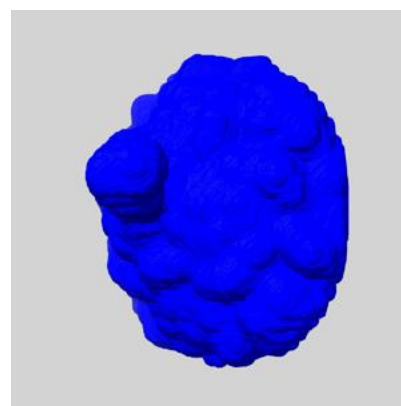
### 6.6.1 emd\_26068\_msk\_1.map [i](#)



X



Y

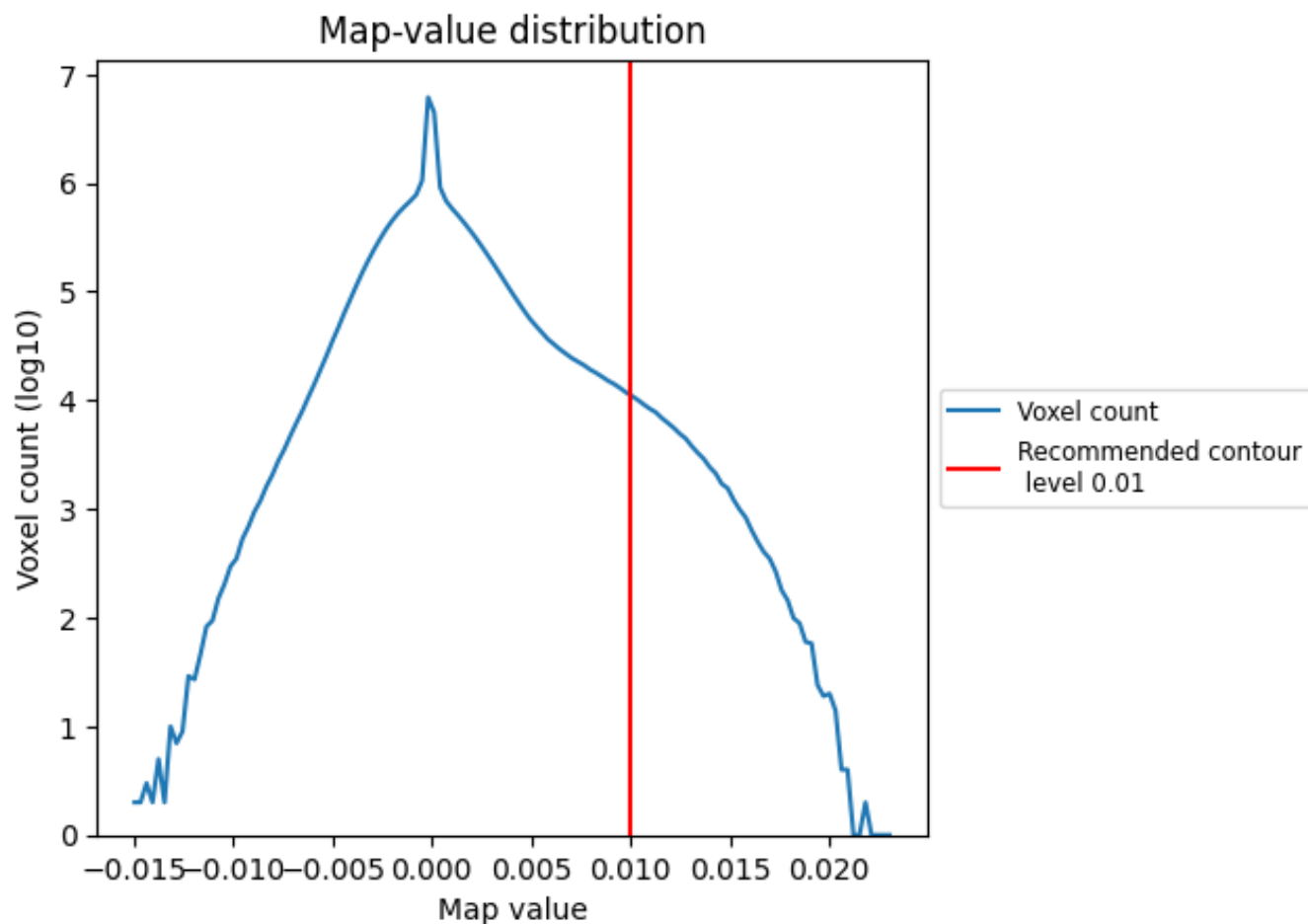


Z

