



## Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 04:34 pm GMT

PDB ID : 8BFL  
EMDB ID : EMD-13862  
Title : Jumbo Phage phi-kp24 empty capsid hexamers  
Authors : Ouyang, R.  
Deposited on : 2022-10-26  
Resolution : 4.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

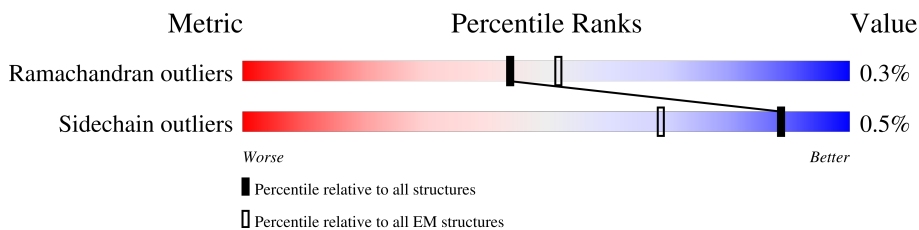
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 4.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	570	14% (red), 99% (green), . (grey)
1	B	570	11% (red), 99% (green), . (grey)
1	C	570	12% (red), 99% (green), . (grey)
1	D	570	14% (red), 100% (green)
1	E	570	12% (red), 99% (green), . (grey)
1	F	570	14% (red), 99% (green), . (grey)
1	G	570	12% (red), 99% (green), . (grey)
1	H	570	10% (red), 99% (green), . (grey)
1	I	570	10% (red), 99% (green), . (grey)

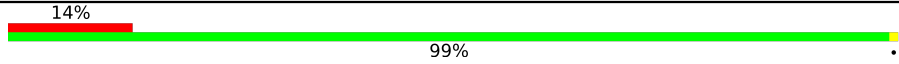
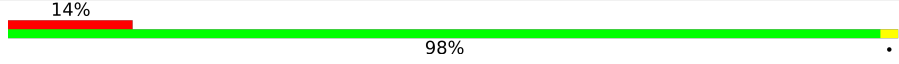
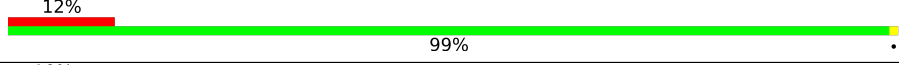
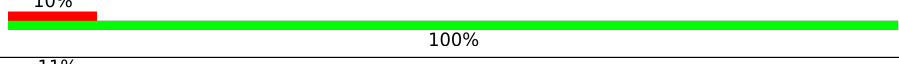
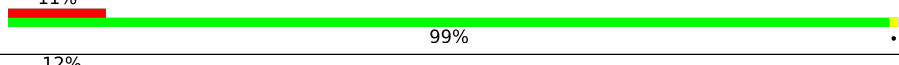
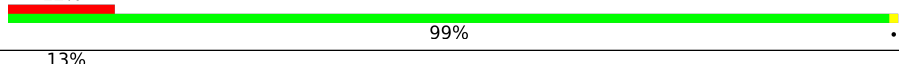
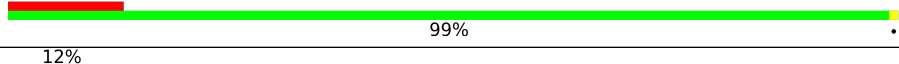
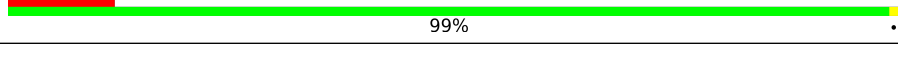
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Mol	Chain	Length	Quality of chain
1	J	570	10% 99%
1	K	570	11% 99%
1	L	570	11% 99%
1	M	570	12% 99%
1	N	570	14% 99%
1	O	570	14% 99%
1	P	570	11% 99%
1	Q	570	13% 99%
1	R	570	14% 99%
1	S	570	11% 99%
1	T	570	11% 99%
1	U	570	12% 99%
1	V	570	9% 100%
1	W	570	11% 99%
1	X	570	12% 100%
1	Y	570	9% 99%
1	Z	570	9% 100%
1	a	570	12% 99%
1	b	570	10% 99%
1	c	570	10% 99%
1	d	570	12% 99%
1	e	570	14% 99%
1	f	570	13% 99%
1	g	570	14% 99%
1	h	570	13% 99%

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Mol	Chain	Length	Quality of chain
1	i	570	 14% 99%
1	j	570	 14% 98%
1	k	570	 12% 99%
1	l	570	 10% 100%
1	m	570	 11% 99%
1	n	570	 12% 99%
1	o	570	 13% 99%
1	p	570	 12% 99%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 188286 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 Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	570	4483	2835	761	873	14	0	0
1	B	570	4483	2835	761	873	14	0	0
1	C	570	4483	2835	761	873	14	0	0
1	D	570	4483	2835	761	873	14	0	0
1	E	570	4483	2835	761	873	14	0	0
1	F	570	4483	2835	761	873	14	0	0
1	G	570	4483	2835	761	873	14	0	0
1	H	570	4483	2835	761	873	14	0	0
1	I	570	4483	2835	761	873	14	0	0
1	J	570	4483	2835	761	873	14	0	0
1	K	570	4483	2835	761	873	14	0	0
1	L	570	4483	2835	761	873	14	0	0
1	M	570	4483	2835	761	873	14	0	0
1	N	570	4483	2835	761	873	14	0	0
1	O	570	4483	2835	761	873	14	0	0
1	P	570	4483	2835	761	873	14	0	0
1	Q	570	4483	2835	761	873	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	S	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	T	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	U	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	V	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	W	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	X	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	Y	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	Z	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	a	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	b	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	c	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	d	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	e	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	f	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	g	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	h	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	i	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	j	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	k	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	l	570	Total 4483	C 2835	N 761	O 873	S 14	0	0

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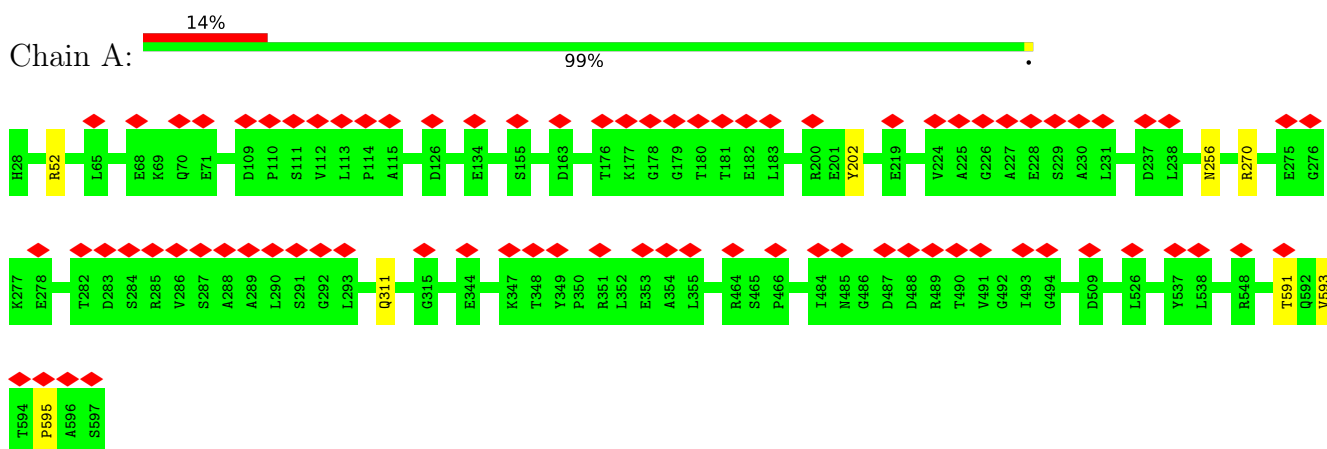
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>AltConf</b>	<b>Trace</b>
1	m	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	n	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
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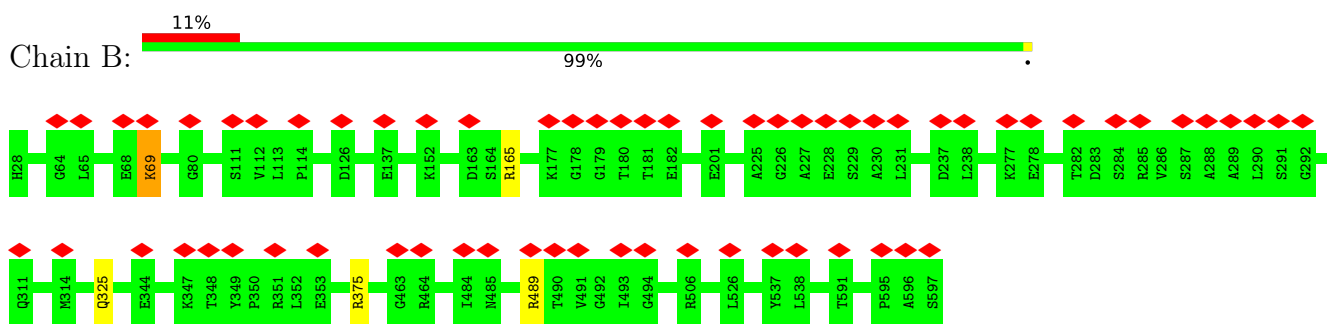
### 3 Residue-property plots [i](#)

