



## wwPDB EM Validation Summary Report ⓘ

Jun 17, 2025 – 09:29 AM JST

PDB ID : 8ZDO / pdb\_00008zdo  
EMDB ID : EMD-39996  
Title : Cryo-EM structure of Mycobacteriophage Douge baseplate (gp13, gp17, gp23, gp16, gp18 and gp20)  
Authors : Maharana, J.; Wang, C.H.; Tsai, L.A.; Lowary, T.L.; Ho, M.C.  
Deposited on : 2024-05-02  
Resolution : 2.97 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

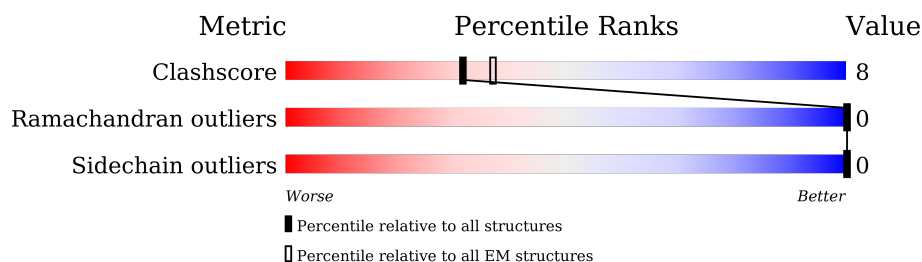
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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.


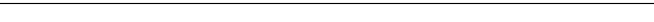

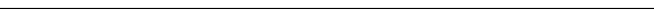

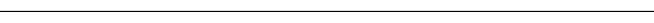
Mol	Chain	Length	Quality of chain
1	G	300	<div> <div>12%</div> <div>80%</div> <div>20%</div> </div>
1	H	300	<div> <div>11%</div> <div>81%</div> <div>19%</div> </div>
1	I	300	<div> <div>11%</div> <div>79%</div> <div>21%</div> </div>
1	J	300	<div> <div>11%</div> <div>81%</div> <div>19%</div> </div>
1	K	300	<div> <div>12%</div> <div>79%</div> <div>21%</div> </div>
1	L	300	<div> <div>9%</div> <div>81%</div> <div>19%</div> </div>
1	M	300	<div> <div>10%</div> <div>82%</div> <div>18%</div> </div>
1	N	300	<div> <div>10%</div> <div>81%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	300	<div> <div>10%</div> <div>81%</div> <div>19%</div> </div>
1	P	300	<div> <div>10%</div> <div>84%</div> <div>16%</div> </div>
1	Q	300	<div> <div>11%</div> <div>82%</div> <div>18%</div> </div>
1	R	300	<div> <div>9%</div> <div>80%</div> <div>20%</div> </div>
2	S	1699	<div> <div>98%</div> </div>
2	T	1699	<div> <div>98%</div> </div>
2	U	1699	<div> <div>98%</div> </div>
3	a	311	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
3	b	311	<div> <div>84%</div> <div>16%</div> </div>
3	c	311	<div> <div>82%</div> <div>18%</div> </div>
3	d	311	<div> <div>82%</div> <div>18%</div> </div>
3	e	311	<div> <div>81%</div> <div>19%</div> </div>
3	f	311	<div> <div>80%</div> <div>20%</div> </div>
3	g	311	<div> <div>84%</div> <div>16%</div> </div>
3	h	311	<div> <div>80%</div> <div>20%</div> </div>
3	i	311	<div> <div>5%</div> <div>83%</div> <div>17%</div> </div>
3	j	311	<div> <div>82%</div> <div>18%</div> </div>
3	k	311	<div> <div>83%</div> <div>17%</div> </div>
3	l	311	<div> <div>80%</div> <div>20%</div> </div>
4	m	295	<div> <div>75%</div> <div>23%</div> </div>
4	n	295	<div> <div>70%</div> <div>28%</div> </div>
4	o	295	<div> <div>75%</div> <div>23%</div> </div>
4	p	295	<div> <div>74%</div> <div>24%</div> </div>
4	q	295	<div> <div>74%</div> <div>24%</div> </div>
4	r	295	<div> <div>74%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
5	s	587	
5	t	587	
5	u	587	
6	v	878	
6	w	878	
6	x	878	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 86910 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 Tail tube protein (gp13).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	H	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	I	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	J	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	K	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	L	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	M	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	N	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	O	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	P	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	Q	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		
1	R	299	Total	C	N	O	S	0	0
			2256	1438	367	448	3		

- Molecule 2 is a protein called Tape measure protein (gp16).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	42	Total	C	N	O	0	0
			327	201	62	64		
2	T	42	Total	C	N	O	0	0
			327	201	62	64		
2	U	42	Total	C	N	O	0	0
			327	201	62	64		

- Molecule 3 is a protein called Baseplate upper protein (gp23).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	b	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	c	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	d	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	e	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	f	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	g	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	h	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	i	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	j	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	k	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		
3	l	311	Total	C	N	O	S	0	0
			2372	1519	388	453	12		

- Molecule 4 is a protein called Distal tail protein (gp17).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	m	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		
4	n	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		
4	o	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		
4	p	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		
4	q	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		
4	r	290	Total	C	N	O	S	0	0
			2343	1497	397	440	9		

- Molecule 5 is a protein called Baseplate hub protein (gp18).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	s	586	Total	C	N	O	S	0	0
			4582	2937	768	863	14		
5	t	586	Total	C	N	O	S	0	0
			4582	2937	768	863	14		
5	u	586	Total	C	N	O	S	0	0
			4582	2937	768	863	14		

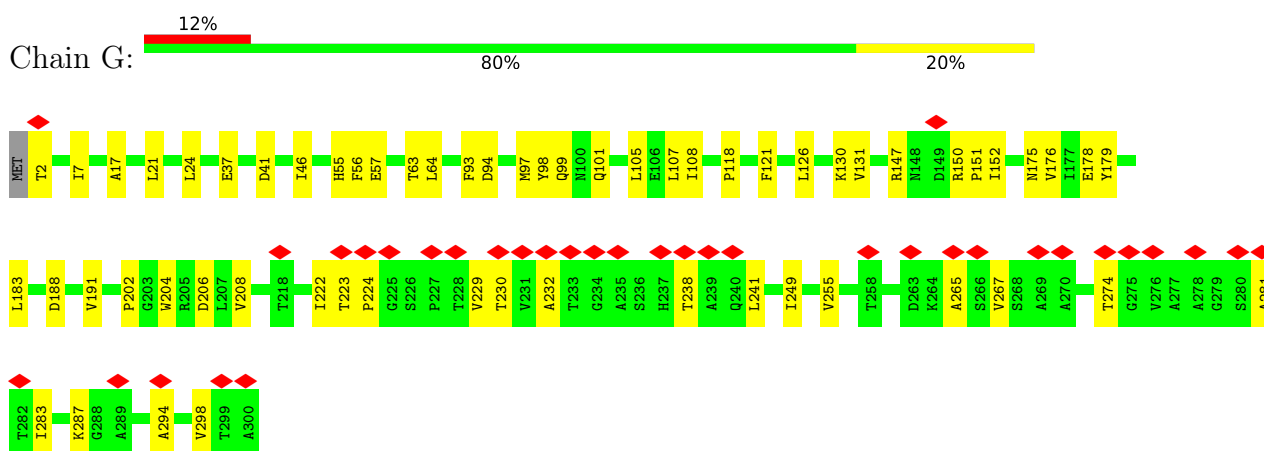
- Molecule 6 is a protein called Central fiber protein (gp20).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	v	115	Total	C	N	O	S	0	0
			863	547	143	171	2		
6	w	115	Total	C	N	O	S	0	0
			863	547	143	171	2		
6	x	115	Total	C	N	O	S	0	0
			863	547	143	171	2		

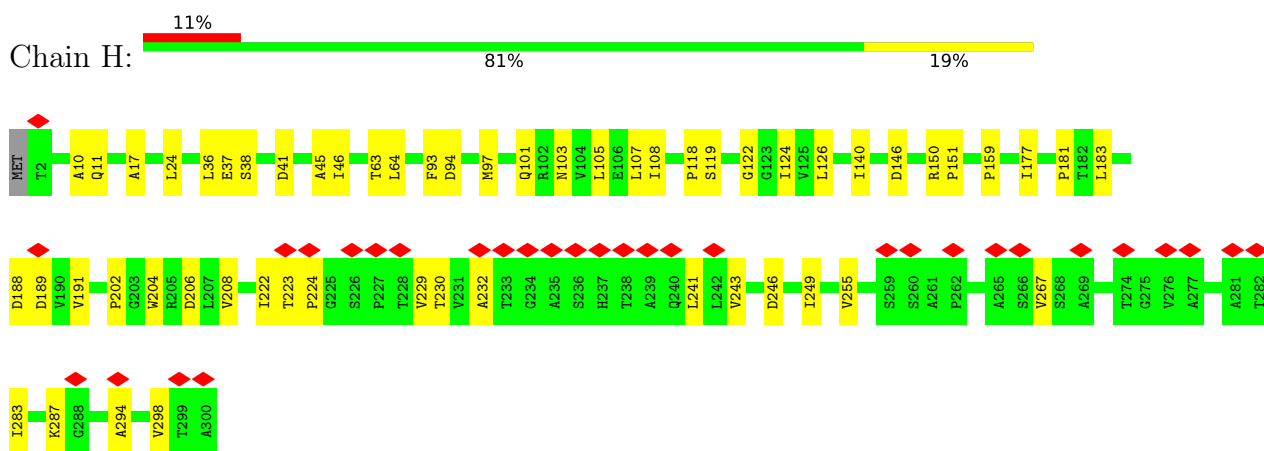
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

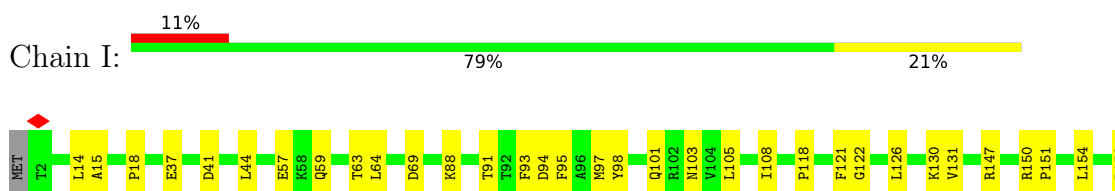
- Molecule 1: Tail tube protein (gp13)



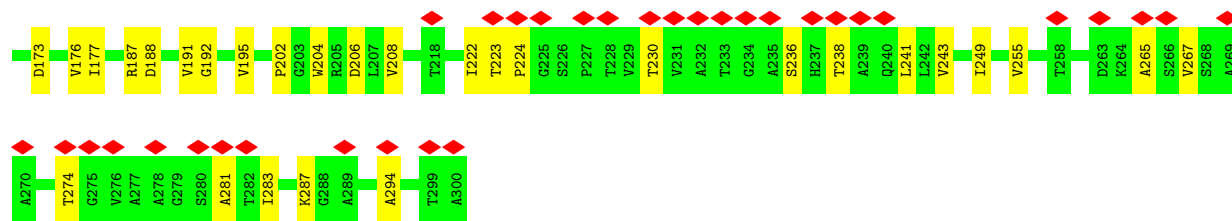
- Molecule 1: Tail tube protein (gp13)



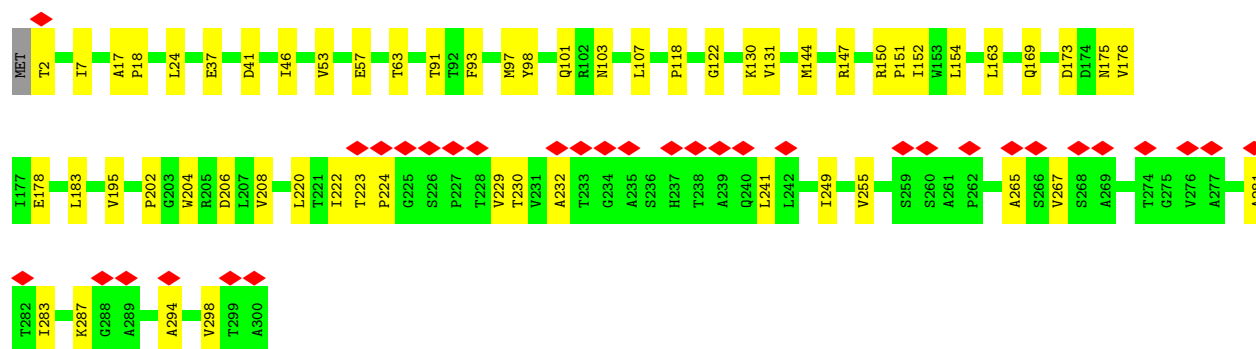
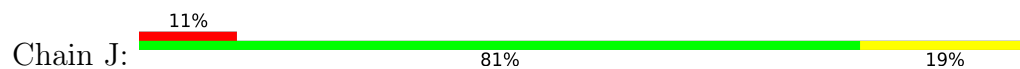
- Molecule 1: Tail tube protein (gp13)



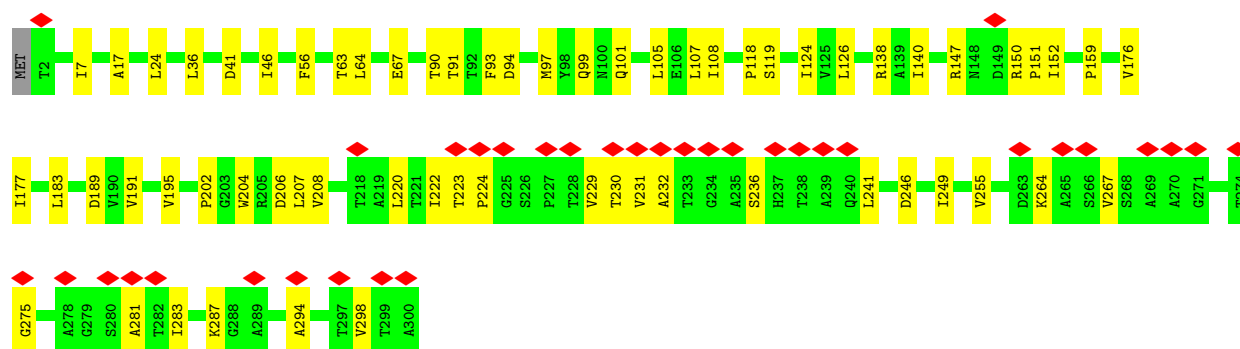
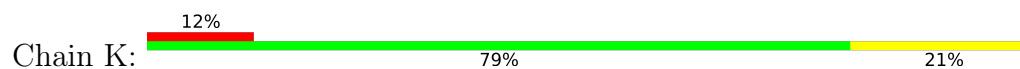