## 7 Map analysis [i](#)

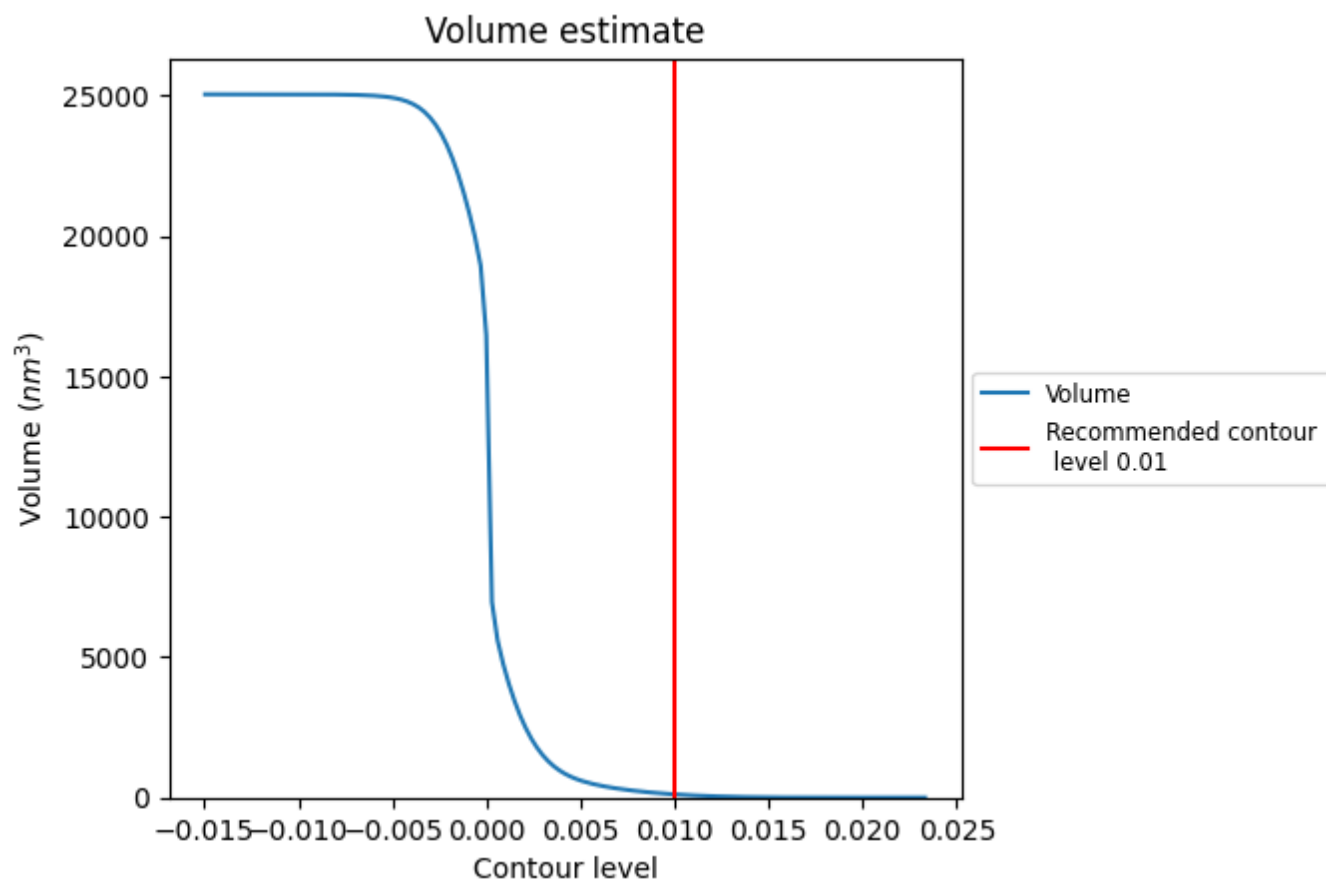
This section contains the results of statistical analysis of the map.

