



## wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 01:42 pm BST

PDB ID : 8RK3  
EMDB ID : EMD-19256  
Title : Bacteriophage JBD30 baseplate - composite structure  
Authors : Valentova, L.; Fuzik, T.; Plevka, P.  
Deposited on : 2023-12-23  
Resolution : 4.46 Å (reported)

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

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

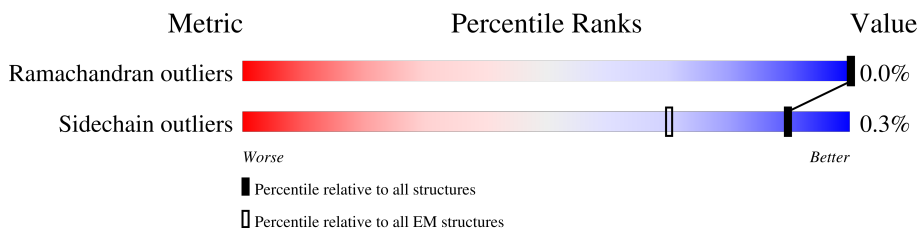
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1158	97%
1	B	1158	97%
1	C	1158	97%
2	O	273	99%
2	P	273	99%
2	g	273	99%
3	D	567	10% 98%
3	U	567	8% 98%
3	r	567	10% 98%

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Mol	Chain	Length	Quality of chain
4	E	382	31% 97%
4	F	382	31% 97%
4	I	382	30% 97%
4	J	382	42% 97%
4	M	382	31% 97%
4	N	382	28% 97%
4	W	382	18% 97%
4	a	382	27% 97%
4	e	382	26% 97%
5	b	735	98%
5	d	735	98%
5	o	735	98%
6	K	318	62% 99%
6	L	318	45% 99%
6	Q	318	65% 99%
6	R	318	44% 99%
6	T	318	65% 99%
6	V	318	61% 99%
6	c	318	13% 99%
6	i	318	24% 99%
6	k	318	14% 99%
7	G	307	46% 99%
7	H	307	49% 99%
7	S	307	16% 99%
7	X	307	47% 99%

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Mol	Chain	Length	Quality of chain
7	Y	307	<p>29% 99%</p>
7	Z	307	<p>65% 99%</p>
7	m	307	<p>21% 99%</p>
7	n	307	<p>74% 99%</p>
7	p	307	<p>60% 99%</p>
8	f	256	<p>7% 98%</p>
8	h	256	<p>8% 98%</p>
8	j	256	<p>7% 98%</p>
8	l	256	<p>8% 98%</p>
8	q	256	<p>7% 98%</p>
8	s	256	<p>5% 98%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 116259 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 Tape measure protein N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	32	256	161	47	46	2	0	0
1	B	32	256	161	47	46	2	0	0
1	C	32	256	161	47	46	2	0	0

- Molecule 2 is a protein called DUF2163 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	g	272	2099	1311	360	417	11	0	0
2	O	272	2099	1311	360	417	11	0	0
2	P	272	2099	1311	360	417	11	0	0

- Molecule 3 is a protein called Virion structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	554	4278	2692	760	813	13	0	0
3	r	554	4278	2692	760	813	13	0	0
3	D	554	4278	2692	760	813	13	0	0

- Molecule 4 is a protein called DUF2793 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	373	2791	1771	485	521	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	e	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	I	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	E	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	M	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	J	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	F	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		
4	N	373	Total	C	N	O	S	0	0
			2791	1771	485	521	14		

- Molecule 5 is a protein called Tip attachment protein J domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	o	727	Total	C	N	O	S	0	0
			5581	3515	988	1067	11		
5	b	727	Total	C	N	O	S	0	0
			5581	3515	988	1067	11		
5	d	727	Total	C	N	O	S	0	0
			5581	3515	988	1067	11		

- Molecule 6 is a protein called Virion structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	i	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	k	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	K	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	Q	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	T	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	R	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		
6	V	317	Total	C	N	O	S	0	0
			2470	1580	425	459	6		

- Molecule 7 is a protein called Virion structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	Y	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	m	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	n	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	G	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	X	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	p	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	H	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		
7	Z	305	Total	C	N	O	S	0	0
			2338	1479	407	442	10		

- Molecule 8 is a protein called Virion structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	q	252	Total	C	N	O	S	0	0
			1871	1199	309	360	3		
8	s	252	Total	C	N	O	S	0	0
			1871	1199	309	360	3		
8	f	252	Total	C	N	O	S	0	0
			1871	1199	309	360	3		
8	j	252	Total	C	N	O	S	0	0
			1871	1199	309	360	3		
8	h	252	Total	C	N	O	S	0	0
			1871	1199	309	360	3		

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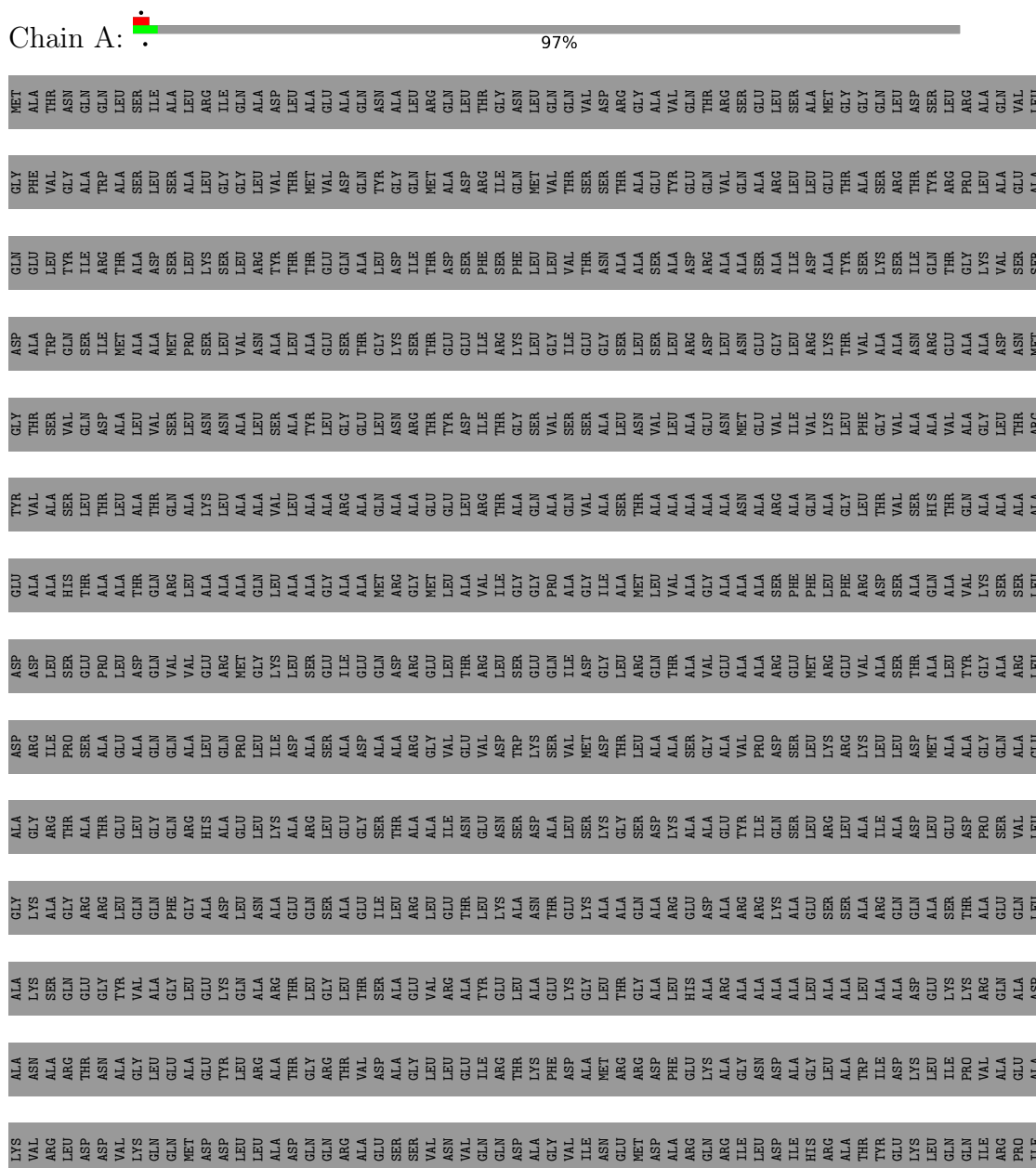
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1	252	1871	1199	309	360	3	0	0

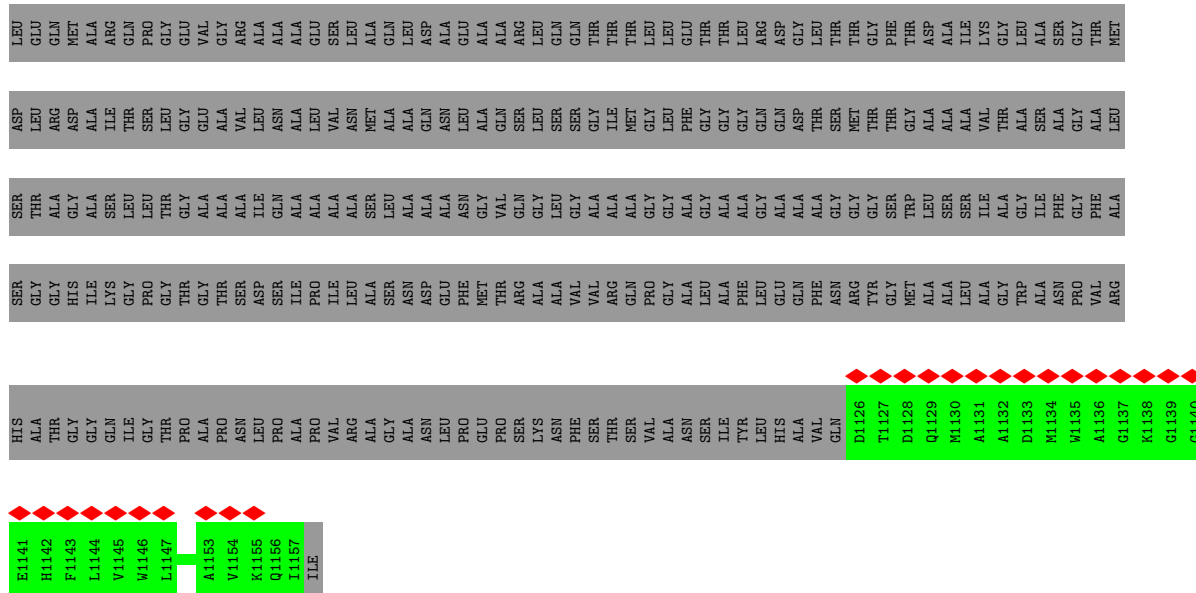


### 3 Residue-property plots

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.

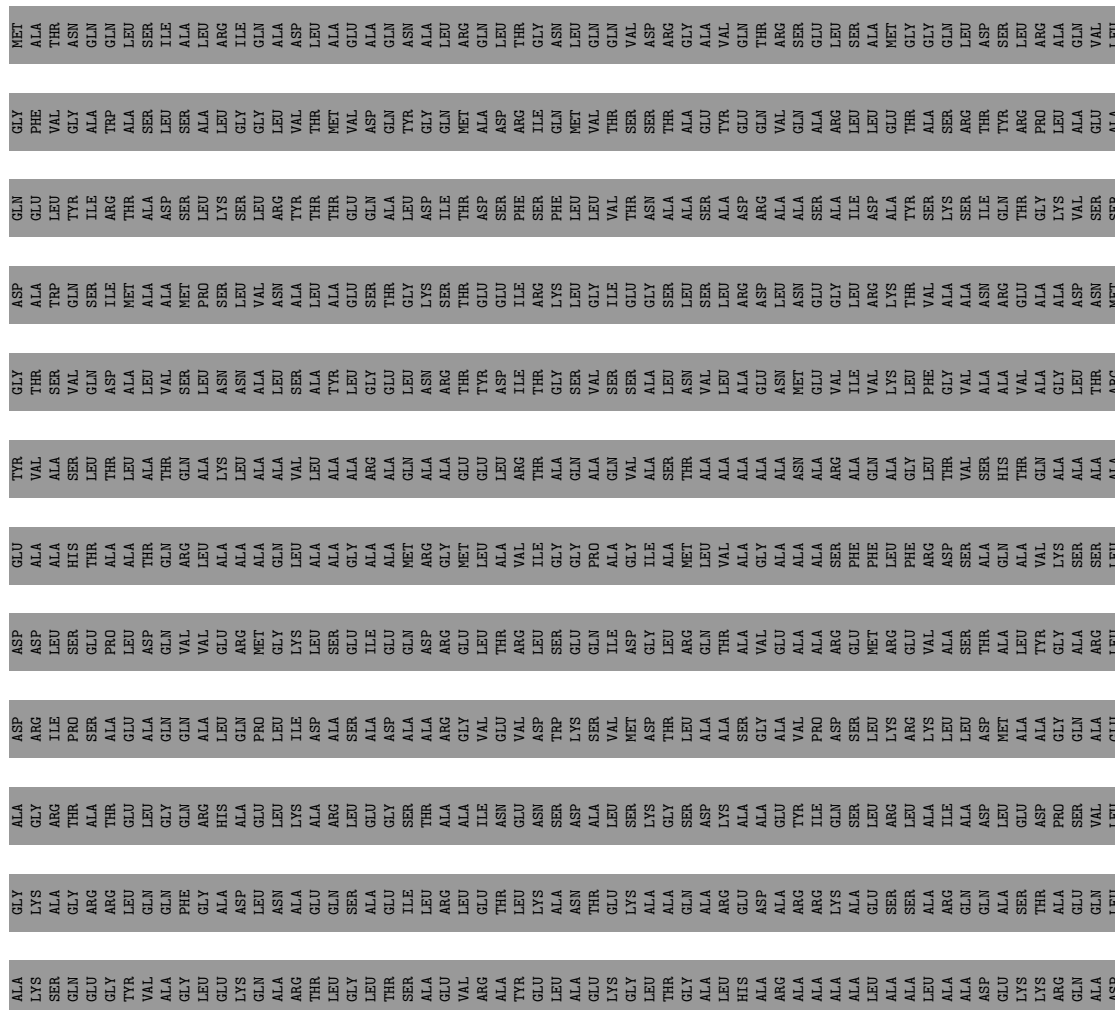
- Molecule 1: Tape measure protein N-terminal domain-containing protein