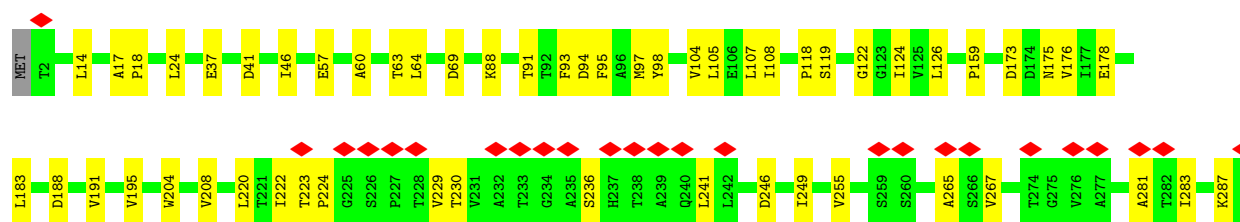
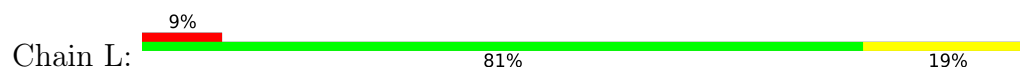
• Molecule 1: Tail tube protein (gp13)

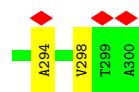


• Molecule 1: Tail tube protein (gp13)

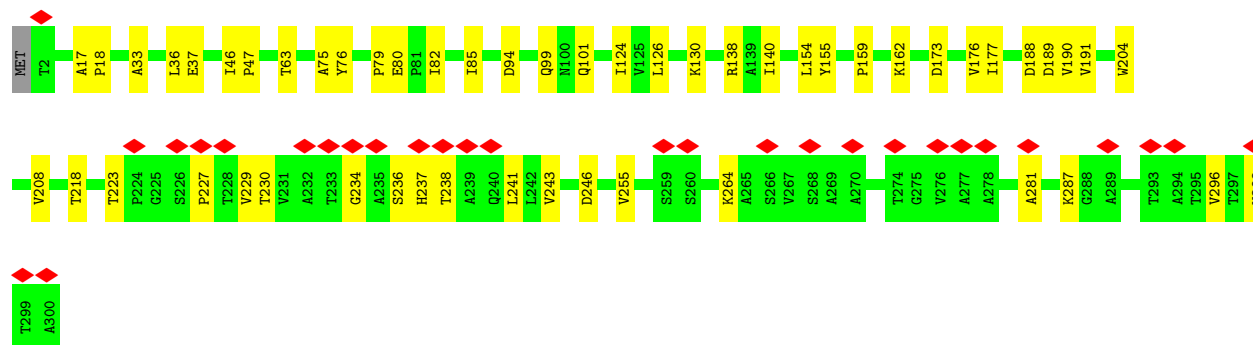
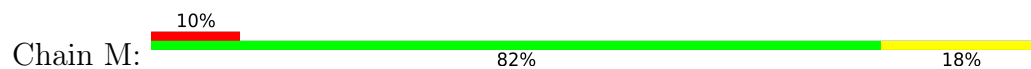


• Molecule 1: Tail tube protein (gp13)

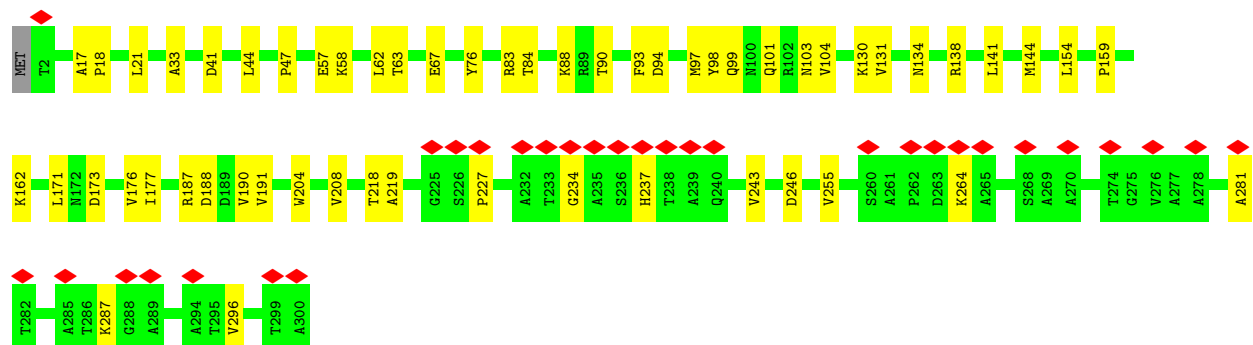
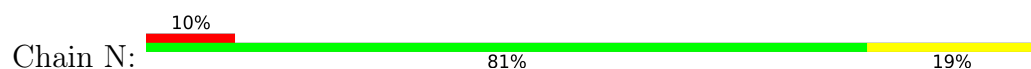




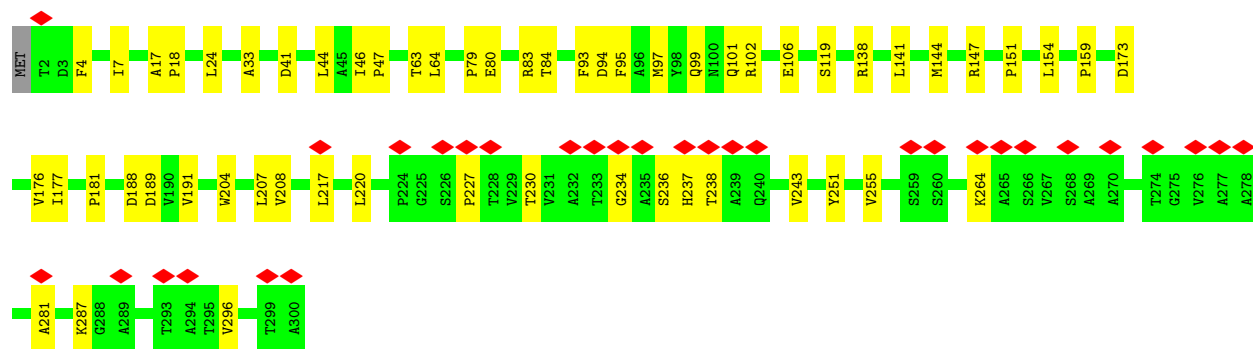
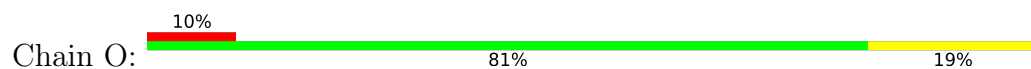
- Molecule 1: Tail tube protein (gp13)



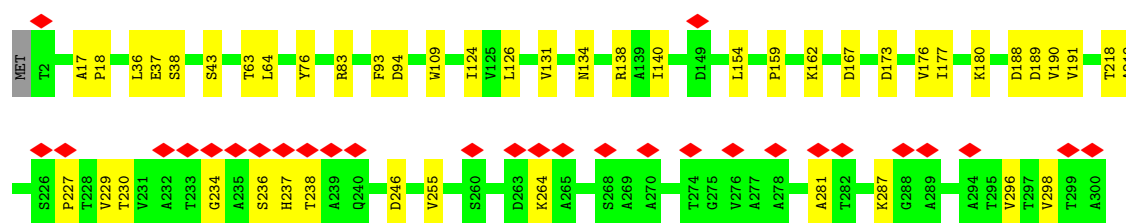
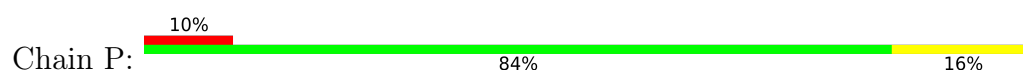
- Molecule 1: Tail tube protein (gp13)



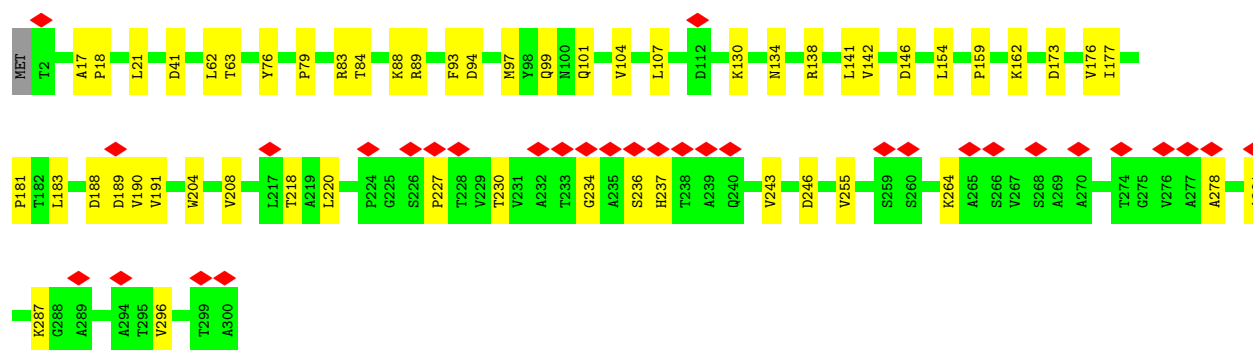
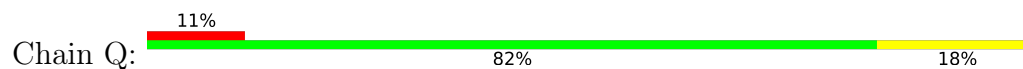
- Molecule 1: Tail tube protein (gp13)



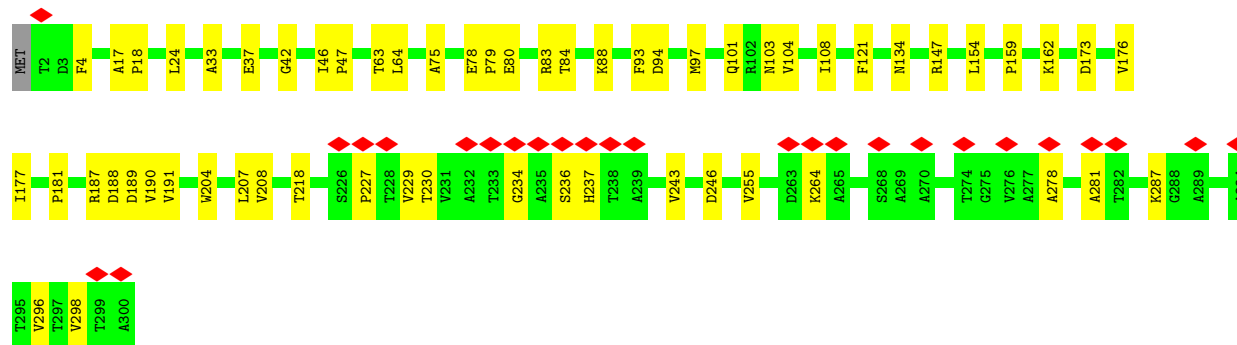
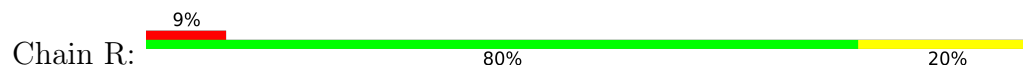
- Molecule 1: Tail tube protein (gp13)



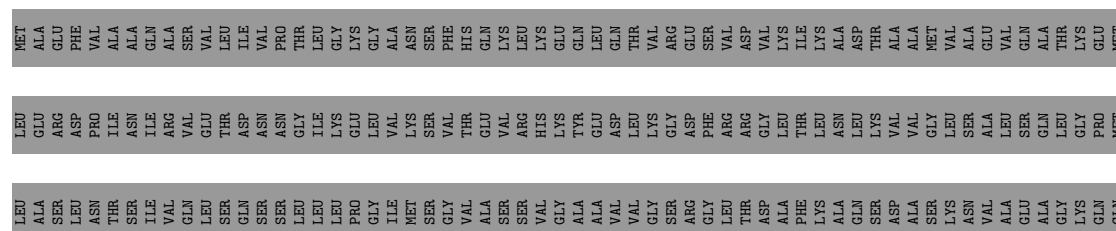
• Molecule 1: Tail tube protein (gp13)



• Molecule 1: Tail tube protein (gp13)



