



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:12 AM UTC

PDB ID : 7TQS / pdb_00007tqs
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

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>.

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

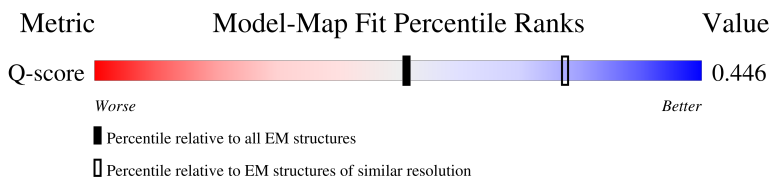
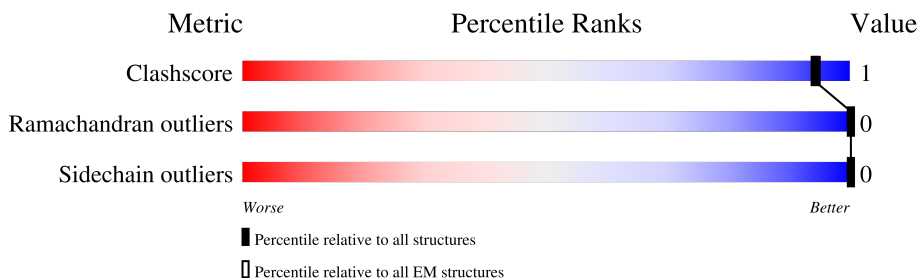
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	95% 98% .
2	H	106	66% 98% .
3	a	298	67% 83% 12% 5%
3	e	298	69% 85% 10% 5%

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Mol	Chain	Length	Quality of chain
3	i	298	73% 89% 6% 5%
3	m	298	73% 87% 8% 5%
3	q	298	68% 88% 7% 5%
4	b	272	60% 92% 5% .
4	f	272	64% 90% 6% .
4	j	272	76% 86% 10% .
4	n	272	72% 90% 6% 5%
4	r	272	60% 90% 5% 5%
5	c	240	64% 93% 7%
5	g	240	60% 90% 9%
5	k	240	72% 90% 8% .
5	o	240	79% 90% 9%
5	s	240	68% 90% 10%
6	d	69	78% 96% . .
6	h	69	78% 91% 6% ..
6	l	69	87% 84% 14% .
6	p	69	88% 88% 10% .
6	t	69	83% 91% 7% .

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.

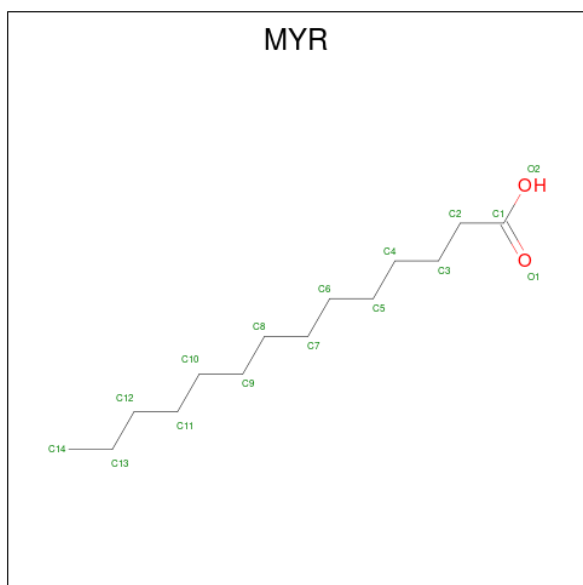
Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	h	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	l	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

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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 (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

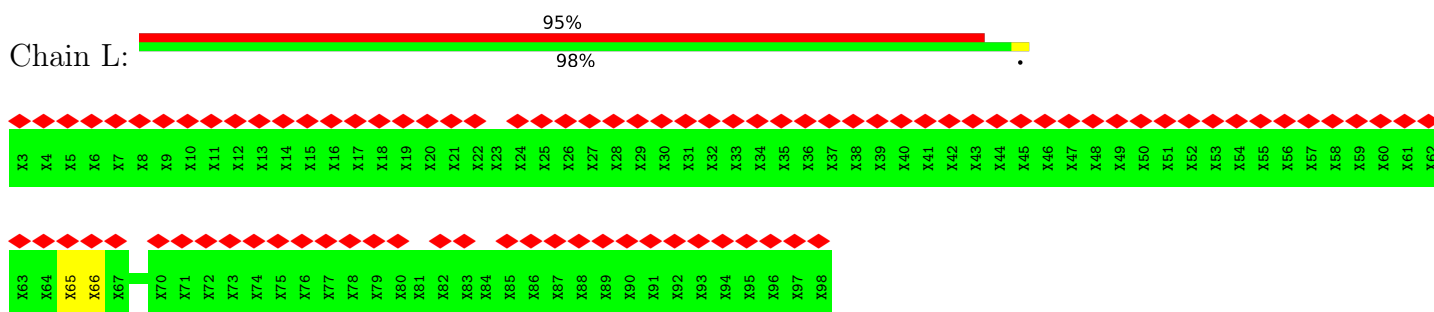


Mol	Chain	Residues	Atoms			AltConf
7	a	1	Total	C	O	0
			16	14	2	
7	e	1	Total	C	O	0
			16	14	2	
7	i	1	Total	C	O	0
			16	14	2	
7	m	1	Total	C	O	0
			16	14	2	
7	q	1	Total	C	O	0
			16	14	2	

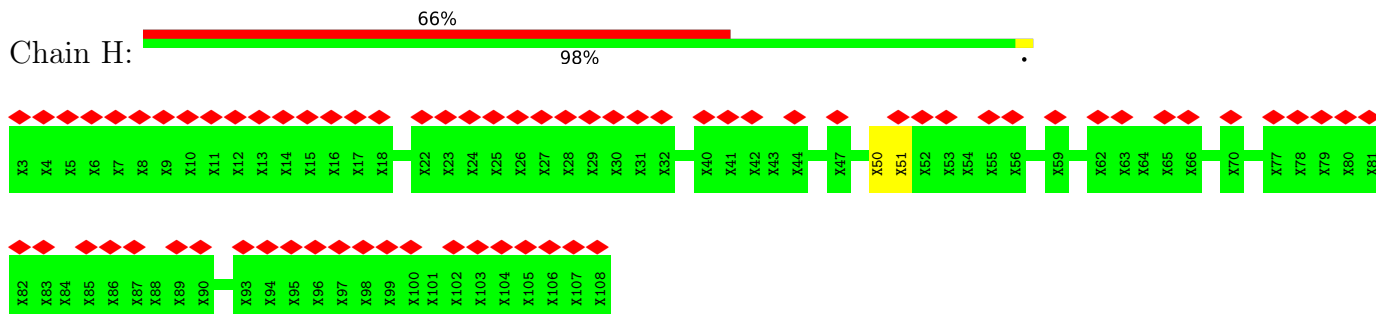
3 Residue-property plots [i](#)

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.

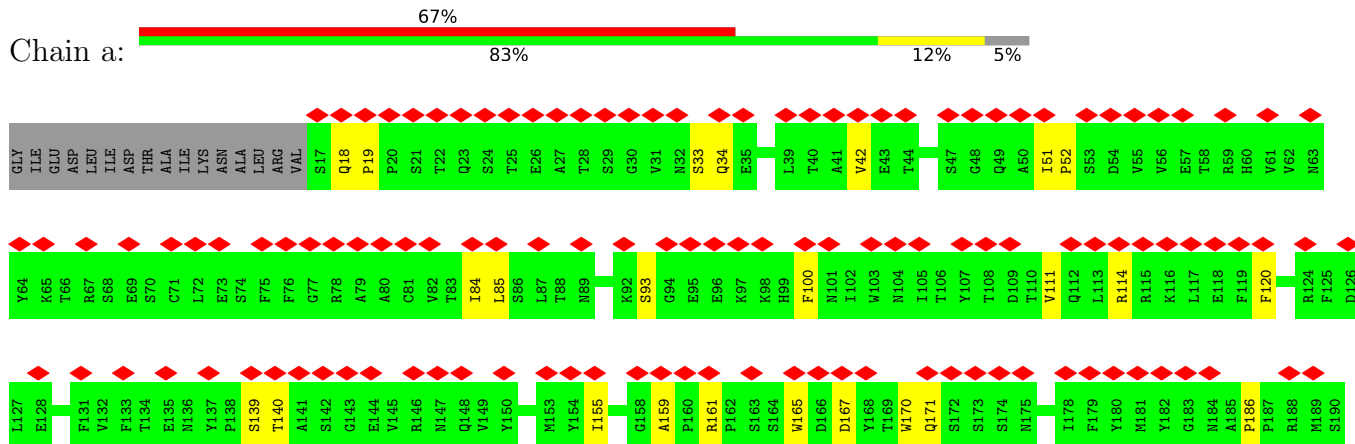
- Molecule 1: pAbC-3 light chain



- Molecule 2: pAbC-3 heavy chain

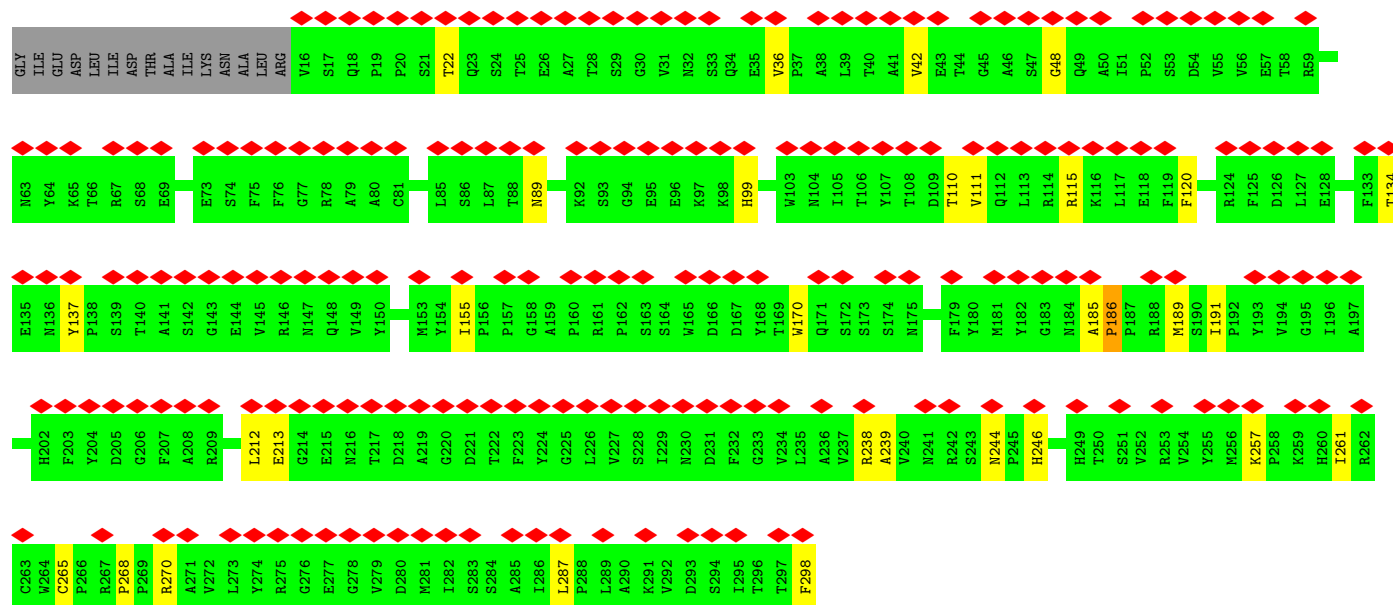
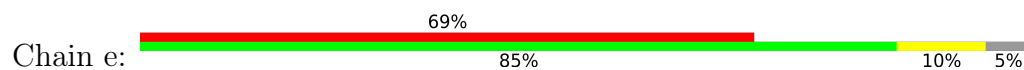


- Molecule 3: VP1

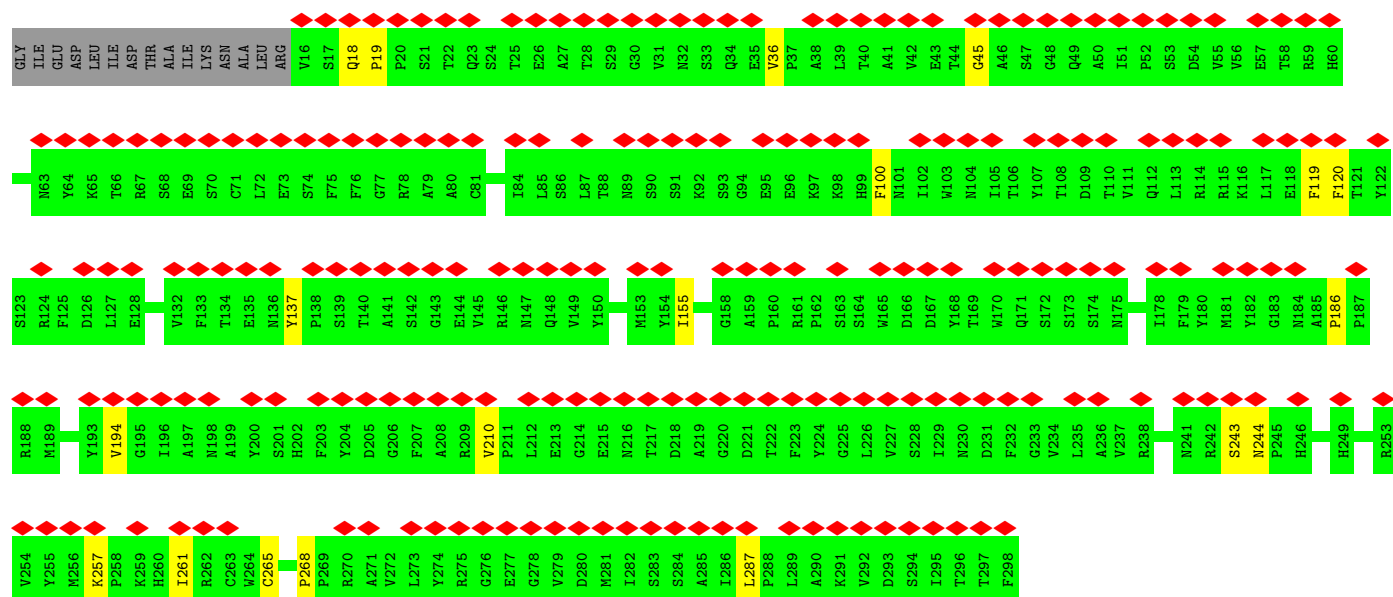
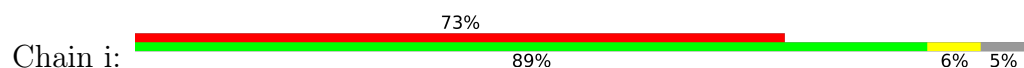