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.

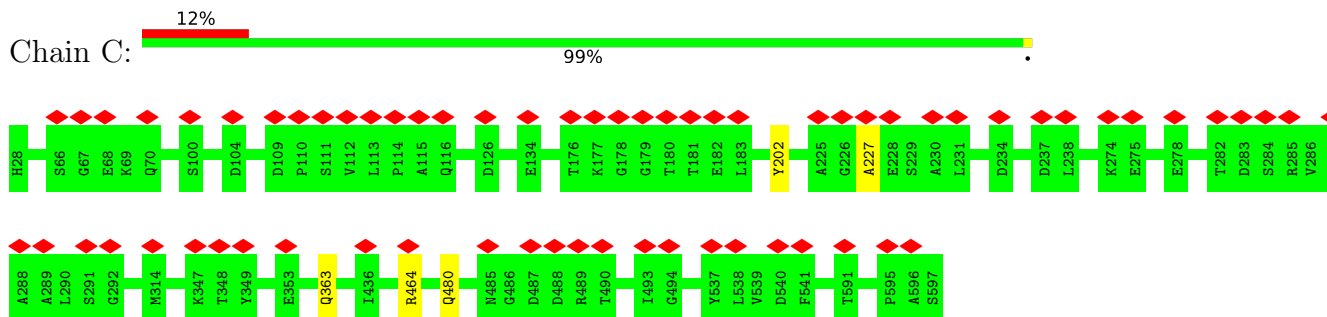
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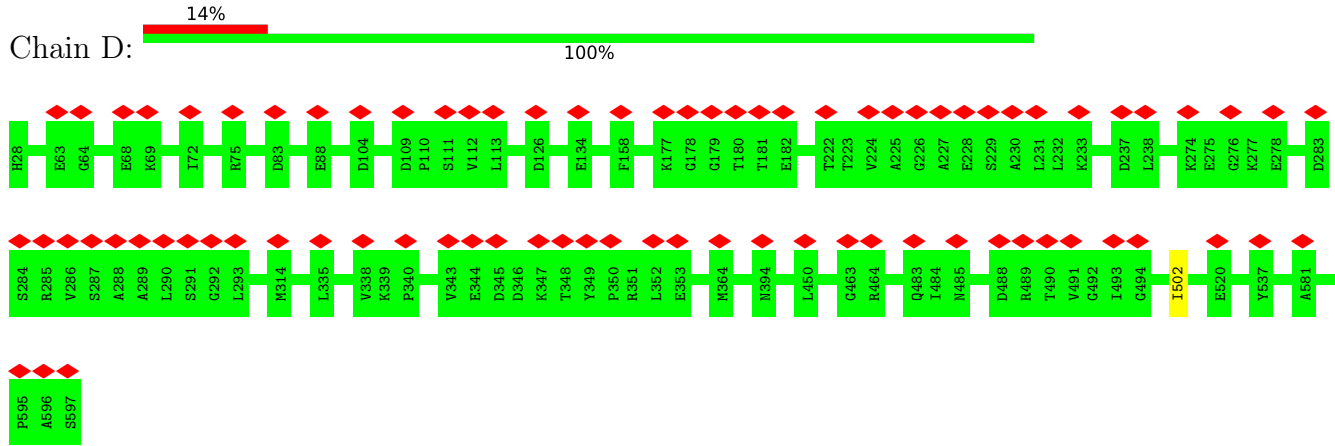