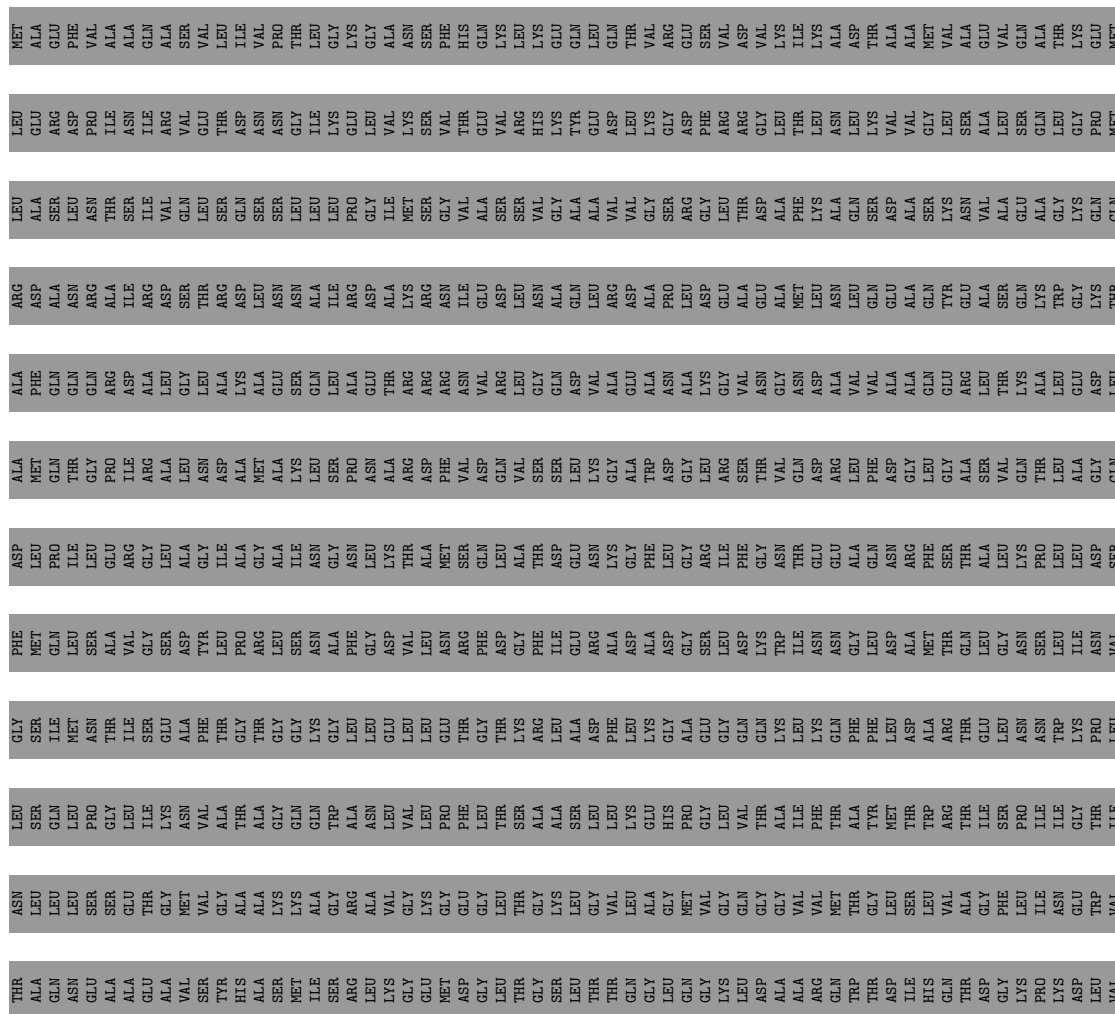
• Molecule 2: Tape measure protein (gp16)





- Molecule 2: Tape measure protein (gp16)

Chain T:  98%

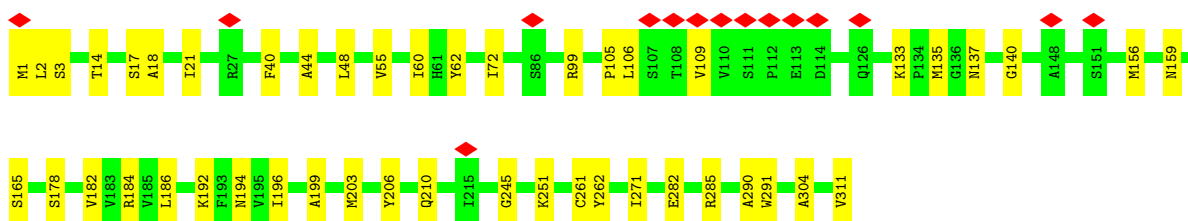


- Molecule 2: Tape measure protein (gp16)

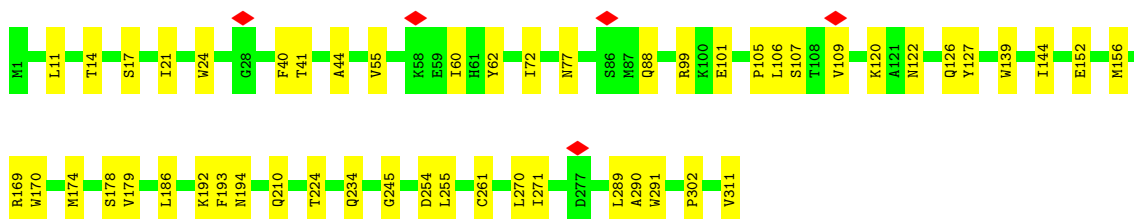


THR	GLY	ALA	GLY	LEU	ASN	ILE	LEU	SER	SER	SER	LEU	VAL	GLY	SER	ALA	PRO	PRO	SER	THR	GLY	THR	THR	GLN	SER	ALA	TYR	GLY	GLY	ALA	ALA	PRO	PRO	VAL	LEU	PRO	GLN	GLY	PRO	PRO	GLN	S1658	P1663	V1666	N1667	N1668	Y1669	I1672	H1673	T1674	Y1677	E1688	A1689	Q1692	P1697	V1698
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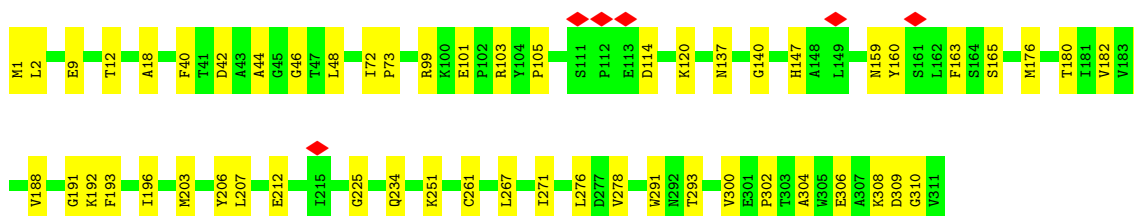
Chain a: 



Chain b:  84% 16%




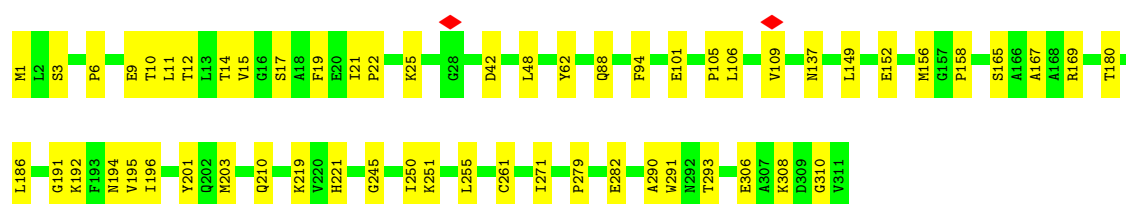
Chain c:  82% 18%






- Molecule 3: Baseplate upper protein (gp23)

Chain d:  82% 18%




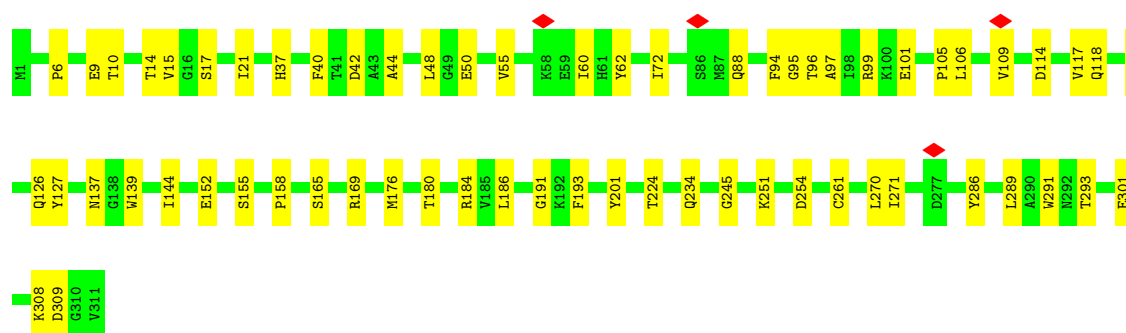
- Molecule 3: Baseplate upper protein (gp23)

Chain e:  81% 19%




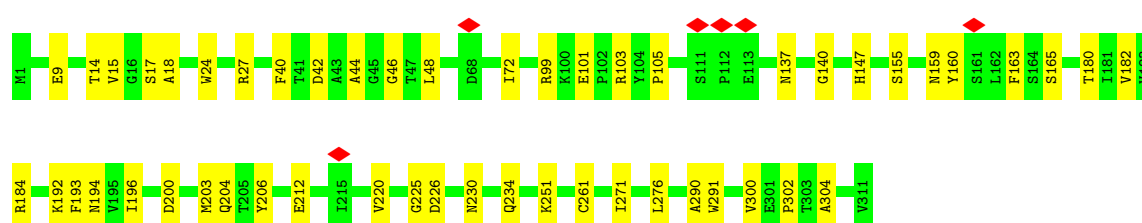
- Molecule 3: Baseplate upper protein (gp23)

Chain f:  80% 20%




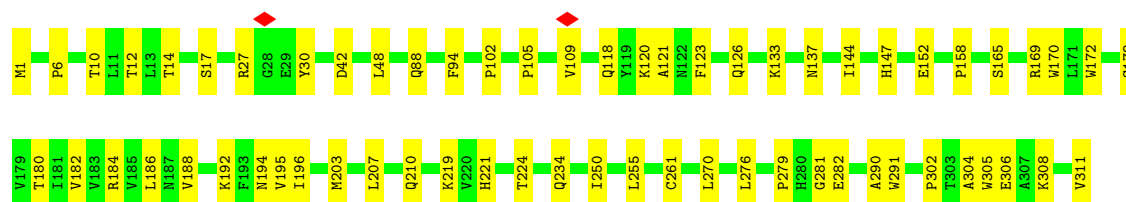
- Molecule 3: Baseplate upper protein (gp23)

Chain g:  84% 16%




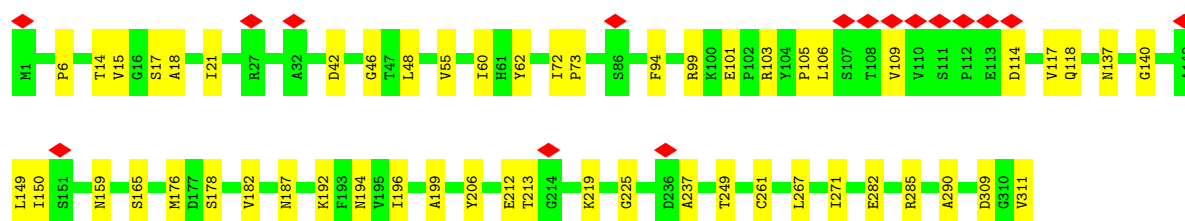
- Molecule 3: Baseplate upper protein (gp23)

Chain h:  80% 20%




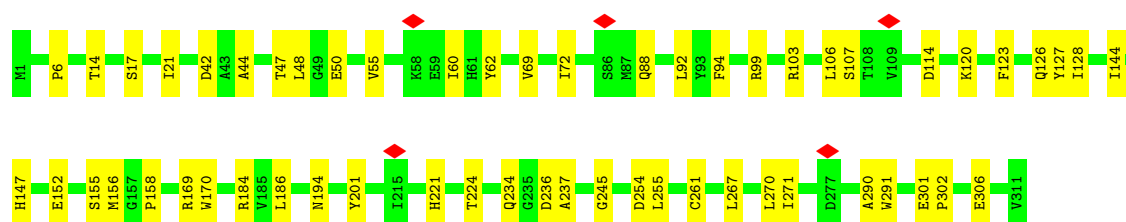
- Molecule 3: Baseplate upper protein (gp23)

Chain i:  5% 83% 17%




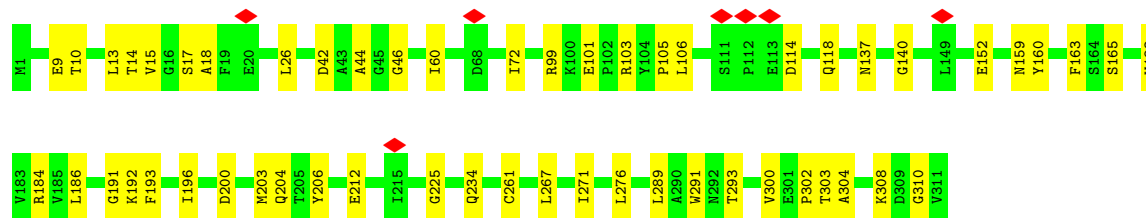
- Molecule 3: Baseplate upper protein (gp23)

Chain j:  82% 18%




- Molecule 3: Baseplate upper protein (gp23)

Chain k:  83% 17%



- Molecule 3: Baseplate upper protein (gp23)

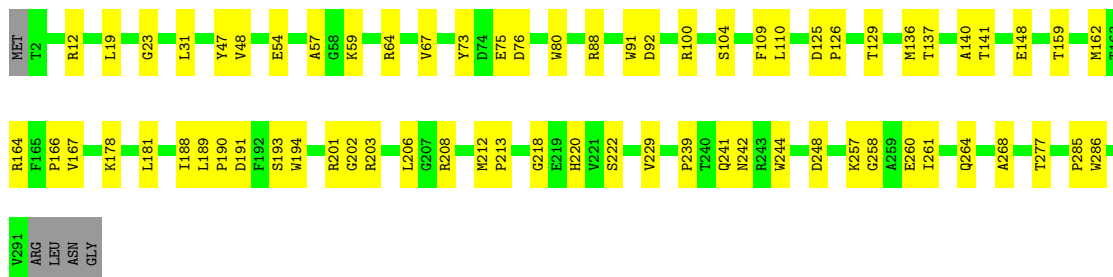
Chain l:  80% 20%





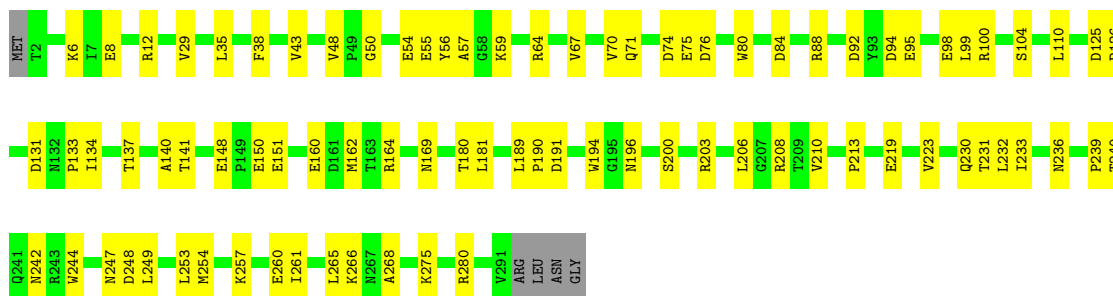
• Molecule 4: Distal tail protein (gp17)