● Molecule 1: Tape measure protein N-terminal domain-containing protein

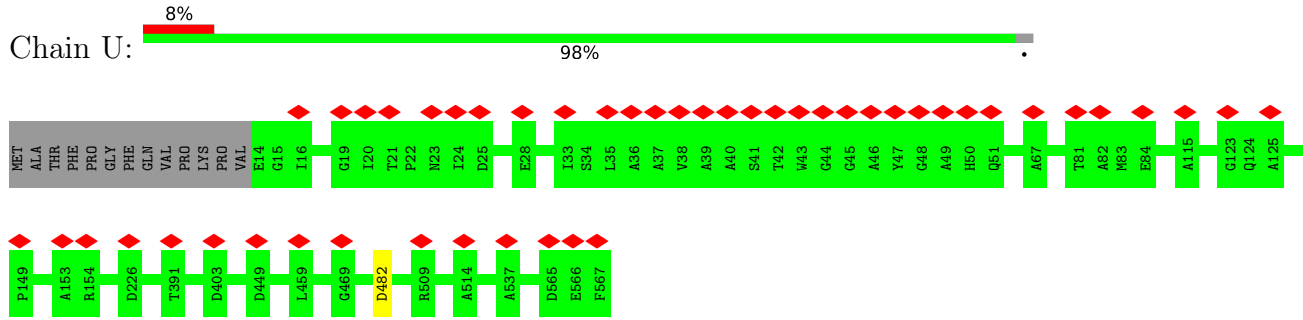
Chain B: 97%



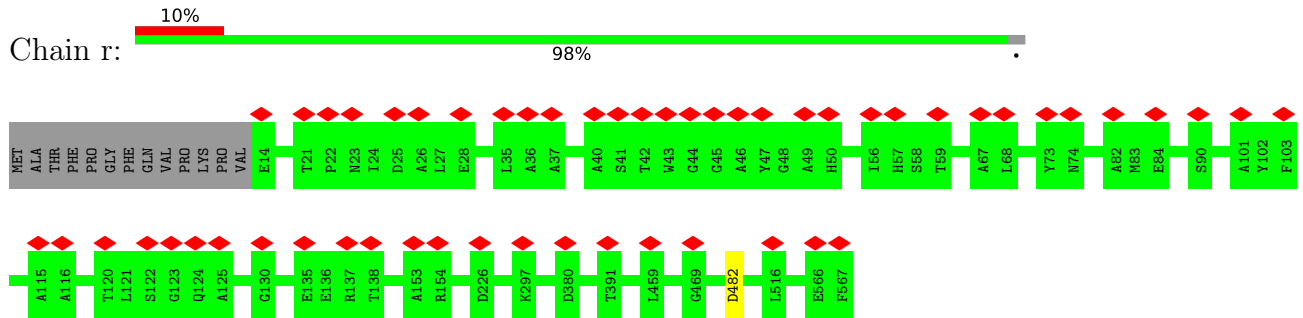




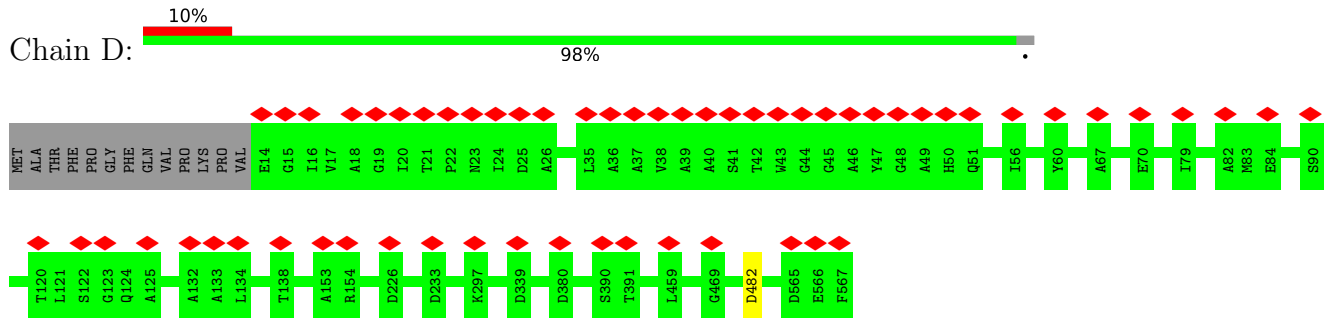
• Molecule 3: Virion structural protein



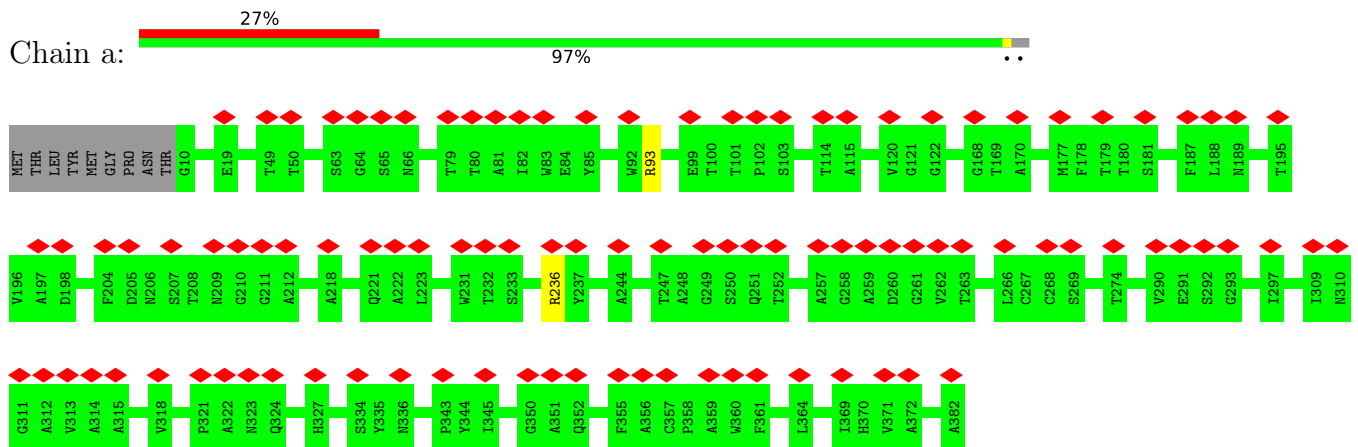
• Molecule 3: Virion structural protein



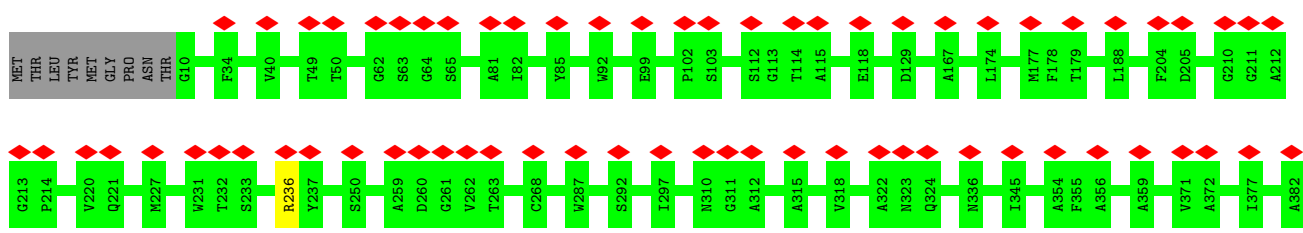
• Molecule 3: Virion structural protein



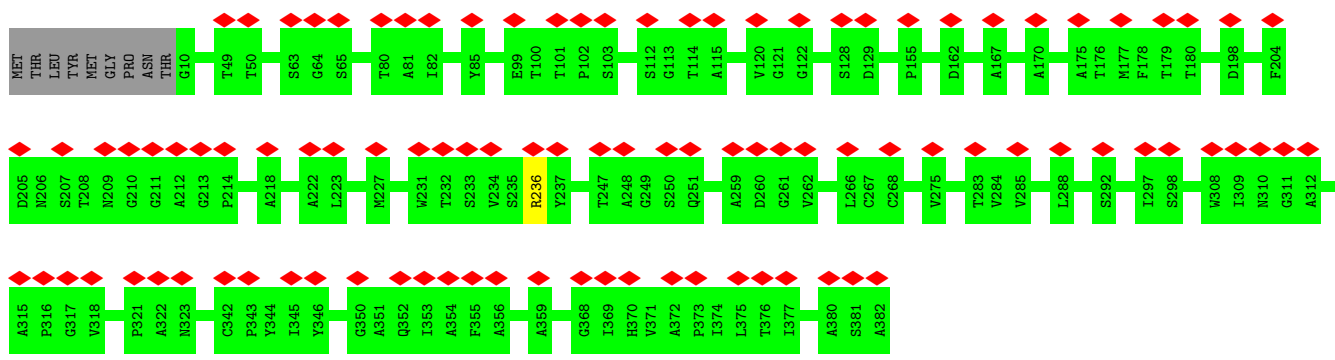
• Molecule 4: DUF2793 domain-containing protein



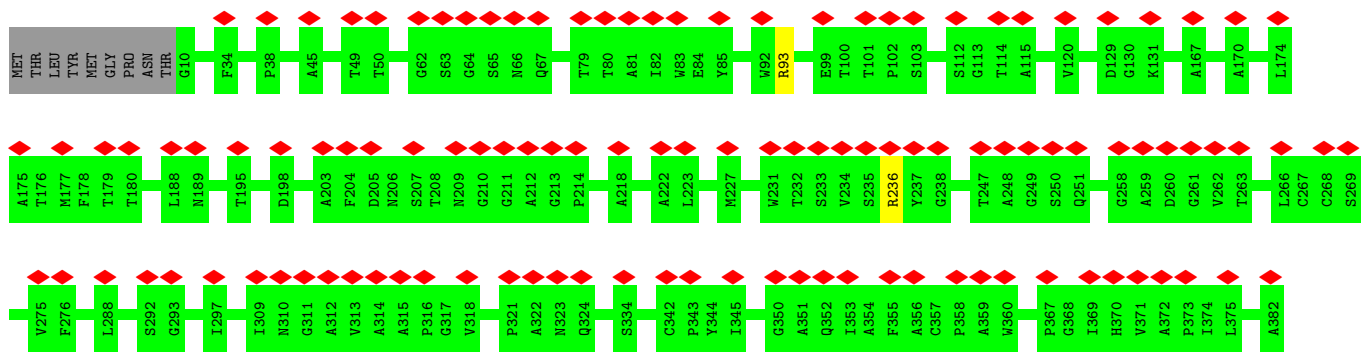
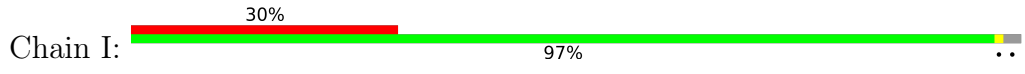
• Molecule 4: DUF2793 domain-containing protein



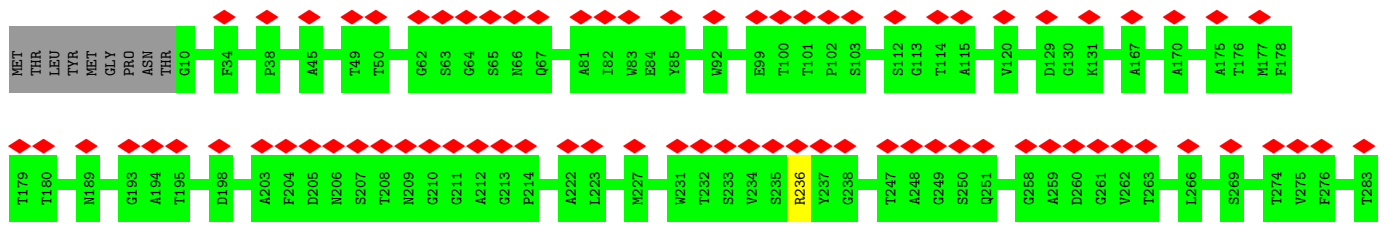
• Molecule 4: DUF2793 domain-containing protein