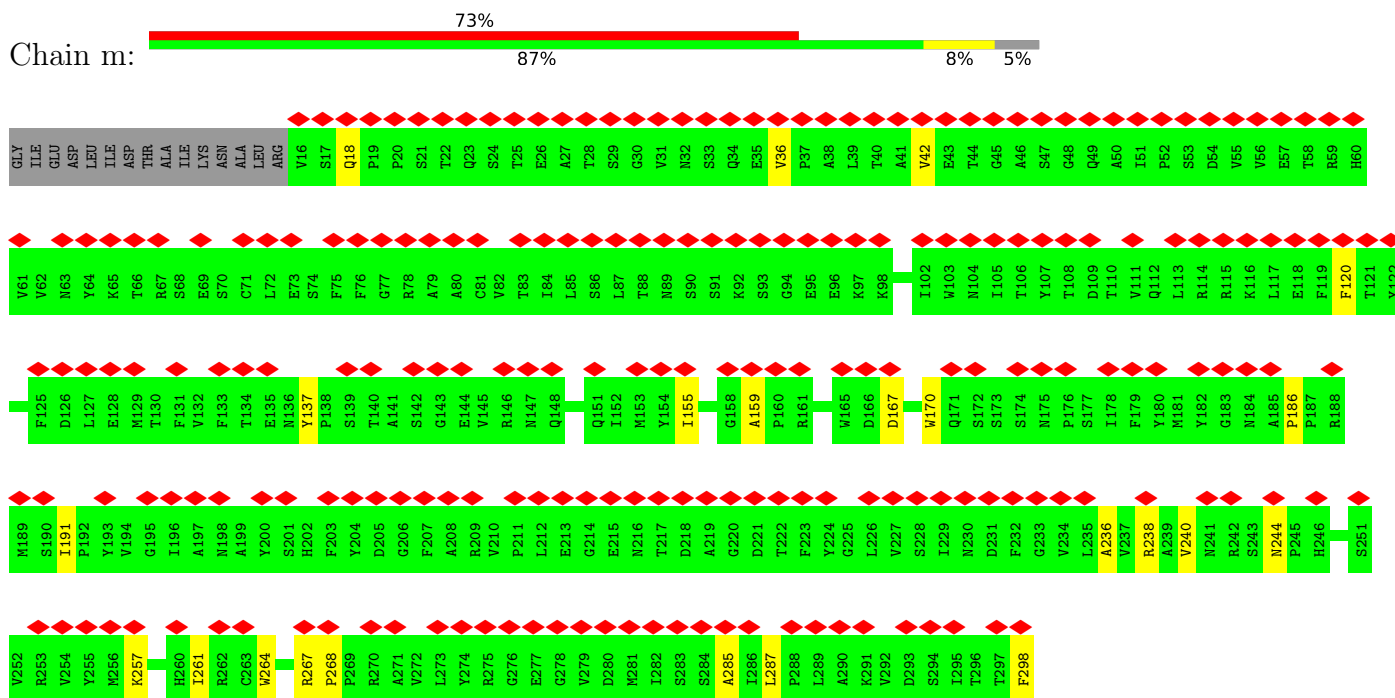
• Molecule 3: VP1



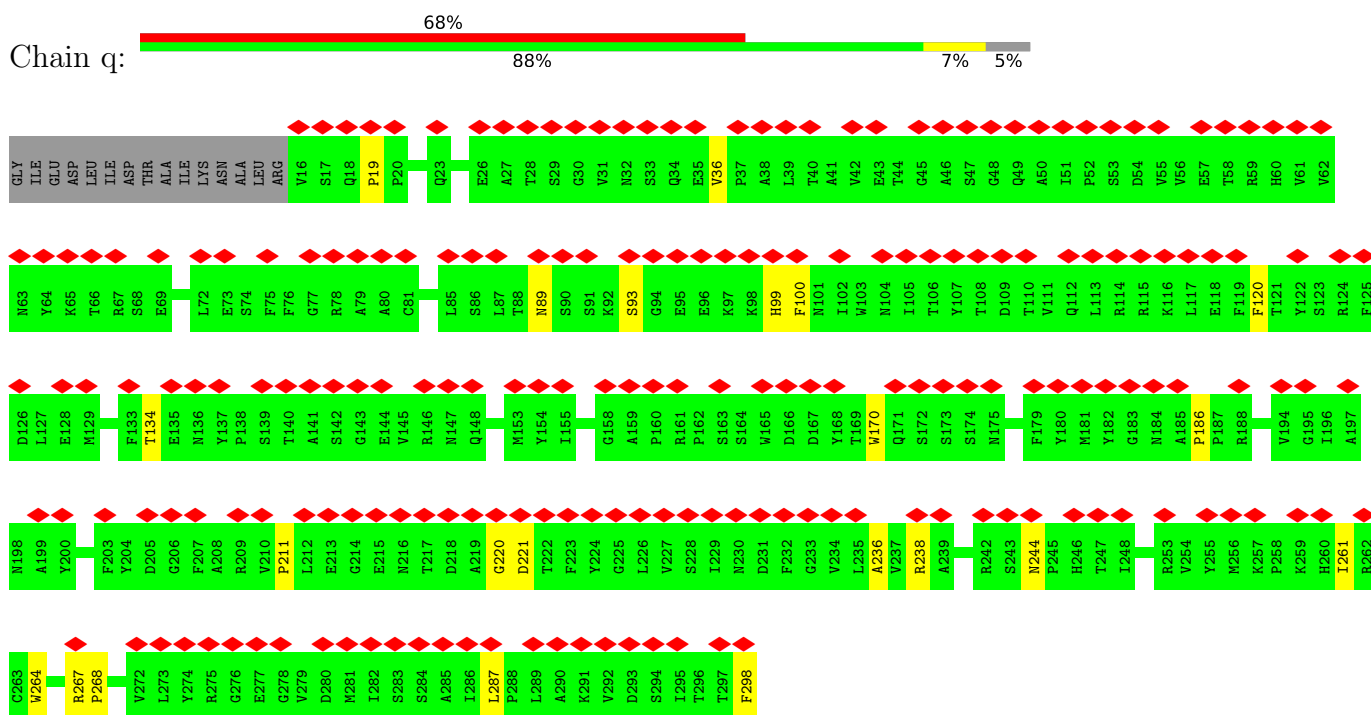
• Molecule 3: VP1



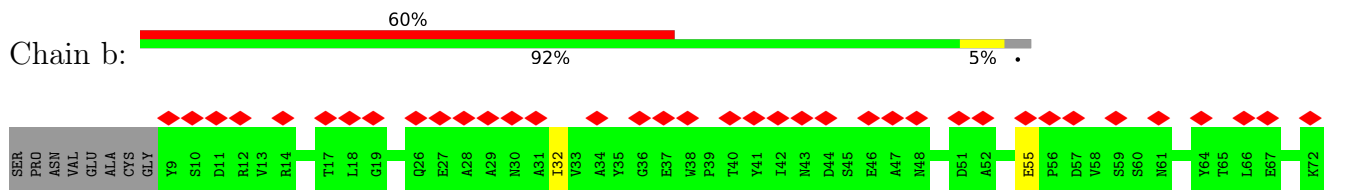
• Molecule 3: VP1

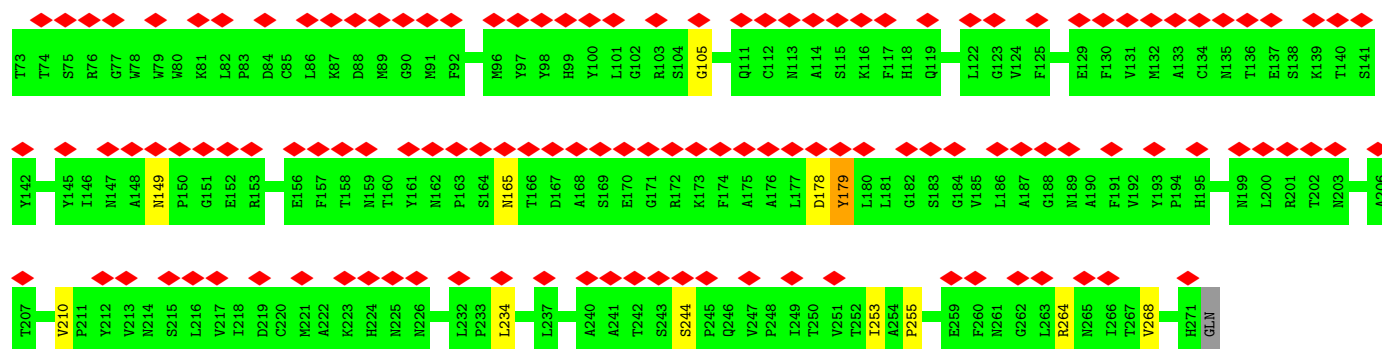


• Molecule 3: VP1

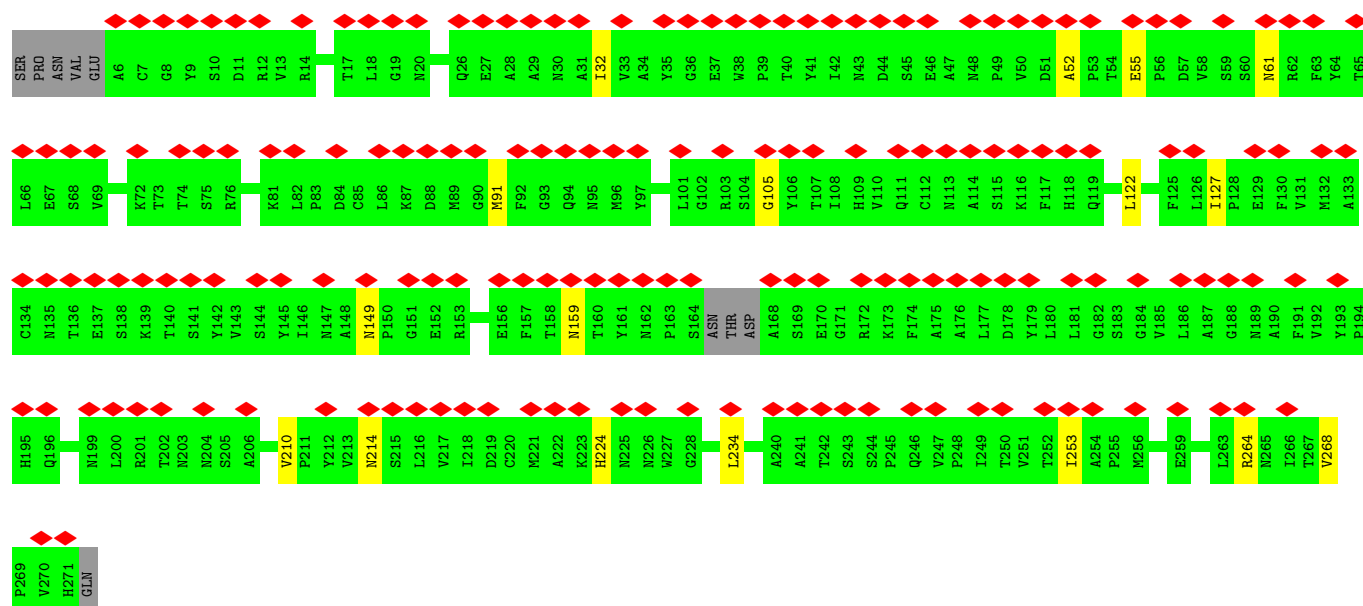
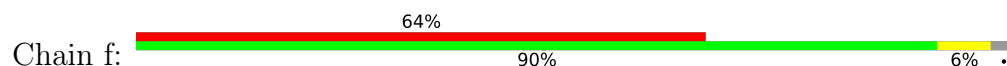


• Molecule 4: VP2

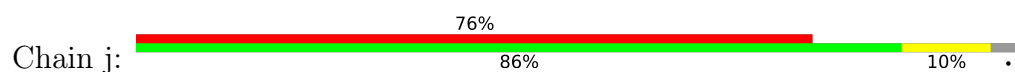




• Molecule 4: VP2

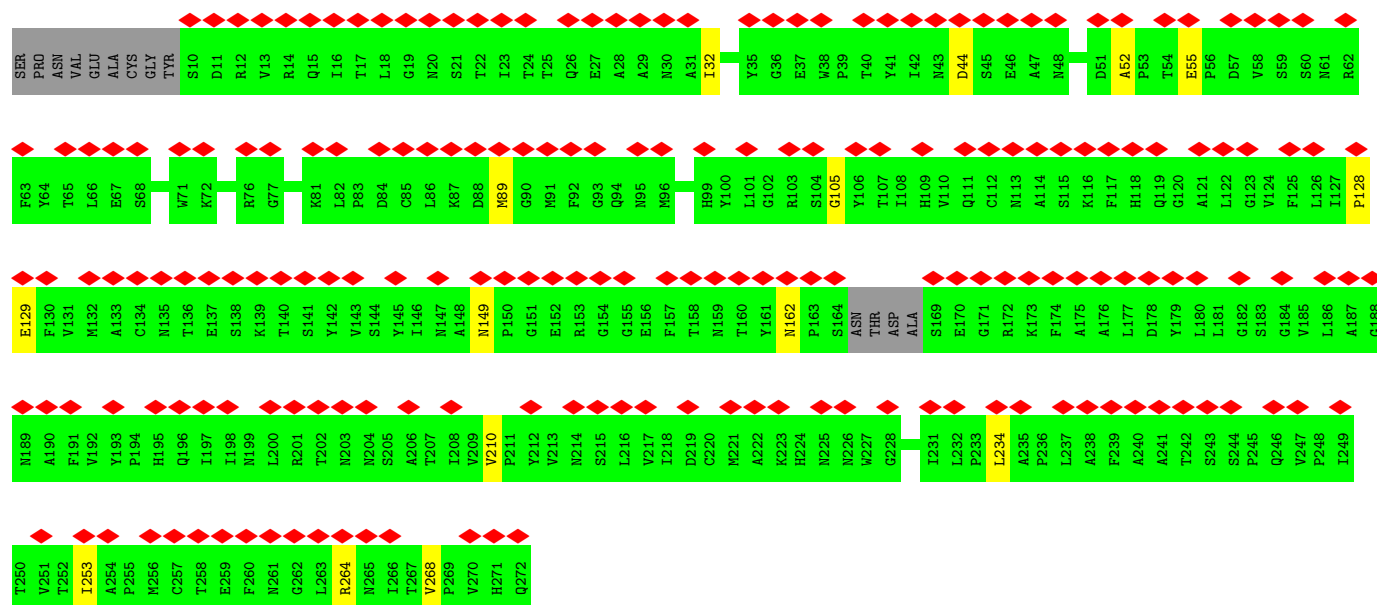
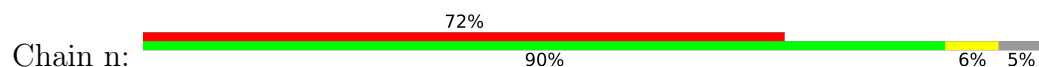


• Molecule 4: VP2

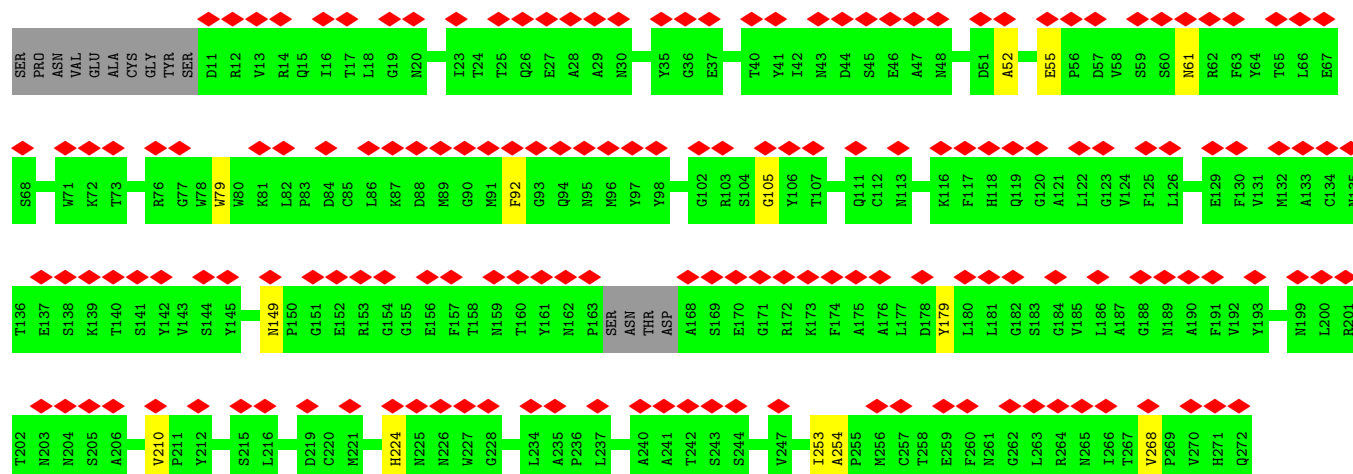
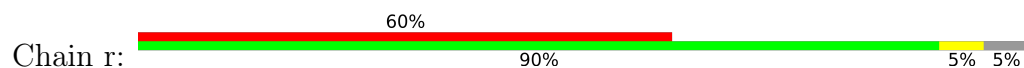