- Molecule 1: Major head protein

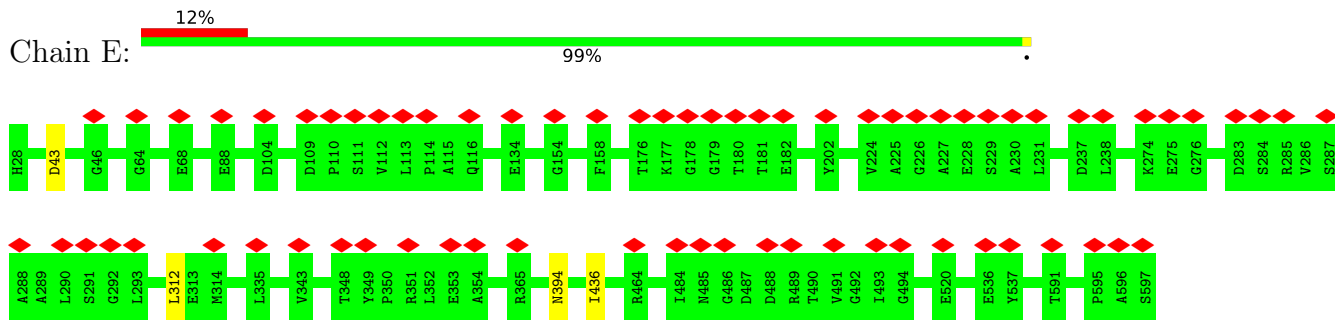




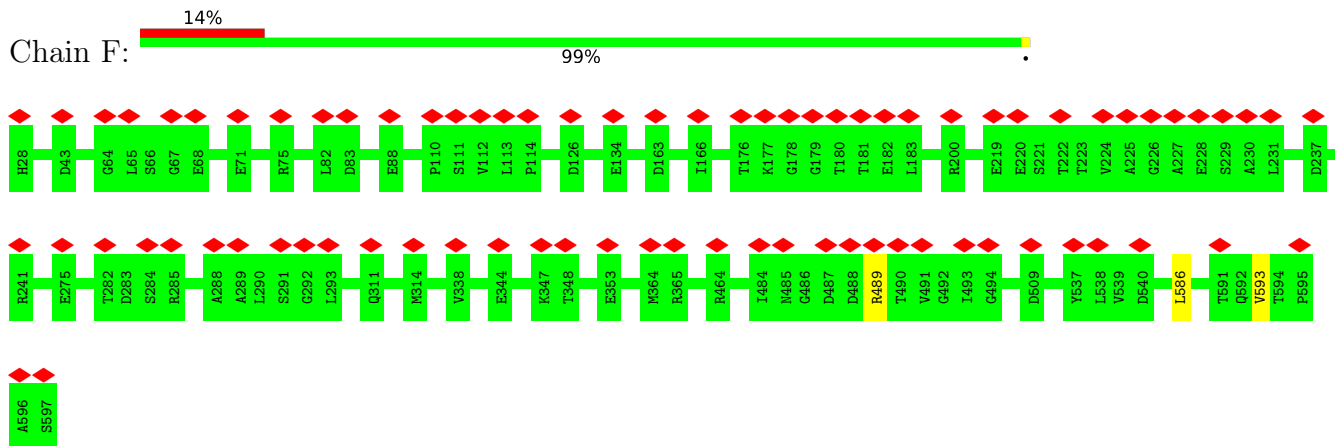
• Molecule 1: Major head protein



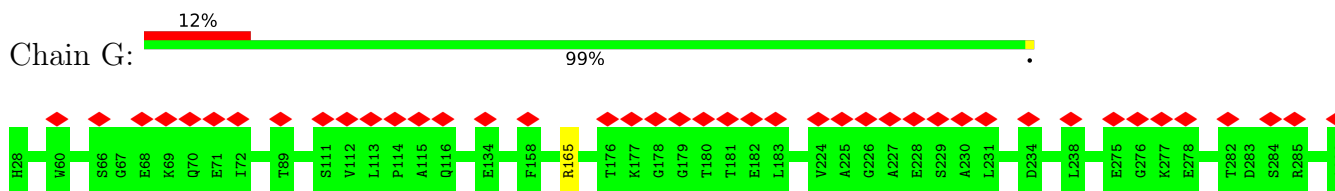
• Molecule 1: Major head protein

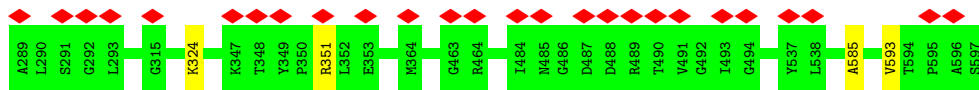


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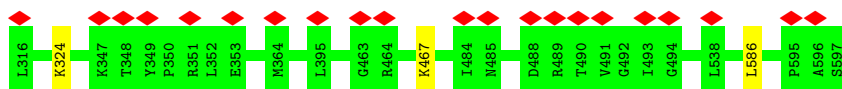
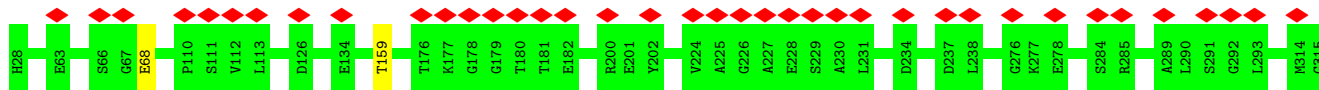


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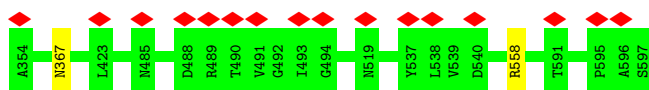
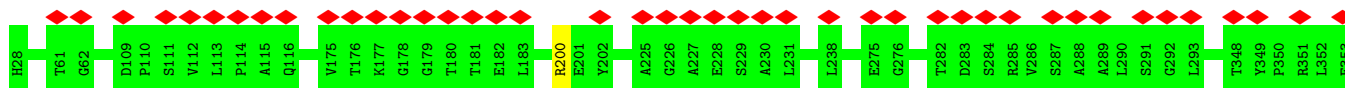