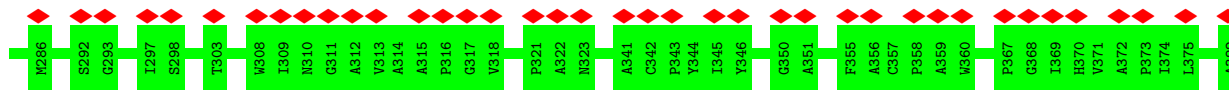


• Molecule 4: DUF2793 domain-containing protein

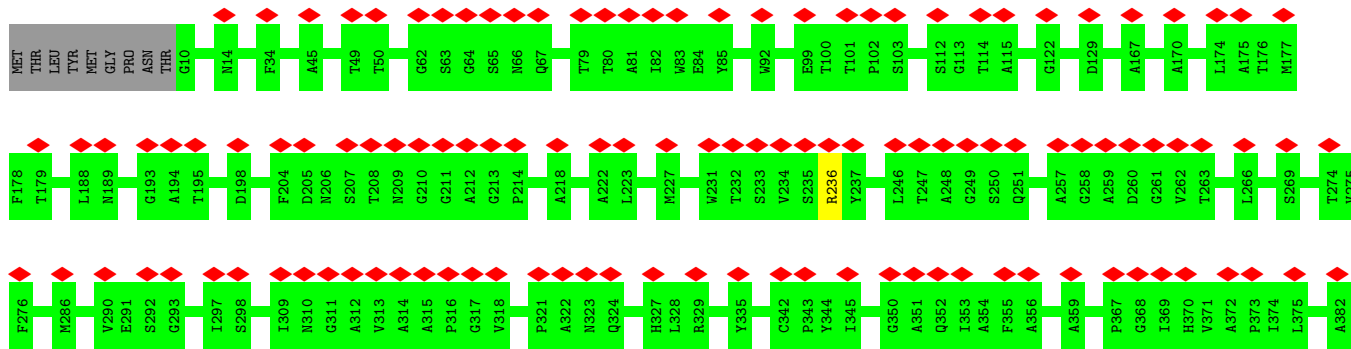


• Molecule 4: DUF2793 domain-containing protein

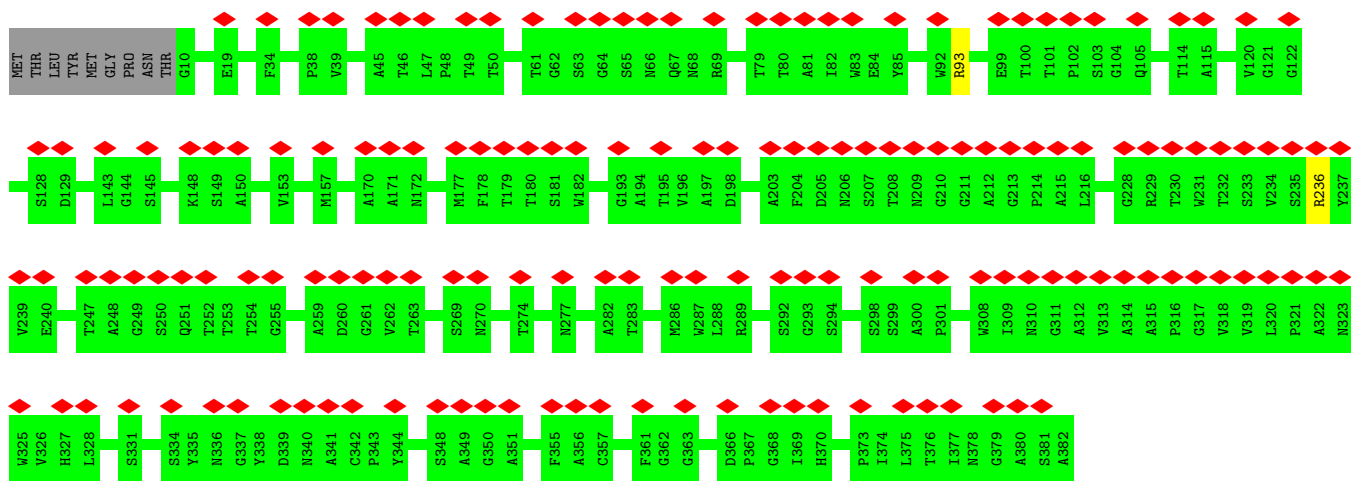
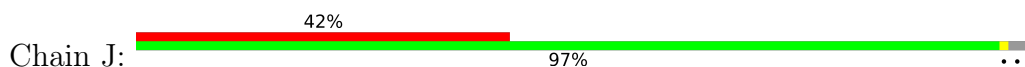




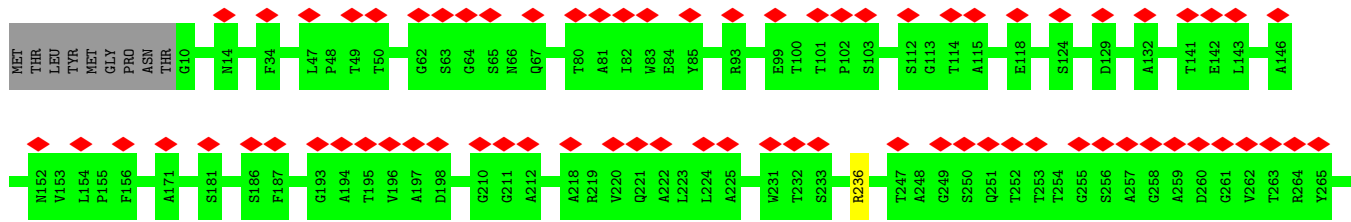
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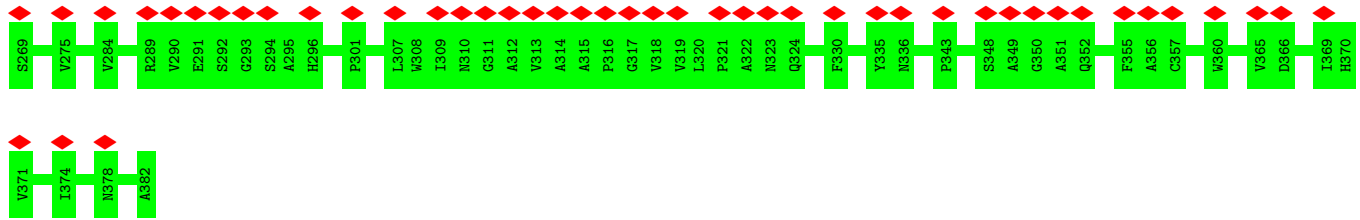


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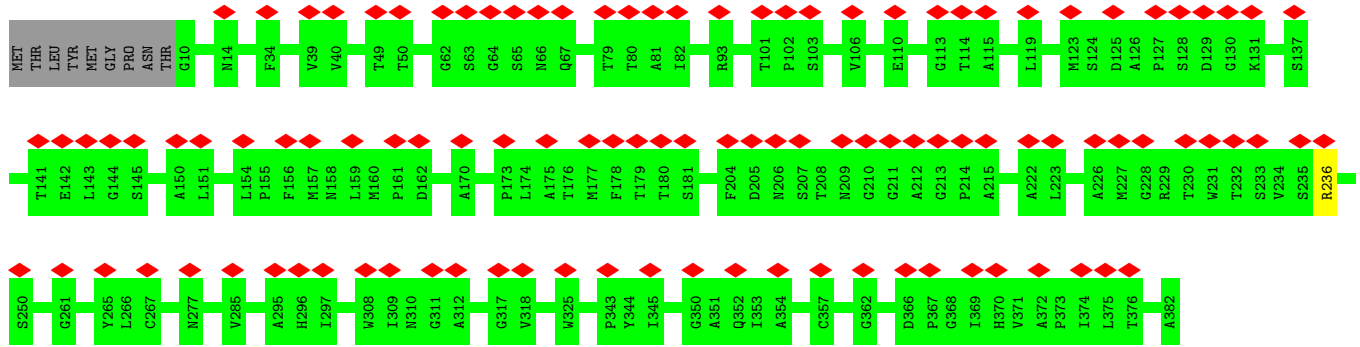


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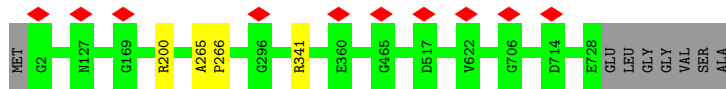




• Molecule 4: DUF2793 domain-containing protein



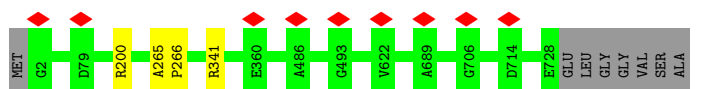
• Molecule 5: Tip attachment protein J domain-containing protein



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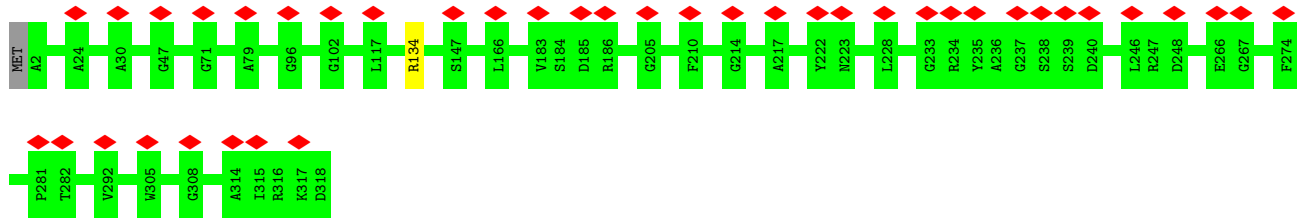
• Molecule 5: Tip attachment protein J domain-containing protein



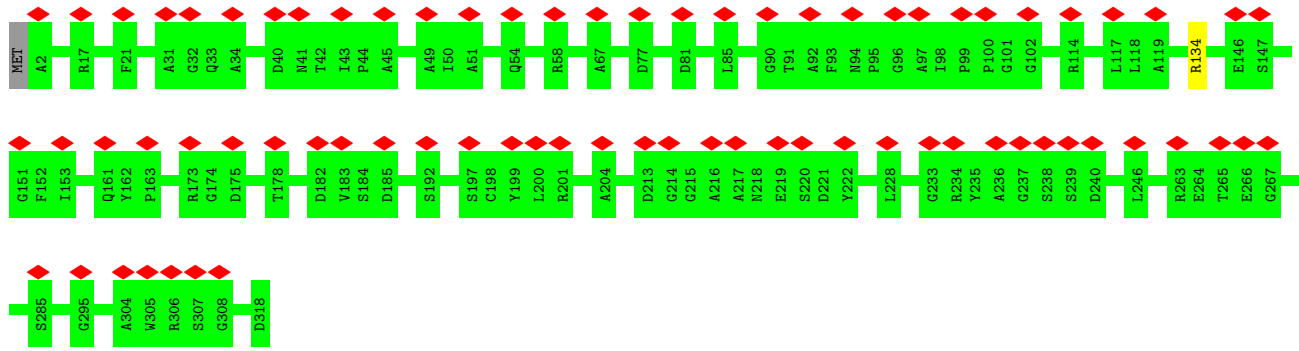
• Molecule 6: Virion structural protein



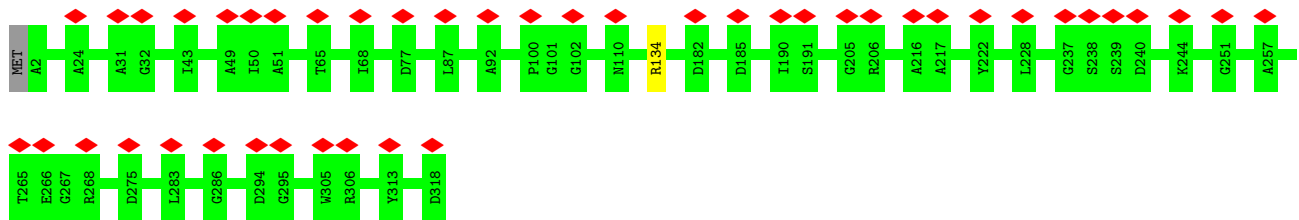




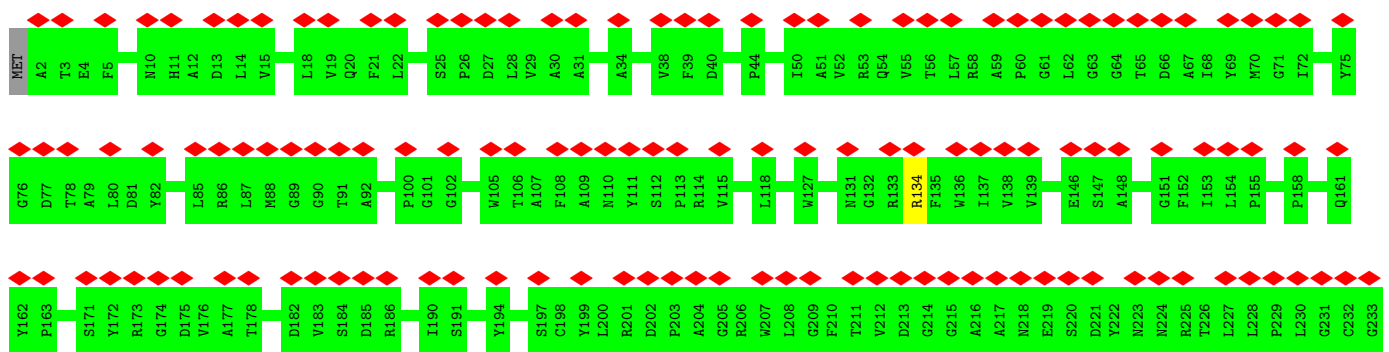
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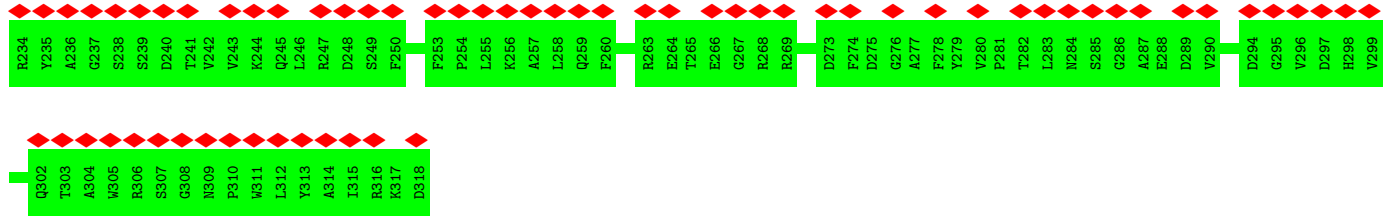