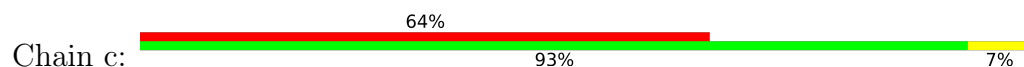
• Molecule 4: VP2

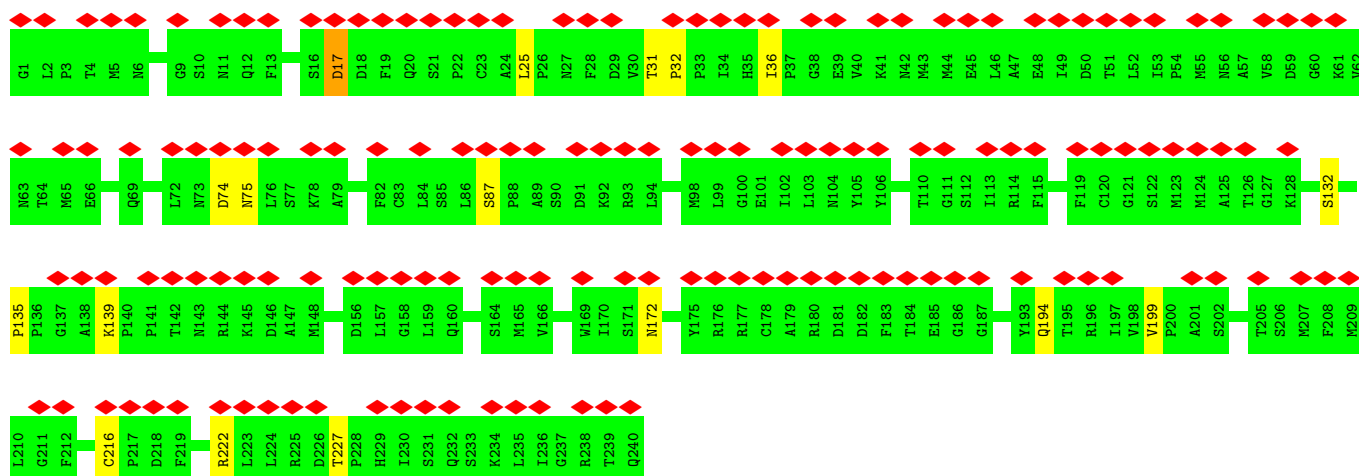


• Molecule 4: VP2

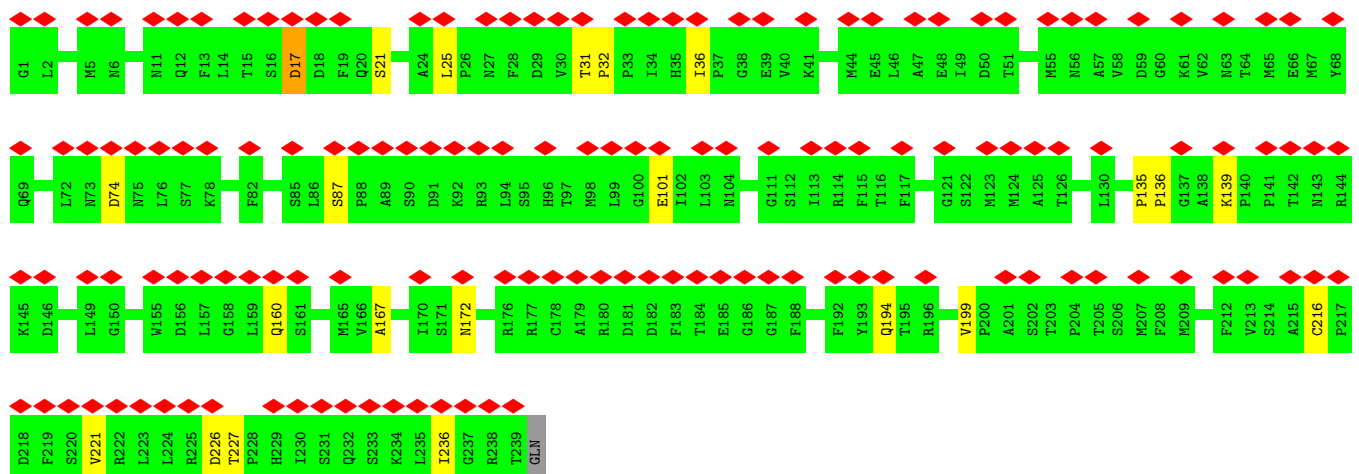
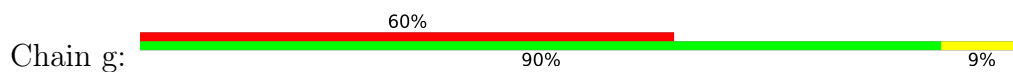


• Molecule 5: VP3

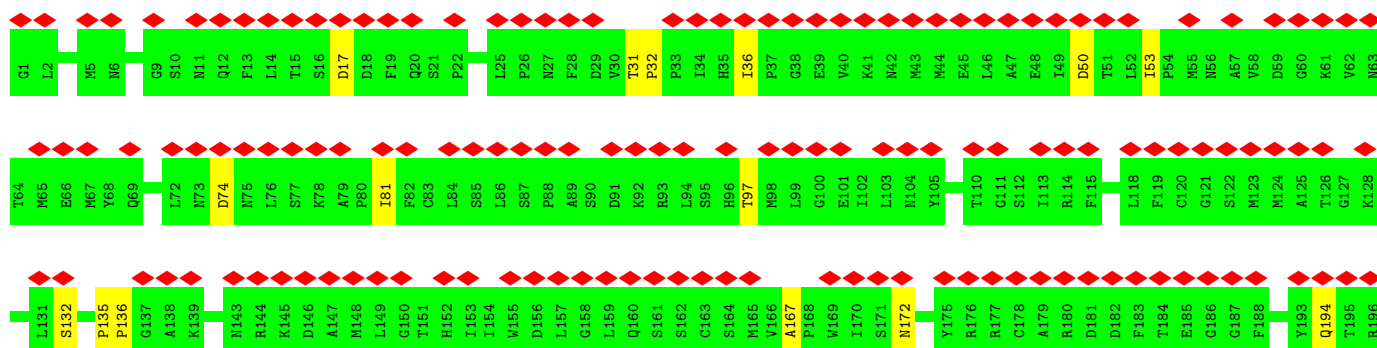
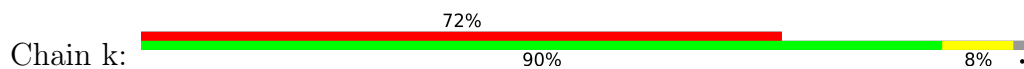




• Molecule 5: VP3

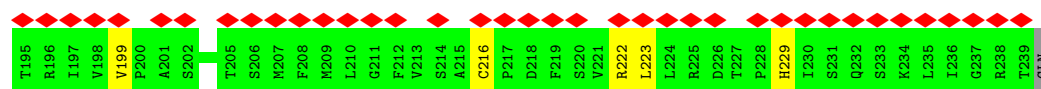
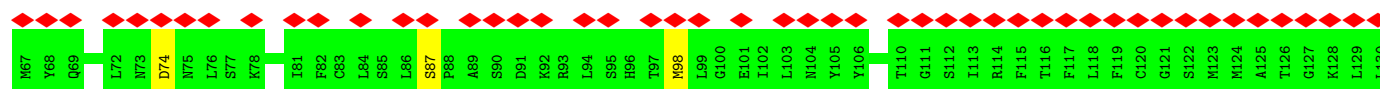
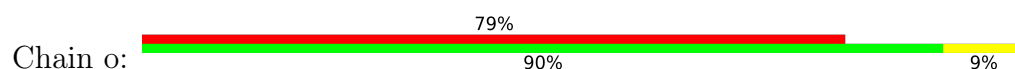


• Molecule 5: VP3

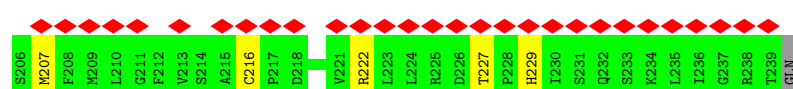
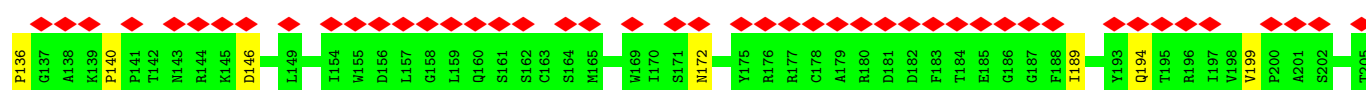
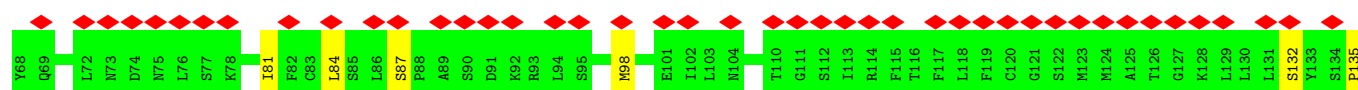
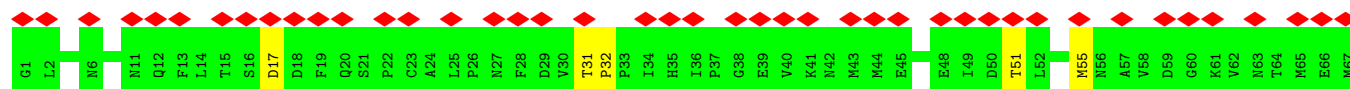
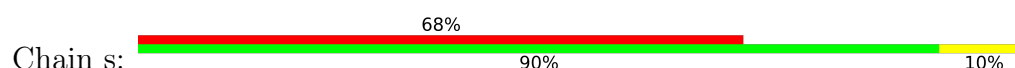




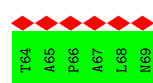
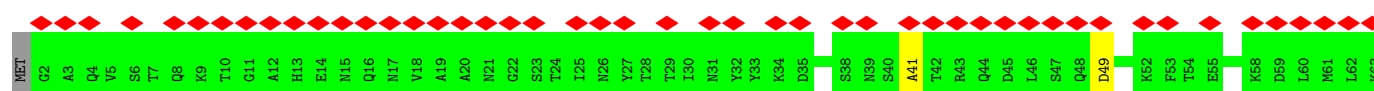
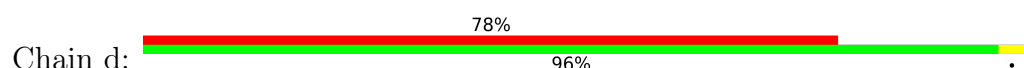
• Molecule 5: VP3



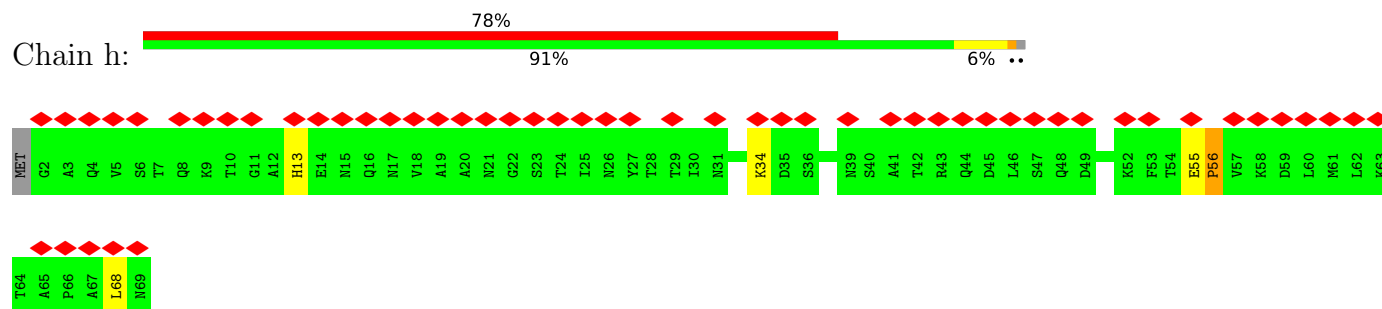
• Molecule 5: VP3



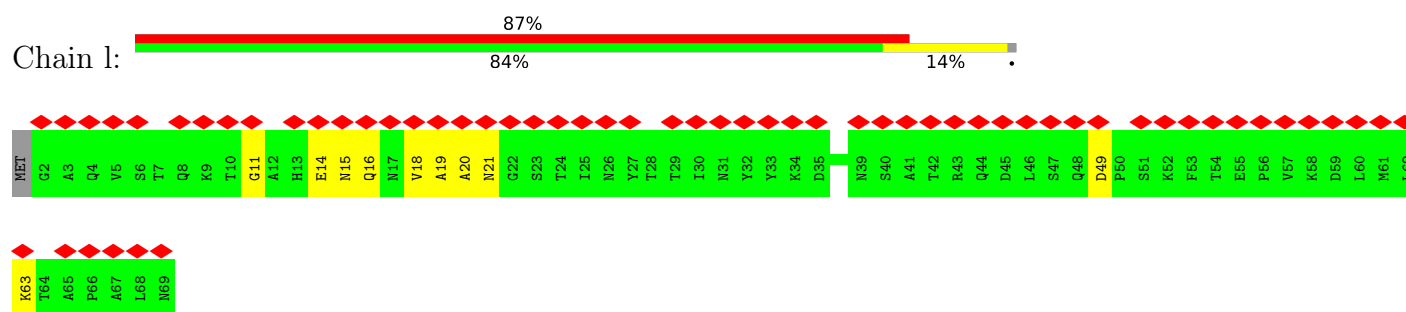
• Molecule 6: VP4



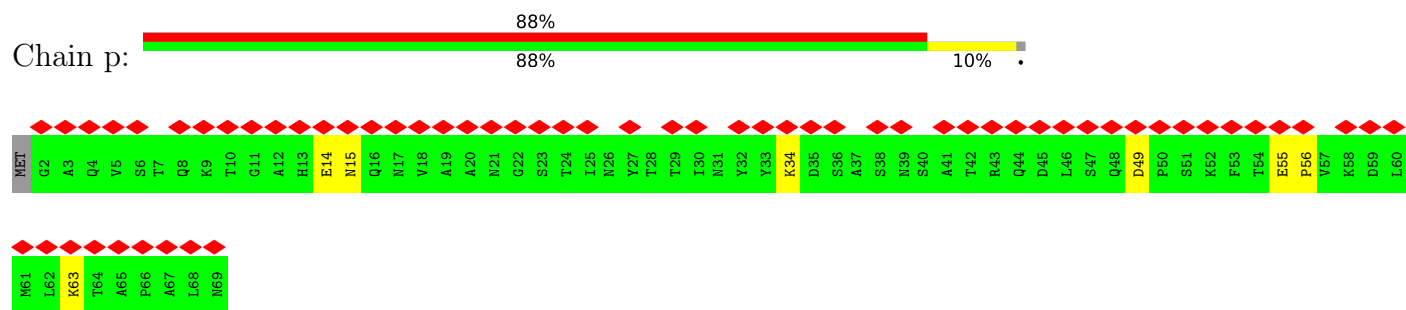
● Molecule 6: VP4



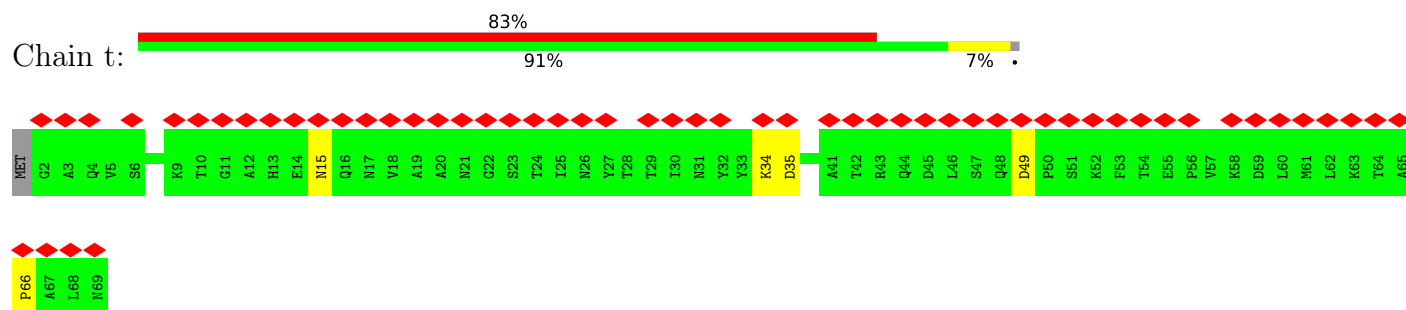
● Molecule 6: VP4



● 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 [i](#)