Chain m: 75% 23%



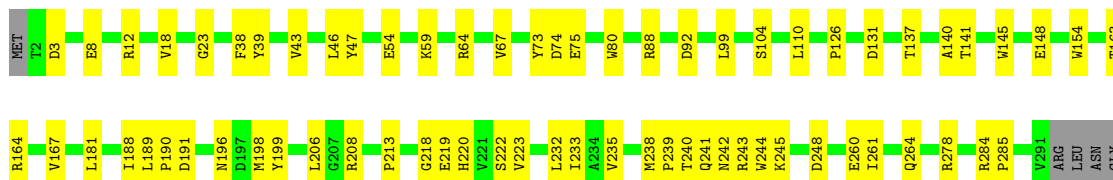
• Molecule 4: Distal tail protein (gp17)

Chain n: 70% 28%



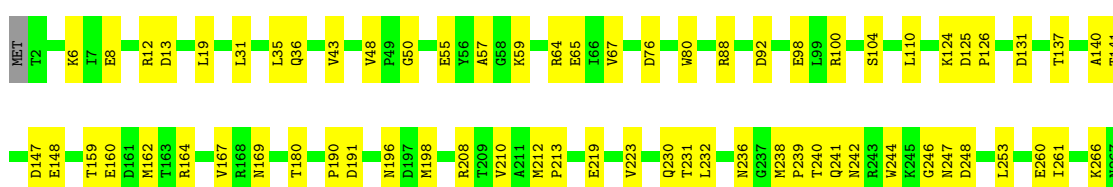
• Molecule 4: Distal tail protein (gp17)

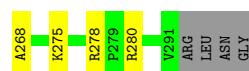
Chain o: 75% 23%



• Molecule 4: Distal tail protein (gp17)

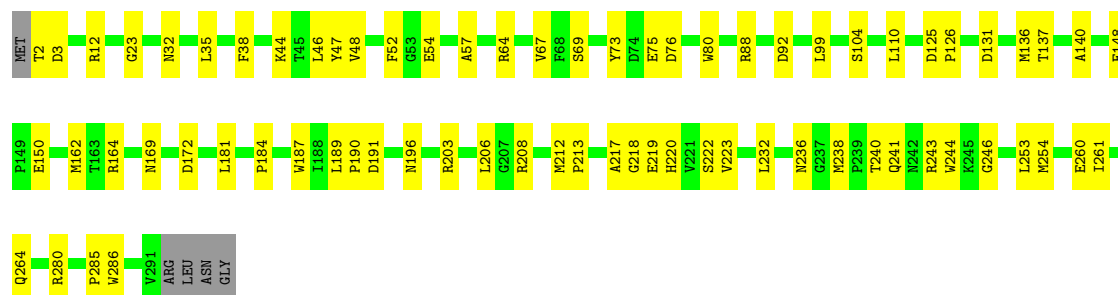
Chain p: 74% 24%





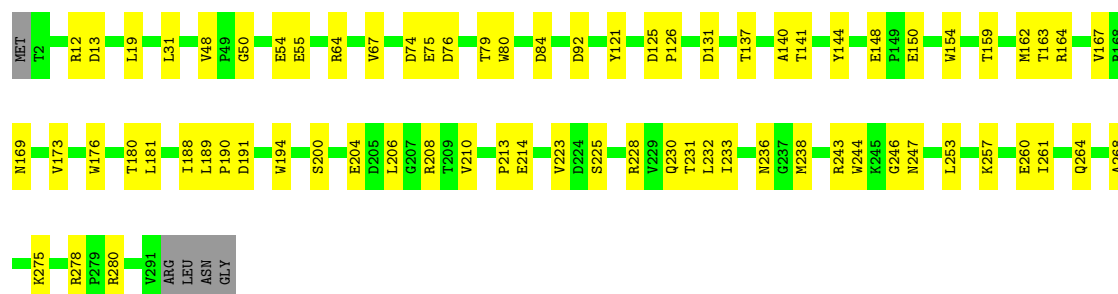
• Molecule 4: Distal tail protein (gp17)

Chain q: 74% 24%



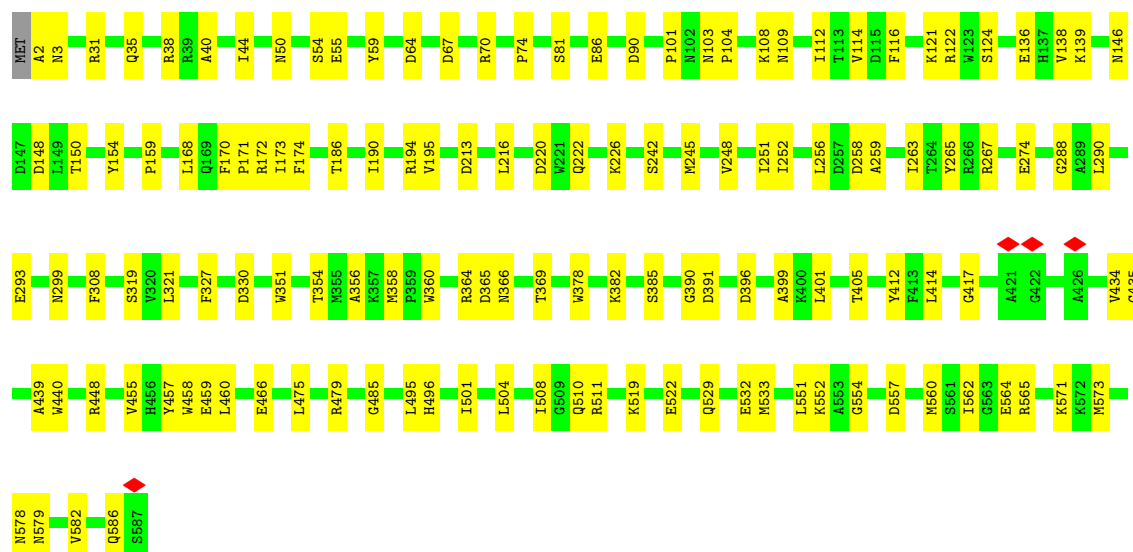
• Molecule 4: Distal tail protein (gp17)

Chain r: 74% 24%

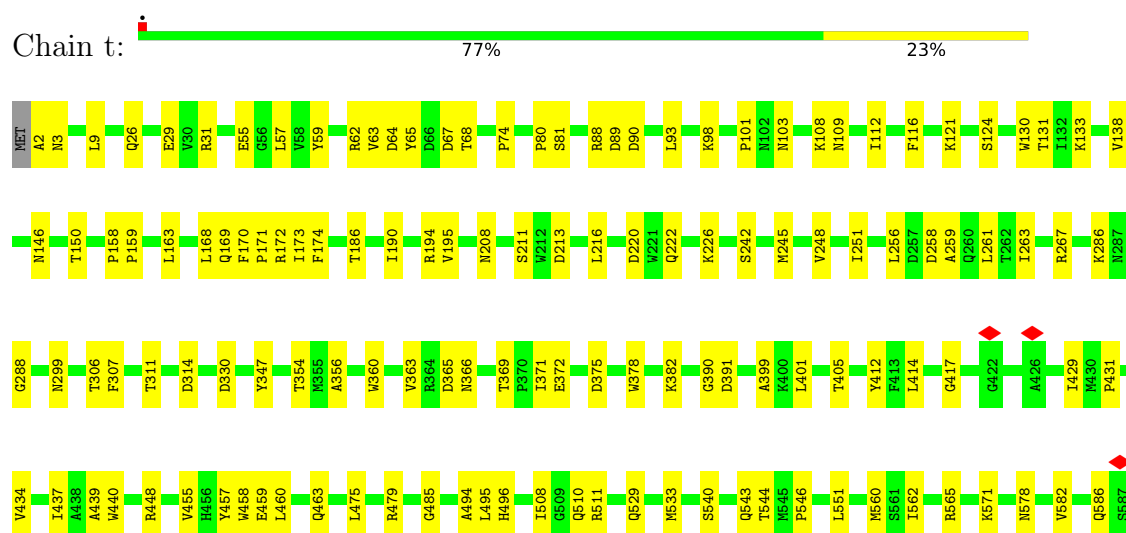


• Molecule 5: Baseplate hub protein (gp18)

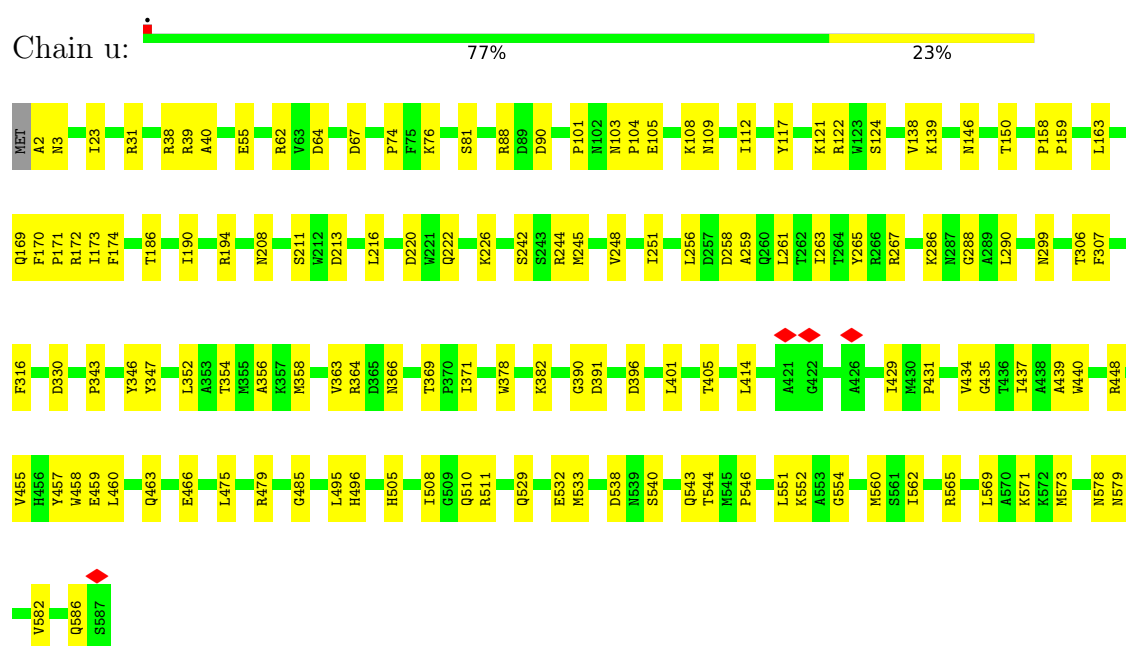
Chain s: 77% 23%



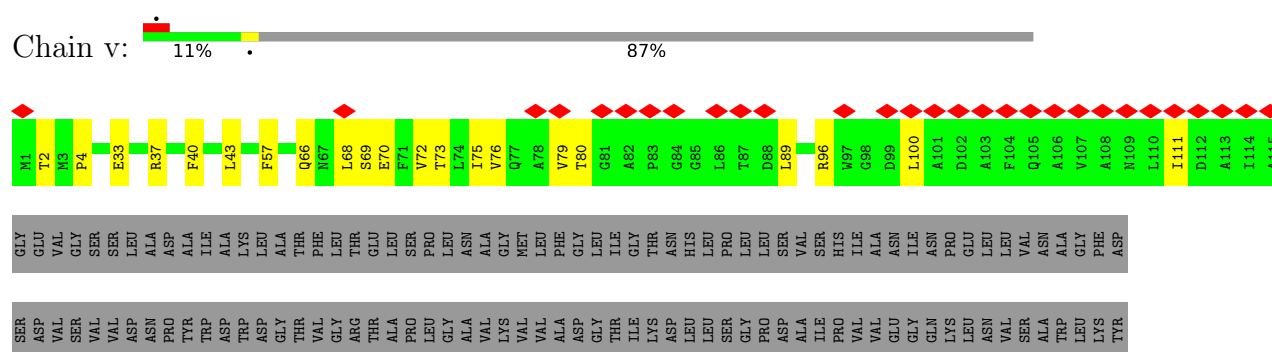
• Molecule 5: Baseplate hub protein (gp18)



• Molecule 5: Baseplate hub protein (gp18)



• Molecule 6: Central fiber protein (gp20)