### 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.

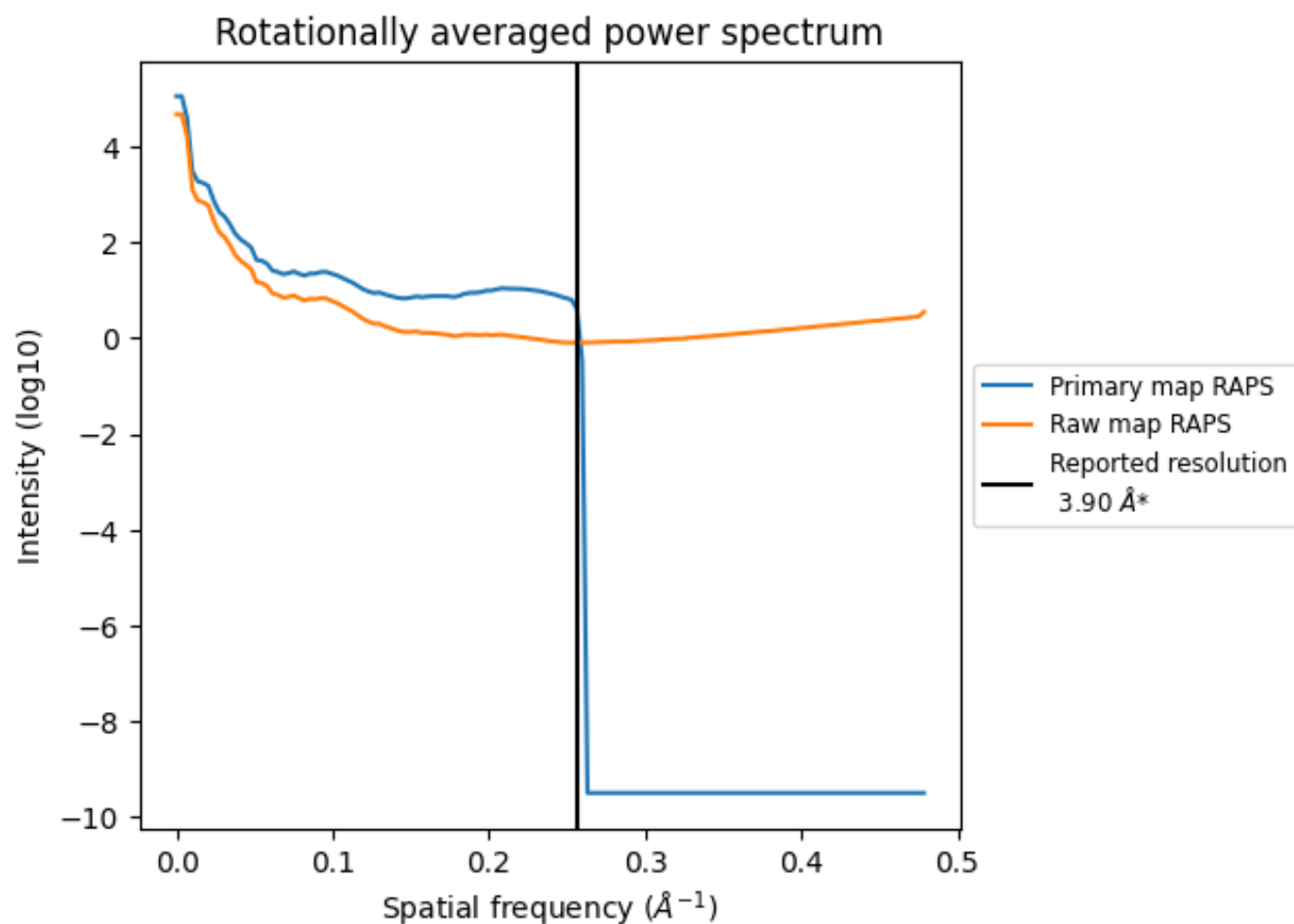
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm<sup>3</sup>; this corresponds to an approximate mass of 103 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 ⓘ