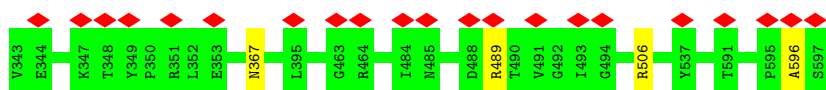
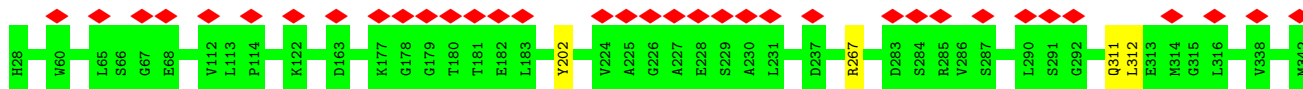
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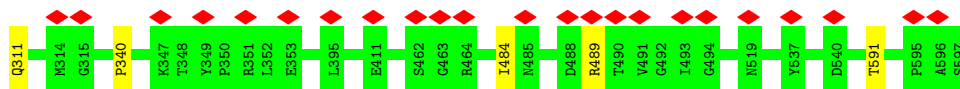
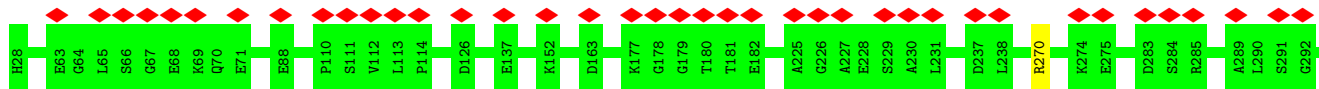
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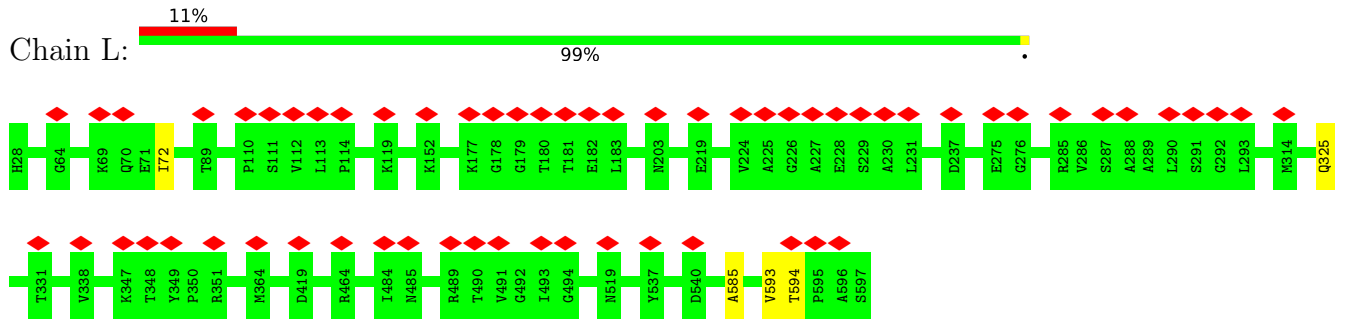
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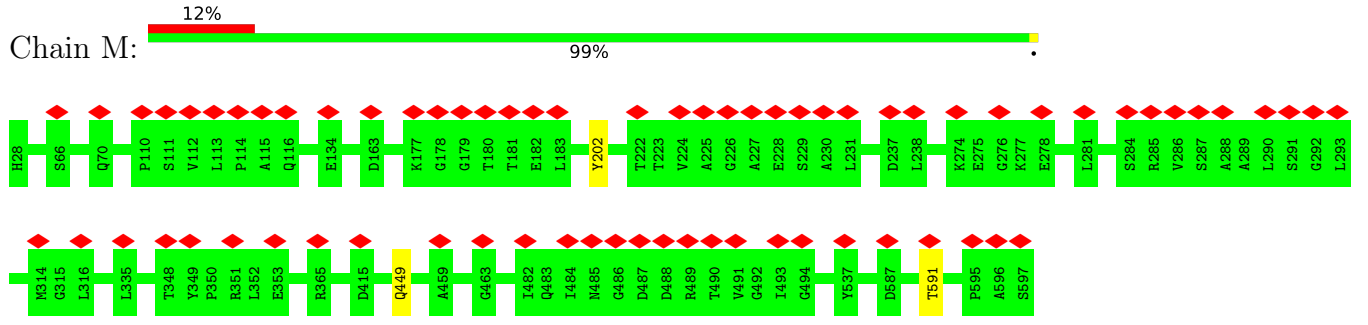
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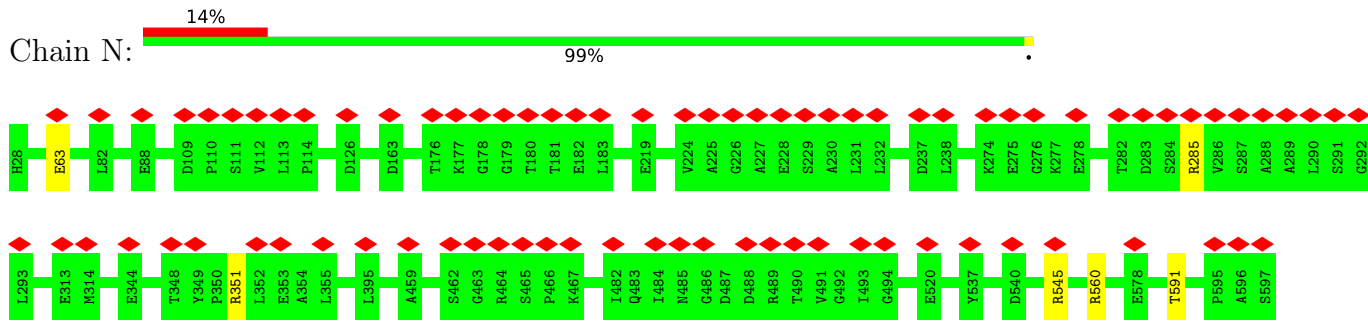
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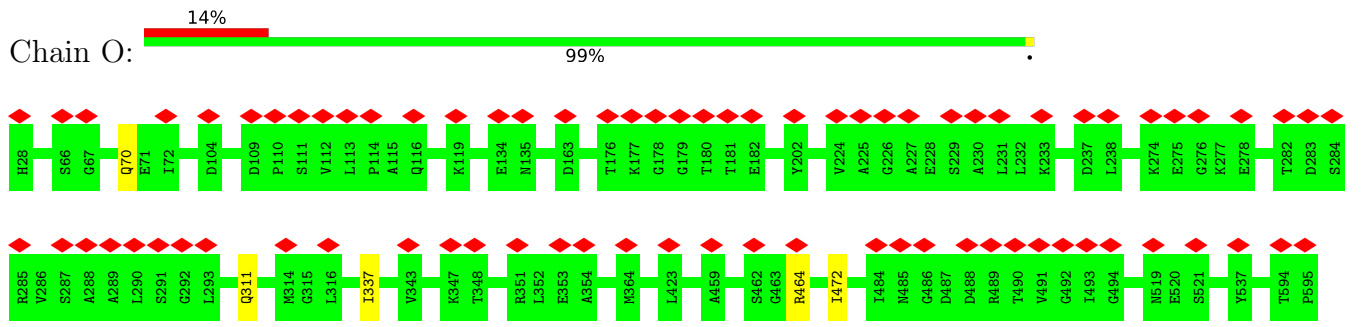
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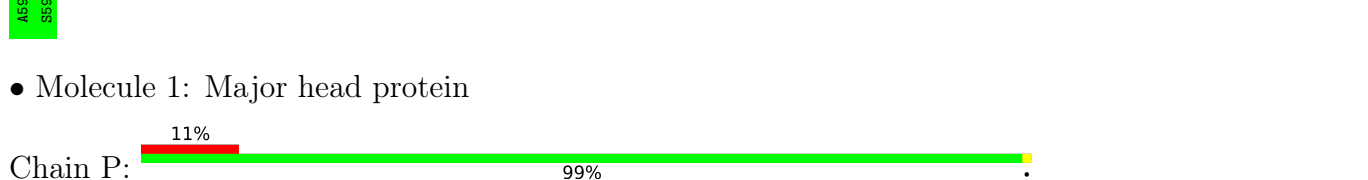
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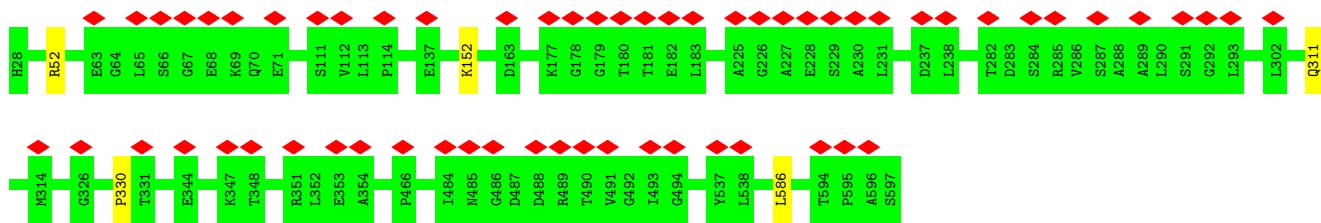
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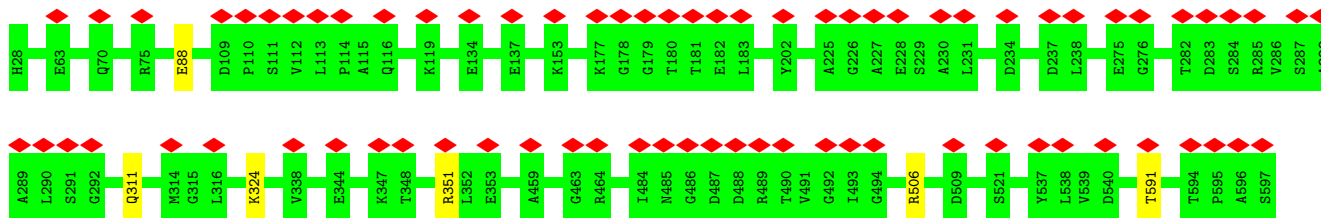
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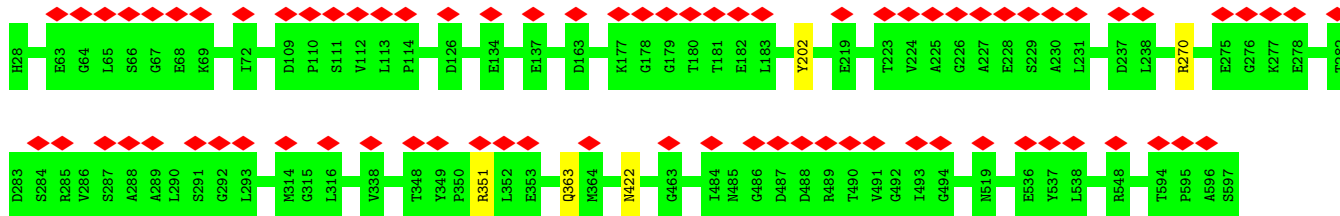
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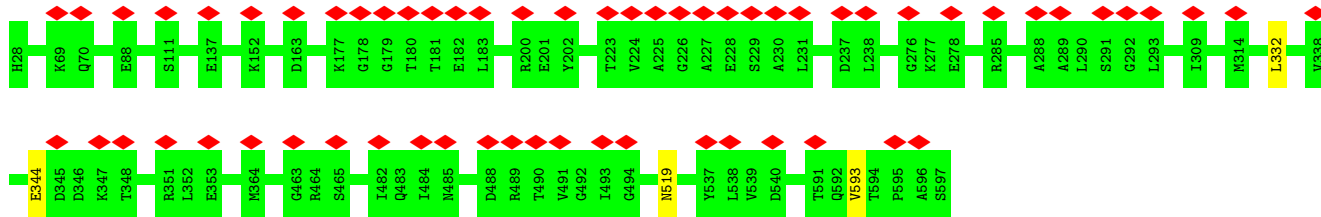
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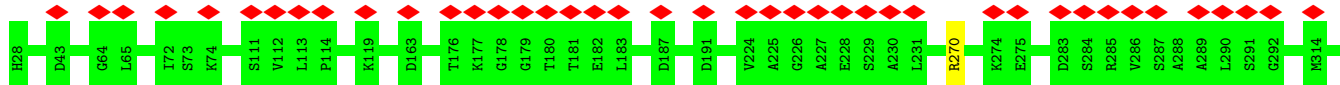
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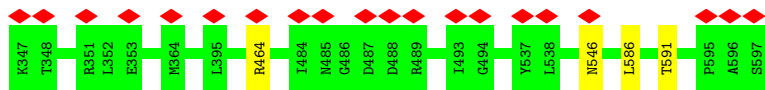