5.1 Standard geometry [i](#)

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	1.17	1/2281 (0.0%)	1.38	34/3111 (1.1%)
3	e	1.16	2/2288 (0.1%)	1.35	27/3121 (0.9%)
3	i	1.14	1/2288 (0.0%)	1.37	29/3121 (0.9%)
3	m	1.15	1/2288 (0.0%)	1.34	29/3121 (0.9%)
3	q	1.16	2/2288 (0.1%)	1.36	27/3121 (0.9%)
4	b	1.19	1/2101 (0.0%)	1.32	17/2876 (0.6%)
4	f	1.15	2/2092 (0.1%)	1.30	18/2861 (0.6%)
4	j	1.16	2/2086 (0.1%)	1.30	18/2852 (0.6%)
4	n	1.17	1/2068 (0.0%)	1.31	20/2827 (0.7%)
4	r	1.20	2/2061 (0.1%)	1.28	18/2818 (0.6%)
5	c	1.14	0/1906	1.35	24/2594 (0.9%)
5	g	1.15	0/1897	1.36	29/2582 (1.1%)
5	k	1.13	0/1859	1.35	22/2531 (0.9%)
5	o	1.16	1/1897 (0.1%)	1.35	19/2582 (0.7%)
5	s	1.14	1/1897 (0.1%)	1.38	25/2582 (1.0%)
6	d	1.04	0/519	1.20	2/705 (0.3%)
6	h	1.10	0/519	1.18	2/705 (0.3%)
6	l	1.02	0/519	1.12	3/705 (0.4%)
6	p	1.08	0/519	1.21	4/705 (0.6%)
6	t	1.11	0/519	1.20	4/705 (0.6%)
All	All	1.15	17/33892 (0.1%)	1.33	371/46225 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	j	224	HIS	CB-CG	-8.37	1.38	1.50
4	r	224	HIS	CB-CG	-7.29	1.40	1.50
3	i	100	PHE	CB-CG	-7.23	1.34	1.50
3	q	100	PHE	CB-CG	-7.04	1.34	1.50
4	f	224	HIS	CB-CG	-6.91	1.40	1.50
4	r	179	TYR	CB-CG	-6.77	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	m	298	PHE	CG-CD1	5.85	1.51	1.38
5	s	207	MET	CG-SD	-5.83	1.66	1.80
4	b	179	TYR	CB-CG	-5.67	1.39	1.51
3	a	114	ARG	CD-NE	-5.47	1.38	1.46
5	o	222	ARG	CG-CD	-5.43	1.36	1.52
4	f	122	LEU	C-N	-5.33	1.30	1.33
4	n	129	GLU	CG-CD	-5.33	1.38	1.52
3	e	298	PHE	CG-CD2	5.21	1.49	1.38
4	j	176	ALA	CA-C	-5.09	1.46	1.52
3	q	298	PHE	CG-CD1	5.04	1.49	1.38
3	e	246	HIS	CB-CG	-5.01	1.43	1.50

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	221	VAL	N-CA-C	11.67	124.42	113.10
5	o	135	PRO	CA-C-N	9.80	129.62	120.21
5	o	135	PRO	C-N-CA	9.80	129.62	120.21
5	k	135	PRO	CA-C-N	9.33	129.17	120.21
5	k	135	PRO	C-N-CA	9.33	129.17	120.21
5	s	135	PRO	CA-C-N	9.30	129.13	120.21
5	s	135	PRO	C-N-CA	9.30	129.13	120.21
4	b	234	LEU	N-CA-C	-9.24	102.52	113.88
5	g	135	PRO	CA-C-N	9.02	128.87	120.21
5	g	135	PRO	C-N-CA	9.02	128.87	120.21
3	i	36	VAL	CA-C-N	8.81	128.54	119.56
3	i	36	VAL	C-N-CA	8.81	128.54	119.56
3	e	99	HIS	CA-CB-CG	8.68	122.48	113.80
4	n	149	ASN	CA-C-N	8.63	128.36	119.56
4	n	149	ASN	C-N-CA	8.63	128.36	119.56
5	o	222	ARG	N-CA-C	8.52	124.17	113.43
4	f	234	LEU	N-CA-C	-8.52	103.40	113.88
3	m	267	ARG	CA-C-N	8.34	125.75	119.66
3	m	267	ARG	C-N-CA	8.34	125.75	119.66
4	n	268	VAL	CA-C-N	8.26	128.70	120.52
4	n	268	VAL	C-N-CA	8.26	128.70	120.52
4	j	268	VAL	CA-C-N	8.18	128.68	119.92
4	j	268	VAL	C-N-CA	8.18	128.68	119.92
3	a	261	ILE	N-CA-C	7.97	120.09	108.53
4	r	268	VAL	CA-C-N	7.93	128.38	120.52
4	r	268	VAL	C-N-CA	7.93	128.38	120.52
4	b	268	VAL	CA-C-N	7.90	128.37	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	268	VAL	C-N-CA	7.90	128.37	119.92
4	j	240	ALA	N-CA-C	7.84	119.83	111.28
3	a	264	TRP	N-CA-C	7.83	122.98	112.88
3	i	155	ILE	CA-C-N	7.66	125.25	119.66
3	i	155	ILE	C-N-CA	7.66	125.25	119.66
5	s	222	ARG	N-CA-C	7.56	122.95	113.43
5	c	31	THR	CA-C-N	7.47	125.12	119.66
5	c	31	THR	C-N-CA	7.47	125.12	119.66
4	b	149	ASN	CA-C-N	7.45	127.62	119.87
4	b	149	ASN	C-N-CA	7.45	127.62	119.87
3	q	287	LEU	CA-C-N	7.44	127.15	119.56
3	q	287	LEU	C-N-CA	7.44	127.15	119.56
3	q	99	HIS	CA-CB-CG	7.43	121.23	113.80
4	r	149	ASN	CA-C-N	7.34	126.97	119.56
4	r	149	ASN	C-N-CA	7.34	126.97	119.56
3	i	261	ILE	N-CA-C	7.30	118.39	108.17
5	s	216	CYS	CA-C-N	7.21	126.89	119.82
5	s	216	CYS	C-N-CA	7.21	126.89	119.82
4	n	55	GLU	CA-C-N	7.18	126.89	119.56
4	n	55	GLU	C-N-CA	7.18	126.89	119.56
6	h	56	PRO	N-CA-C	-7.16	99.95	111.19
5	o	32	PRO	CA-C-N	7.11	127.27	120.31
5	o	32	PRO	C-N-CA	7.11	127.27	120.31
3	m	42	VAL	N-CA-C	-7.08	106.41	113.20
3	e	42	VAL	N-CA-C	-7.07	106.41	113.20
3	q	100	PHE	CA-CB-CG	7.04	120.84	113.80
3	q	220	GLY	N-CA-C	-7.03	105.53	115.43
4	n	128	PRO	N-CA-C	-7.00	100.21	111.19
4	b	55	GLU	CA-C-N	6.99	126.69	119.56
4	b	55	GLU	C-N-CA	6.99	126.69	119.56
3	m	261	ILE	N-CA-C	6.97	117.92	108.17
3	m	287	LEU	CA-C-N	6.95	126.58	119.56
3	m	287	LEU	C-N-CA	6.95	126.58	119.56
3	m	268	PRO	CA-C-N	6.94	126.86	119.85
3	m	268	PRO	C-N-CA	6.94	126.86	119.85
5	k	31	THR	CA-C-N	6.93	124.72	119.66
5	k	31	THR	C-N-CA	6.93	124.72	119.66
3	m	36	VAL	CA-C-N	6.92	127.06	119.87
3	m	36	VAL	C-N-CA	6.92	127.06	119.87
3	e	261	ILE	N-CA-C	6.90	117.83	108.17
5	o	199	VAL	CA-C-N	6.87	126.81	120.21
5	o	199	VAL	C-N-CA	6.87	126.81	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	264	TRP	N-CA-C	6.85	122.60	112.94
3	a	42	VAL	N-CA-C	-6.84	106.47	113.10
3	a	287	LEU	CA-C-N	6.81	126.44	119.56
3	a	287	LEU	C-N-CA	6.81	126.44	119.56
4	f	52	ALA	CA-C-N	6.79	126.97	120.31
4	f	52	ALA	C-N-CA	6.79	126.97	120.31
3	e	36	VAL	CA-C-N	6.78	126.41	119.56
3	e	36	VAL	C-N-CA	6.78	126.41	119.56
5	s	199	VAL	CA-C-N	6.77	127.23	120.52
5	s	199	VAL	C-N-CA	6.77	127.23	120.52
3	e	244	ASN	CA-C-N	6.75	126.45	119.56
3	e	244	ASN	C-N-CA	6.75	126.45	119.56
4	b	165	ASN	N-CA-C	-6.72	101.65	110.53
3	q	244	ASN	CA-C-N	6.70	126.39	119.56
3	q	244	ASN	C-N-CA	6.70	126.39	119.56
5	g	25	LEU	CA-C-N	6.69	126.61	119.85
5	g	25	LEU	C-N-CA	6.69	126.61	119.85
3	a	214	GLY	N-CA-C	-6.68	106.43	113.58
3	q	267	ARG	CA-C-N	6.67	124.53	119.66
3	q	267	ARG	C-N-CA	6.67	124.53	119.66
5	s	32	PRO	CA-C-N	6.67	126.64	120.03
5	s	32	PRO	C-N-CA	6.67	126.64	120.03
4	j	52	ALA	CA-C-N	6.65	126.83	120.31
4	j	52	ALA	C-N-CA	6.65	126.83	120.31
4	j	149	ASN	CA-C-N	6.56	126.70	119.87
4	j	149	ASN	C-N-CA	6.56	126.70	119.87
3	m	264	TRP	N-CA-C	6.56	121.44	113.38
5	k	199	VAL	CA-C-N	6.55	126.50	120.21
5	k	199	VAL	C-N-CA	6.55	126.50	120.21
5	s	229	HIS	CA-C-N	-6.53	115.09	123.19
5	s	229	HIS	C-N-CA	-6.53	115.09	123.19
3	i	244	ASN	CA-C-N	6.45	126.14	119.56
3	i	244	ASN	C-N-CA	6.45	126.14	119.56
5	o	229	HIS	N-CA-C	-6.44	105.05	114.39
3	i	186	PRO	CA-C-N	6.42	126.33	119.85
3	i	186	PRO	C-N-CA	6.42	126.33	119.85
3	a	244	ASN	CA-C-N	6.40	126.09	119.56
3	a	244	ASN	C-N-CA	6.40	126.09	119.56
3	m	18	GLN	CA-C-N	6.38	124.26	119.66
3	m	18	GLN	C-N-CA	6.38	124.26	119.66
5	s	87	SER	CA-C-N	6.36	125.98	119.56
5	s	87	SER	C-N-CA	6.36	125.98	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	261	ILE	N-CA-C	6.34	117.73	108.53
3	a	93	SER	N-CA-C	6.34	117.99	111.14
4	r	254	ALA	CA-C-N	6.34	126.25	119.85
4	r	254	ALA	C-N-CA	6.34	126.25	119.85
5	g	199	VAL	CA-C-N	6.33	126.69	119.92
5	g	199	VAL	C-N-CA	6.33	126.69	119.92
5	o	216	CYS	CA-C-N	6.32	126.01	119.56
5	o	216	CYS	C-N-CA	6.32	126.01	119.56
3	q	36	VAL	CA-C-N	6.32	126.44	119.87
3	q	36	VAL	C-N-CA	6.32	126.44	119.87
4	n	52	ALA	CA-C-N	6.30	126.49	120.31
4	n	52	ALA	C-N-CA	6.30	126.49	120.31
3	i	194	VAL	N-CA-C	6.29	118.54	111.88
4	b	105	GLY	N-CA-C	-6.25	103.04	112.60
5	k	218	ASP	N-CA-C	-6.25	104.41	114.09
5	c	222	ARG	N-CA-C	6.23	120.06	111.71
3	q	19	PRO	CA-C-N	6.22	126.19	119.78
3	q	19	PRO	C-N-CA	6.22	126.19	119.78
5	g	32	PRO	CA-C-N	6.22	126.40	120.31
5	g	32	PRO	C-N-CA	6.22	126.40	120.31
4	r	52	ALA	CA-C-N	6.20	126.39	120.31
4	r	52	ALA	C-N-CA	6.20	126.39	120.31
6	d	49	ASP	CA-C-N	6.20	125.82	119.56
6	d	49	ASP	C-N-CA	6.20	125.82	119.56
5	g	236	ILE	N-CA-C	6.19	116.89	111.56
3	a	84	ILE	N-CA-C	6.17	117.11	111.81
3	e	287	LEU	CA-C-N	6.17	125.79	119.56
3	e	287	LEU	C-N-CA	6.17	125.79	119.56
4	j	57	ASP	N-CA-C	6.14	117.67	110.97
3	m	36	VAL	N-CA-C	6.14	114.17	107.60
3	i	265	CYS	CA-C-N	6.13	126.04	119.85
3	i	265	CYS	C-N-CA	6.13	126.04	119.85
5	c	25	LEU	CA-C-N	6.12	126.03	119.85
5	c	25	LEU	C-N-CA	6.12	126.03	119.85
4	f	61	ASN	CA-CB-CG	6.11	118.71	112.60
5	c	199	VAL	CA-C-N	6.11	127.52	120.98
5	c	199	VAL	C-N-CA	6.11	127.52	120.98
4	r	61	ASN	CA-CB-CG	6.09	118.69	112.60
3	a	120	PHE	CA-CB-CG	-6.08	107.72	113.80
5	s	194	GLN	N-CA-C	-6.07	104.95	112.90
3	q	220	GLY	CA-C-N	6.06	129.01	120.28
3	q	220	GLY	C-N-CA	6.06	129.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	227	THR	CA-C-N	6.06	126.58	120.04
5	k	227	THR	C-N-CA	6.06	126.58	120.04
4	n	234	LEU	N-CA-C	-6.06	106.02	113.41
5	c	216	CYS	CA-C-N	6.04	125.72	119.56
5	c	216	CYS	C-N-CA	6.04	125.72	119.56
5	c	194	GLN	N-CA-C	-6.03	105.00	112.90
3	i	100	PHE	CA-CB-CG	6.02	119.82	113.80
4	j	105	GLY	N-CA-C	-6.01	103.08	112.58
4	n	210	VAL	CA-C-N	6.00	125.97	120.03
4	n	210	VAL	C-N-CA	6.00	125.97	120.03
4	b	244	SER	CA-C-N	5.99	125.96	120.03
4	b	244	SER	C-N-CA	5.99	125.96	120.03
5	s	55	MET	N-CA-C	5.99	117.81	111.28
4	f	149	ASN	CA-C-N	5.99	126.10	119.87
4	f	149	ASN	C-N-CA	5.99	126.10	119.87
4	j	122	LEU	CA-C-N	-5.96	115.78	121.57
4	j	122	LEU	C-N-CA	-5.96	115.78	121.57
3	e	268	PRO	CA-C-N	5.96	125.92	120.03
3	e	268	PRO	C-N-CA	5.96	125.92	120.03
4	j	210	VAL	CA-C-N	5.95	126.14	120.31
4	j	210	VAL	C-N-CA	5.95	126.14	120.31
5	c	36	ILE	CA-C-N	5.95	125.91	119.78
5	c	36	ILE	C-N-CA	5.95	125.91	119.78
4	f	268	VAL	CA-C-N	5.94	125.91	120.03
4	f	268	VAL	C-N-CA	5.94	125.91	120.03
5	c	135	PRO	CA-C-N	5.93	127.26	119.84
5	c	135	PRO	C-N-CA	5.93	127.26	119.84
5	c	87	SER	CA-C-N	5.93	125.61	119.56
5	c	87	SER	C-N-CA	5.93	125.61	119.56
4	j	254	ALA	CA-C-N	5.93	125.89	119.78
4	j	254	ALA	C-N-CA	5.93	125.89	119.78
5	k	132	SER	N-CA-C	5.93	119.14	109.06
6	l	49	ASP	CA-C-N	5.93	125.80	119.28
6	l	49	ASP	C-N-CA	5.93	125.80	119.28
5	c	32	PRO	CA-C-N	5.91	125.82	119.85
5	c	32	PRO	C-N-CA	5.91	125.82	119.85
4	n	105	GLY	N-CA-C	-5.91	103.25	112.58
3	m	186	PRO	CA-C-N	5.90	125.81	119.85
3	m	186	PRO	C-N-CA	5.90	125.81	119.85
5	o	87	SER	CA-C-N	5.90	126.31	119.47
5	o	87	SER	C-N-CA	5.90	126.31	119.47
5	o	194	GLN	N-CA-C	-5.90	105.18	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	159	ALA	CA-C-N	5.86	125.80	119.76
3	m	159	ALA	C-N-CA	5.86	125.80	119.76
3	a	161	ARG	CA-C-N	5.85	125.75	119.85
3	a	161	ARG	C-N-CA	5.85	125.75	119.85
5	o	140	PRO	N-CA-C	-5.84	103.57	110.70
3	a	186	PRO	CA-C-N	5.83	125.74	119.85
3	a	186	PRO	C-N-CA	5.83	125.74	119.85
3	q	100	PHE	N-CA-CB	-5.83	101.56	110.65
4	f	55	GLU	CA-C-N	5.82	125.49	119.56
4	f	55	GLU	C-N-CA	5.82	125.49	119.56
4	b	32	ILE	N-CA-C	5.81	116.31	108.17
5	s	132	SER	N-CA-C	5.81	118.68	108.75
6	p	34	LYS	N-CA-C	5.81	118.39	111.71
3	a	111	VAL	N-CA-C	5.80	118.34	111.09
3	i	287	LEU	CA-C-N	5.79	125.41	119.56
3	i	287	LEU	C-N-CA	5.79	125.41	119.56
3	q	93	SER	N-CA-C	5.79	118.37	111.71
5	g	87	SER	CA-C-N	5.79	126.18	119.47
5	g	87	SER	C-N-CA	5.79	126.18	119.47
4	f	32	ILE	N-CA-C	5.79	116.27	108.17
3	m	137	TYR	CA-C-N	5.79	125.40	119.56
3	m	137	TYR	C-N-CA	5.79	125.40	119.56
3	a	159	ALA	CA-C-N	5.78	125.72	119.76
3	a	159	ALA	C-N-CA	5.78	125.72	119.76
4	n	253	ILE	N-CA-C	5.77	116.43	108.12
5	k	167	ALA	CA-C-N	5.77	125.74	120.03
5	k	167	ALA	C-N-CA	5.77	125.74	120.03
4	b	255	PRO	N-CA-C	-5.76	102.06	111.68
4	n	162	ASN	CA-C-N	5.75	125.66	119.85
4	n	162	ASN	C-N-CA	5.75	125.66	119.85
3	e	137	TYR	N-CA-C	-5.74	102.55	109.72
6	p	63	LYS	N-CA-C	5.73	117.52	111.28
5	g	227	THR	CA-C-N	5.72	126.67	120.83
5	g	227	THR	C-N-CA	5.72	126.67	120.83
3	m	244	ASN	CA-C-N	5.72	125.39	119.56
3	m	244	ASN	C-N-CA	5.72	125.39	119.56
3	i	268	PRO	CA-C-N	5.71	125.90	120.31
3	i	268	PRO	C-N-CA	5.71	125.90	120.31
3	i	194	VAL	CB-CA-C	-5.71	104.54	112.36
3	e	120	PHE	CA-CB-CG	-5.70	108.10	113.80
6	t	49	ASP	CA-C-N	5.69	125.36	119.56
6	t	49	ASP	C-N-CA	5.69	125.36	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	55	GLU	CA-C-N	5.68	125.36	119.56
4	r	55	GLU	C-N-CA	5.68	125.36	119.56
3	m	191	ILE	CA-C-N	5.68	125.63	119.78
3	m	191	ILE	C-N-CA	5.68	125.63	119.78
3	a	268	PRO	CA-C-N	5.67	125.58	119.85
3	a	268	PRO	C-N-CA	5.67	125.58	119.85
6	p	49	ASP	CA-C-N	5.65	125.32	119.56
6	p	49	ASP	C-N-CA	5.65	125.32	119.56
5	o	178	CYS	N-CA-C	-5.64	105.21	111.36
5	s	81	ILE	N-CA-C	-5.64	105.35	110.82
5	k	81	ILE	N-CA-C	-5.63	104.86	111.00
5	g	31	THR	CA-C-N	5.62	123.71	119.66
5	g	31	THR	C-N-CA	5.62	123.71	119.66
3	q	36	VAL	N-CA-C	5.62	113.71	108.15
3	i	120	PHE	CA-CB-CG	-5.60	108.20	113.80
3	q	268	PRO	CA-C-N	5.59	125.57	120.03
3	q	268	PRO	C-N-CA	5.59	125.57	120.03
3	e	22	THR	N-CA-C	-5.58	103.55	110.41
4	f	210	VAL	CA-C-N	5.57	125.77	120.31
4	f	210	VAL	C-N-CA	5.57	125.77	120.31
5	c	132	SER	N-CA-C	5.57	117.53	109.07
5	s	17	ASP	CA-CB-CG	5.54	118.14	112.60
5	k	53	ILE	CB-CA-C	-5.53	104.42	110.78
3	e	111	VAL	CA-C-N	-5.51	112.90	120.28
3	e	111	VAL	C-N-CA	-5.51	112.90	120.28
3	e	239	ALA	CA-C-N	-5.51	115.22	122.16
3	e	239	ALA	C-N-CA	-5.51	115.22	122.16
5	g	216	CYS	CA-C-N	5.50	125.17	119.56
5	g	216	CYS	C-N-CA	5.50	125.17	119.56
3	i	100	PHE	N-CA-CB	-5.50	102.08	110.65
4	f	253	ILE	N-CA-C	5.50	116.03	108.12
5	k	32	PRO	CA-C-N	5.49	125.47	120.03
5	k	32	PRO	C-N-CA	5.49	125.47	120.03
5	g	17	ASP	CA-CB-CG	5.48	118.08	112.60
6	t	66	PRO	N-CA-C	-5.48	102.58	111.03
4	r	253	ILE	N-CA-C	5.48	116.63	108.46
5	g	226	ASP	CA-CB-CG	5.46	118.06	112.60
3	i	18	GLN	CA-C-N	5.46	123.59	119.66
3	i	18	GLN	C-N-CA	5.46	123.59	119.66
5	c	17	ASP	CA-CB-CG	5.43	118.03	112.60
4	f	105	GLY	N-CA-C	-5.40	104.04	112.58
5	g	194	GLN	N-CA-C	-5.39	105.84	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	21	SER	CA-C-N	5.39	125.29	119.85
5	g	21	SER	C-N-CA	5.39	125.29	119.85
6	h	34	LYS	N-CA-C	5.38	117.90	111.71
5	k	74	ASP	CA-CB-CG	5.36	117.96	112.60
3	a	85	LEU	N-CA-C	5.36	118.78	111.39
3	q	120	PHE	CA-CB-CG	-5.35	108.45	113.80
3	m	120	PHE	CA-CB-CG	-5.35	108.45	113.80
5	s	227	THR	CA-C-N	5.35	125.43	119.87
5	s	227	THR	C-N-CA	5.35	125.43	119.87
3	a	85	LEU	CB-CA-C	-5.34	104.30	111.89
5	k	36	ILE	CA-C-N	5.34	125.28	119.78
5	k	36	ILE	C-N-CA	5.34	125.28	119.78
3	q	211	PRO	N-CA-C	-5.34	102.81	111.19
4	r	210	VAL	CA-C-N	5.33	125.53	120.31
4	r	210	VAL	C-N-CA	5.33	125.53	120.31
3	e	48	GLY	N-CA-C	-5.31	105.29	112.14
5	o	36	ILE	CA-C-N	5.30	125.24	119.78
5	o	36	ILE	C-N-CA	5.30	125.24	119.78
5	g	36	ILE	CA-C-N	5.29	125.26	120.03
5	g	36	ILE	C-N-CA	5.29	125.26	120.03
5	k	97	THR	N-CA-C	-5.28	103.71	110.53
3	q	100	PHE	N-CA-C	5.27	117.00	108.41
5	k	194	GLN	N-CA-C	-5.27	105.13	112.45
4	j	128	PRO	N-CA-C	-5.26	103.01	111.38
5	c	227	THR	CA-C-N	5.26	126.29	120.45
5	c	227	THR	C-N-CA	5.26	126.29	120.45
4	b	253	ILE	N-CA-C	5.25	116.29	108.46
4	r	224	HIS	N-CA-C	5.25	117.64	108.76
3	e	186	PRO	CA-C-N	5.25	125.16	119.85
3	e	186	PRO	C-N-CA	5.25	125.16	119.85
3	e	265	CYS	CA-C-N	5.25	125.15	119.85
3	e	265	CYS	C-N-CA	5.25	125.15	119.85
3	a	268	PRO	N-CA-C	-5.25	104.97	110.58
3	m	155	ILE	CA-C-N	5.24	125.78	120.38
3	m	155	ILE	C-N-CA	5.24	125.78	120.38
3	a	18	GLN	CA-C-N	5.23	123.43	119.66
3	a	18	GLN	C-N-CA	5.23	123.43	119.66
3	a	191	ILE	CA-C-N	5.23	125.21	120.03
3	a	191	ILE	C-N-CA	5.23	125.21	120.03
3	i	210	VAL	CB-CA-C	-5.22	104.77	110.78
4	f	127	ILE	N-CA-C	5.21	113.67	107.73
3	i	19	PRO	CA-C-N	5.21	125.12	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	i	19	PRO	C-N-CA	5.21	125.12	119.76
6	l	63	LYS	N-CA-C	5.21	116.64	111.07
3	q	186	PRO	CA-C-N	5.21	125.11	119.85
3	q	186	PRO	C-N-CA	5.21	125.11	119.85
5	k	50	ASP	CA-CB-CG	5.21	117.81	112.60
4	b	210	VAL	CA-C-N	5.20	125.41	120.31
4	b	210	VAL	C-N-CA	5.20	125.41	120.31
5	s	140	PRO	CA-C-N	5.20	126.34	119.84
5	s	140	PRO	C-N-CA	5.20	126.34	119.84
4	n	89	MET	N-CA-C	5.19	116.98	108.52
6	t	15	ASN	CA-CB-CG	-5.18	107.42	112.60
4	j	235	ALA	N-CA-C	-5.16	102.34	110.14
5	g	167	ALA	CA-C-N	5.16	125.14	120.03
5	g	167	ALA	C-N-CA	5.16	125.14	120.03
5	s	31	THR	CA-C-N	5.15	123.42	119.66
5	s	31	THR	C-N-CA	5.15	123.42	119.66
5	o	223	LEU	CB-CA-C	-5.15	102.85	110.62
5	o	132	SER	N-CA-C	5.14	116.88	109.07
5	c	139	LYS	CA-C-N	5.14	123.41	119.66
5	c	139	LYS	C-N-CA	5.14	123.41	119.66
4	r	92	PHE	N-CA-C	-5.12	105.61	111.14
3	i	243	SER	N-CA-C	5.10	117.63	110.23
3	a	19	PRO	CA-C-N	5.10	125.00	119.85
3	a	19	PRO	C-N-CA	5.10	125.00	119.85
3	e	155	ILE	CA-C-N	5.09	125.62	120.38
3	e	155	ILE	C-N-CA	5.09	125.62	120.38
4	f	214	ASN	CA-CB-CG	5.09	117.69	112.60
4	r	79	TRP	N-CA-C	5.09	116.98	108.99
3	i	119	PHE	CA-CB-CG	5.07	118.87	113.80
4	n	32	ILE	N-CA-C	5.07	115.89	108.53
3	e	191	ILE	CA-C-N	5.07	125.05	120.03
3	e	191	ILE	C-N-CA	5.07	125.05	120.03
5	g	139	LYS	CA-C-N	5.06	123.36	119.66
5	g	139	LYS	C-N-CA	5.06	123.36	119.66
3	a	111	VAL	CA-C-N	-5.06	113.11	120.29
3	a	111	VAL	C-N-CA	-5.06	113.11	120.29
4	r	105	GLY	N-CA-C	-5.04	104.62	112.58
4	n	210	VAL	N-CA-CB	-5.04	104.71	111.86
4	b	210	VAL	N-CA-CB	-5.04	104.71	111.86
4	f	91	MET	N-CA-C	-5.04	108.88	114.62
3	m	285	ALA	CA-C-N	5.03	129.26	120.86
3	m	285	ALA	C-N-CA	5.03	129.26	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	n	44	ASP	CA-CB-CG	-5.03	107.58	112.60
3	a	297	THR	N-CA-C	5.02	119.12	112.89
3	i	137	TYR	CA-C-N	5.02	125.46	120.04
3	i	137	TYR	C-N-CA	5.02	125.46	120.04
4	j	79	TRP	N-CA-C	5.02	116.87	108.99
5	s	146	ASP	N-CA-C	-5.02	105.48	112.45
3	a	155	ILE	CA-C-N	5.00	125.53	120.38
3	a	155	ILE	C-N-CA	5.00	125.53	120.38