• Molecule 6: Virion structural protein

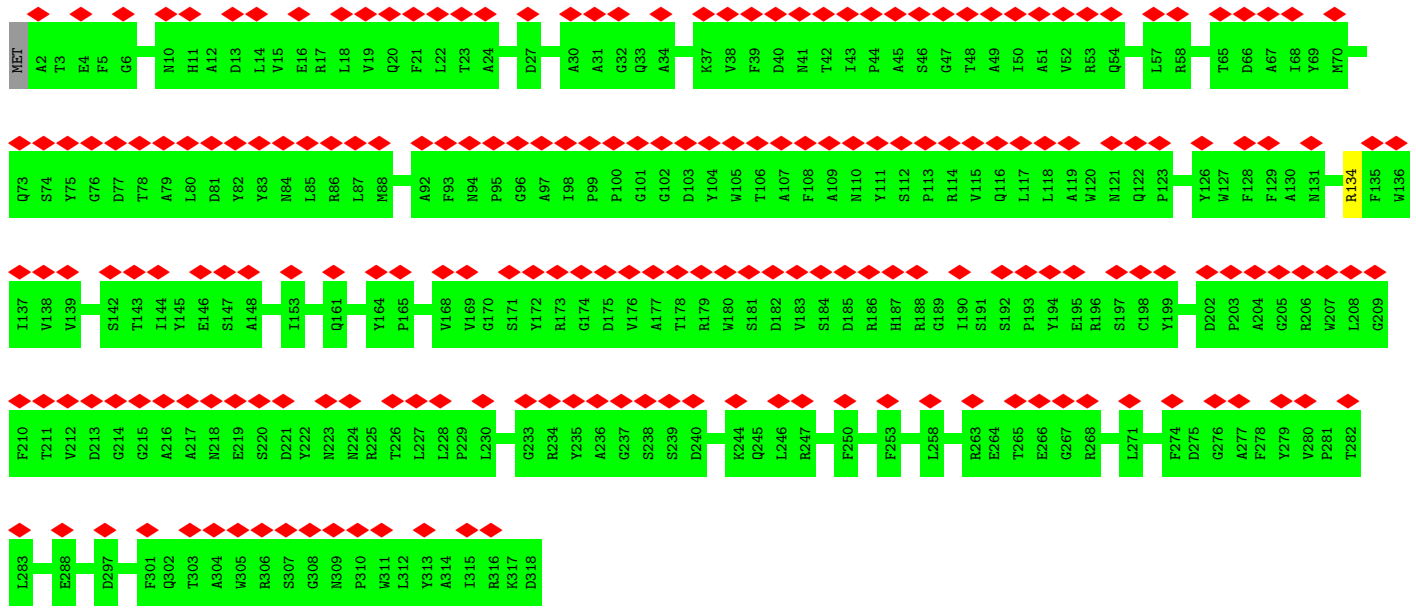


• Molecule 6: Virion structural protein

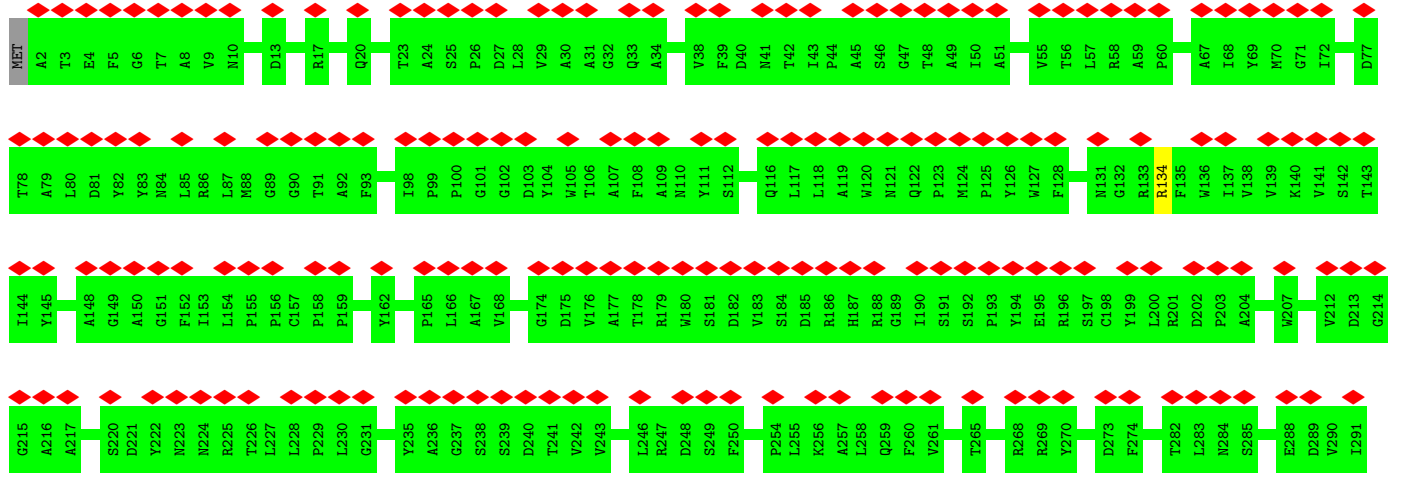


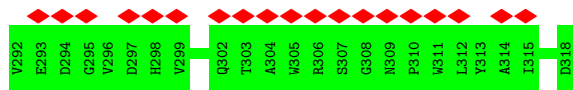


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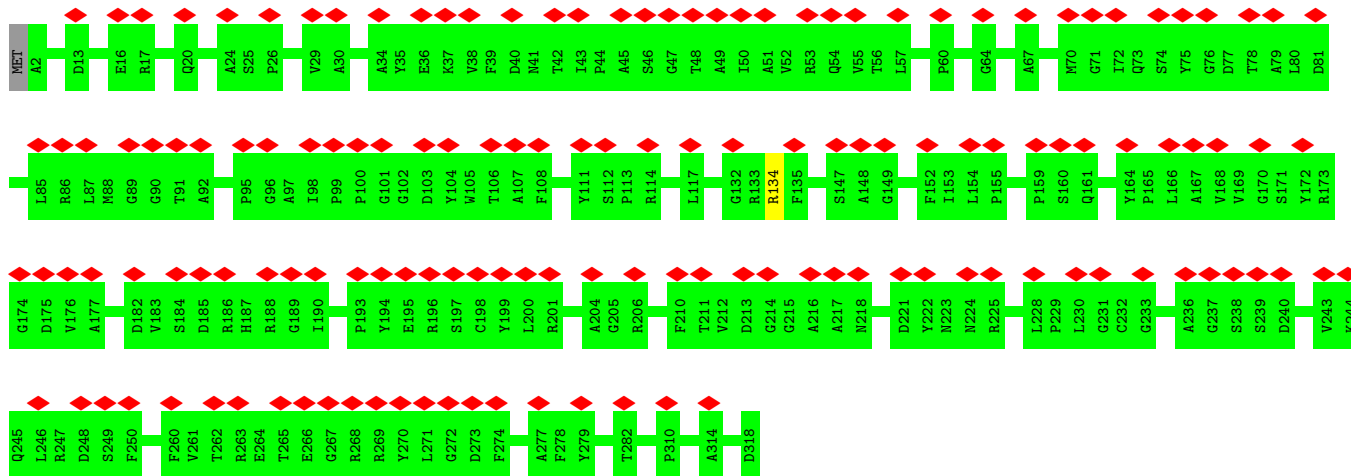
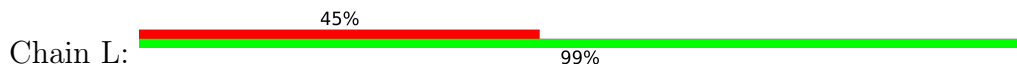


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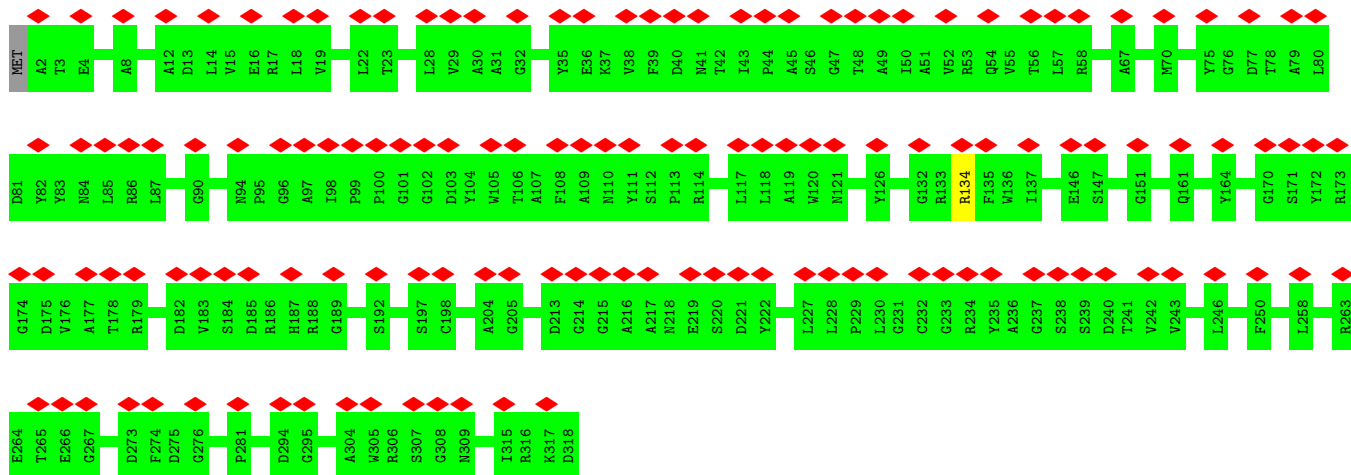
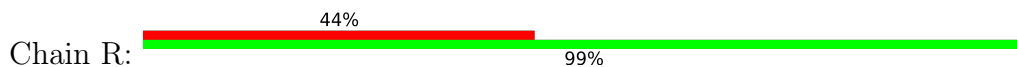




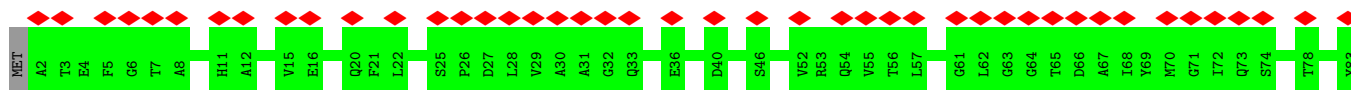
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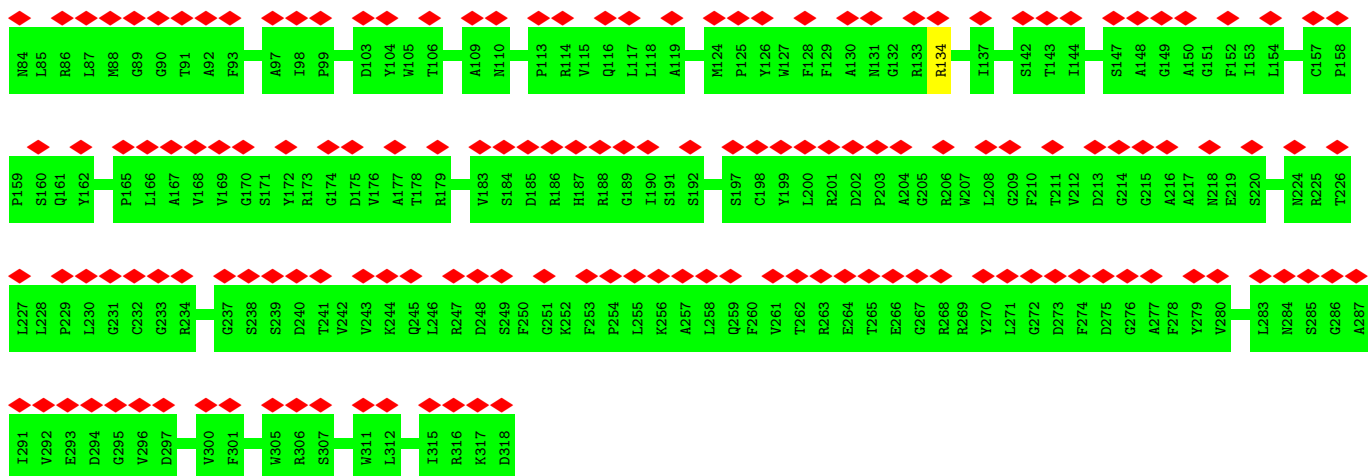


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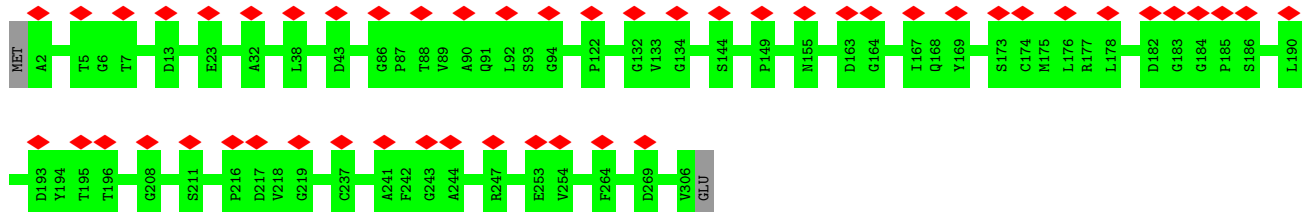