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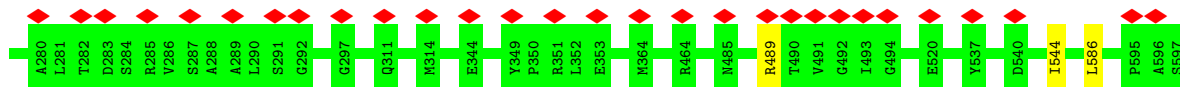
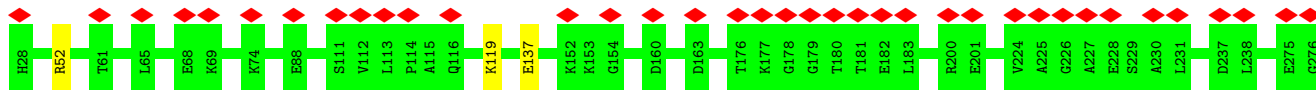


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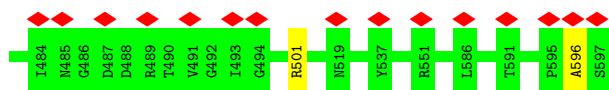
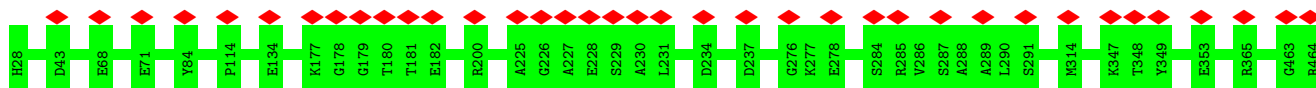




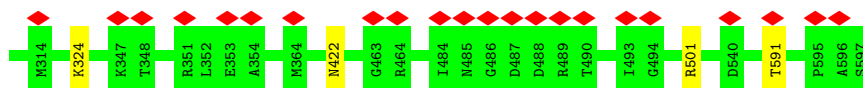
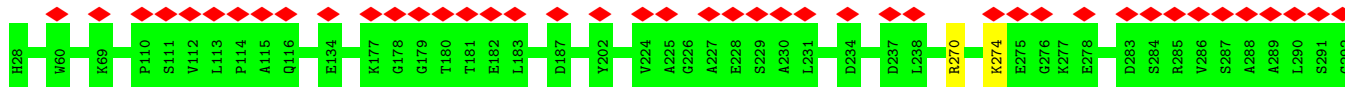
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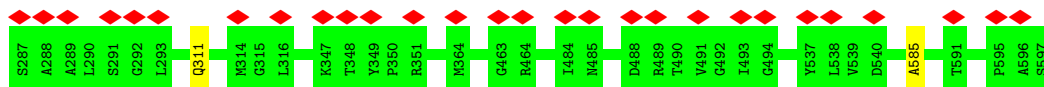
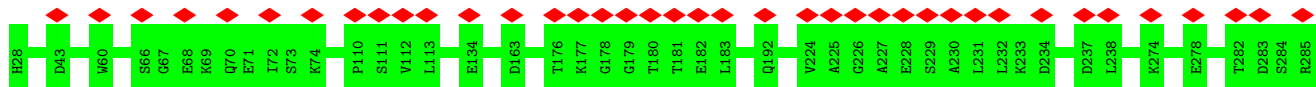
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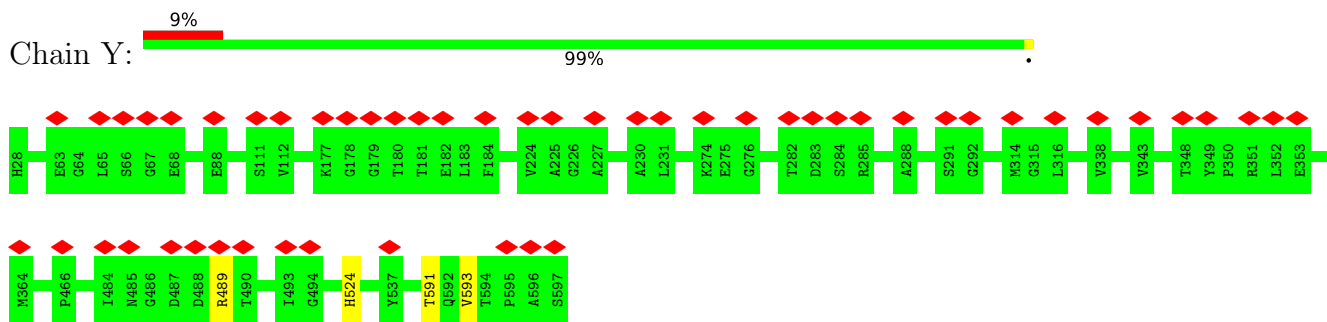
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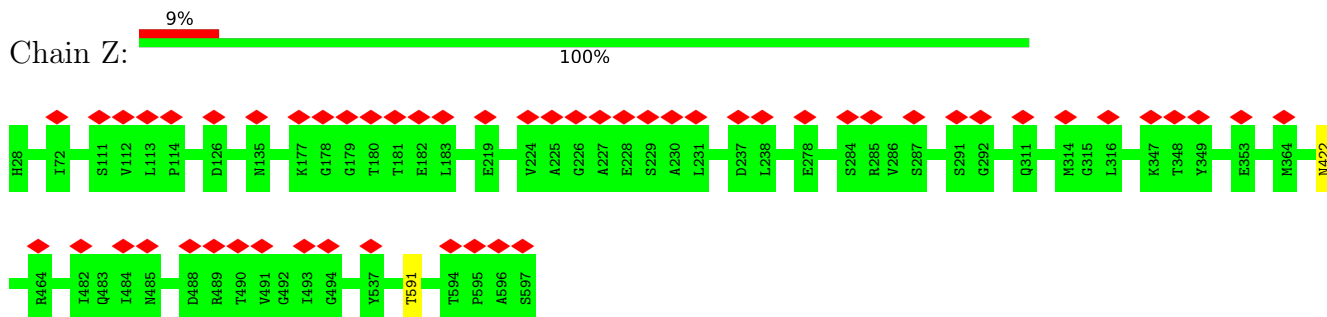
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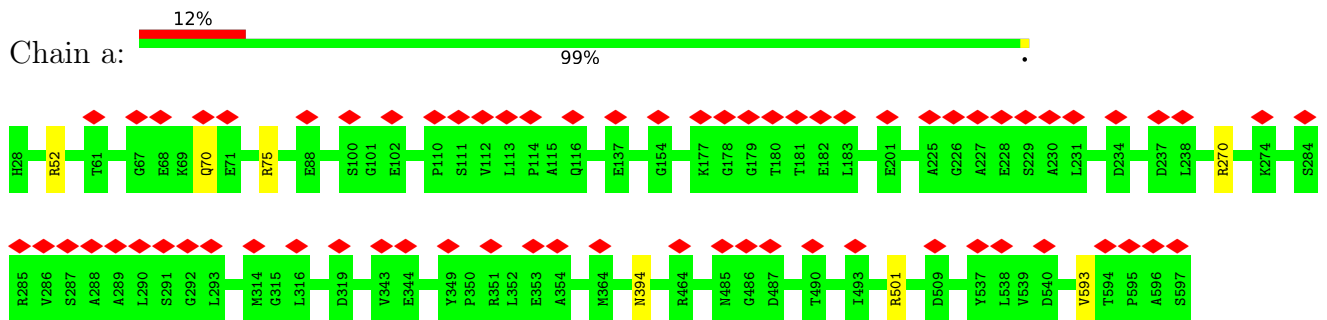
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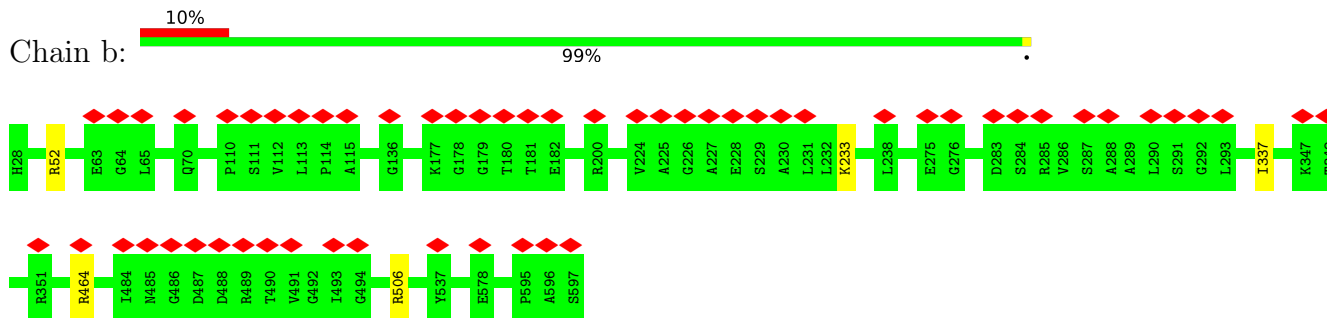
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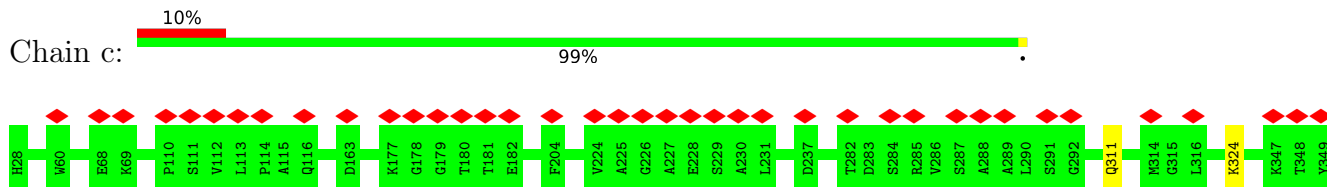
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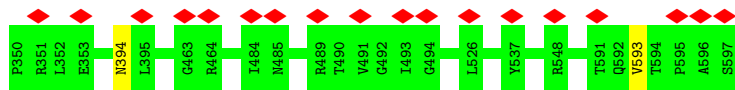