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	11	0
3	e	2226	0	2146	10	0
3	i	2226	0	2146	2	0
3	m	2226	0	2146	5	0
3	q	2226	0	2146	7	0
4	b	2044	0	1967	2	0
4	f	2036	0	1962	2	0
4	j	2030	0	1957	9	0
4	n	2013	0	1943	1	0
4	r	2006	0	1938	0	0
5	c	1857	0	1844	4	0
5	g	1848	0	1836	6	0
5	k	1810	0	1791	3	0
5	o	1848	0	1836	7	0
5	s	1848	0	1836	4	0
6	d	512	0	493	1	0
6	h	512	0	493	3	0
6	l	512	0	493	11	0
6	p	512	0	493	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	t	512	0	493	2	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	80	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 (80) 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)
4:j:88:ASP:C	4:j:89:MET:HE2	2.22	0.64
5:o:155:TRP:CG	5:o:163:CYS:HG	2.22	0.57
6:l:15:ASN:HB3	6:l:21:ASN:ND2	2.19	0.57
6:l:15:ASN:HD21	6:l:19:ALA:HA	1.69	0.57
6:l:15:ASN:HB3	6:l:21:ASN:CB	2.36	0.56
3:q:221:ASP:N	3:q:221:ASP:OD1	2.36	0.55
6:d:41:ALA:O	6:t:34:LYS:NZ	2.41	0.54
3:i:257:LYS:NZ	5:k:17:ASP:O	2.41	0.53
6:l:15:ASN:HB3	6:l:21:ASN:HD22	1.73	0.53
3:q:170:TRP:CH2	3:q:236:ALA:HB1	2.44	0.53
1:L:65:UNK:O	1:L:66:UNK:C	2.57	0.52
3:q:170:TRP:CH2	3:q:238:ARG:HB3	2.45	0.51
4:j:89:MET:HE2	4:j:89:MET:N	2.25	0.51
3:q:170:TRP:CE2	3:q:238:ARG:HD3	2.45	0.51
3:q:170:TRP:CD2	3:q:238:ARG:HD3	2.46	0.51
3:m:167:ASP:O	3:m:170:TRP:HD1	1.94	0.51
3:e:170:TRP:CD2	3:e:238:ARG:HD2	2.46	0.51
3:m:257:LYS:NZ	5:o:17:ASP:O	2.44	0.51
3:a:170:TRP:CH2	3:a:236:ALA:HB1	2.47	0.50
3:e:257:LYS:NZ	5:g:17:ASP:O	2.45	0.50
4:j:178:ASP:OD1	4:j:178:ASP:N	2.43	0.49
6:l:16:GLN:C	6:l:18:VAL:H	2.19	0.49
3:e:115:ARG:NH2	5:g:101:GLU:OE1	2.46	0.49
3:a:257:LYS:NZ	5:c:17:ASP:O	2.46	0.49
5:g:160:GLN:HE22	6:h:68:LEU:H	1.60	0.49
6:p:14:GLU:HG3	6:p:15:ASN:H	1.77	0.49
5:o:172:ASN:N	5:o:172:ASN:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:264:ARG:NH1	5:g:136:PRO:O	2.46	0.48
5:k:172:ASN:OD1	5:k:172:ASN:N	2.43	0.48
3:a:240:VAL:HG23	3:e:134:THR:HG21	1.96	0.48
4:f:264:ARG:NH1	5:k:136:PRO:O	2.47	0.48
4:j:64:TYR:HB3	4:j:89:MET:SD	2.53	0.47
6:l:18:VAL:HG23	6:l:20:ALA:H	1.78	0.47
5:o:74:ASP:N	5:o:74:ASP:OD1	2.42	0.47
3:i:45:GLY:H	4:j:32:ILE:HD11	1.80	0.47
3:a:100:PHE:O	3:a:100:PHE:CG	2.68	0.46
2:H:50:UNK:O	2:H:51:UNK:C	2.64	0.46
4:n:264:ARG:NH1	5:s:136:PRO:O	2.49	0.46
4:j:81:LYS:NZ	4:j:130:PHE:O	2.48	0.46
5:s:51:THR:HG21	5:s:98:MET:H	1.82	0.45
5:c:172:ASN:OD1	5:c:172:ASN:N	2.49	0.45
3:m:240:VAL:HG23	3:q:134:THR:HG21	1.99	0.45
3:e:189:MET:N	3:e:189:MET:SD	2.90	0.44
6:l:15:ASN:CB	6:l:21:ASN:HB2	2.48	0.44
3:e:212:LEU:O	3:e:213:GLU:C	2.61	0.44
3:m:170:TRP:CE2	3:m:238:ARG:HD3	2.53	0.44
5:g:74:ASP:OD1	5:g:74:ASP:N	2.48	0.43
4:j:91:MET:O	4:j:92:PHE:HB3	2.18	0.43
3:e:185:ALA:O	3:e:186:PRO:C	2.61	0.43
3:a:139:SER:OG	3:a:140:THR:N	2.51	0.43
6:l:15:ASN:CB	6:l:21:ASN:CB	2.97	0.43
5:o:51:THR:HG21	5:o:98:MET:H	1.83	0.43
3:q:89:ASN:C	3:q:89:ASN:OD1	2.60	0.43
3:a:167:ASP:O	3:a:170:TRP:HD1	2.02	0.43
6:h:55:GLU:N	6:h:56:PRO:CD	2.81	0.42
5:c:74:ASP:OD1	5:c:74:ASP:N	2.49	0.42
3:a:262:ARG:HE	6:h:13:HIS:CE1	2.37	0.42
3:m:170:TRP:CH2	3:m:236:ALA:HB1	2.54	0.42
5:o:59:ASP:OD1	5:o:60:GLY:N	2.53	0.42
5:o:135:PRO:HA	5:o:136:PRO:HD3	1.80	0.42
5:s:84:LEU:HB3	5:s:189:ILE:HG23	2.02	0.42
5:s:172:ASN:N	5:s:172:ASN:OD1	2.52	0.42
6:p:55:GLU:N	6:p:56:PRO:HD3	2.35	0.41
3:a:51:ILE:HB	3:a:52:PRO:HD2	2.02	0.41
3:e:89:ASN:C	3:e:89:ASN:OD1	2.63	0.41
6:t:35:ASP:C	6:t:35:ASP:OD1	2.61	0.41
3:a:100:PHE:HB3	3:a:165:TRP:HB3	2.02	0.41
6:l:11:GLY:H	6:l:14:GLU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:p:55:GLU:N	6:p:56:PRO:CD	2.83	0.41
4:j:82:LEU:HD21	4:j:106:TYR:CD1	2.56	0.41
4:j:86:LEU:O	4:j:89:MET:HG2	2.21	0.41
3:a:171:GLN:CD	3:e:110:THR:HG23	2.46	0.41
3:e:115:ARG:NH1	3:e:270:ARG:O	2.54	0.41
4:f:159:ASN:OD1	4:f:159:ASN:N	2.50	0.41
6:l:16:GLN:C	6:l:18:VAL:N	2.78	0.40
5:g:172:ASN:OD1	5:g:172:ASN:N	2.48	0.40
3:a:33:SER:OG	3:a:34:GLN:N	2.54	0.40
5:c:74:ASP:OD1	5:c:75:ASN:N	2.54	0.40
6:l:15:ASN:OD1	6:l:15:ASN:N	2.55	0.40
4:b:178:ASP:OD1	4:b:179:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
3	e	248/260 (95%)	248 (100%)	0	100	100
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%)	223 (100%)	0	100	100
4	f	221/230 (96%)	221 (100%)	0	100	100
4	j	221/230 (96%)	221 (100%)	0	100	100
4	n	220/230 (96%)	220 (100%)	0	100	100
4	r	218/230 (95%)	218 (100%)	0	100	100
5	c	213/213 (100%)	213 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	3684 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	a	49	GLN
4	b	94	GLN
4	b	111	GLN
4	b	204	ASN
4	b	265	ASN
5	c	96	HIS
6	d	69	ASN
4	f	15	GLN
4	f	26	GLN
4	f	265	ASN
5	g	11	ASN
6	h	17	ASN
6	h	26	ASN
6	h	69	ASN
3	i	198	ASN
3	i	246	HIS
4	j	246	GLN
5	k	6	ASN
6	l	15	ASN
6	l	17	ASN
3	m	147	ASN
4	n	30	ASN
4	n	94	GLN