• Molecule 6: Virion structural protein

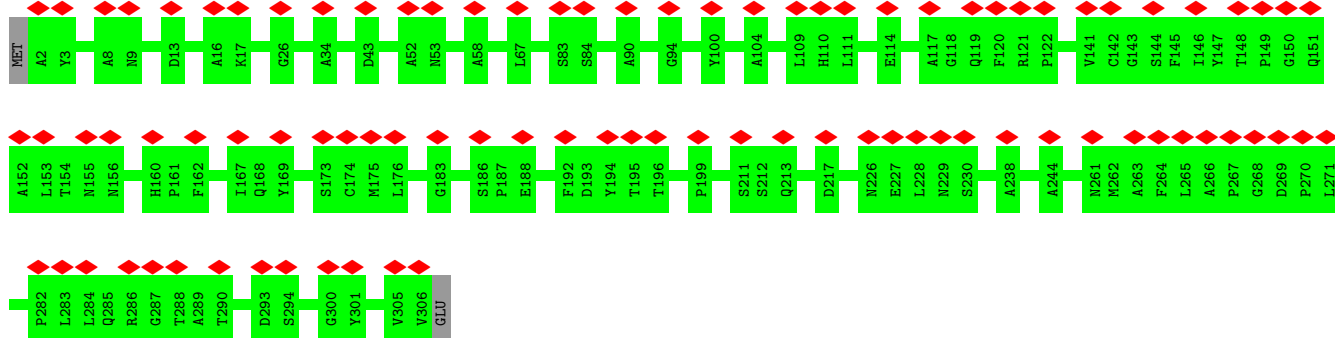




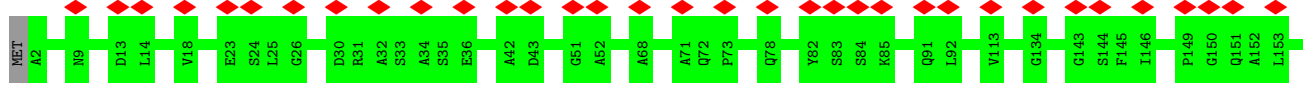
• Molecule 7: Virion structural protein

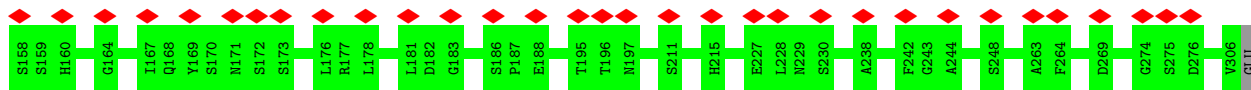


• Molecule 7: Virion structural protein

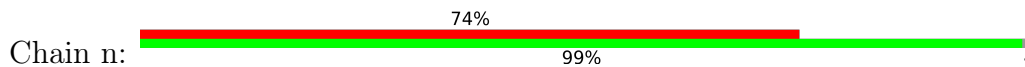


• Molecule 7: Virion structural protein

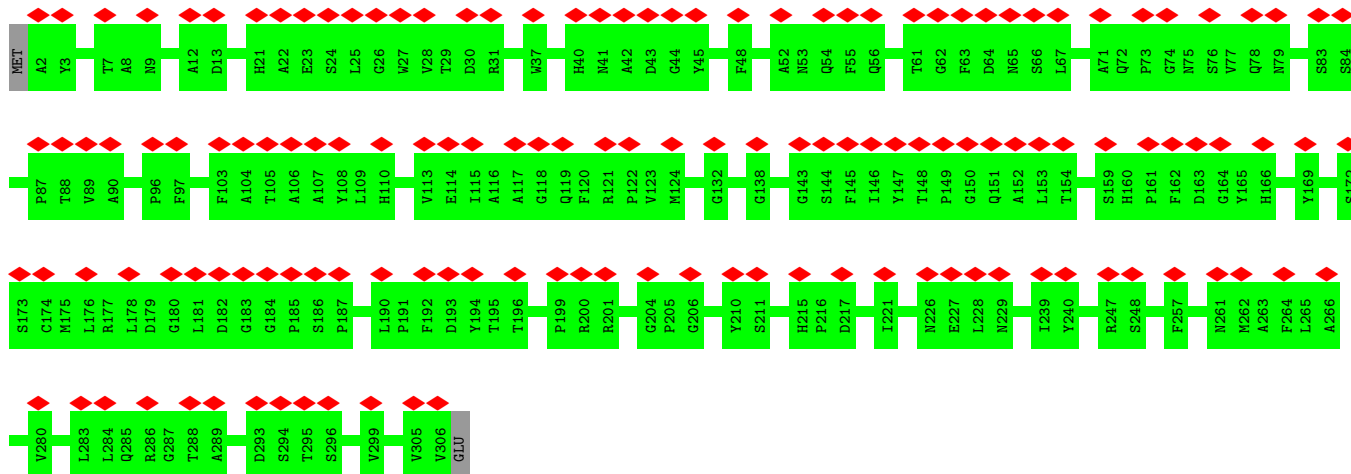




• Molecule 7: Virion structural protein



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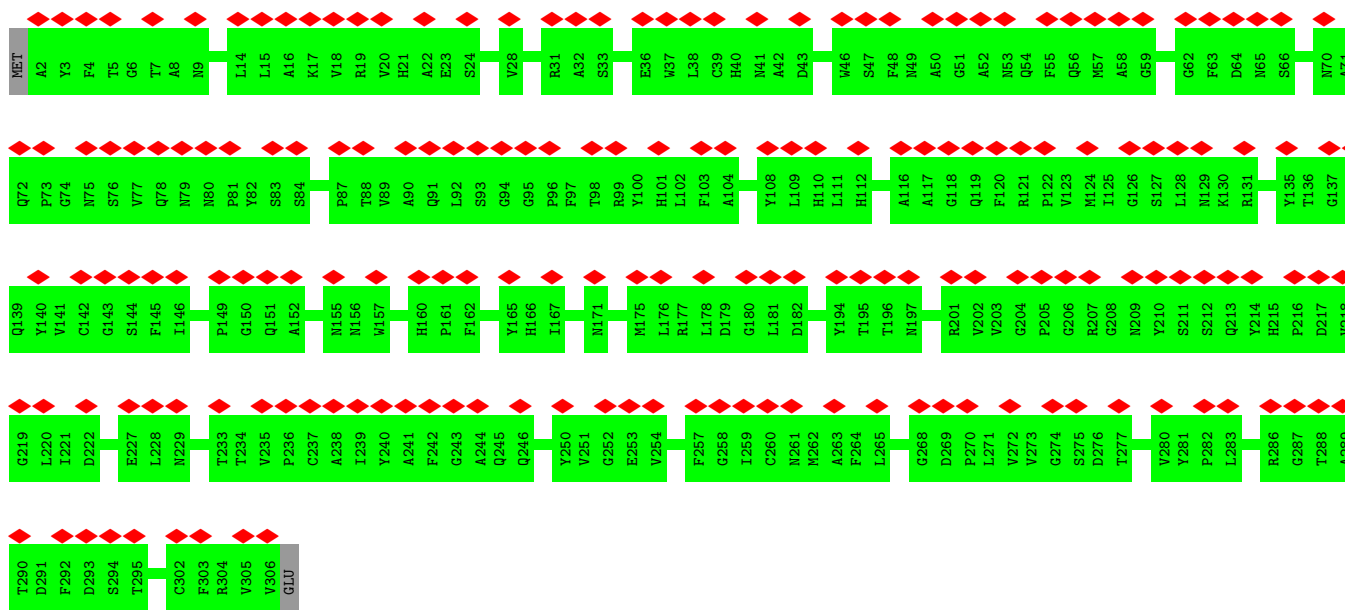


• Molecule 7: Virion structural protein

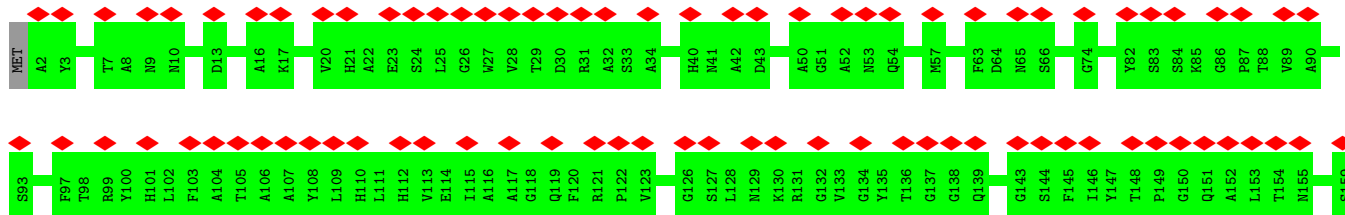


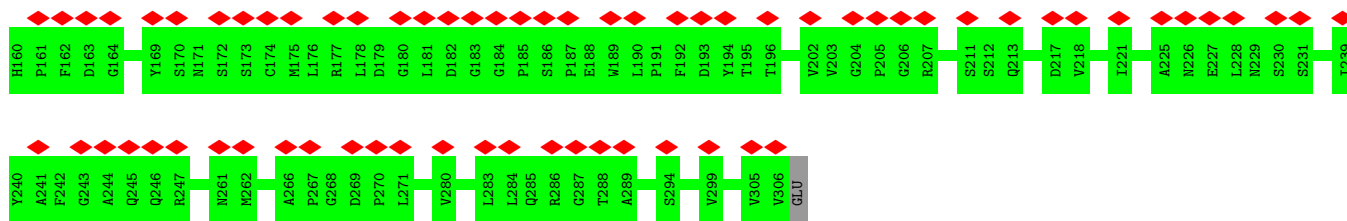


• Molecule 7: Virion structural protein

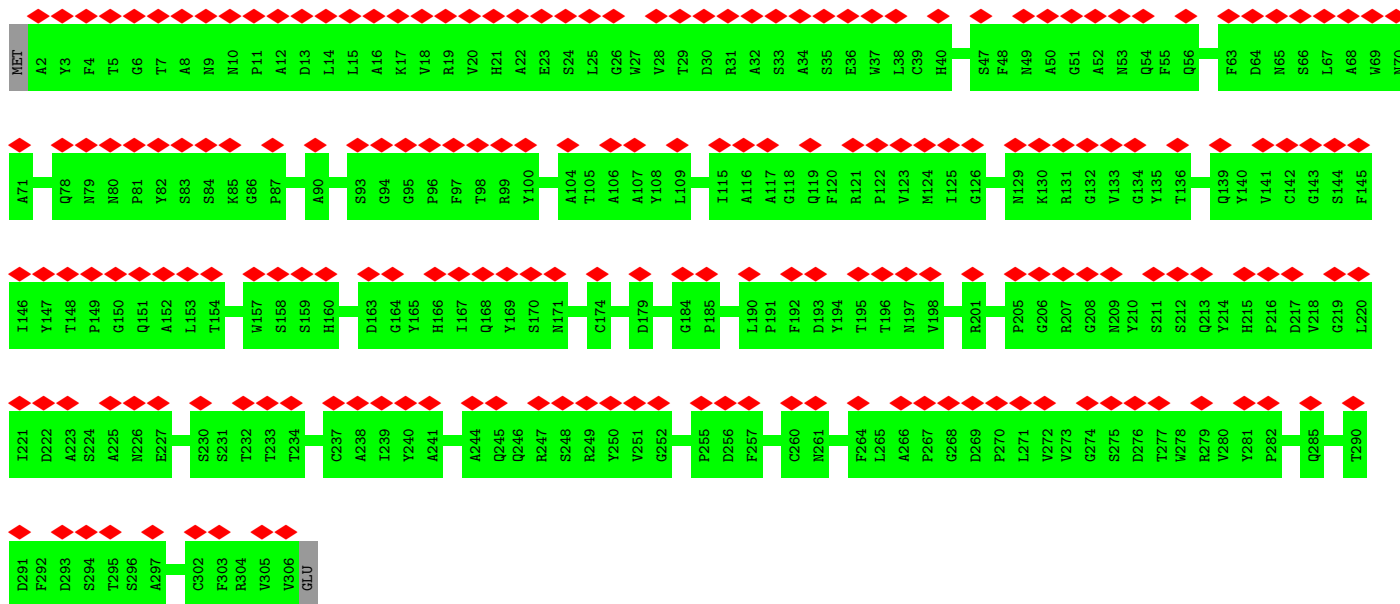


• Molecule 7: Virion structural protein





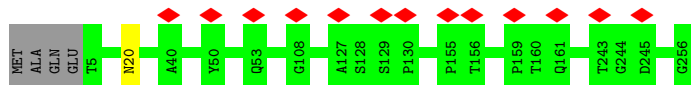
• Molecule 7: Virion structural protein



• Molecule 8: Virion structural protein

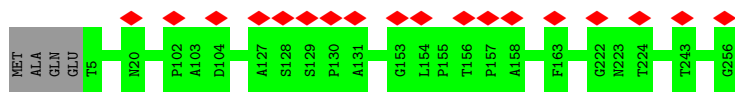


• Molecule 8: Virion structural protein

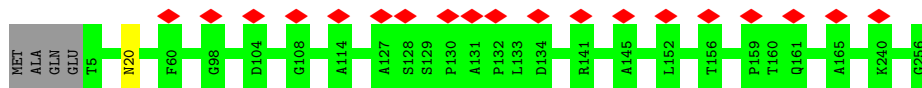


• Molecule 8: Virion structural protein





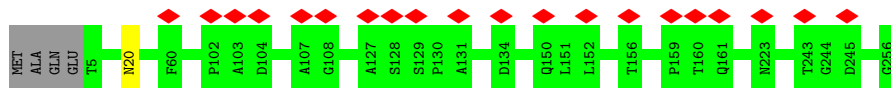
- Molecule 8: Virion structural protein



- Molecule 8: Virion structural protein



- Molecule 8: Virion structural protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	1780	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 ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	36.304	Depositor
Minimum map value	-16.154	Depositor
Average map value	0.060	Depositor
Map value standard deviation	1.061	Depositor
Recommended contour level	5	Depositor
Map size ( $\text{\AA}$ )	450.14398, 450.14398, 450.14398	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8336, 0.8336, 0.8336	Depositor