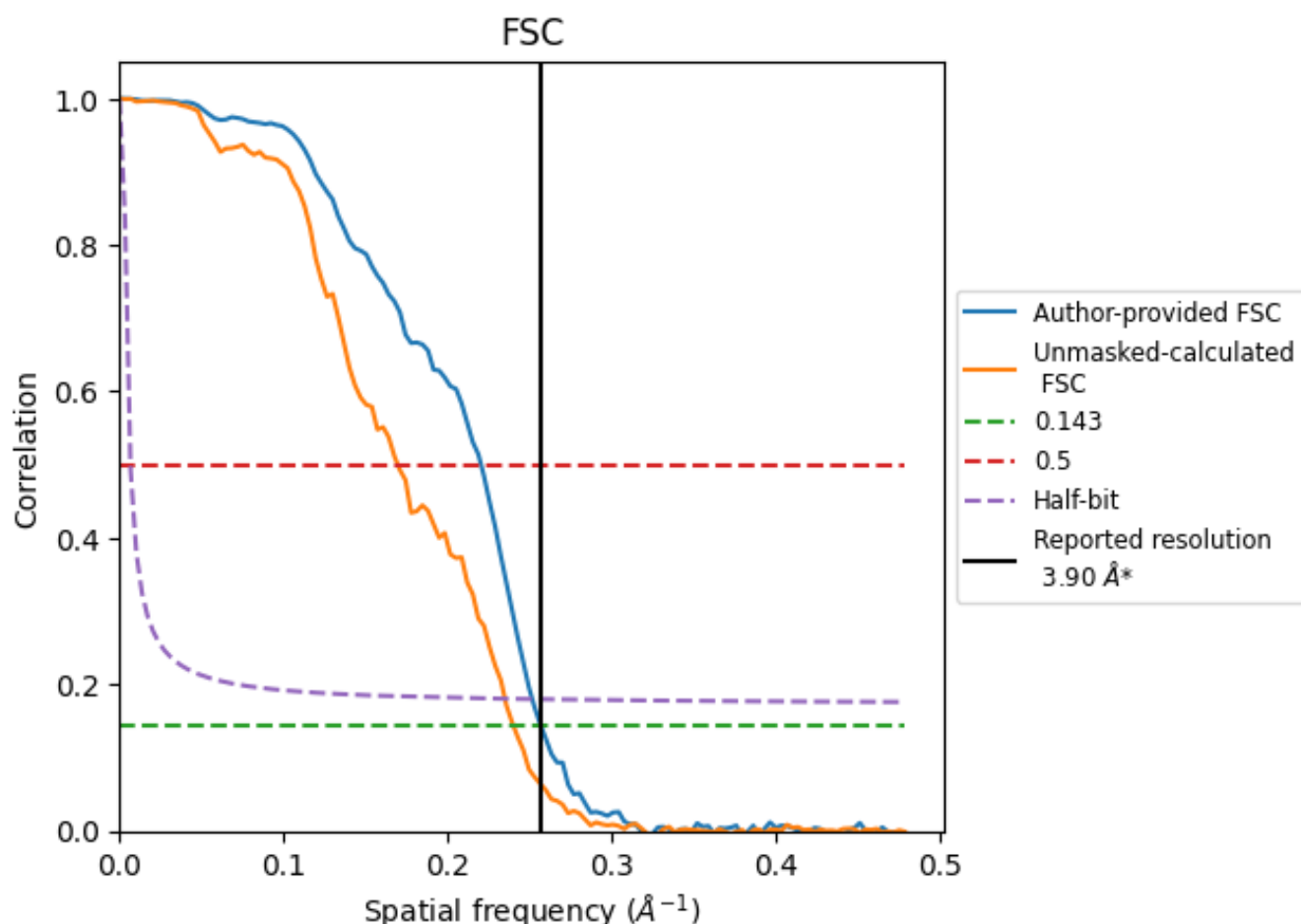


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

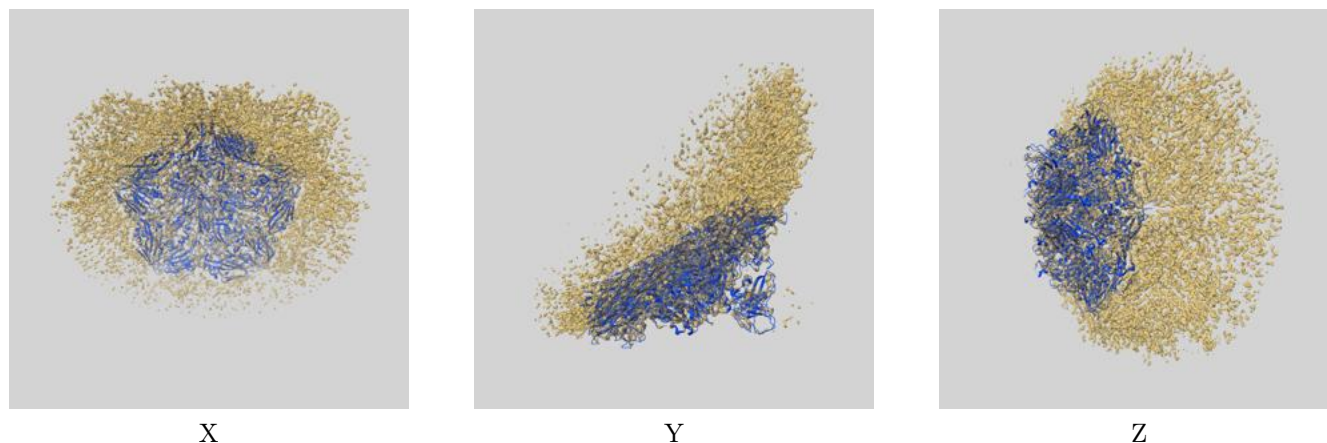
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.54	3.98
Unmasked-calculated*	4.16	5.90	4.26