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Mol	Chain	Res	Type
4	n	118	HIS
4	n	246	GLN
5	o	6	ASN
5	o	194	GLN
3	q	171	GLN
4	r	119	GLN
4	r	135	ASN
4	r	149	ASN
4	r	225	ASN
4	r	246	GLN
4	r	272	GLN
5	s	96	HIS
5	s	194	GLN
6	t	17	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 oligosaccharides 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	a	300	-	15,15,15	1.42	2 (13%)	15,15,15	0.84	1 (6%)
7	MYR	i	300	-	15,15,15	1.51	2 (13%)	15,15,15	1.22	2 (13%)
7	MYR	e	300	-	15,15,15	0.96	0	15,15,15	0.99	2 (13%)
7	MYR	m	300	-	15,15,15	1.53	2 (13%)	15,15,15	1.07	2 (13%)
7	MYR	q	300	-	15,15,15	1.41	2 (13%)	15,15,15	1.07	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	a	300	-	-	3/13/13/13	-
7	MYR	i	300	-	-	2/13/13/13	-
7	MYR	e	300	-	-	7/13/13/13	-
7	MYR	m	300	-	-	4/13/13/13	-
7	MYR	q	300	-	-	2/13/13/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	m	300	MYR	O1-C1	3.28	1.32	1.22
7	m	300	MYR	O2-C1	-3.22	1.20	1.30
7	q	300	MYR	O2-C1	-3.21	1.20	1.30
7	i	300	MYR	O2-C1	-3.14	1.20	1.30
7	i	300	MYR	O1-C1	3.12	1.32	1.22
7	q	300	MYR	O1-C1	3.10	1.32	1.22
7	a	300	MYR	O1-C1	3.10	1.32	1.22
7	a	300	MYR	O2-C1	-2.94	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	-3.30	114.84	123.33
7	i	300	MYR	O2-C1-C2	3.21	124.13	114.00
7	m	300	MYR	O2-C1-C2	2.84	122.96	114.00
7	q	300	MYR	O2-C1-C2	2.82	122.92	114.00
7	e	300	MYR	O2-C1-O1	-2.74	116.29	123.33
7	m	300	MYR	O2-C1-O1	-2.73	116.30	123.33
7	q	300	MYR	O2-C1-O1	-2.68	116.44	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	300	MYR	O2-C1-C2	2.47	121.81	114.00
7	a	300	MYR	O2-C1-O1	-2.36	117.27	123.33

There are no chirality outliers.

All (18) 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
7	m	300	MYR	C4-C5-C6-C7
7	e	300	MYR	C1-C2-C3-C4
7	m	300	MYR	C1-C2-C3-C4
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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

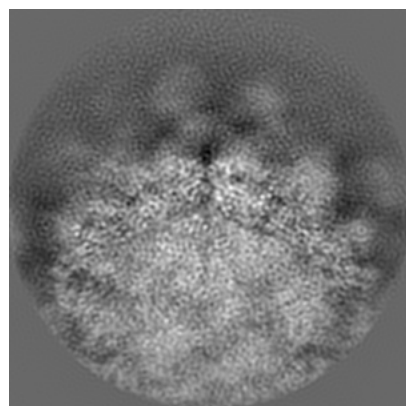
6 Map visualisation [i](#)

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.

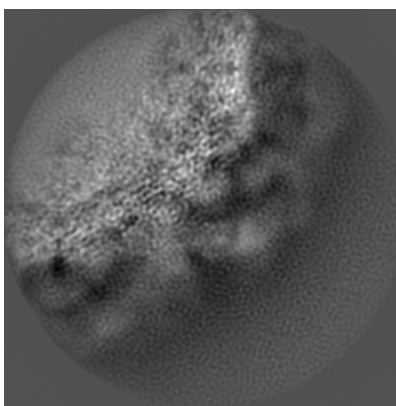
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

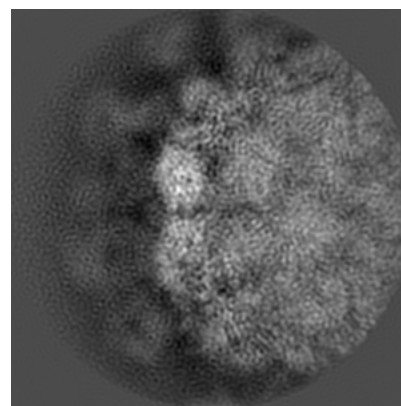
6.1.1 Primary map



X

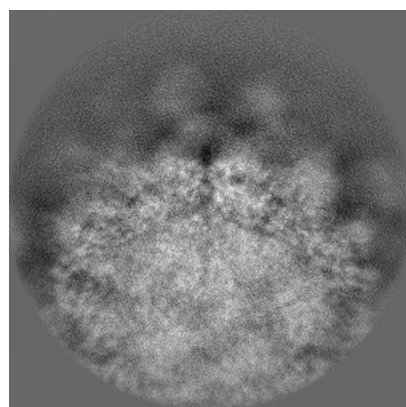


Y

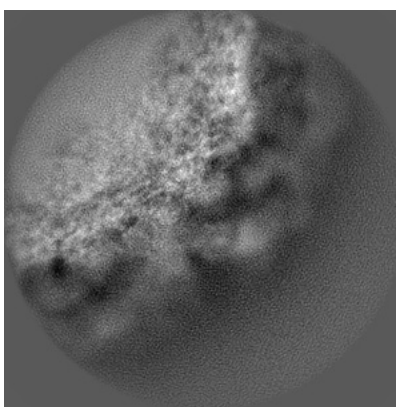


Z

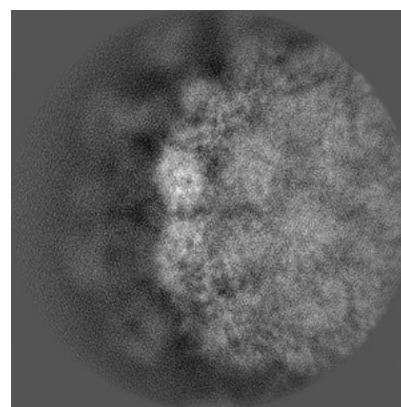
6.1.2 Raw map



X



Y

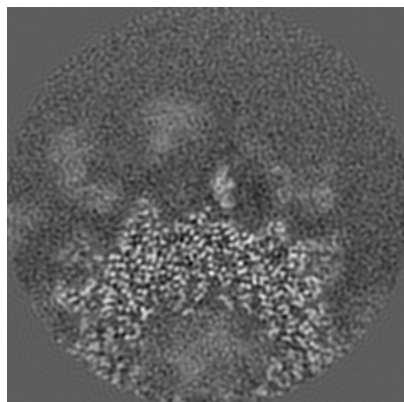


Z

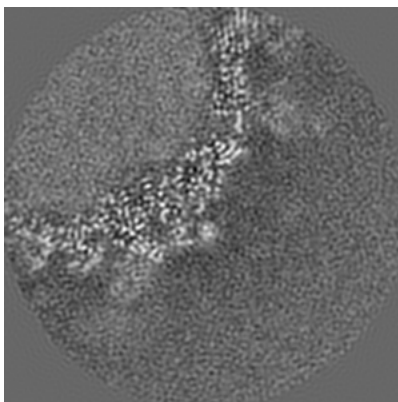
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

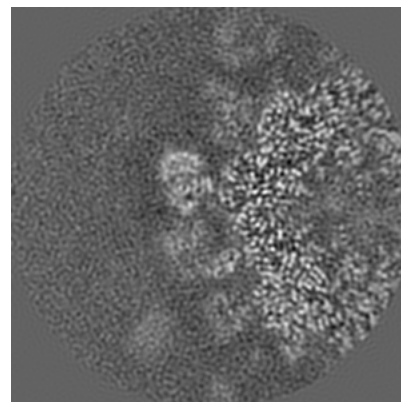
6.2.1 Primary map



X Index: 140

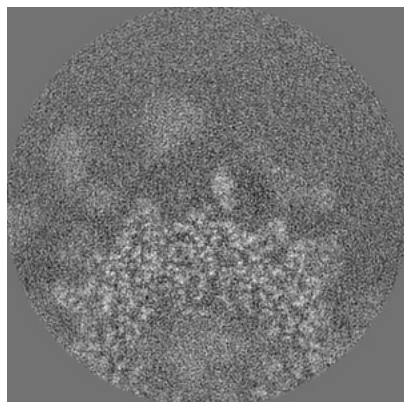


Y Index: 140

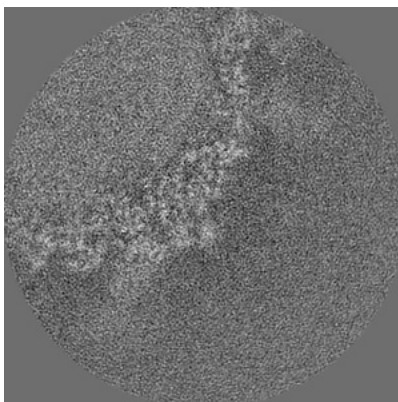


Z Index: 140

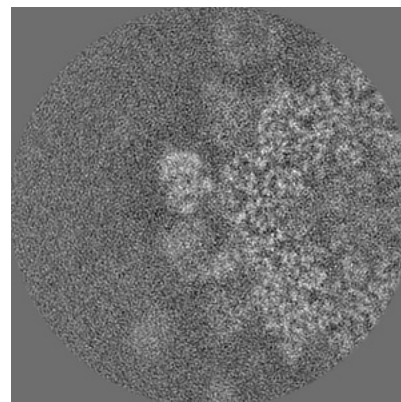
6.2.2 Raw map



X Index: 140



Y Index: 140

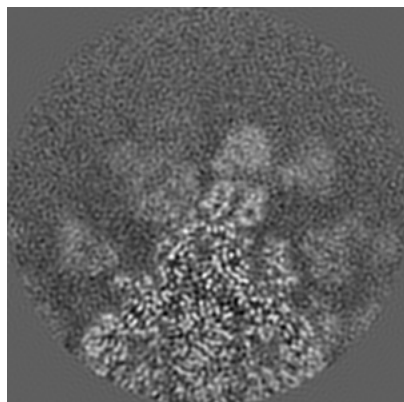


Z Index: 140

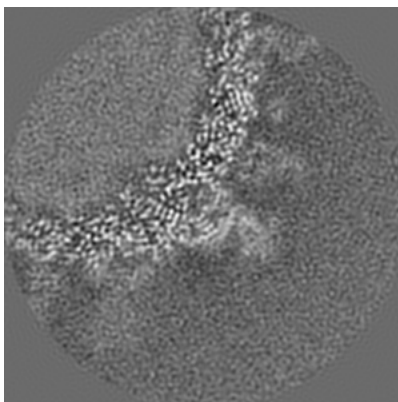
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

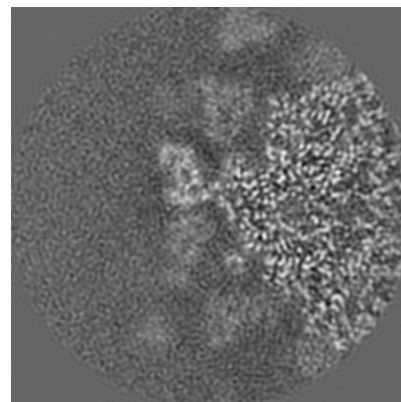
6.3.1 Primary map



X Index: 124

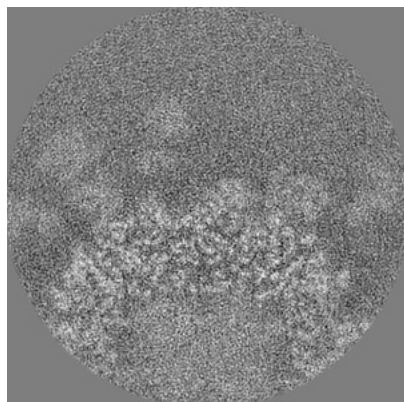


Y Index: 153

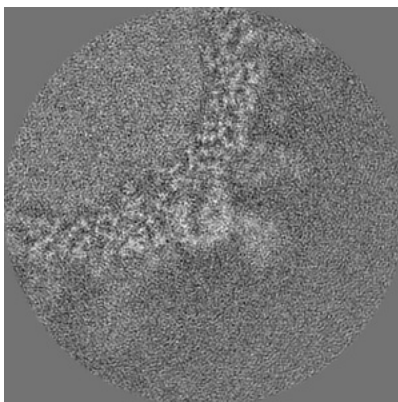


Z Index: 148

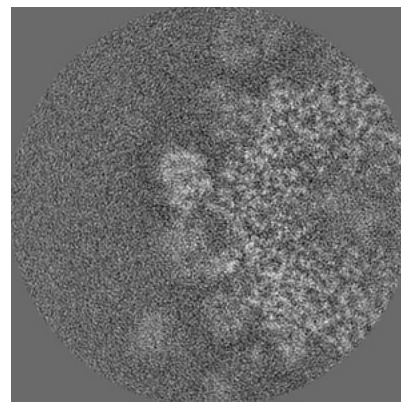
6.3.2 Raw map



X Index: 149



Y Index: 155

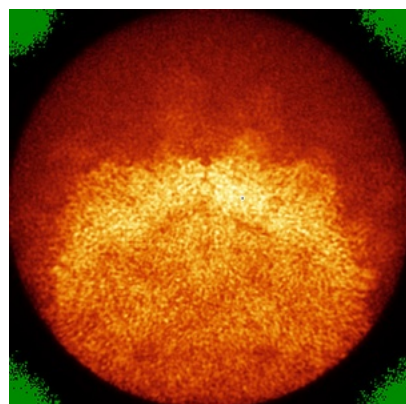


Z Index: 139

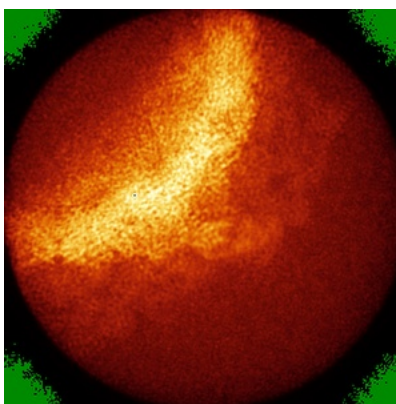
The images above show the largest variance slices of the map in three orthogonal directions.