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/261	0.42	0/350
1	B	0.25	0/261	0.42	0/350
1	C	0.25	0/261	0.42	0/350
2	O	0.61	2/2151 (0.1%)	0.77	6/2934 (0.2%)
2	P	0.61	2/2151 (0.1%)	0.77	6/2934 (0.2%)
2	g	0.61	2/2151 (0.1%)	0.77	6/2934 (0.2%)
3	D	0.24	0/4370	0.54	0/5972
3	U	0.24	0/4370	0.54	0/5972
3	r	0.24	0/4370	0.54	0/5972
4	E	0.25	0/2873	0.50	0/3929
4	F	0.25	0/2873	0.50	0/3929
4	I	0.25	0/2873	0.50	0/3929
4	J	0.25	0/2873	0.50	0/3929
4	M	0.25	0/2873	0.50	0/3929
4	N	0.25	0/2873	0.50	0/3929
4	W	0.25	0/2873	0.50	0/3929
4	a	0.25	0/2873	0.50	0/3929
4	e	0.25	0/2873	0.50	0/3929
5	b	0.26	0/5701	0.53	1/7762 (0.0%)
5	d	0.26	0/5701	0.53	1/7762 (0.0%)
5	o	0.25	0/5701	0.53	1/7762 (0.0%)
6	K	0.25	0/2544	0.52	0/3473
6	L	0.25	0/2544	0.52	0/3473
6	Q	0.25	0/2544	0.52	0/3473
6	R	0.24	0/2544	0.52	0/3473
6	T	0.25	0/2544	0.53	0/3473
6	V	0.25	0/2544	0.53	0/3473
6	c	0.25	0/2544	0.52	0/3473
6	i	0.24	0/2544	0.52	0/3473
6	k	0.24	0/2544	0.53	0/3473
7	G	0.25	0/2412	0.49	0/3299
7	H	0.25	0/2412	0.49	0/3299
7	S	0.25	0/2412	0.49	0/3299
7	X	0.25	0/2412	0.49	0/3299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	Y	0.25	0/2412	0.49	0/3299
7	Z	0.25	0/2412	0.48	0/3299
7	m	0.25	0/2412	0.49	0/3299
7	n	0.25	0/2412	0.49	0/3299
7	p	0.25	0/2412	0.49	0/3299
8	f	0.25	0/1909	0.48	0/2603
8	h	0.25	0/1909	0.48	0/2603
8	j	0.24	0/1909	0.49	0/2603
8	l	0.24	0/1909	0.49	0/2603
8	q	0.25	0/1909	0.48	0/2603
8	s	0.24	0/1909	0.49	0/2603
All	All	0.28	6/119364 (0.0%)	0.53	21/162981 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	62	PRO	CB-CG	20.75	2.53	1.50
2	g	62	PRO	CB-CG	20.75	2.53	1.50
2	P	62	PRO	CB-CG	20.75	2.53	1.50
2	O	62	PRO	CG-CD	-15.25	1.00	1.50
2	g	62	PRO	CG-CD	-15.25	1.00	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	62	PRO	CB-CG-CD	-22.59	18.40	106.50
2	O	62	PRO	CB-CG-CD	-22.59	18.41	106.50
2	g	62	PRO	CB-CG-CD	-22.58	18.44	106.50
2	P	62	PRO	CA-N-CD	-15.69	89.54	111.50
2	O	62	PRO	CA-N-CD	-15.69	89.54	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	30/1158 (3%)	29 (97%)	1 (3%)	0	100	100
1	B	30/1158 (3%)	29 (97%)	1 (3%)	0	100	100
1	C	30/1158 (3%)	29 (97%)	1 (3%)	0	100	100
2	O	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
2	P	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
2	g	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
3	D	552/567 (97%)	499 (90%)	52 (9%)	1 (0%)	44	78
3	U	552/567 (97%)	499 (90%)	52 (9%)	1 (0%)	44	78
3	r	552/567 (97%)	499 (90%)	52 (9%)	1 (0%)	44	78
4	E	371/382 (97%)	353 (95%)	18 (5%)	0	100	100
4	F	371/382 (97%)	352 (95%)	19 (5%)	0	100	100
4	I	371/382 (97%)	352 (95%)	19 (5%)	0	100	100
4	J	371/382 (97%)	352 (95%)	19 (5%)	0	100	100
4	M	371/382 (97%)	357 (96%)	14 (4%)	0	100	100
4	N	371/382 (97%)	357 (96%)	14 (4%)	0	100	100
4	W	371/382 (97%)	353 (95%)	18 (5%)	0	100	100
4	a	371/382 (97%)	352 (95%)	19 (5%)	0	100	100
4	e	371/382 (97%)	357 (96%)	14 (4%)	0	100	100
5	b	725/735 (99%)	696 (96%)	28 (4%)	1 (0%)	48	83
5	d	725/735 (99%)	696 (96%)	28 (4%)	1 (0%)	48	83
5	o	725/735 (99%)	696 (96%)	28 (4%)	1 (0%)	48	83
6	K	315/318 (99%)	305 (97%)	10 (3%)	0	100	100
6	L	315/318 (99%)	305 (97%)	10 (3%)	0	100	100
6	Q	315/318 (99%)	304 (96%)	11 (4%)	0	100	100
6	R	315/318 (99%)	304 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	315/318 (99%)	299 (95%)	16 (5%)	0	100	100
6	V	315/318 (99%)	299 (95%)	16 (5%)	0	100	100
6	c	315/318 (99%)	305 (97%)	10 (3%)	0	100	100
6	i	315/318 (99%)	304 (96%)	11 (4%)	0	100	100
6	k	315/318 (99%)	299 (95%)	16 (5%)	0	100	100
7	G	303/307 (99%)	293 (97%)	10 (3%)	0	100	100
7	H	303/307 (99%)	293 (97%)	10 (3%)	0	100	100
7	S	303/307 (99%)	288 (95%)	15 (5%)	0	100	100
7	X	303/307 (99%)	286 (94%)	17 (6%)	0	100	100
7	Y	303/307 (99%)	293 (97%)	10 (3%)	0	100	100
7	Z	303/307 (99%)	286 (94%)	17 (6%)	0	100	100
7	m	303/307 (99%)	286 (94%)	17 (6%)	0	100	100
7	n	303/307 (99%)	288 (95%)	15 (5%)	0	100	100
7	p	303/307 (99%)	288 (95%)	15 (5%)	0	100	100
8	f	250/256 (98%)	244 (98%)	6 (2%)	0	100	100
8	h	250/256 (98%)	244 (98%)	6 (2%)	0	100	100
8	j	250/256 (98%)	240 (96%)	10 (4%)	0	100	100
8	l	250/256 (98%)	240 (96%)	10 (4%)	0	100	100
8	q	250/256 (98%)	244 (98%)	6 (2%)	0	100	100
8	s	250/256 (98%)	240 (96%)	10 (4%)	0	100	100
All	All	15132/18798 (80%)	14417 (95%)	709 (5%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	U	482	ASP
3	r	482	ASP
3	D	482	ASP
5	o	265	ALA
5	b	265	ALA

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	25/834 (3%)	25 (100%)	0	100	100
1	B	25/834 (3%)	25 (100%)	0	100	100
1	C	25/834 (3%)	25 (100%)	0	100	100
2	O	226/227 (100%)	226 (100%)	0	100	100
2	P	226/227 (100%)	226 (100%)	0	100	100
2	g	226/227 (100%)	226 (100%)	0	100	100
3	D	450/461 (98%)	450 (100%)	0	100	100
3	U	450/461 (98%)	450 (100%)	0	100	100
3	r	450/461 (98%)	450 (100%)	0	100	100
4	E	278/286 (97%)	277 (100%)	1 (0%)	89	90
4	F	278/286 (97%)	277 (100%)	1 (0%)	89	90
4	I	278/286 (97%)	276 (99%)	2 (1%)	81	87
4	J	278/286 (97%)	276 (99%)	2 (1%)	81	87
4	M	278/286 (97%)	277 (100%)	1 (0%)	89	90
4	N	278/286 (97%)	277 (100%)	1 (0%)	89	90
4	W	278/286 (97%)	277 (100%)	1 (0%)	89	90
4	a	278/286 (97%)	276 (99%)	2 (1%)	81	87
4	e	278/286 (97%)	277 (100%)	1 (0%)	89	90
5	b	585/590 (99%)	583 (100%)	2 (0%)	91	91
5	d	585/590 (99%)	583 (100%)	2 (0%)	91	91
5	o	585/590 (99%)	583 (100%)	2 (0%)	91	91
6	K	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	L	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	Q	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	R	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	T	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	V	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	c	252/253 (100%)	251 (100%)	1 (0%)	89	90
6	i	252/253 (100%)	251 (100%)	1 (0%)	89	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	k	252/253 (100%)	251 (100%)	1 (0%)	89	90
7	G	243/245 (99%)	243 (100%)	0	100	100
7	H	243/245 (99%)	243 (100%)	0	100	100
7	S	243/245 (99%)	243 (100%)	0	100	100
7	X	243/245 (99%)	243 (100%)	0	100	100
7	Y	243/245 (99%)	243 (100%)	0	100	100
7	Z	243/245 (99%)	243 (100%)	0	100	100
7	m	243/245 (99%)	243 (100%)	0	100	100
7	n	243/245 (99%)	243 (100%)	0	100	100
7	p	243/245 (99%)	243 (100%)	0	100	100
8	f	195/198 (98%)	195 (100%)	0	100	100
8	h	195/198 (98%)	195 (100%)	0	100	100
8	j	195/198 (98%)	194 (100%)	1 (0%)	86	89
8	l	195/198 (98%)	194 (100%)	1 (0%)	86	89
8	q	195/198 (98%)	195 (100%)	0	100	100
8	s	195/198 (98%)	194 (100%)	1 (0%)	86	89
All	All	11985/14580 (82%)	11955 (100%)	30 (0%)	90	91

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	200	ARG
6	R	134	ARG
6	Q	134	ARG
8	l	20	ASN
5	d	200	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
7	n	245	GLN
7	X	261	ASN
7	p	245	GLN
6	Q	259	GLN
2	P	271	GLN

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.



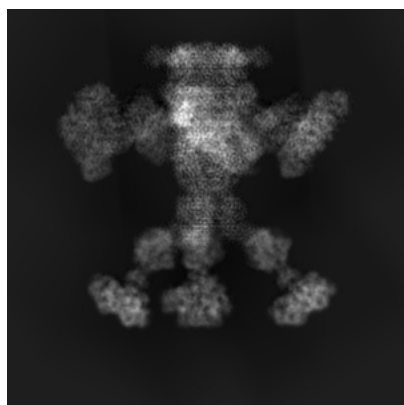
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19256. These allow visual inspection of the internal detail of the map and identification of artifacts.

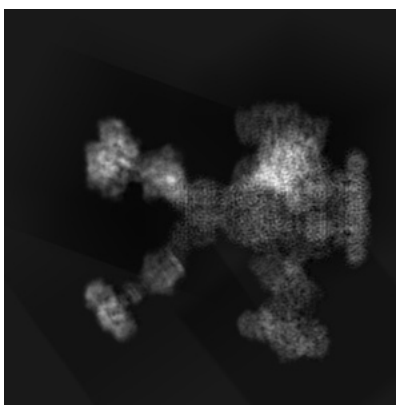
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

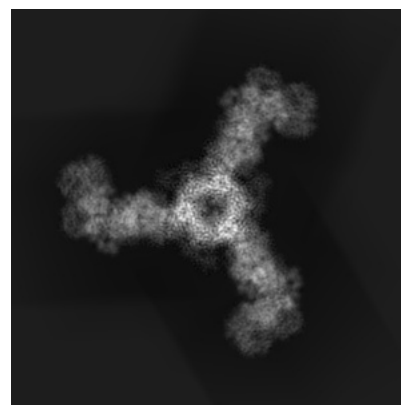
#### 6.1.1 Primary map



X



Y

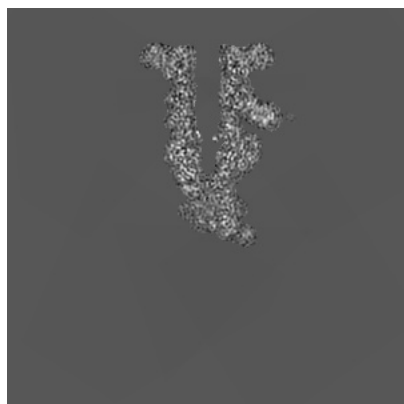


Z

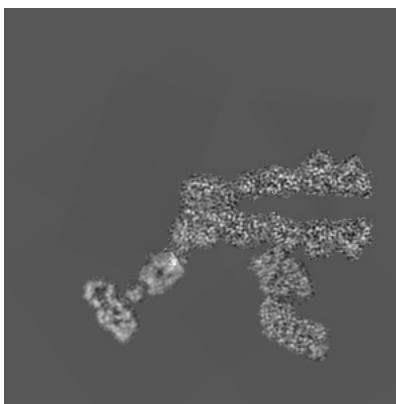
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 270



Y Index: 270

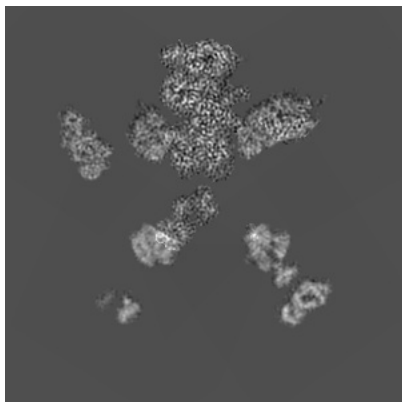


Z Index: 270

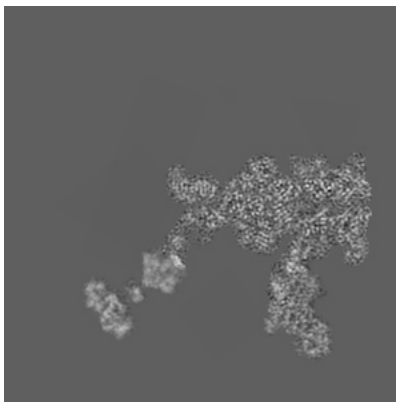
The images above show central slices of the map in three orthogonal directions.