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

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

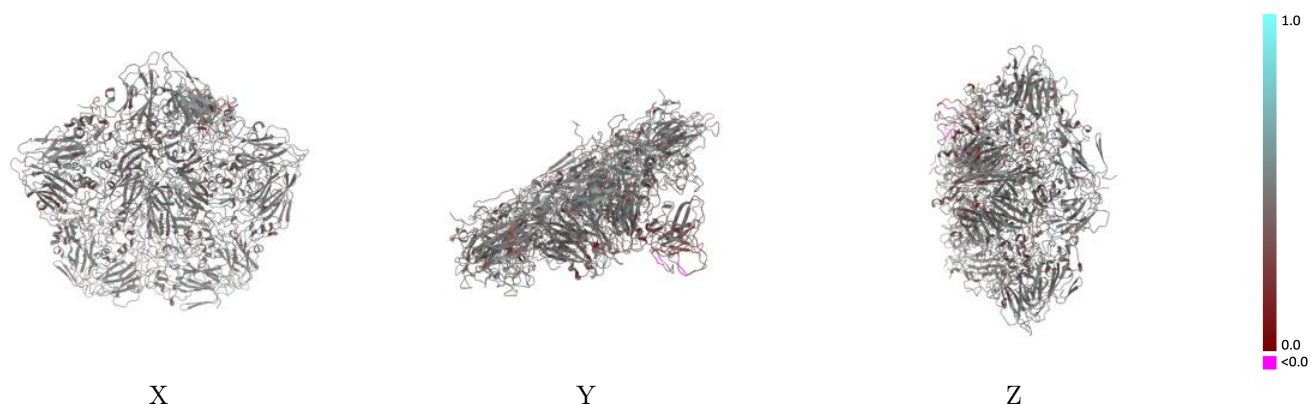
This section contains information regarding the fit between EMDB map EMD-26068 and PDB model 7TQS. Per-residue inclusion information can be found in section 3 on page 7.

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



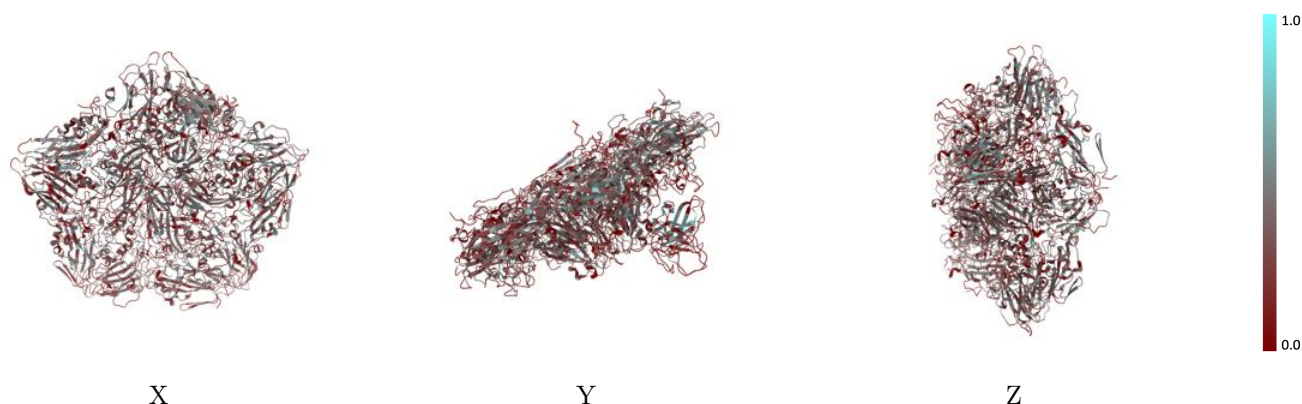
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