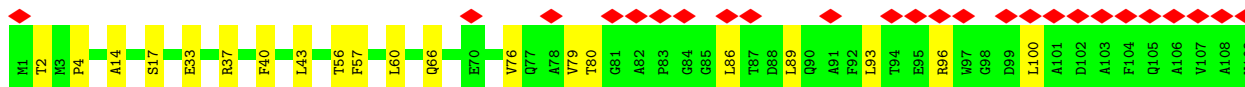




TRP	GLN	VAL	ASN	THR	GLY	TRP
ASP	VAL	VAL	THR	ALA	LYS	LYE
SER	TYR	SER	PHE	SER	ALA	LYS
GLY	GLY	GLY	TYR	TYR	ILE	GLN
SER	GLY	GLY	THR	VAL	GLY	TRP
VAL	VAL	ARG	PRO	GLU	TYR	GLY
VAL	ASN	ALA	ASN	SER	ILE	CYS
ALA	LEU	ALA	GLU	THR	GLY	ARG
HIS	ASN	PHE	VAL	LEU	ILE	TYR
GLY	THR	SER	LEU	PRO	SER	SER
THR	ALA	GLY	THR	ALA	ASP	THR
ASN	LYS	LEU	ALA	GLY	THR	ALA
TYR	ILE	THR	GLN	VAL	THR	PHE
ARG	TYR	ASP	GLY	ILE	ILE	VAL
PHE	THR	GLY	VAL	VAL	VAL	THR
GLY	GLY	ASN	SER	ASN	ASP	PHE
GLY	PRO	GLN	VAL	ALA	THR	PRO
LEU	TRP	ASN	ILE	GLY	ILE	GLU
ARG	ASN	ALA	MET	GLU	ALA	MET
ILE	SER	LEU	PRO	ARG	MET	CYS
SER	LEU	TYR	TRP	TYR	LYS	THR
ARG	THR	ILE	ALA	VAL	MET	ASP
ALA	GLU	ARG	MET	VAL	TYR	TRP
THR	ARG	PRO	MET	ARG	LYS	GLY
PHE	ALA	THR	ALA	MET	THR	PHE
ASN	VAL	GLY	LYS	ASN	GLU	LEU
ALA	SER	ASP	ASN	ALA	SER	GLY
GLY	THR	LYS	LEU	THR	ALA	GLY
ARG	THR	GLN	ALA	THR	ILE	THR
ILE	GLY	TRP	THR	VAL	ASN	THR
ASN	ASN	VAL	THR	ASN	GLY	ALA
ASP	ASP	GLU	GLN	ARG	VAL	GLN
TRP	VAL	ALA	SER	VAL	TYR	GLN
THR	LEU	THR	THR	ARG	LEU	SER
LEU	TRP	LEU	PHE	GLY	GLU	THR
LYS	GLN	THR	SER	VAL	VAL	THR
ASP	MET	GLU	ASP	SER	PHE	THR
TRP	TYR	THR	ASP	VAL	ARG	ALA
ALA	PHE	GLY	PHE	MET	GLU	HIS
	ASP	ILE	ASN	LYS	ASP	THR
	PRO	ALA	ARG	GLU	SER	HIS
	ALA	ALA	SER	LEU	THR	THR
	THR	SER	ALA	VAL	GLY	ASN
	ALA	GLY	MET	GLY	ALA	ASN
	ALA	ARG	GLY	GLY	LEU	LEU
	TYR	ARG	LEU	ARG	THR	ASP
	THR	GLU	GLY	GLU	SER	GLY
	VAL	GLY	PHE	LEU	VAL	ALA
	LEU	LYS	LEU	ILE	GLY	ALA
	ASN	MET	LYS	ARG	VAL	LEU
	GLY	HIS	SER	THR	ASP	GLN
	GLN	ALA	ASP	GLU	VAL	ILE
	ALA	ARG	THR	THR	GLN	ILE
	SER	ARG	THR	ALA	GLY	LEU
	GLY	ASP	THR	THR	GLN	PRO
	THR	LEU	ASN	SER	LEU	ALA

- Molecule 6: Central fiber protein (gp20)

Chain x:  11% 87%

[illegible]

LYS	SER	ASP	THR	GLY	THR	ASN	GLN	GLY	VAL	SER	GLY	GLY	ARG	ALA	ALA	PHE	SER	GLY	LEU	ASN	GLN	ASN	ALA	LEU	TYR	ILE	ARG	PRO	THR	ALA	THR	GLY	GLY	LYS	GLN	TRP	VAL	ASP	GLU	ALA	THR	LEU	TYR	GLU	THR	GLY	ILE	ALA	ALA	GLY	ALA	ARG	GLU	GLY	LEU	LYS								
MET	HIS	ALA	ASN	ARG	ASP	LEU	SER	GLN	VAL	THR	TYR	LEU	GLY	VAL	ASN	LEU	ASN	THR	ALA	LYS	ILE	THR	ASP	TYR	GLY	GLY	PRO	TRP	ASN	ASN	ALA	SER	LEU	THR	ILE	GLU	ARG	PRO	ALA	THR	SER	VAL	THR	LEU	TRP	GLN	TYR	GLU	MET	TYR	THR	PHE	ASP	PRO	ALA	ALA	THR	ALA	ALA	TYR	THR	VAL	LEU	LYS
ASN	GLY	GLN	ALA	SER	GLY	LEU	THR	THR	THR	ASP	SER	GLY	SER	VAL	VAL	ALA	HIS	GLY	PRO	ASN	TYR	ARG	PHE	GLY	GLY	LEU	ARG	ILE	SER	ARG	ALA	THR	PHE	ASN	ALA	GLY	ARG	ILE	ASP	ASN	TRP	THR	LEU	LYS	ASP	TRP	ALA																	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78927	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	430	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.556	Depositor
Minimum map value	-1.951	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	543.232, 543.232, 543.232	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	G	0.15	0/2306	0.27	0/3159
1	H	0.15	0/2306	0.29	0/3159
1	I	0.15	0/2306	0.28	0/3159
1	J	0.15	0/2306	0.28	0/3159
1	K	0.15	0/2306	0.29	0/3159
1	L	0.15	0/2306	0.28	0/3159
1	M	0.15	0/2306	0.29	0/3159
1	N	0.15	0/2306	0.29	0/3159
1	O	0.15	0/2306	0.29	0/3159
1	P	0.15	0/2306	0.28	0/3159
1	Q	0.14	0/2306	0.28	0/3159
1	R	0.15	0/2306	0.29	0/3159
2	S	0.15	0/334	0.43	0/452
2	T	0.14	0/334	0.42	0/452
2	U	0.13	0/334	0.42	0/452
3	a	0.14	0/2439	0.30	0/3333
3	b	0.14	0/2439	0.28	0/3333
3	c	0.14	0/2439	0.28	0/3333
3	d	0.14	0/2439	0.28	0/3333
3	e	0.14	0/2439	0.29	0/3333
3	f	0.14	0/2439	0.29	0/3333
3	g	0.13	0/2439	0.28	0/3333
3	h	0.14	0/2439	0.29	0/3333
3	i	0.14	0/2439	0.29	0/3333
3	j	0.14	0/2439	0.28	0/3333
3	k	0.13	0/2439	0.28	0/3333
3	l	0.14	0/2439	0.28	0/3333
4	m	0.18	0/2418	0.29	0/3307
4	n	0.17	0/2418	0.31	0/3307
4	o	0.19	0/2418	0.31	0/3307
4	p	0.17	0/2418	0.31	0/3307
4	q	0.17	0/2418	0.30	0/3307
4	r	0.18	0/2418	0.30	0/3307
5	s	0.18	0/4700	0.30	0/6413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	t	0.17	0/4700	0.30	0/6413
5	u	0.18	0/4700	0.31	0/6413
6	v	0.13	0/882	0.23	0/1204
6	w	0.13	0/882	0.25	0/1204
6	x	0.14	0/882	0.24	0/1204
All	All	0.16	0/89196	0.29	0/121953

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	G	2256	0	2233	45	0
1	H	2256	0	2233	44	0
1	I	2256	0	2233	46	0
1	J	2256	0	2233	40	0
1	K	2256	0	2233	44	0
1	L	2256	0	2233	43	0
1	M	2256	0	2233	45	0
1	N	2256	0	2233	48	0
1	O	2256	0	2233	44	0
1	P	2256	0	2233	39	0
1	Q	2256	0	2233	46	0
1	R	2256	0	2233	44	0
2	S	327	0	305	15	0
2	T	327	0	305	11	0
2	U	327	0	305	14	0
3	a	2372	0	2294	35	0
3	b	2372	0	2294	35	0
3	c	2372	0	2294	39	0
3	d	2372	0	2294	43	0
3	e	2372	0	2294	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	2372	0	2294	43	0
3	g	2372	0	2294	34	0
3	h	2372	0	2294	42	0
3	i	2372	0	2294	36	0
3	j	2372	0	2294	41	0
3	k	2372	0	2294	41	0
3	l	2372	0	2294	42	0
4	m	2343	0	2248	49	0
4	n	2343	0	2248	59	0
4	o	2343	0	2248	52	0
4	p	2343	0	2248	54	0
4	q	2343	0	2248	54	0
4	r	2343	0	2248	53	0
5	s	4582	0	4473	111	0
5	t	4582	0	4473	103	0
5	u	4582	0	4473	107	0
6	v	863	0	814	21	0
6	w	863	0	814	21	0
6	x	863	0	814	21	0
All	All	86910	0	84588	1449	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 8.

The worst 5 of 1449 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:p:12:ARG:HD2	4:p:92:ASP:HB2	1.58	0.86
5:t:63:VAL:HG23	5:t:93:LEU:HD12	1.63	0.81
6:v:111:ILE:HD11	6:w:110:LEU:HD21	1.64	0.80
2:T:1697:PRO:HG3	5:u:571:LYS:HA	1.65	0.79
6:w:79:VAL:HG23	6:w:80:THR:HG23	1.65	0.78

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	
1	G	297/300 (99%)	292 (98%)	5 (2%)	0	100	100
1	H	297/300 (99%)	289 (97%)	8 (3%)	0	100	100
1	I	297/300 (99%)	289 (97%)	8 (3%)	0	100	100
1	J	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
1	K	297/300 (99%)	289 (97%)	8 (3%)	0	100	100
1	L	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
1	M	297/300 (99%)	291 (98%)	6 (2%)	0	100	100
1	N	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
1	O	297/300 (99%)	289 (97%)	8 (3%)	0	100	100
1	P	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
1	Q	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
1	R	297/300 (99%)	290 (98%)	7 (2%)	0	100	100
2	S	40/1699 (2%)	35 (88%)	5 (12%)	0	100	100
2	T	40/1699 (2%)	35 (88%)	5 (12%)	0	100	100
2	U	40/1699 (2%)	35 (88%)	5 (12%)	0	100	100
3	a	309/311 (99%)	300 (97%)	9 (3%)	0	100	100
3	b	309/311 (99%)	304 (98%)	5 (2%)	0	100	100
3	c	309/311 (99%)	306 (99%)	3 (1%)	0	100	100
3	d	309/311 (99%)	303 (98%)	6 (2%)	0	100	100
3	e	309/311 (99%)	303 (98%)	6 (2%)	0	100	100
3	f	309/311 (99%)	306 (99%)	3 (1%)	0	100	100
3	g	309/311 (99%)	306 (99%)	3 (1%)	0	100	100
3	h	309/311 (99%)	304 (98%)	5 (2%)	0	100	100
3	i	309/311 (99%)	306 (99%)	3 (1%)	0	100	100
3	j	309/311 (99%)	306 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	k	309/311 (99%)	306 (99%)	3 (1%)	0	100	100
3	l	309/311 (99%)	302 (98%)	7 (2%)	0	100	100
4	m	288/295 (98%)	276 (96%)	12 (4%)	0	100	100
4	n	288/295 (98%)	280 (97%)	8 (3%)	0	100	100
4	o	288/295 (98%)	277 (96%)	11 (4%)	0	100	100
4	p	288/295 (98%)	276 (96%)	12 (4%)	0	100	100
4	q	288/295 (98%)	278 (96%)	10 (4%)	0	100	100
4	r	288/295 (98%)	276 (96%)	12 (4%)	0	100	100
5	s	584/587 (100%)	563 (96%)	21 (4%)	0	100	100
5	t	584/587 (100%)	564 (97%)	20 (3%)	0	100	100
5	u	584/587 (100%)	567 (97%)	17 (3%)	0	100	100
6	v	113/878 (13%)	110 (97%)	3 (3%)	0	100	100
6	w	113/878 (13%)	109 (96%)	4 (4%)	0	100	100
6	x	113/878 (13%)	110 (97%)	3 (3%)	0	100	100
All	All	11211/18594 (60%)	10922 (97%)	289 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	242/243 (100%)	242 (100%)	0	100	100
1	H	242/243 (100%)	242 (100%)	0	100	100
1	I	242/243 (100%)	242 (100%)	0	100	100
1	J	242/243 (100%)	242 (100%)	0	100	100
1	K	242/243 (100%)	242 (100%)	0	100	100
1	L	242/243 (100%)	242 (100%)	0	100	100
1	M	242/243 (100%)	242 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	242/243 (100%)	242 (100%)	0	100	100
1	O	242/243 (100%)	242 (100%)	0	100	100
1	P	242/243 (100%)	242 (100%)	0	100	100
1	Q	242/243 (100%)	242 (100%)	0	100	100
1	R	242/243 (100%)	242 (100%)	0	100	100
2	S	33/1284 (3%)	33 (100%)	0	100	100
2	T	33/1284 (3%)	33 (100%)	0	100	100
2	U	33/1284 (3%)	33 (100%)	0	100	100
3	a	253/253 (100%)	253 (100%)	0	100	100
3	b	253/253 (100%)	253 (100%)	0	100	100
3	c	253/253 (100%)	253 (100%)	0	100	100
3	d	253/253 (100%)	253 (100%)	0	100	100
3	e	253/253 (100%)	253 (100%)	0	100	100
3	f	253/253 (100%)	253 (100%)	0	100	100
3	g	253/253 (100%)	253 (100%)	0	100	100
3	h	253/253 (100%)	253 (100%)	0	100	100
3	i	253/253 (100%)	253 (100%)	0	100	100
3	j	253/253 (100%)	253 (100%)	0	100	100
3	k	253/253 (100%)	253 (100%)	0	100	100
3	l	253/253 (100%)	253 (100%)	0	100	100
4	m	254/258 (98%)	254 (100%)	0	100	100
4	n	254/258 (98%)	254 (100%)	0	100	100
4	o	254/258 (98%)	254 (100%)	0	100	100
4	p	254/258 (98%)	254 (100%)	0	100	100
4	q	254/258 (98%)	254 (100%)	0	100	100
4	r	254/258 (98%)	254 (100%)	0	100	100
5	s	487/488 (100%)	487 (100%)	0	100	100
5	t	487/488 (100%)	487 (100%)	0	100	100
5	u	487/488 (100%)	487 (100%)	0	100	100
6	v	87/691 (13%)	87 (100%)	0	100	100
6	w	87/691 (13%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	x	87/691 (13%)	87 (100%)	0	100	100
All	All	9285/14889 (62%)	9285 (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. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
3	k	202	GLN
4	q	264	GLN
3	l	64	GLN
4	o	16	HIS
4	r	264	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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.



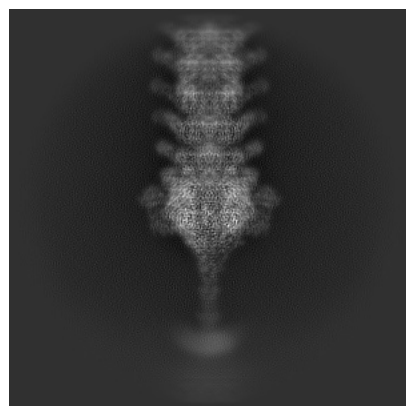
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39996. These allow visual inspection of the internal detail of the map and identification of artifacts.