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

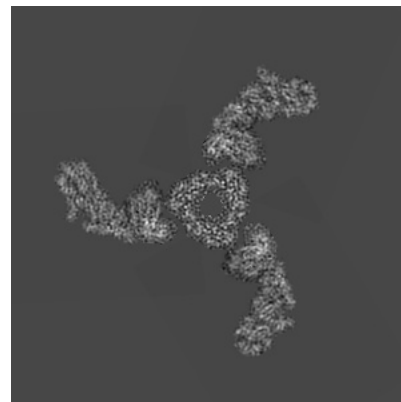
### 6.3.1 Primary map



X Index: 308



Y Index: 246

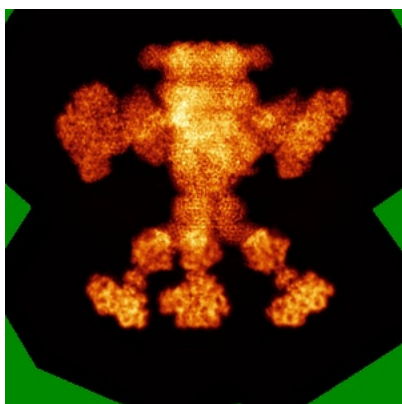


Z Index: 386

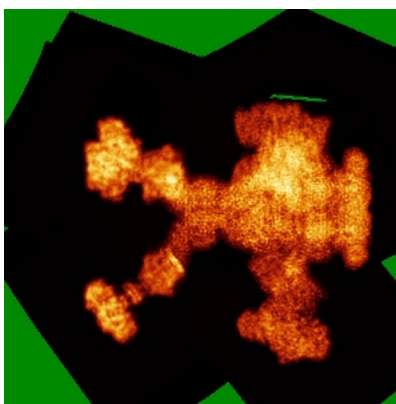
The images above show the largest variance slices of the map in three orthogonal directions.

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

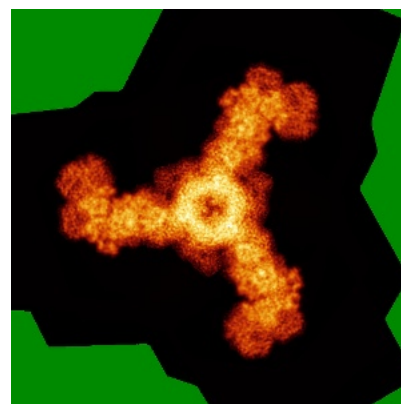
### 6.4.1 Primary map



X



Y

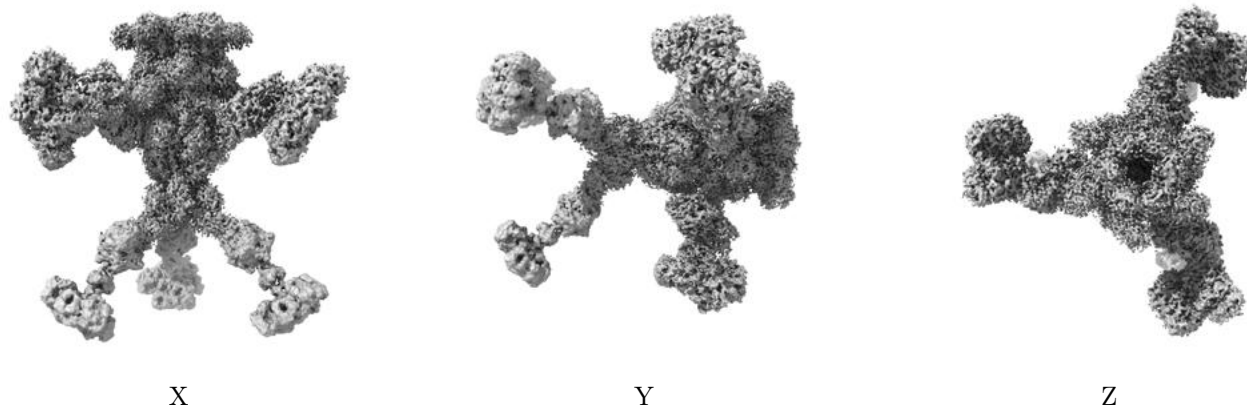


Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

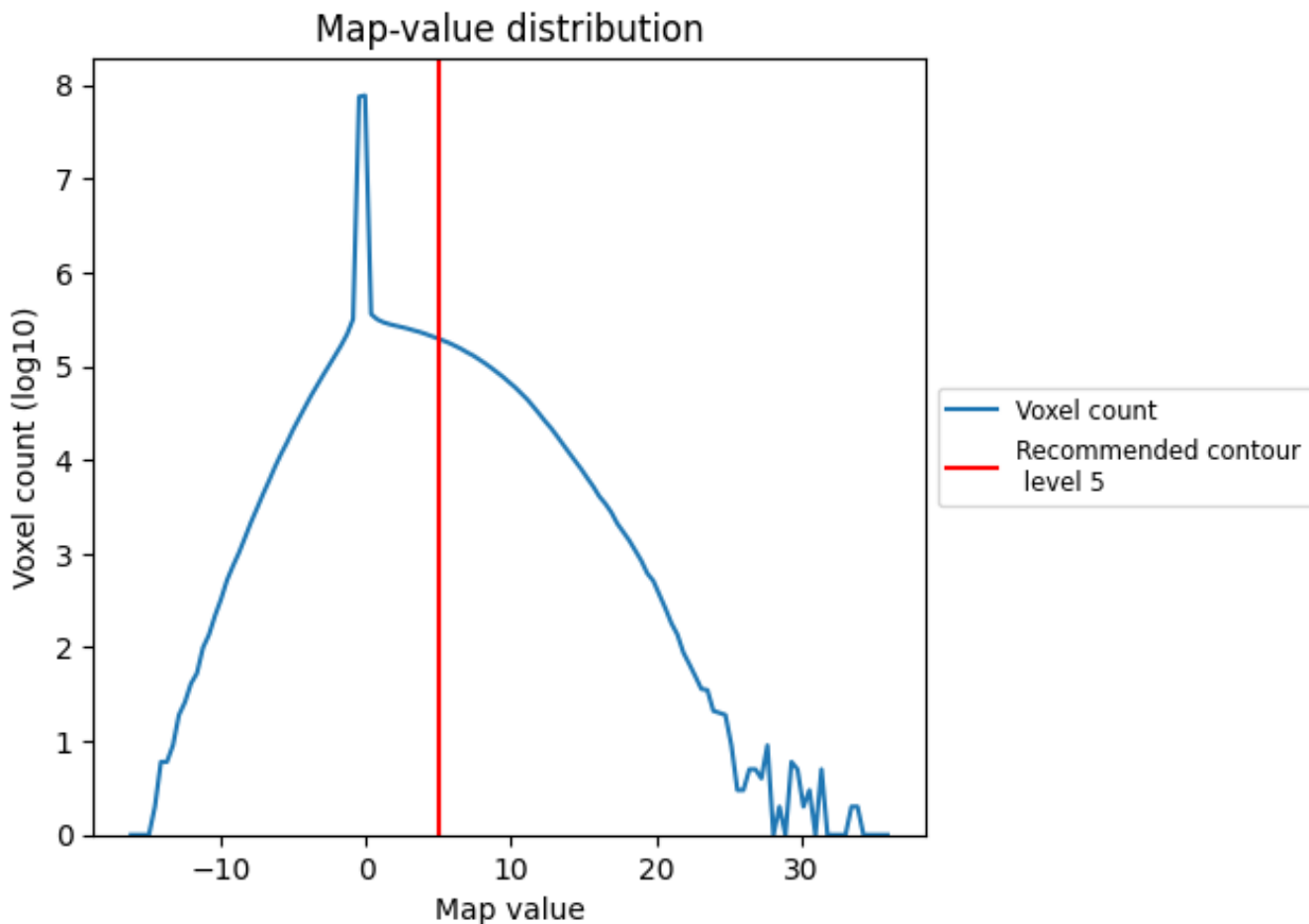
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

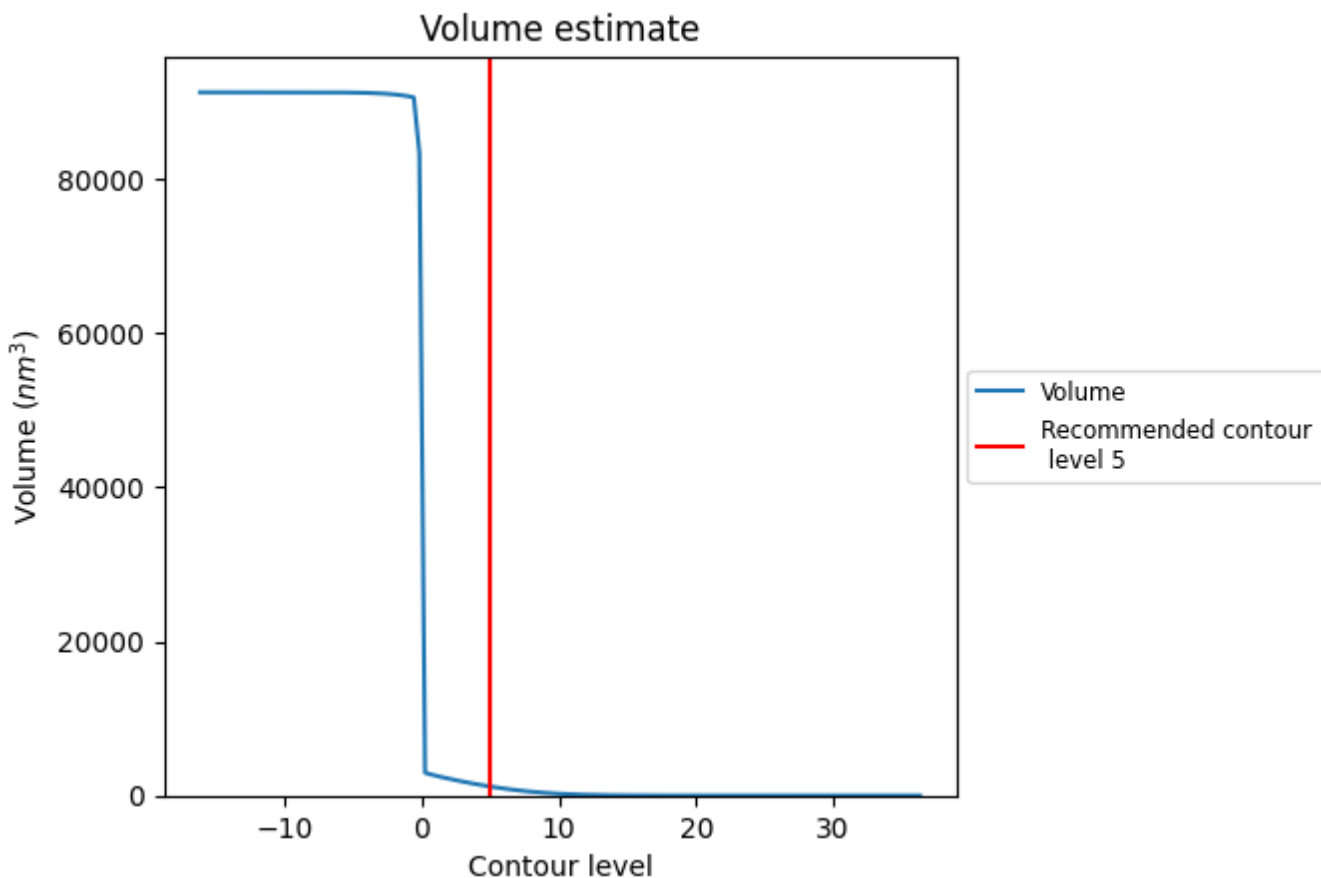
This section contains the results of statistical analysis of the map.