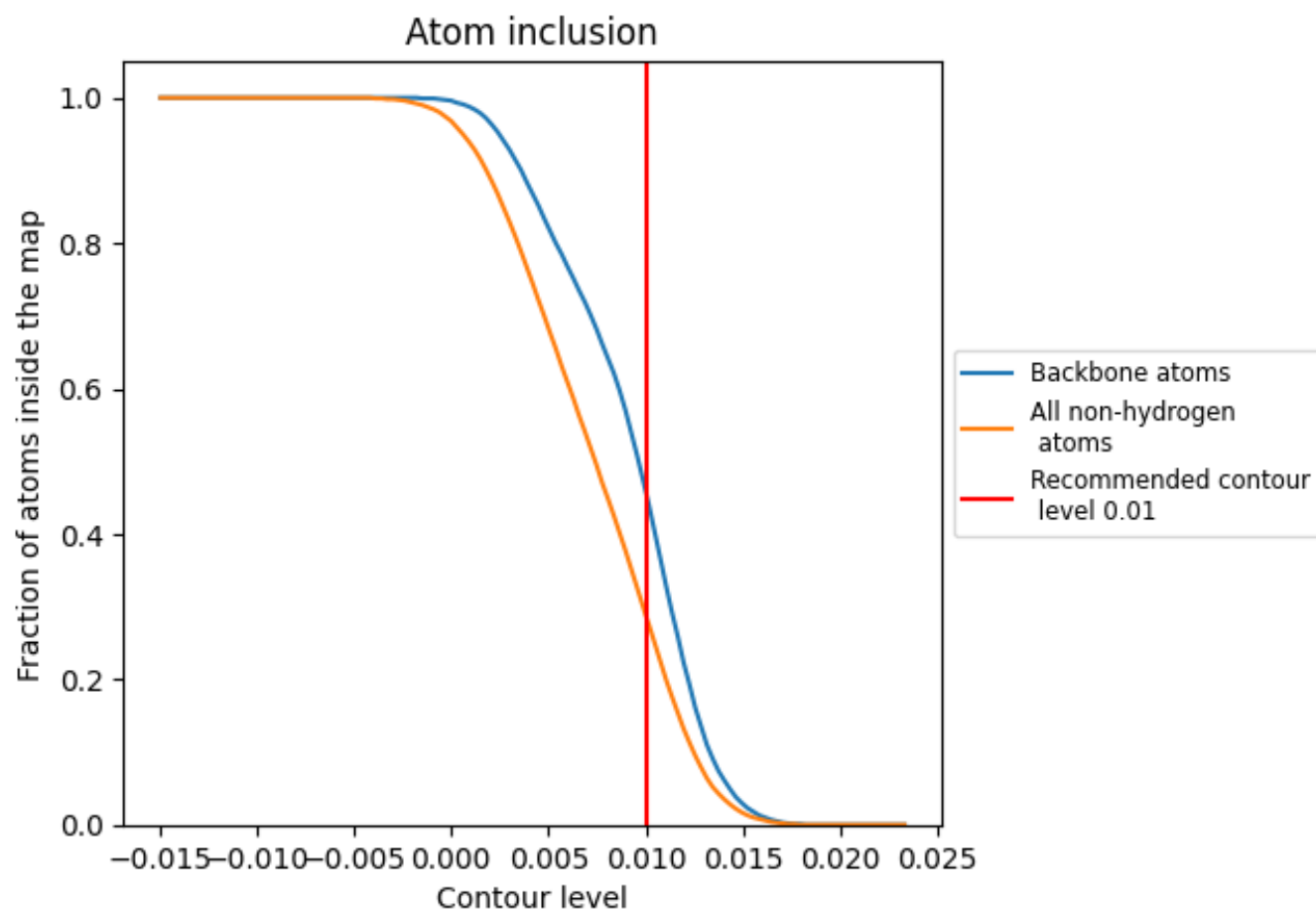
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.2880	 0.4460
H	 0.3360	 0.4200
L	 0.1190	 0.3000
a	 0.3010	 0.4510
b	 0.3310	 0.4540
c	 0.3340	 0.4550
d	 0.1700	 0.4260
e	 0.3000	 0.4490
f	 0.3200	 0.4550
g	 0.3320	 0.4560
h	 0.1910	 0.4380
i	 0.2730	 0.4410
j	 0.2550	 0.4380
k	 0.3110	 0.4510
l	 0.1440	 0.4140
m	 0.2680	 0.4440
n	 0.2870	 0.4540
o	 0.2620	 0.4430
p	 0.1420	 0.4290
q	 0.2950	 0.4450
r	 0.3360	 0.4560
s	 0.3150	 0.4590
t	 0.1790	 0.4350