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

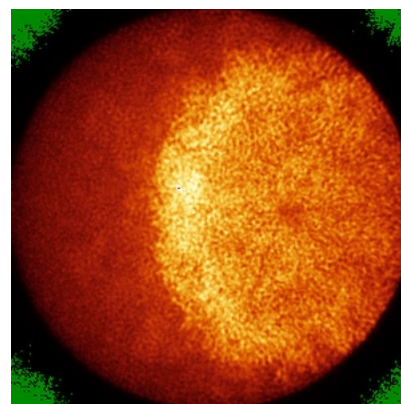
6.4.1 Primary map



X

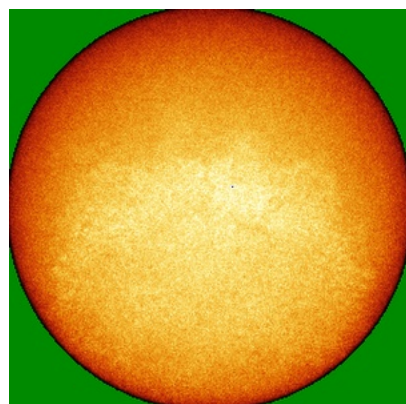


Y

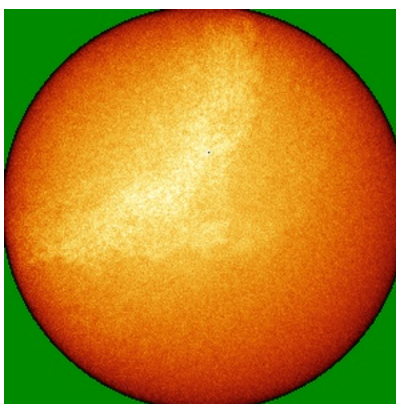


Z

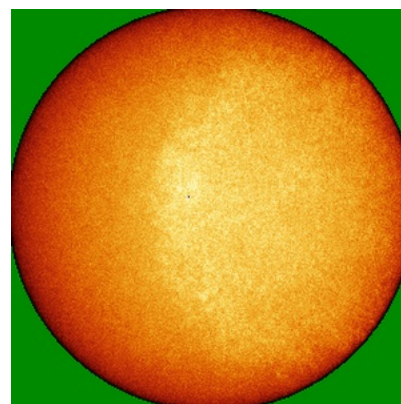
6.4.2 Raw map



X



Y

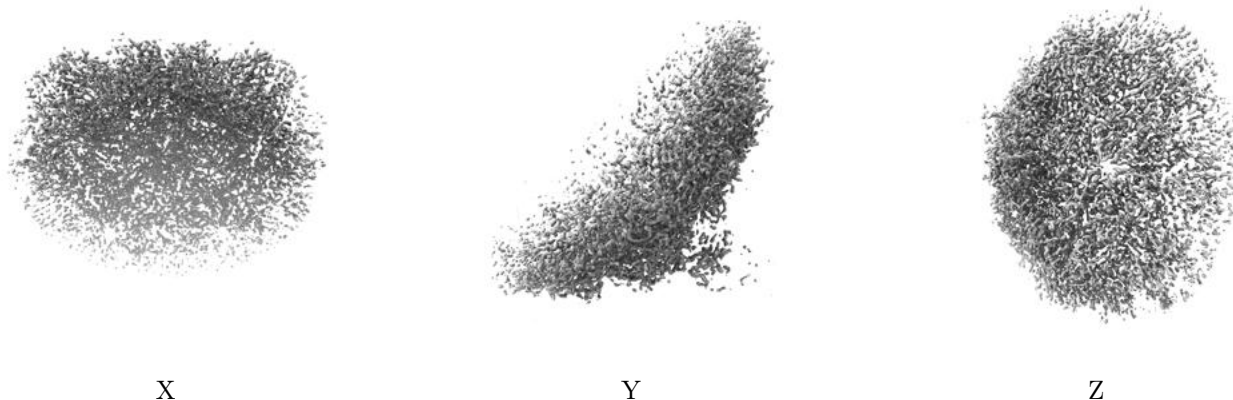


Z

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.

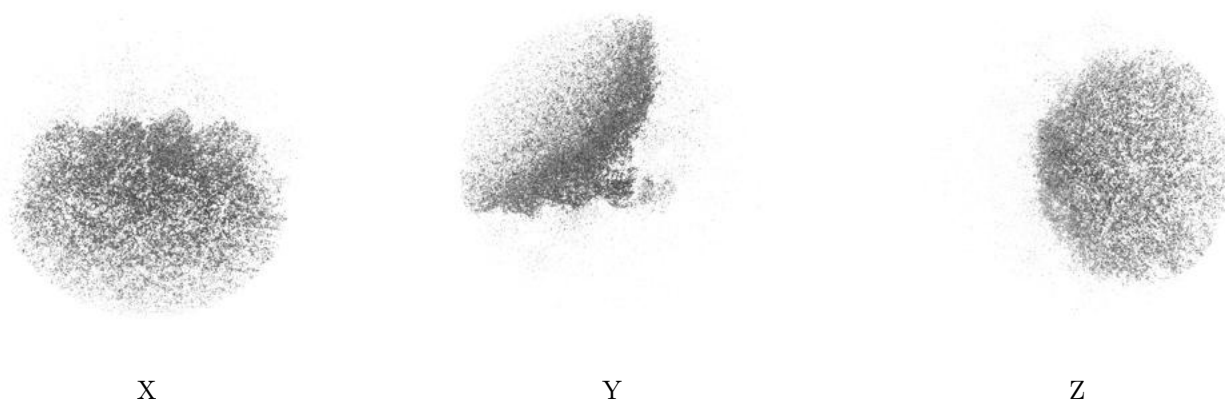
6.5 Orthogonal surface views [i](#)

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.

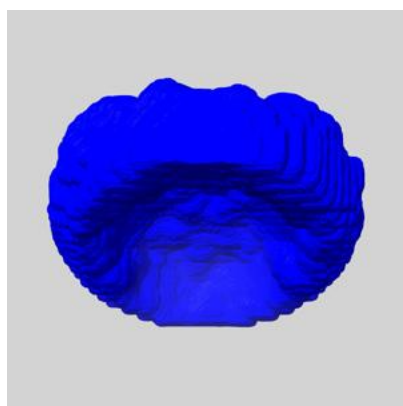
6.6 Mask visualisation [i](#)

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

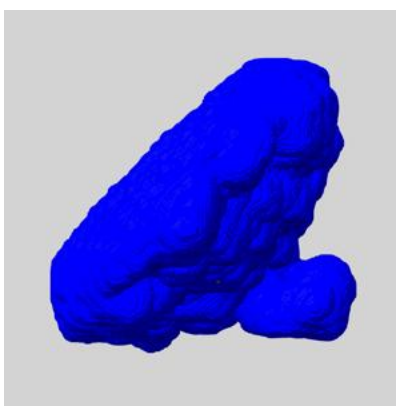
A mask typically either:

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

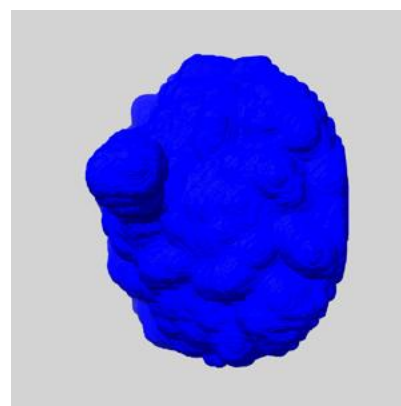
6.6.1 emd_26068_msk_1.map [i](#)



X



Y

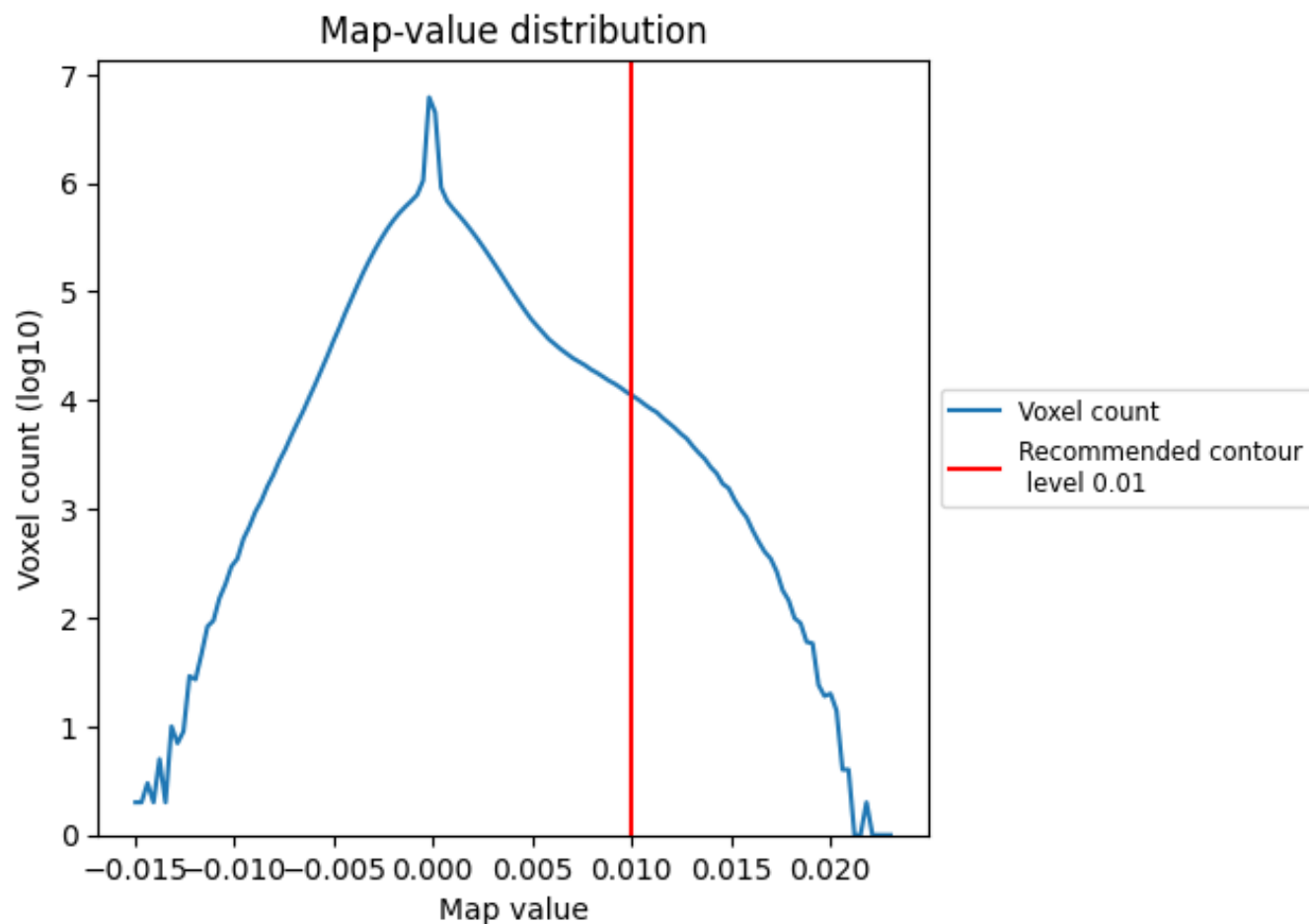


Z

7 Map analysis [i](#)

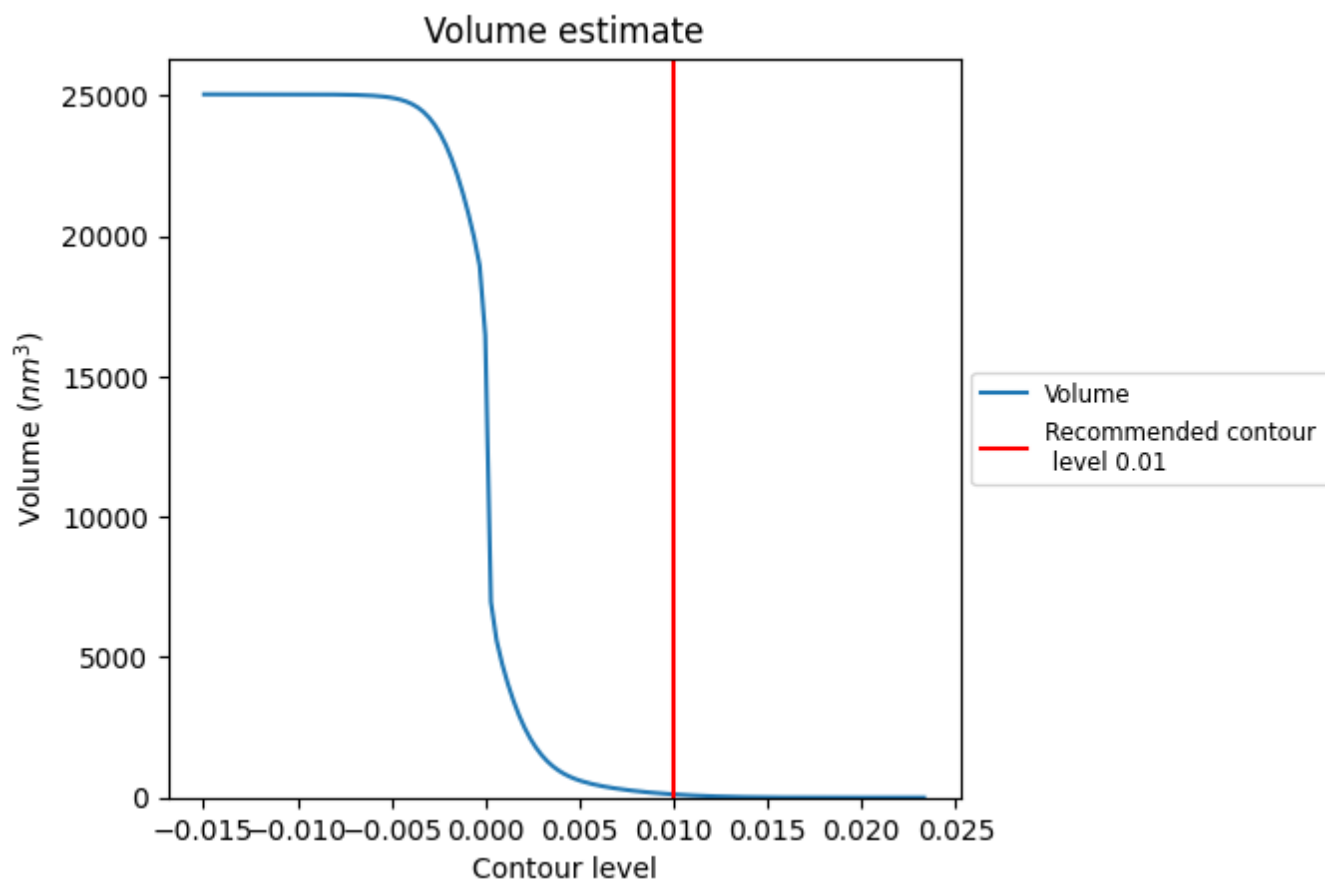
This section contains the results of statistical analysis of the map.

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.