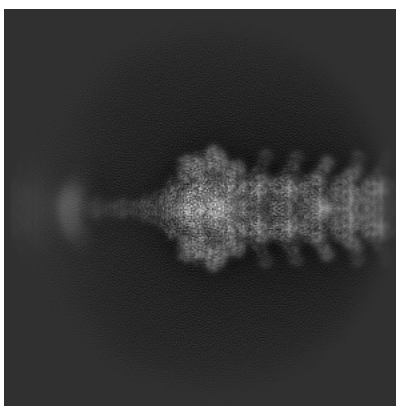
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

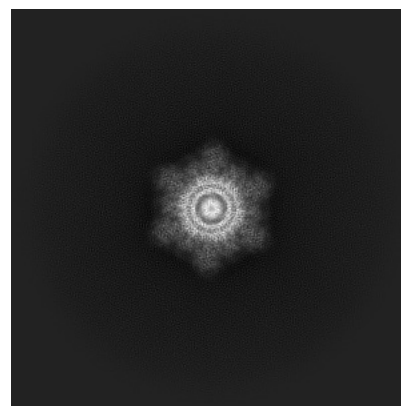
#### 6.1.1 Primary map



X

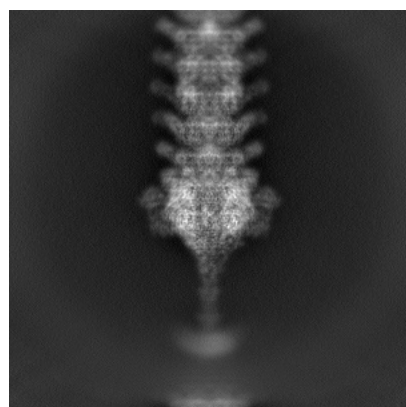


Y

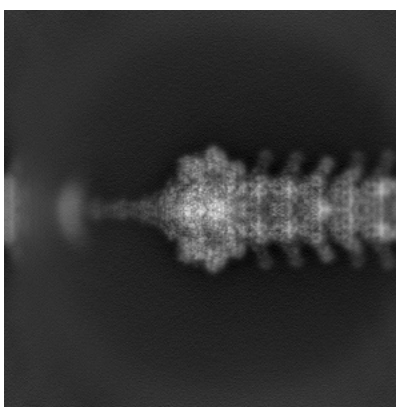


Z

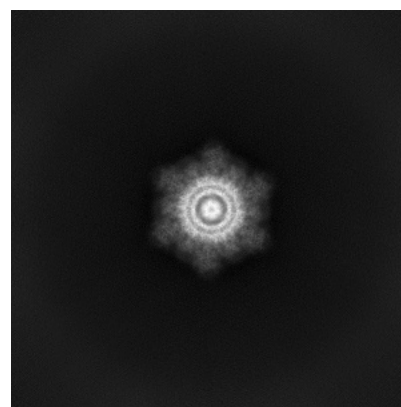
#### 6.1.2 Raw map



X



Y

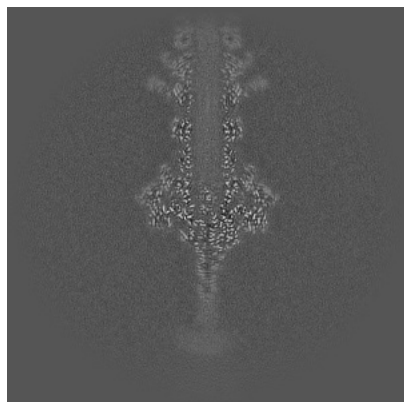


Z

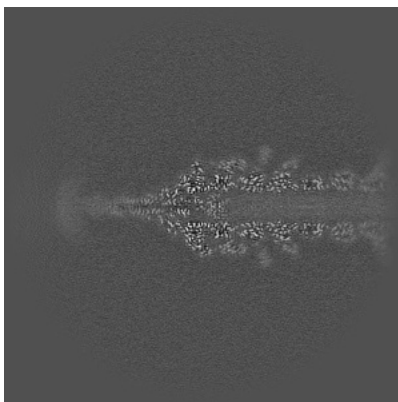
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

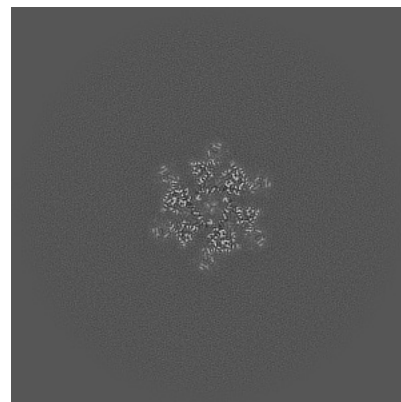
### 6.2.1 Primary map



X Index: 256

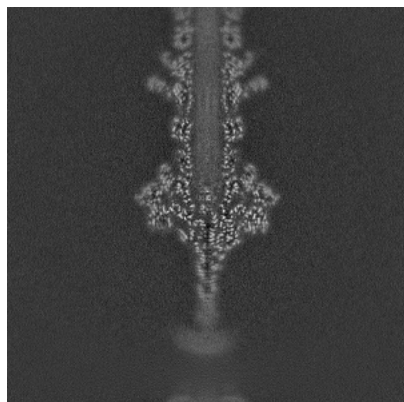


Y Index: 256

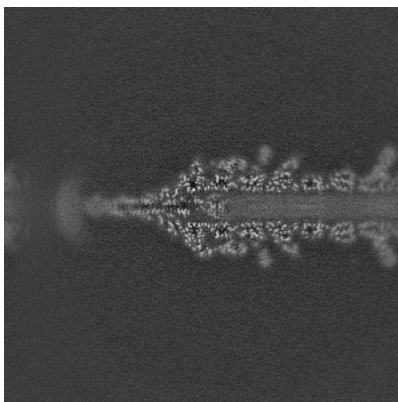


Z Index: 256

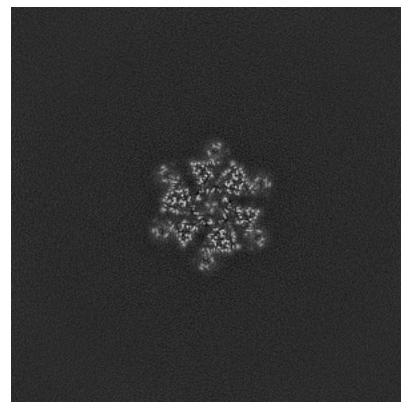
### 6.2.2 Raw map



X Index: 256



Y Index: 256

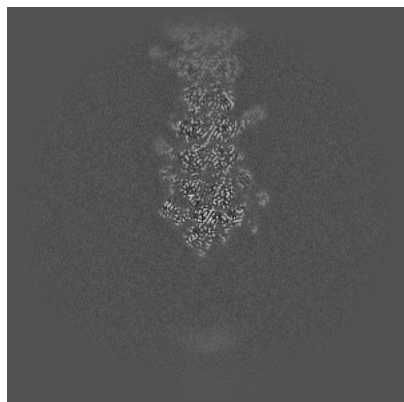


Z Index: 256

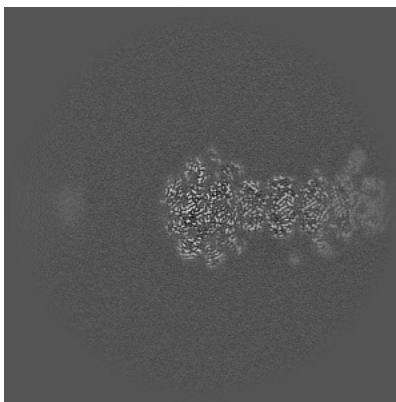
The images above show central slices of the map in three orthogonal directions.

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

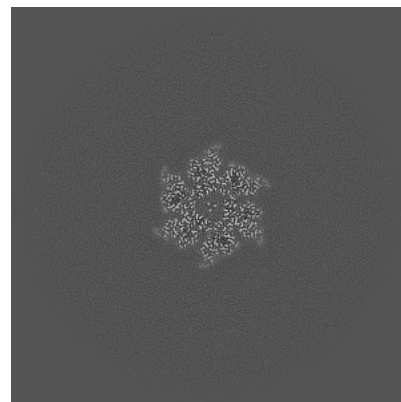
### 6.3.1 Primary map



X Index: 277

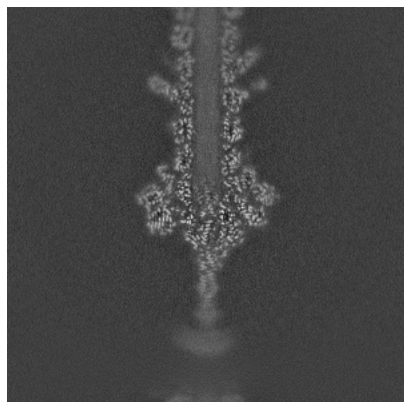


Y Index: 234

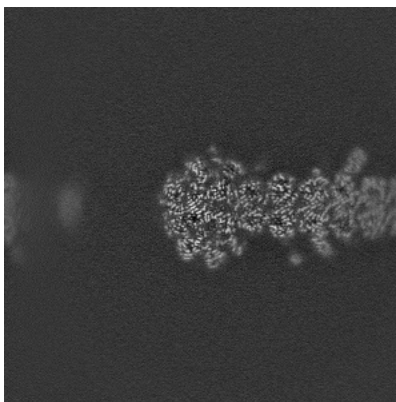


Z Index: 250

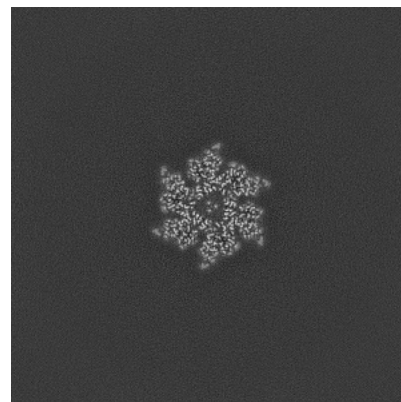
### 6.3.2 Raw map



X Index: 251



Y Index: 235

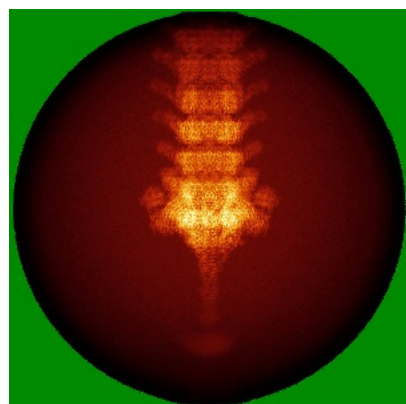


Z Index: 251

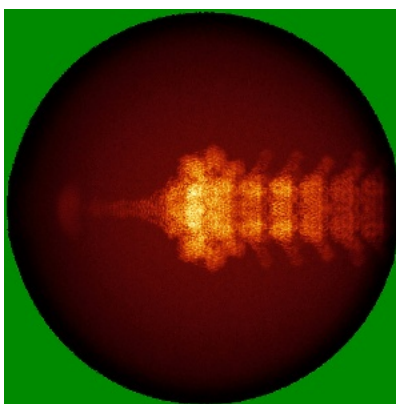
The images above show the largest variance slices of the map in three orthogonal directions.