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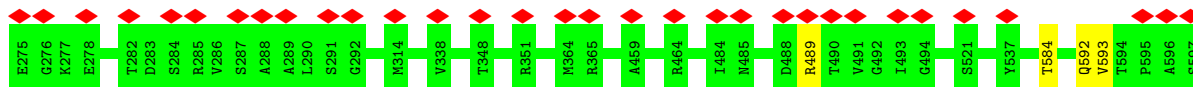
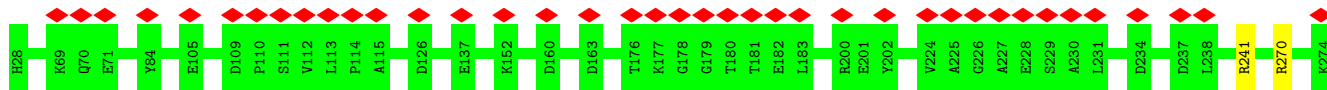


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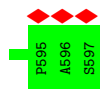
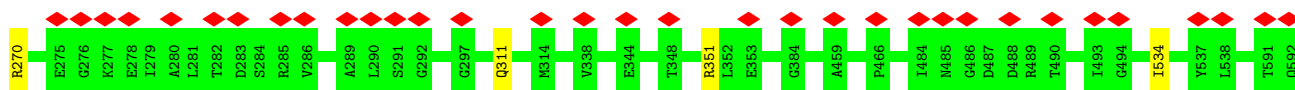
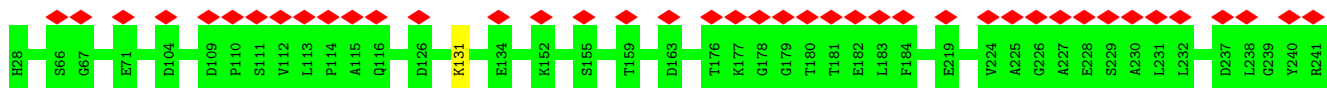




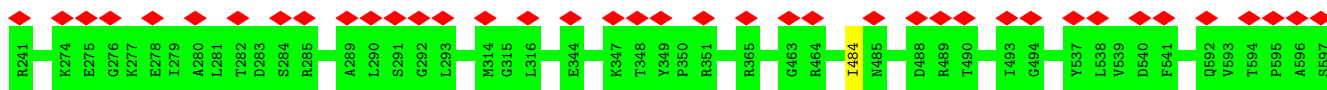
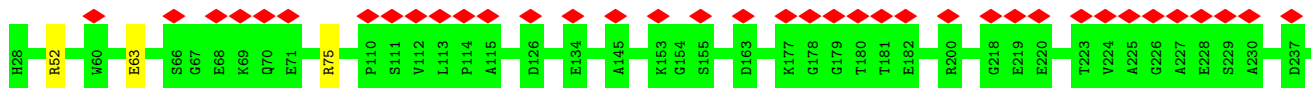
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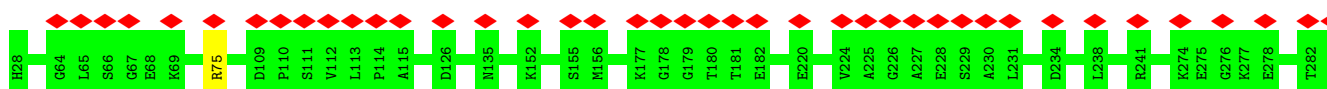
• Molecule 1: Major head protein