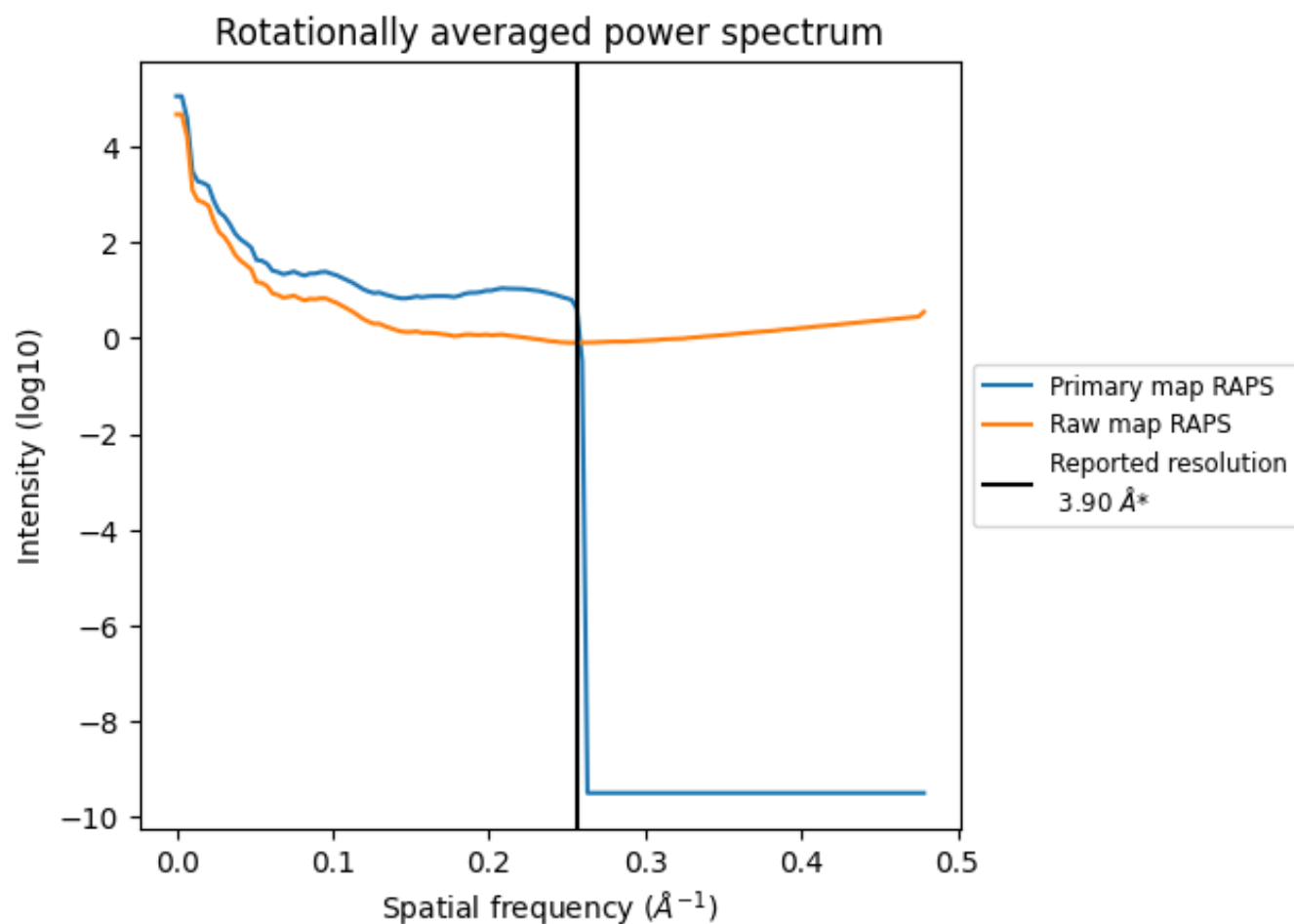
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; 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 ⓘ

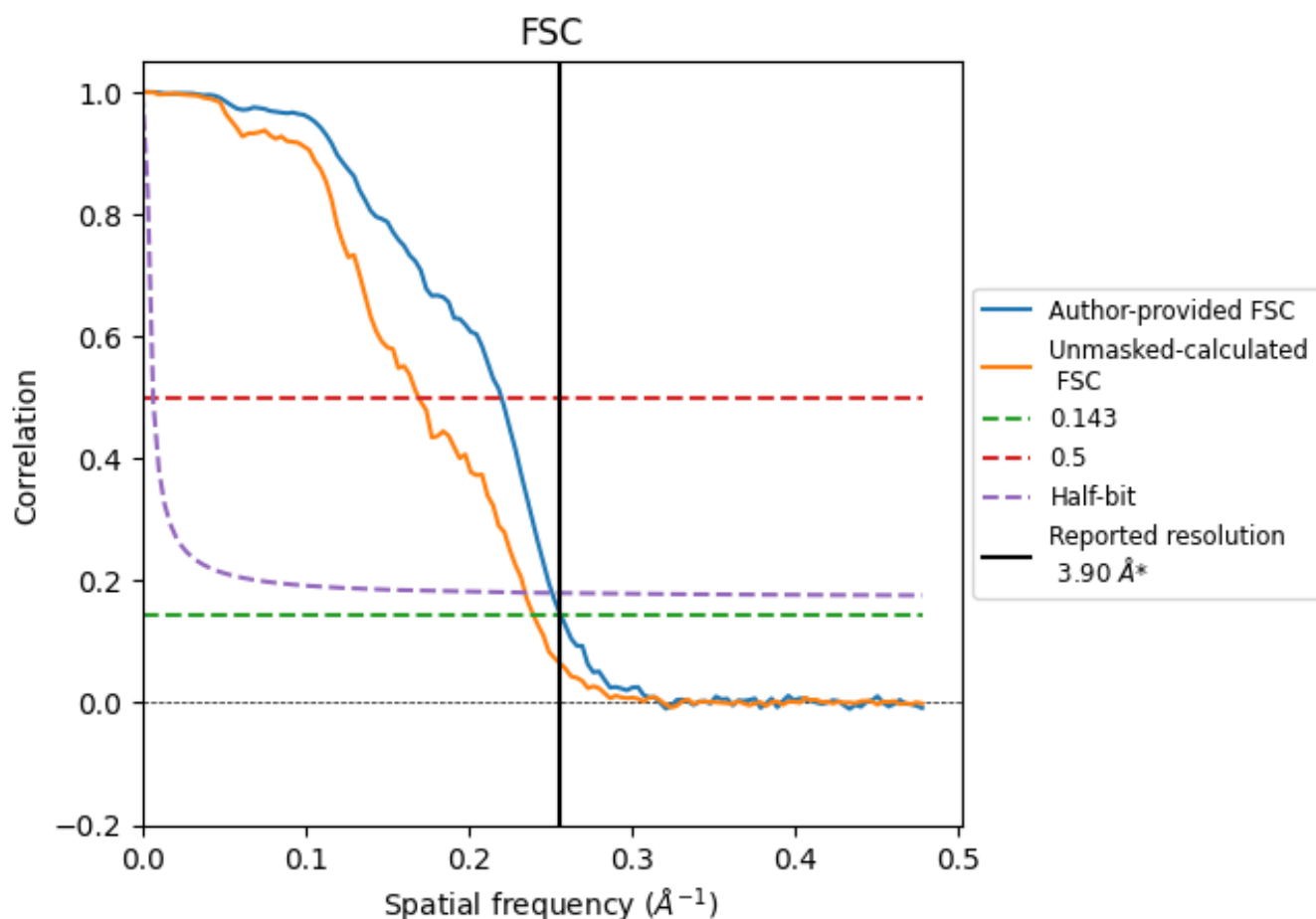


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

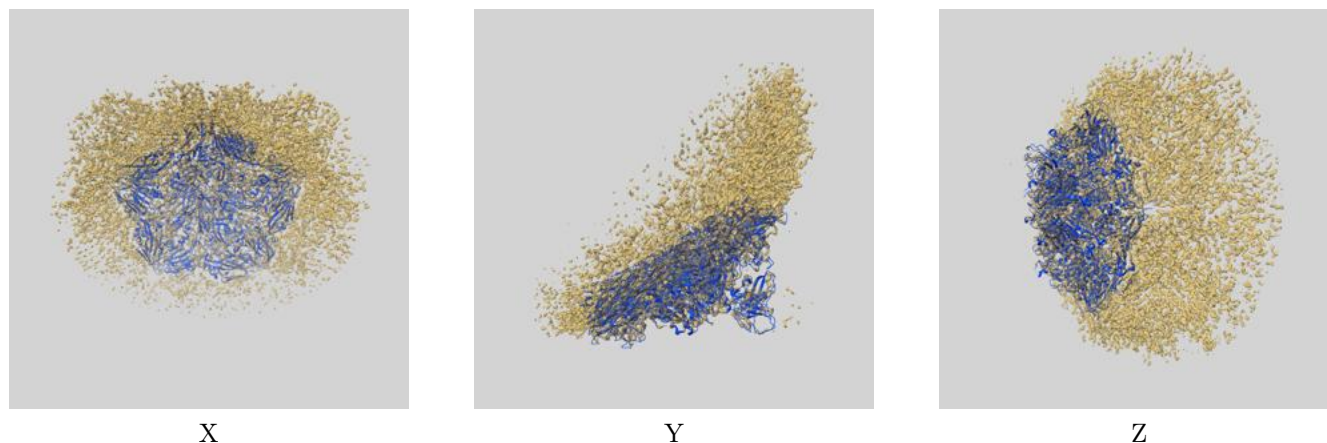
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.54	3.98
Unmasked-calculated*	4.16	5.90	4.26

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

9 Map-model fit [i](#)

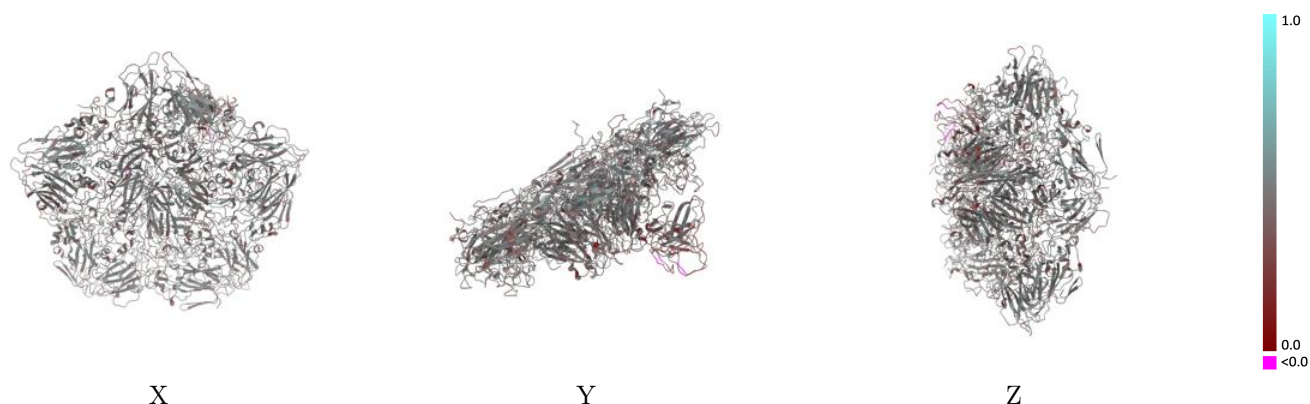
This section contains information regarding the fit between EMDB map EMD-26068 and PDB model 7TQS. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



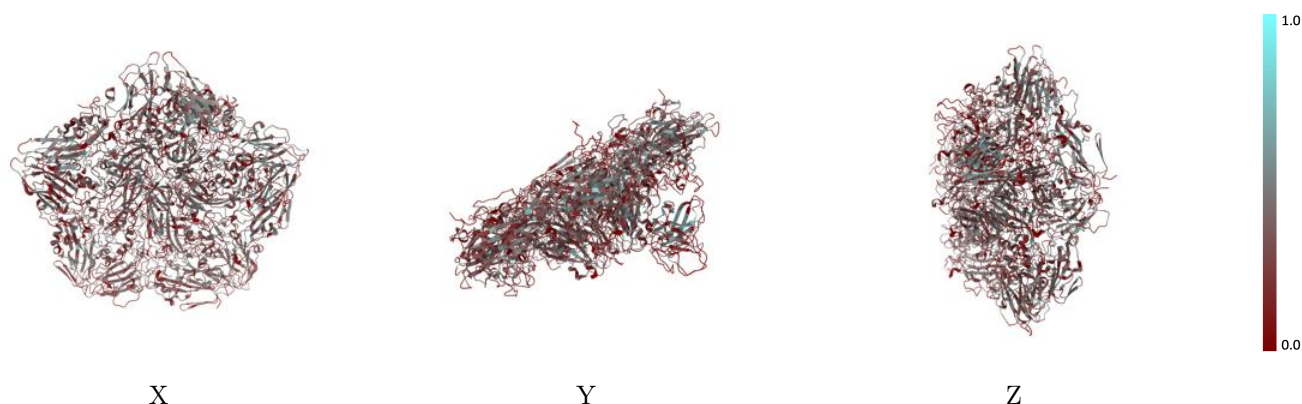
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



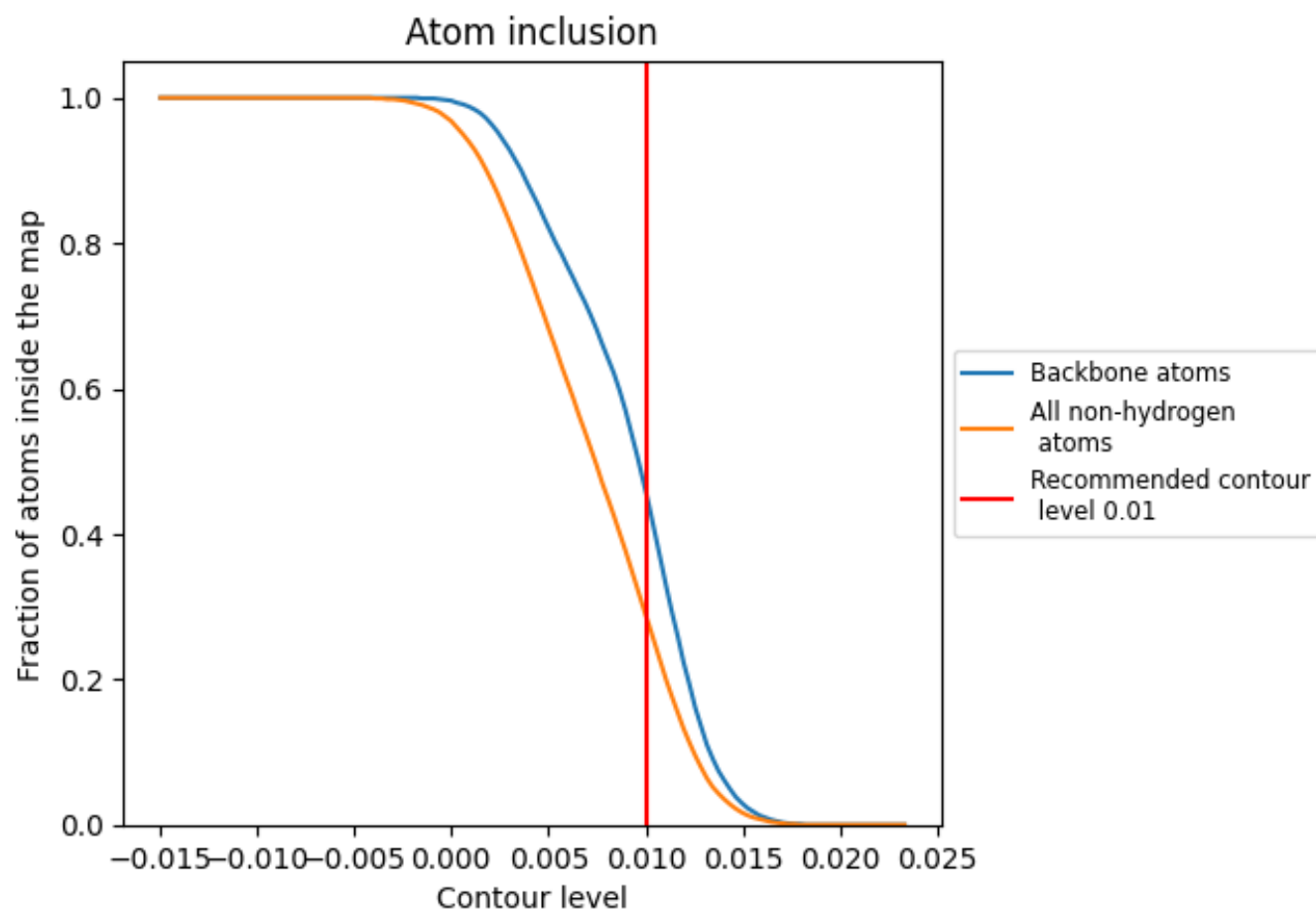
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (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