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

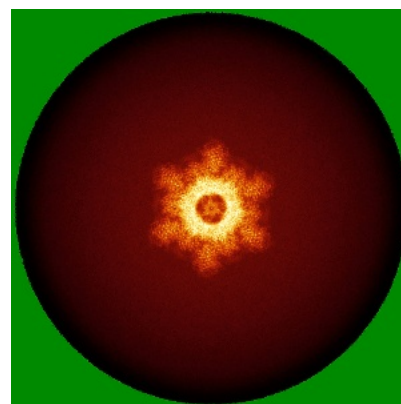
### 6.4.1 Primary map



X

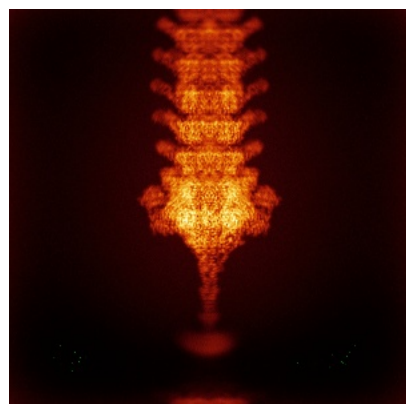


Y

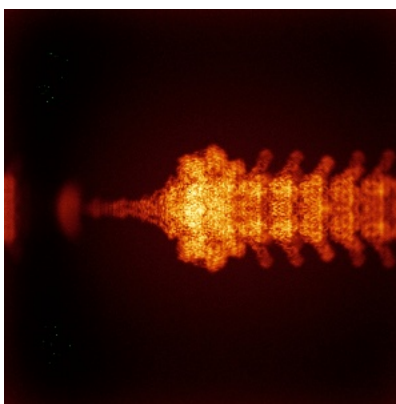


Z

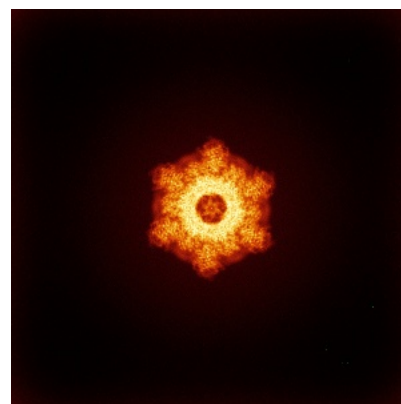
### 6.4.2 Raw map



X



Y



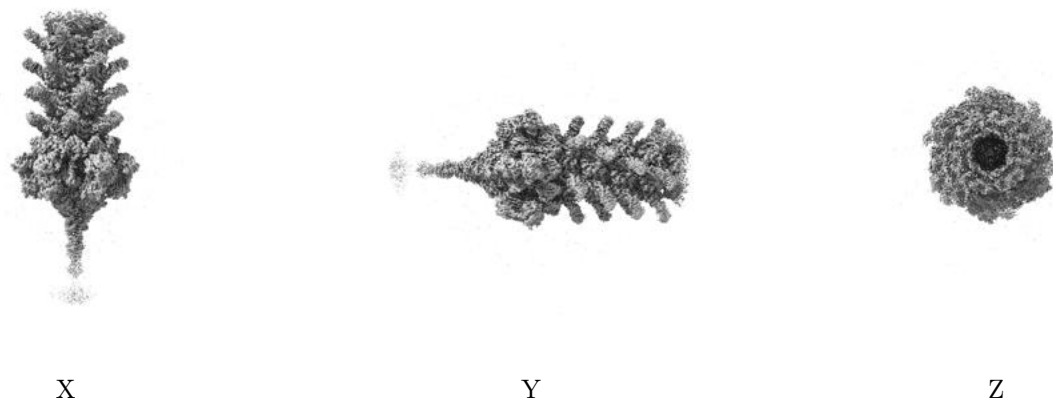
Z

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



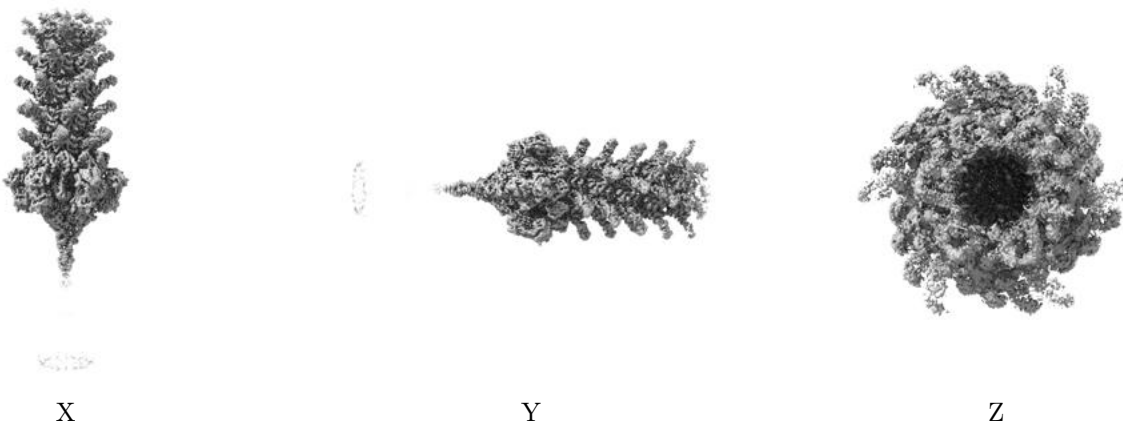
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

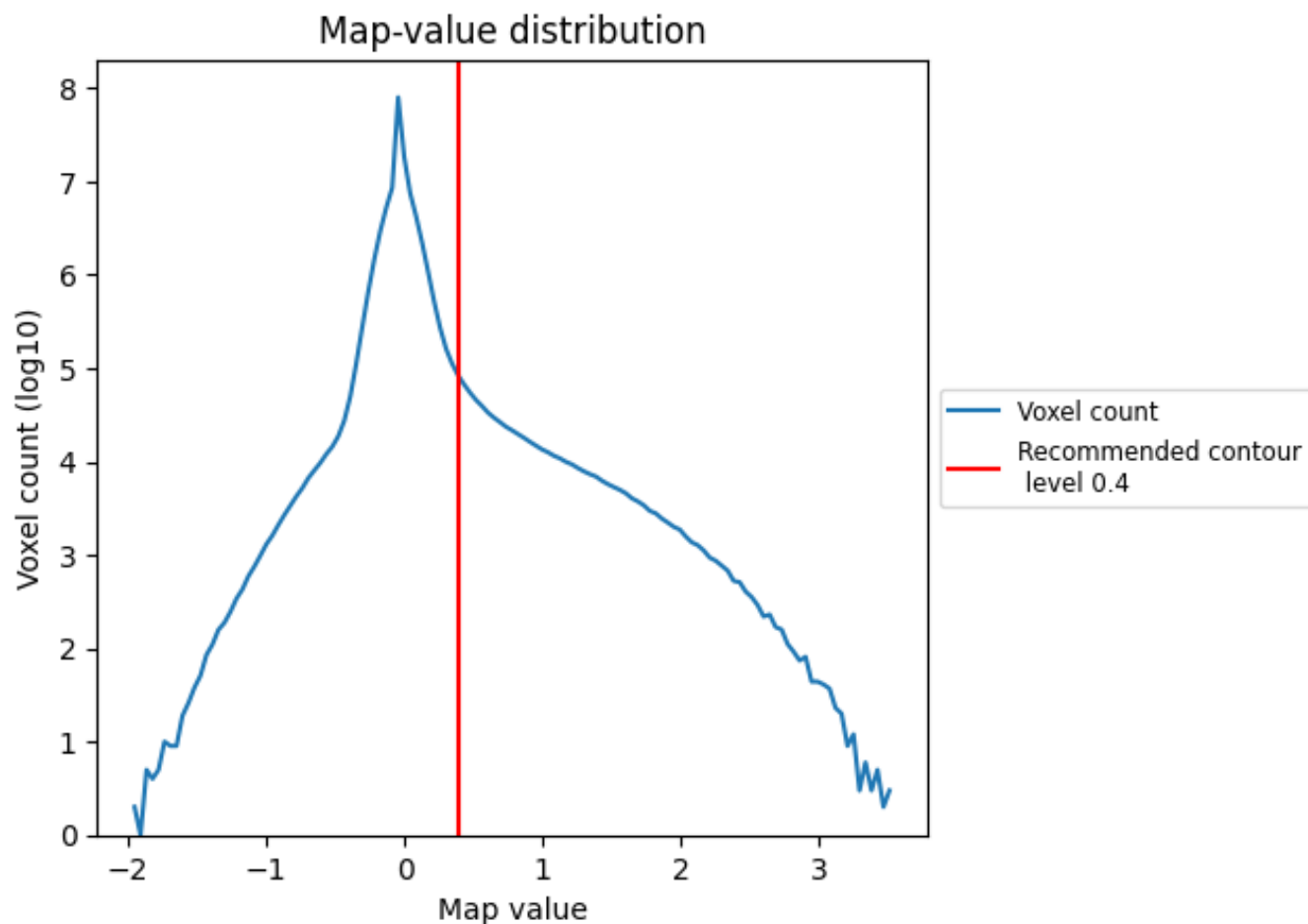
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

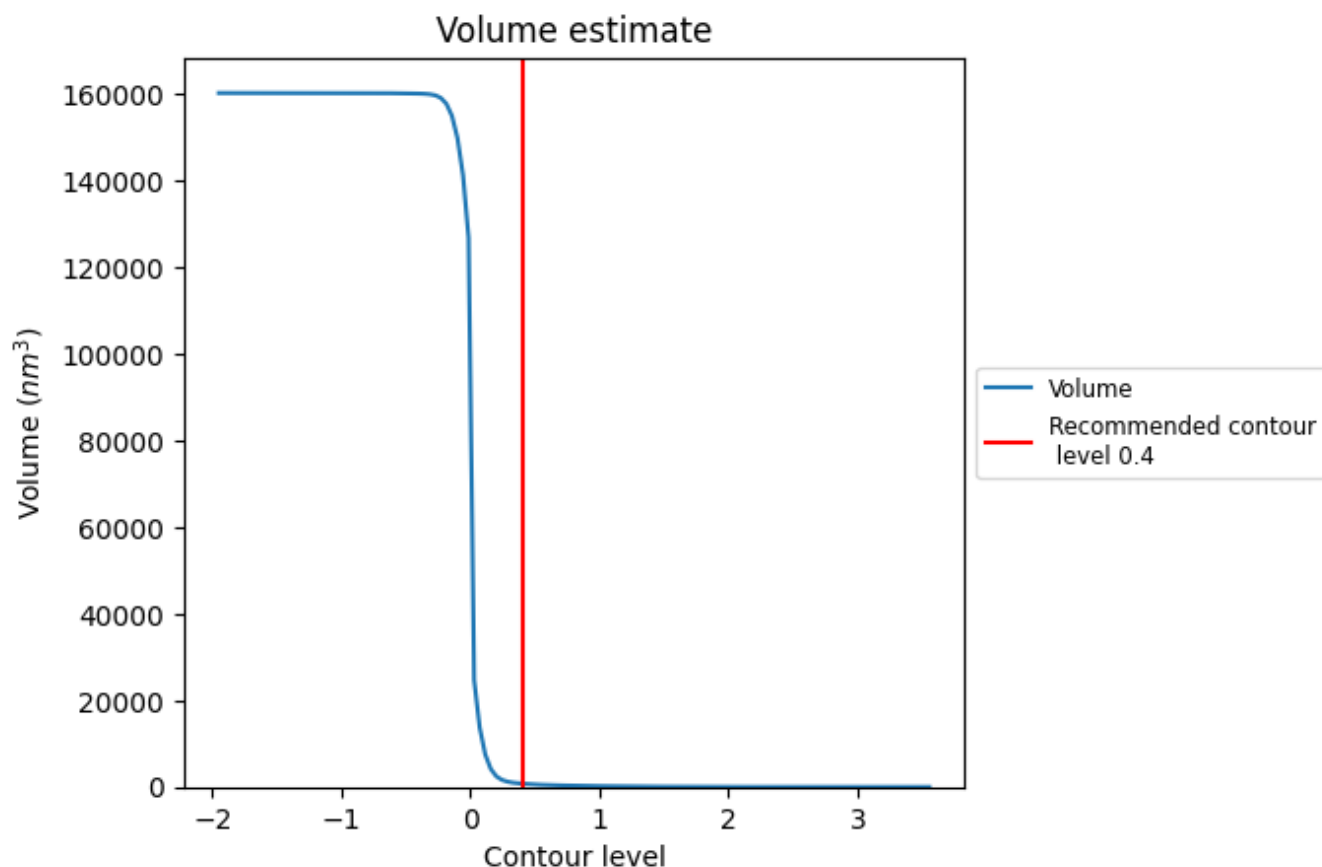
This section contains the results of statistical analysis of the map.

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



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

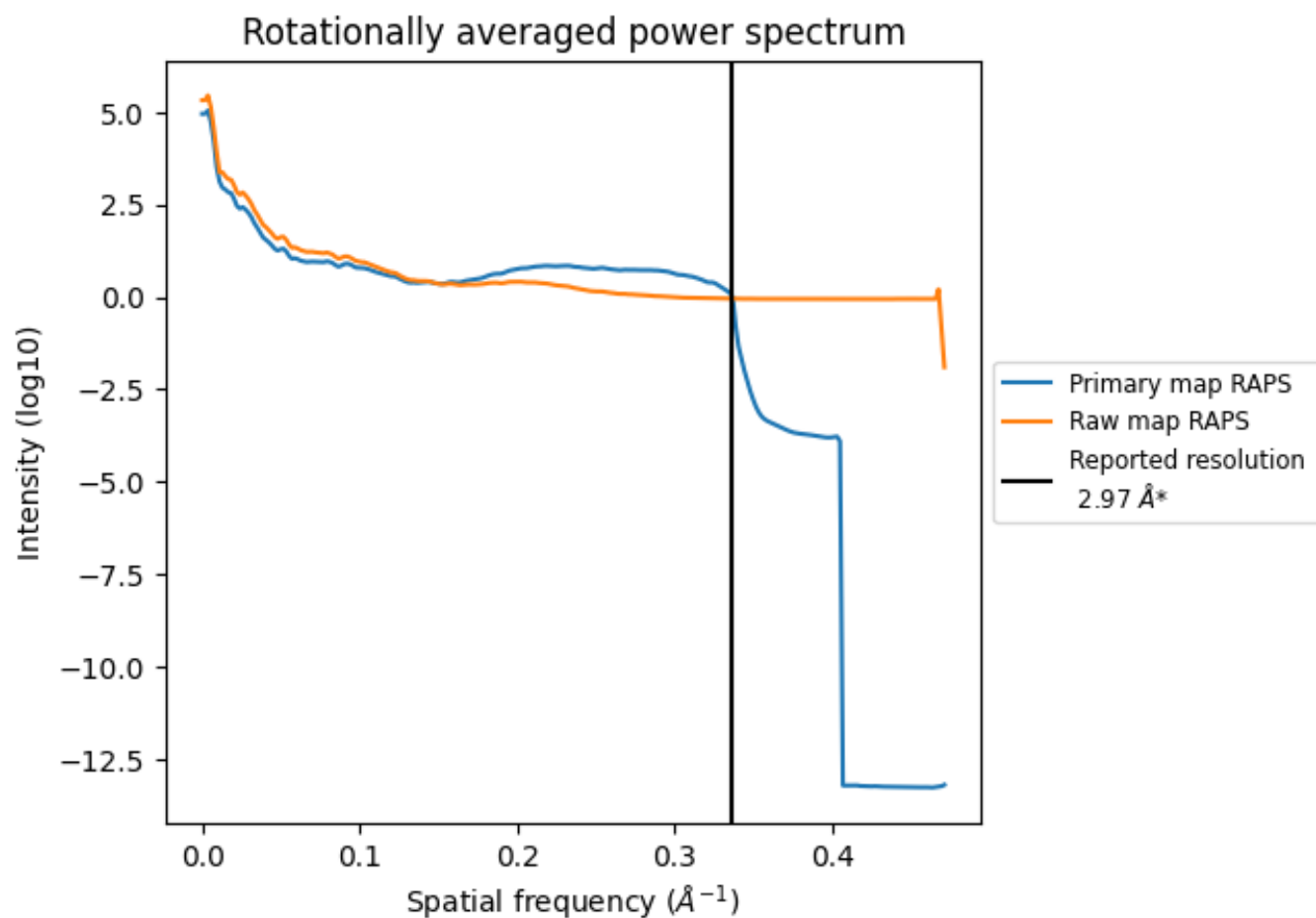
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm<sup>3</sup>; this corresponds to an approximate mass of 690 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 ⓘ