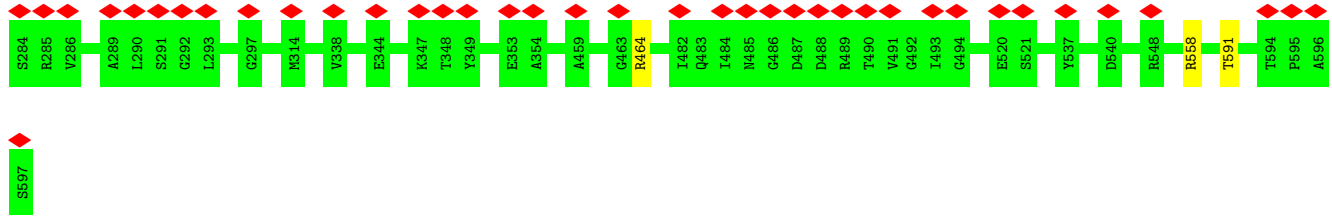


• Molecule 1: Major head protein

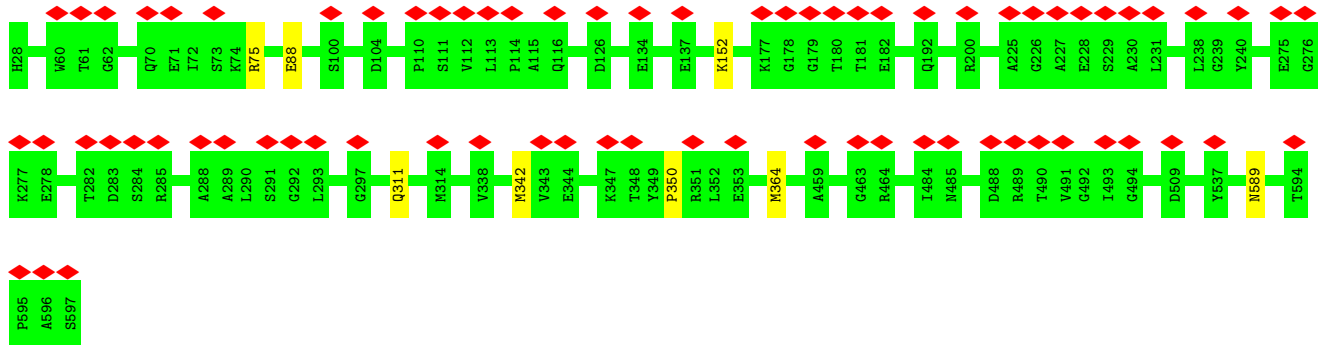


• Molecule 1: Major head protein

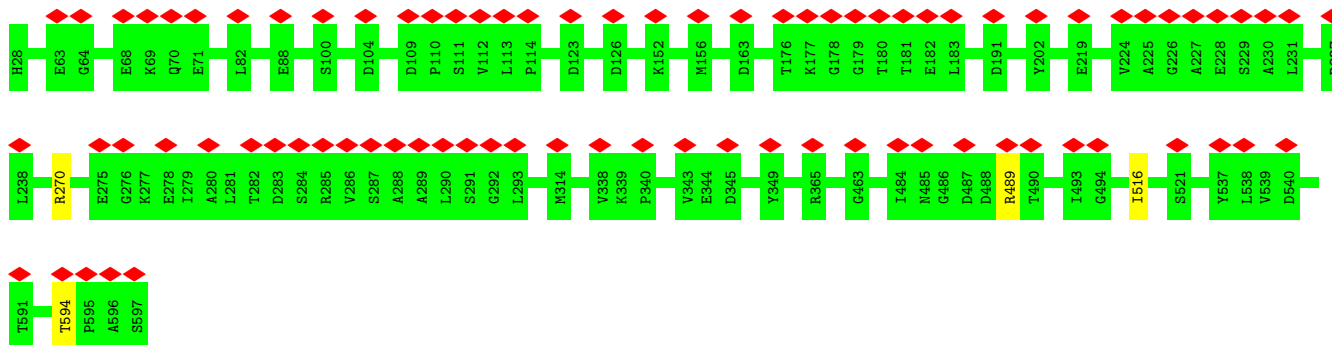




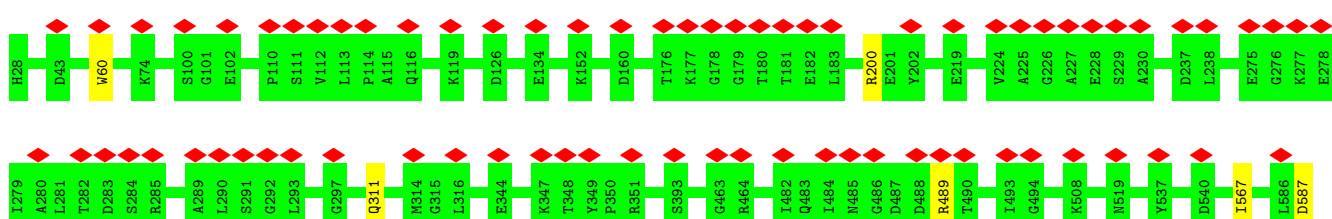
• Molecule 1: Major head protein



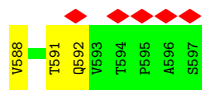
• Molecule 1: Major head protein



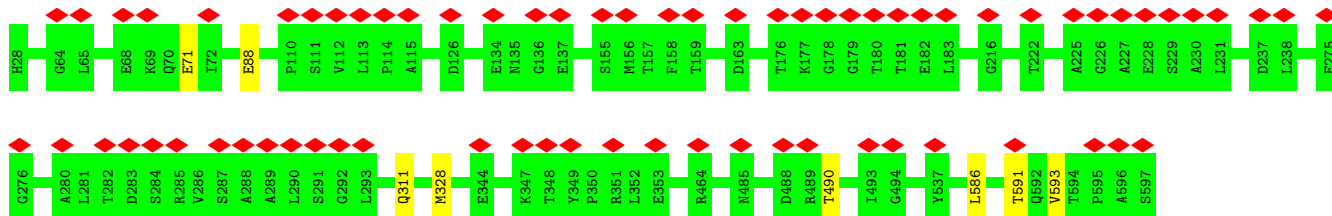
• Molecule 1: Major head protein



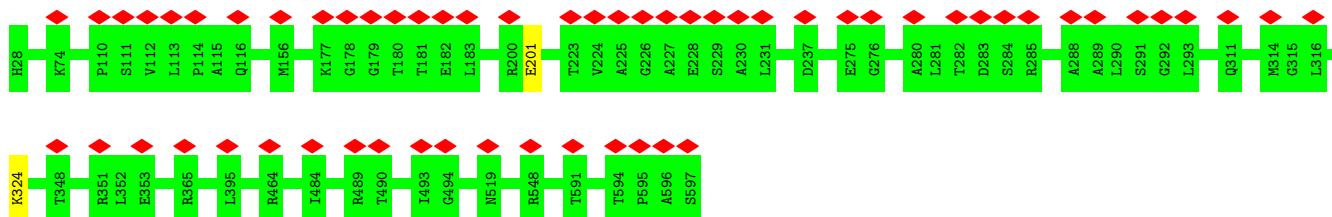




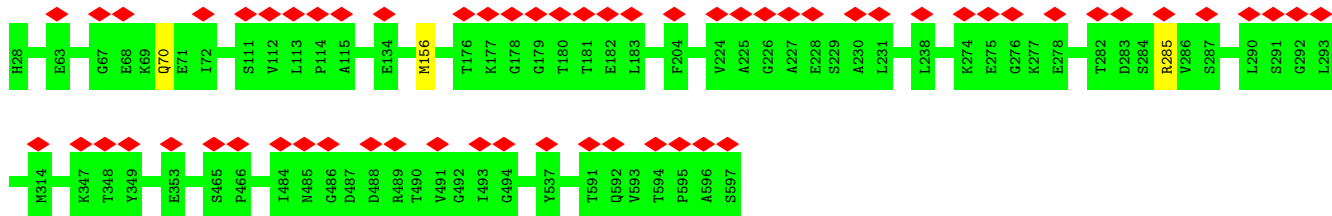
• Molecule 1: Major head protein



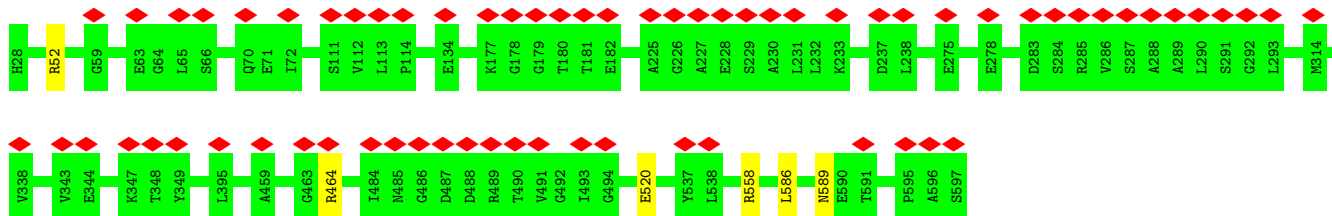
• Molecule 1: Major head protein



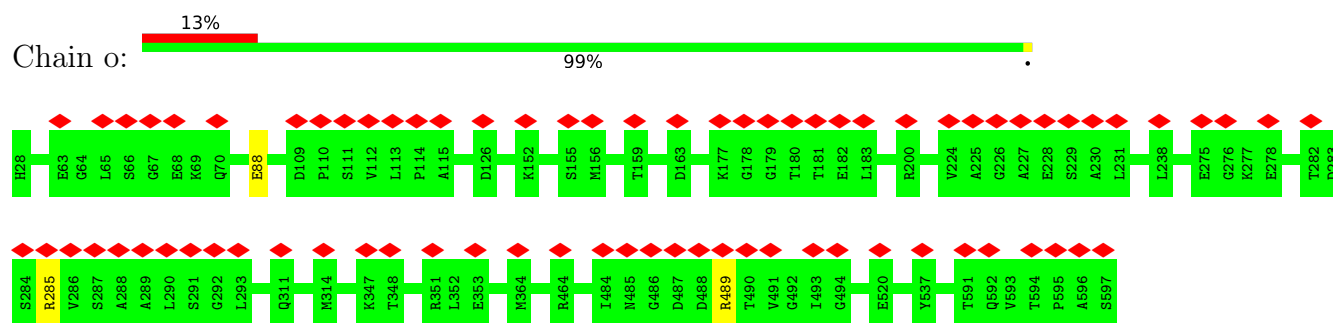
• Molecule 1: Major head protein



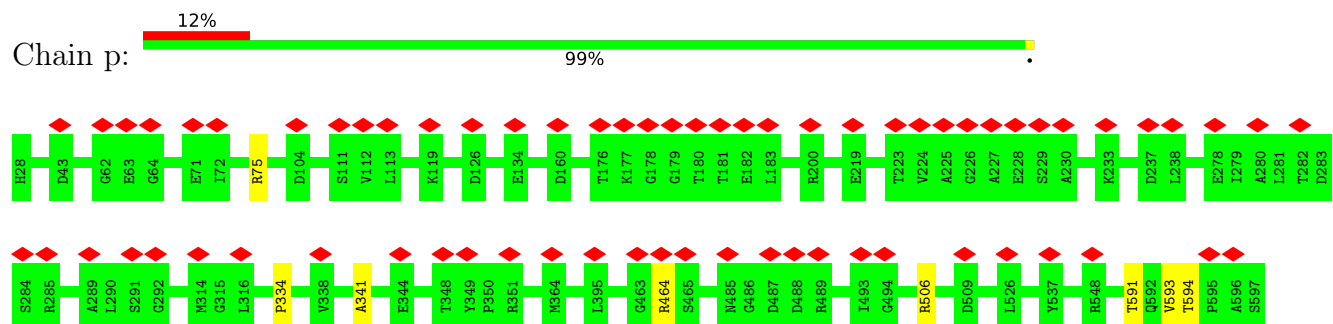
• Molecule 1: Major head protein



• Molecule 1: Major head protein



- Molecule 1: Major head protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19193	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	1644.0, 1644.0, 1644.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.055, 2.055, 2.055	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	0.28	0/4559	0.58	1/6184 (0.0%)
1	B	0.28	0/4559	0.56	0/6184
1	C	0.28	0/4559	0.56	0/6184
1	D	0.28	0/4559	0.55	0/6184
1	E	0.28	0/4559	0.56	1/6184 (0.0%)
1	F	0.28	0/4559	0.58	1/6184 (0.0%)
1	G	0.28	0/4559	0.57	1/6184 (0.0%)
1	H	0.28	0/4559	0.55	0/6184
1	I	0.28	0/4559	0.56	0/6184
1	J	0.28	0/4559	0.56	1/6184 (0.0%)
1	K	0.28	0/4559	0.56	1/6184 (0.0%)
1	L	0.27	0/4559	0.55	1/6184 (0.0%)
1	M	0.27	0/4559	0.54	0/6184
1	N	0.28	0/4559	0.56	0/6184
1	O	0.27	0/4559	0.55	0/6184
1	P	0.27	0/4559	0.57	1/6184 (0.0%)
1	Q	0.28	0/4559	0.55	0/6184
1	R	0.27	0/4559	0.54	0/6184
1	S	0.27	0/4559	0.57	2/6184 (0.0%)
1	T	0.28	0/4559	0.54	0/6184
1	U	0.28	0/4559	0.55	0/6184
1	V	0.28	0/4559	0.55	0/6184
1	W	0.28	0/4559	0.54	0/6184
1	X	0.28	0/4559	0.56	0/6184
1	Y	0.27	0/4559	0.56	1/6184 (0.0%)
1	Z	0.28	0/4559	0.56	0/6184
1	a	0.28	0/4559	0.56	1/6184 (0.0%)
1	b	0.28	0/4559	0.55	0/6184
1	c	0.28	0/4559	0.55	1/6184 (0.0%)
1	d	0.28	0/4559	0.56	1/6184 (0.0%)
1	e	0.28	0/4559	0.56	0/6184