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



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

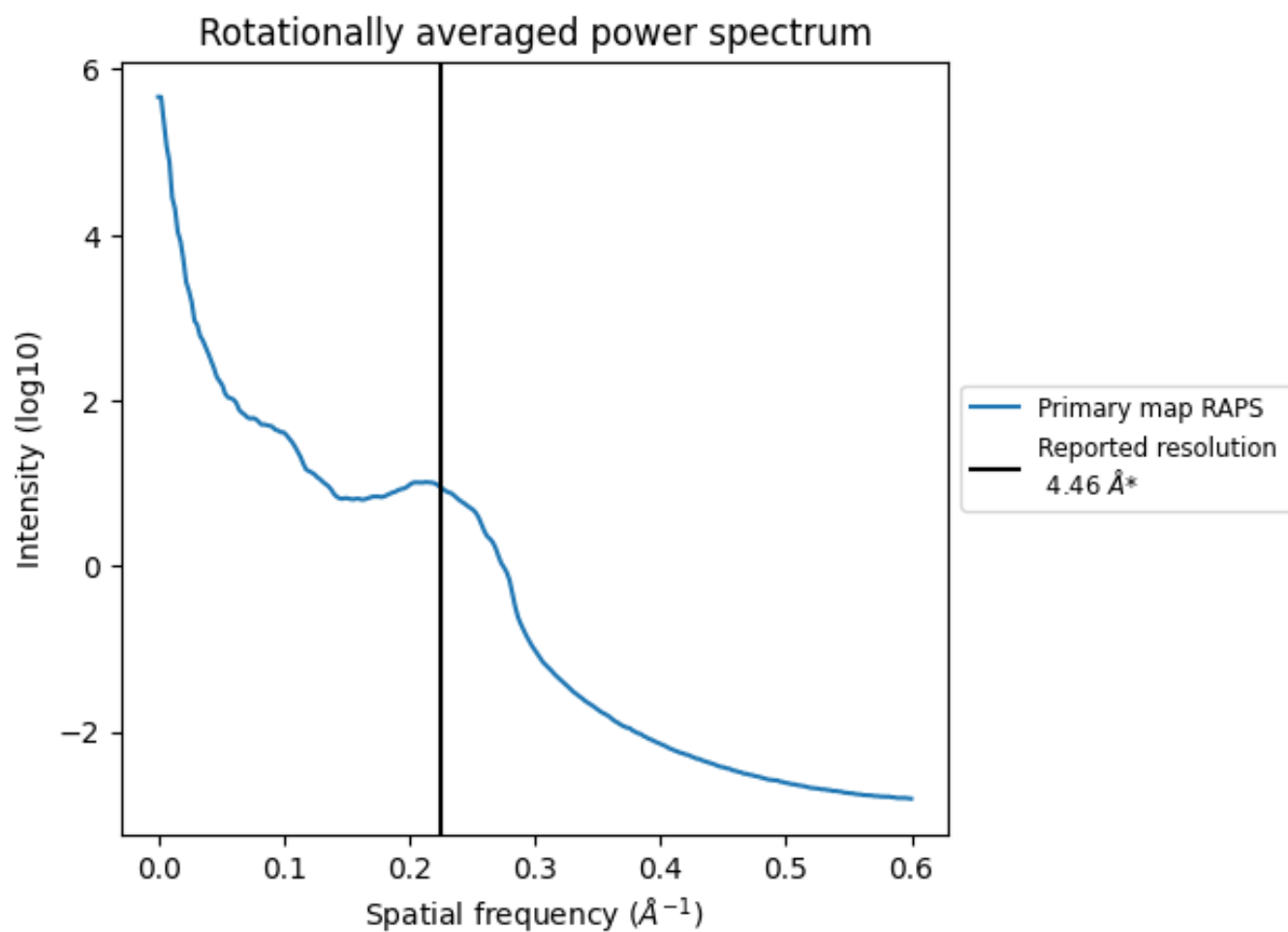
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1167  $\text{nm}^3$ ; this corresponds to an approximate mass of 1054 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.224 Å<sup>-1</sup>

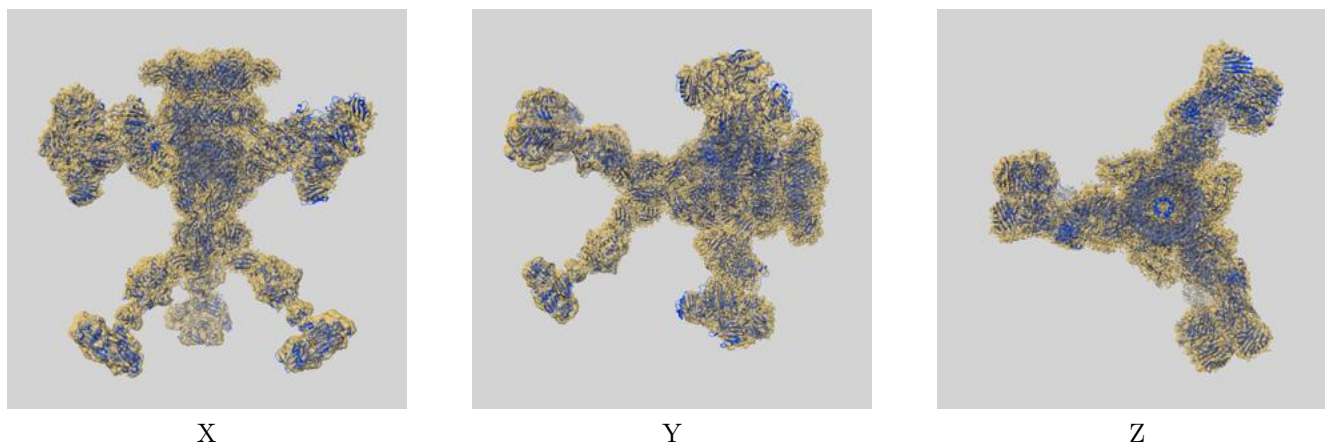
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-19256 and PDB model 8RK3. Per-residue inclusion information can be found in section 3 on page 9.

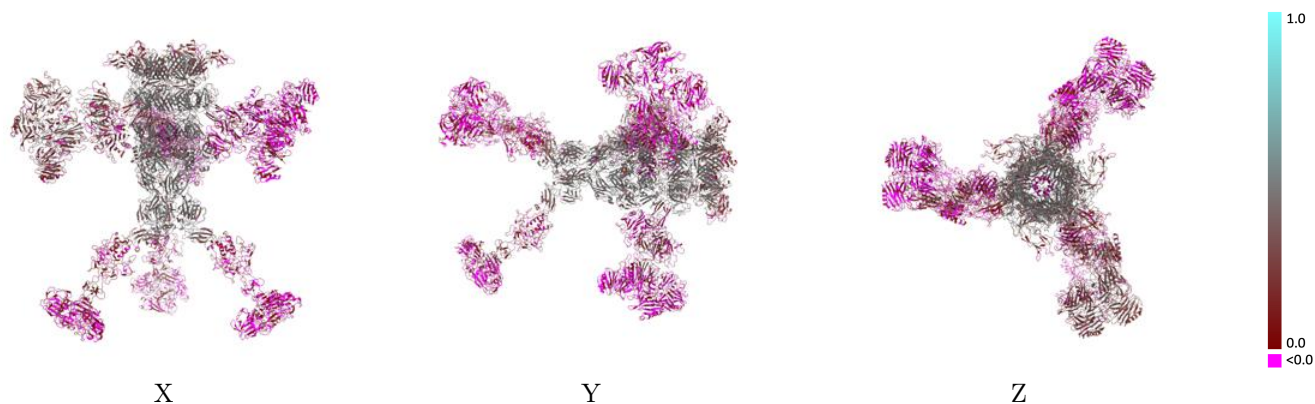
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

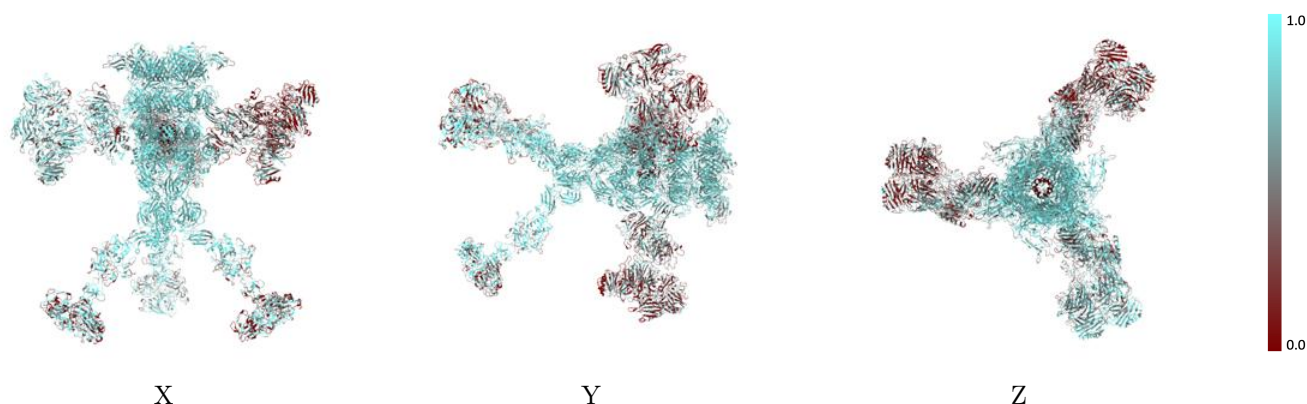


## 9.2 Q-score mapped to coordinate model [i](#)



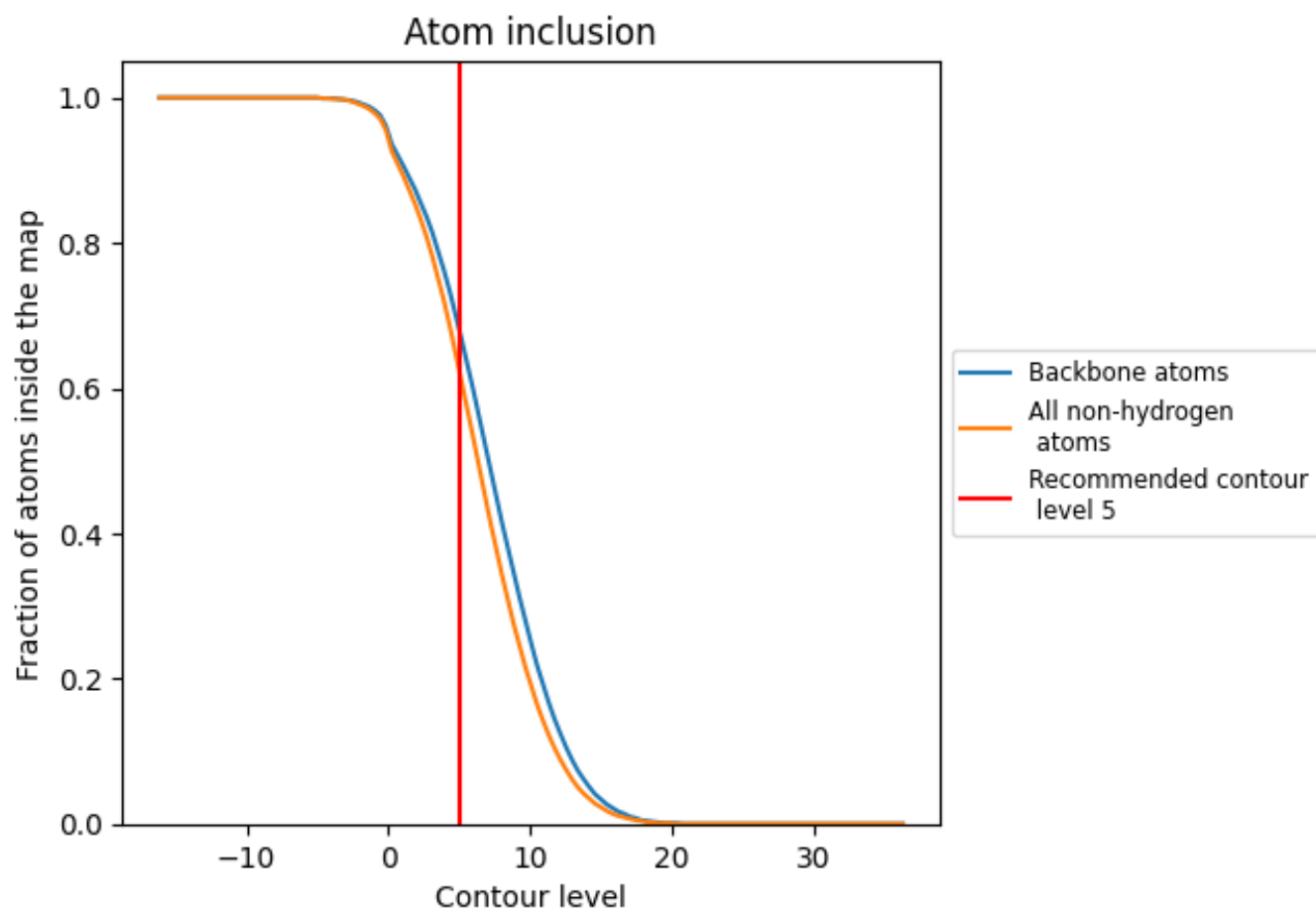
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.2020
A	 0.1670	 0.0230
B	 0.1670	 0.0300
C	 0.1630	 0.0520
D	 0.7290	 0.3320
E	 0.6060	 0.0530
F	 0.6070	 0.0380
G	 0.4370	 0.0630
H	 0.4440	 0.0620
I	 0.6050	 0.0610
J	 0.5200	 0.0260
K	 0.3500	 -0.0010
L	 0.4550	 0.0620
M	 0.6080	 0.0670
N	 0.6190	 0.0430
O	 0.8200	 0.4180
P	 0.8080	 0.4150
Q	 0.3180	 0.0050
R	 0.4830	 0.1380
S	 0.6590	 0.2860
T	 0.3070	 -0.0140
U	 0.7890	 0.3530
V	 0.3560	 0.0030
W	 0.7250	 0.0990
X	 0.4310	 0.0400
Y	 0.5630	 0.1730
Z	 0.3000	 -0.0120
a	 0.6430	 0.0710
b	 0.8290	 0.4100
c	 0.6920	 0.2930
d	 0.8150	 0.4110
e	 0.6380	 0.0750
f	 0.7350	 0.3150
g	 0.8450	 0.4290
h	 0.7410	 0.3210



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Chain	Atom inclusion	Q-score
i	 0.6190	 0.2530
j	 0.6960	 0.3180
k	 0.6680	 0.2540
l	 0.7330	 0.3230
m	 0.6210	 0.2040
n	 0.2260	 -0.0050
o	 0.8480	 0.4240
p	 0.3470	 -0.0060
q	 0.7410	 0.3460
r	 0.7450	 0.3230
s	 0.7780	 0.3400