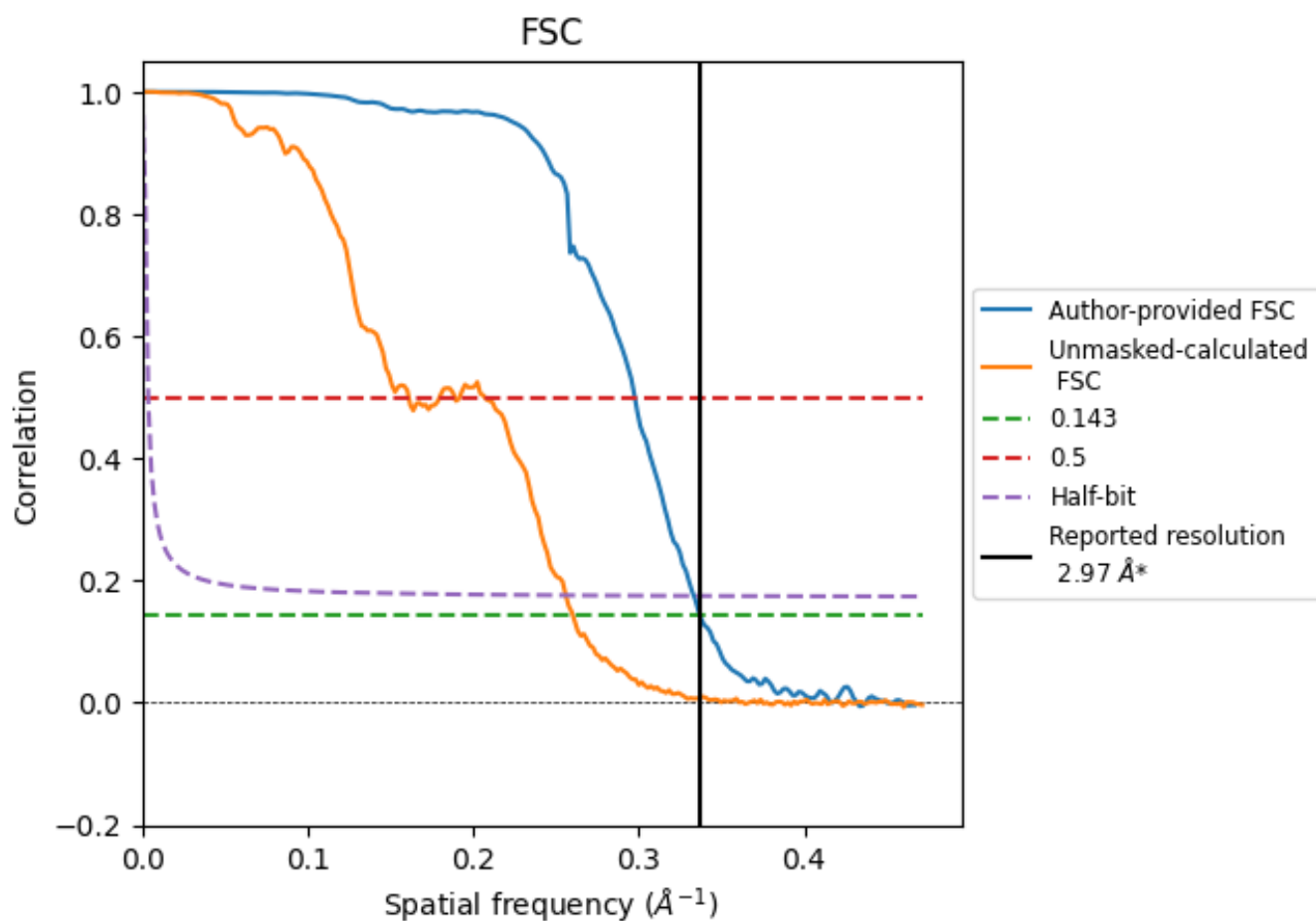
\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>



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

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.337 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

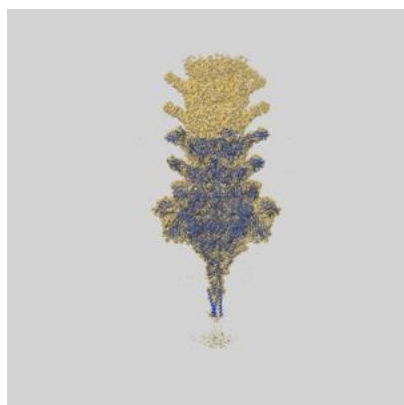
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.36	3.00
Unmasked-calculated*	3.84	6.21	3.91

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 2.97 by more than 10 %

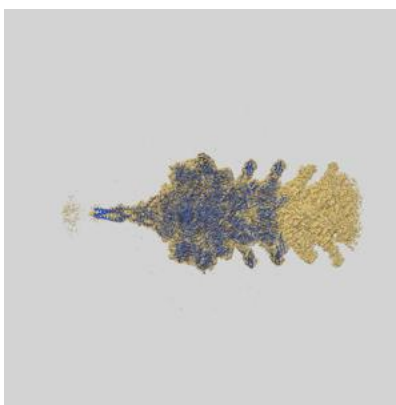
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39996 and PDB model 8ZDO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

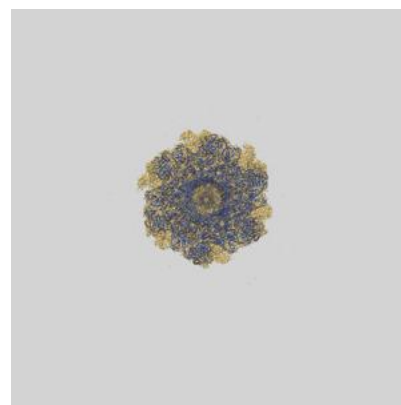
### 9.1 Map-model overlay [i](#)



X



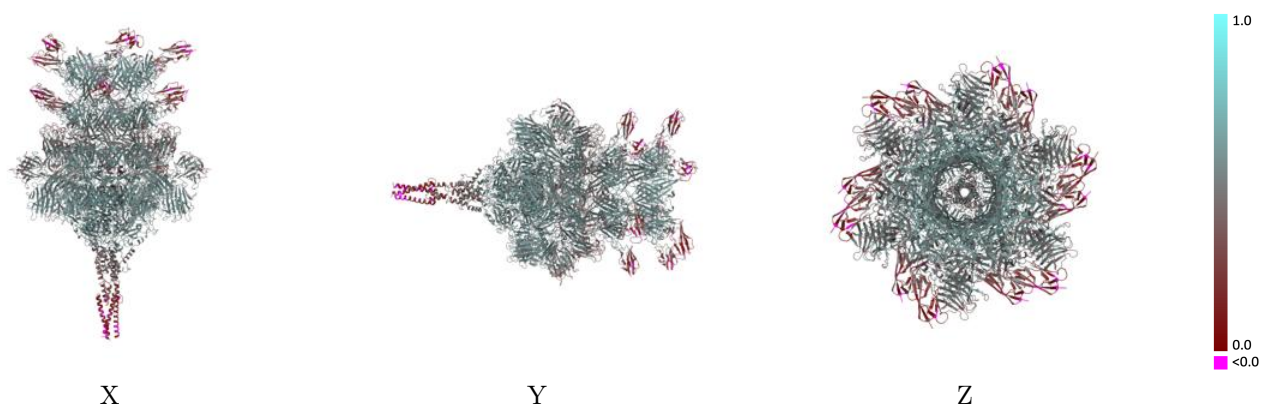
Y



Z

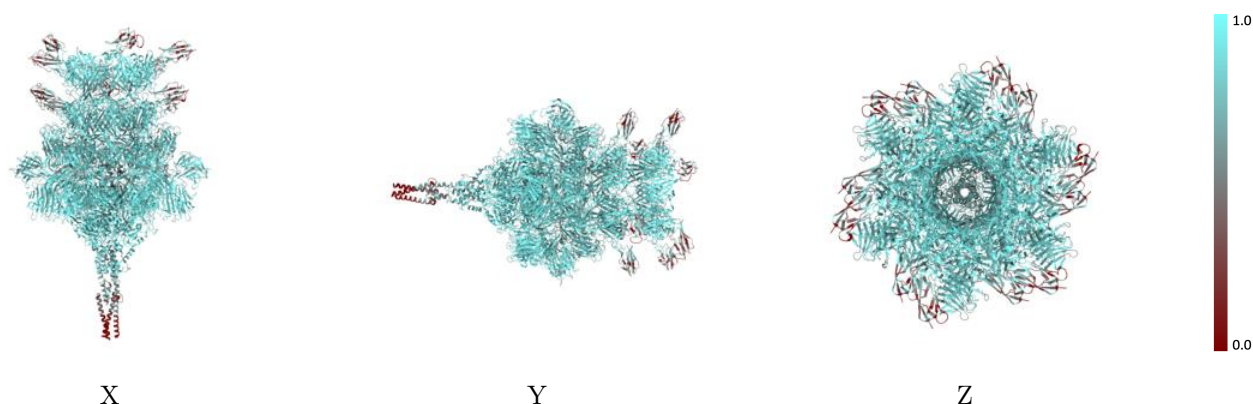
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



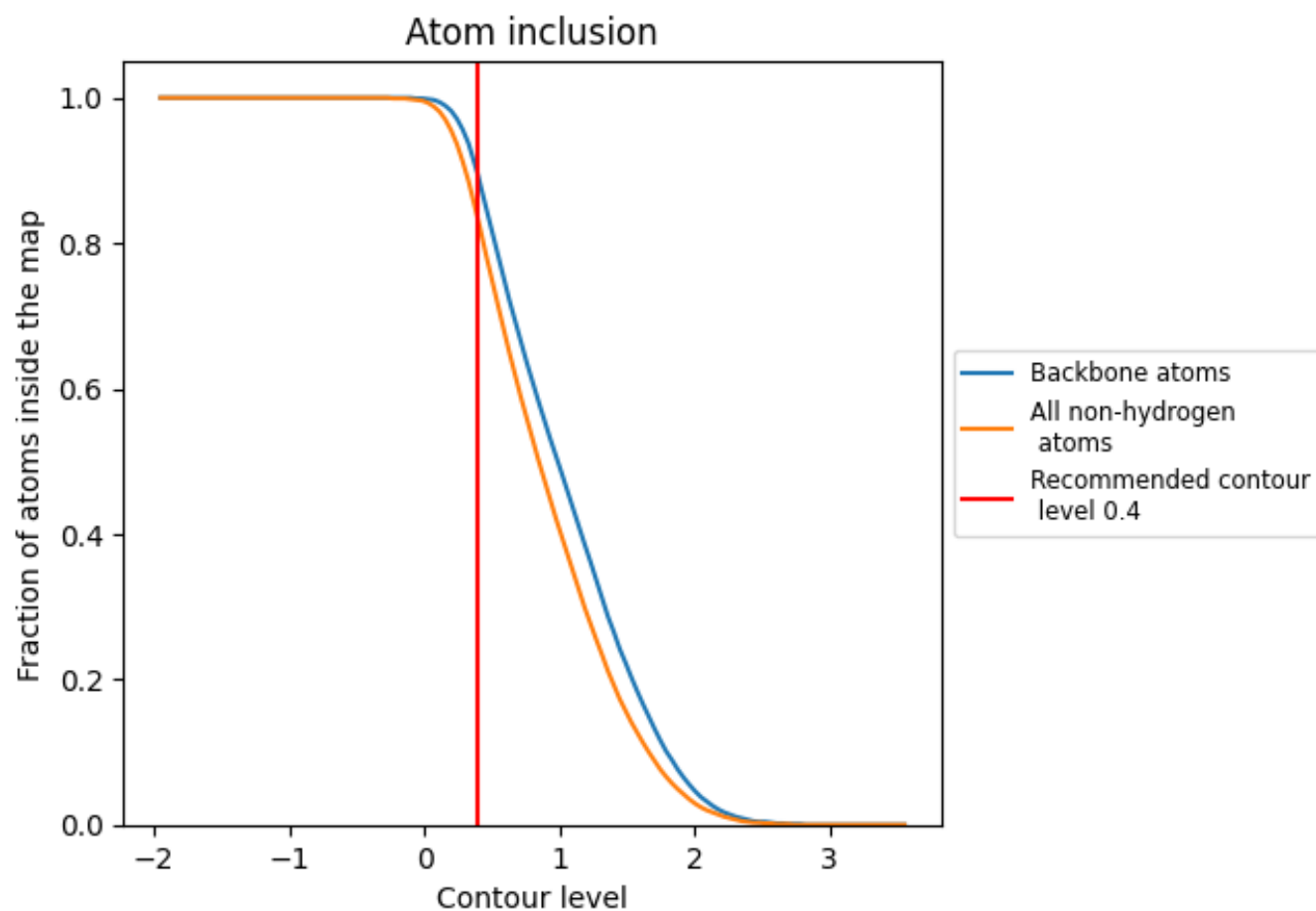
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.5120
G	 0.7860	 0.4900
H	 0.7920	 0.4920
I	 0.7880	 0.4900
J	 0.7890	 0.4930
K	 0.7890	 0.4910
L	 0.7950	 0.4940
M	 0.7760	 0.4810
N	 0.7780	 0.4820
O	 0.7750	 0.4800
P	 0.7830	 0.4830
Q	 0.7770	 0.4810
R	 0.7800	 0.4860
S	 0.7800	 0.4750
T	 0.7580	 0.4850
U	 0.7640	 0.4820
a	 0.7900	 0.4620
b	 0.8480	 0.5050
c	 0.8120	 0.4800
d	 0.8570	 0.5170
e	 0.7900	 0.4610
f	 0.8440	 0.5060
g	 0.8120	 0.4830
h	 0.8590	 0.5190
i	 0.7900	 0.4660
j	 0.8530	 0.5120
k	 0.8040	 0.4830
l	 0.8590	 0.5190
m	 0.9160	 0.5820
n	 0.9190	 0.5770
o	 0.9130	 0.5780
p	 0.9140	 0.5770
q	 0.9160	 0.5840
r	 0.9190	 0.5800
s	 0.9010	 0.5690



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
t	 0.8980	 0.5690
u	 0.8960	 0.5680
v	 0.6090	 0.3360
w	 0.5990	 0.3280
x	 0.6050	 0.3290