1	f	0.28	0/4559	0.58	0/6184
1	g	0.28	0/4559	0.54	0/6184
1	h	0.28	0/4559	0.55	1/6184 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	i	0.28	0/4559	0.54	0/6184
1	j	0.27	0/4559	0.55	0/6184
1	k	0.27	0/4559	0.55	1/6184 (0.0%)
1	l	0.28	0/4559	0.55	0/6184
1	m	0.27	0/4559	0.55	0/6184
1	n	0.27	0/4559	0.54	0/6184
1	o	0.28	0/4559	0.55	0/6184
1	p	0.29	0/4559	0.57	3/6184 (0.0%)
All	All	0.28	0/191478	0.56	19/259728 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	G	0	1
1	K	0	1
1	L	0	2
1	M	0	1
1	N	0	1
1	Q	0	1
1	T	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	d	0	2
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	3
1	k	0	2
1	n	0	1
1	p	0	3
All	All	0	29

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	593	VAL	C-N-CA	17.38	165.16	121.70
1	A	593	VAL	C-N-CA	15.04	159.30	121.70
1	S	593	VAL	C-N-CA	11.55	150.59	121.70
1	p	334	PRO	CA-N-CD	-10.32	97.06	111.50
1	G	593	VAL	C-N-CA	8.96	144.10	121.70
1	c	593	VAL	C-N-CA	8.29	142.41	121.70
1	Y	593	VAL	C-N-CA	7.44	140.30	121.70
1	L	593	VAL	C-N-CA	7.10	139.46	121.70
1	k	593	VAL	C-N-CA	7.01	139.24	121.70
1	p	334	PRO	N-CD-CG	-6.67	93.19	103.20
1	d	593	VAL	C-N-CA	6.00	136.69	121.70
1	E	312	LEU	CA-CB-CG	5.85	128.76	115.30
1	P	330	PRO	CA-N-CD	-5.56	103.72	111.50
1	a	593	VAL	C-N-CA	5.36	135.10	121.70
1	J	312	LEU	CA-CB-CG	5.28	127.44	115.30
1	h	364	MET	CA-CB-CG	5.27	122.26	113.30
1	p	593	VAL	C-N-CA	5.15	134.58	121.70
1	K	340	PRO	CA-N-CD	-5.14	104.31	111.50
1	S	332	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	591	THR	Peptide
1	B	69	LYS	Peptide
1	C	363	GLN	Peptide
1	G	585	ALA	Peptide
1	K	591	THR	Peptide
1	L	585	ALA	Peptide
1	L	594	THR	Peptide
1	M	591	THR	Peptide
1	N	591	THR	Peptide
1	Q	591	THR	Peptide
1	T	591	THR	Peptide
1	W	591	THR	Peptide
1	X	585	ALA	Peptide
1	Y	591	THR	Peptide
1	Z	591	THR	Peptide
1	d	584	THR	Peptide
1	d	592	GLN	Peptide
1	g	591	THR	Peptide
1	h	589	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	i	594	THR	Peptide
1	j	591	THR	Peptide
1	j	592	GLN	Peptide
1	j	60	TRP	Peptide
1	k	328	MET	Peptide
1	k	591	THR	Peptide
1	n	589	ASN	Peptide
1	p	341	ALA	Peptide
1	p	591	THR	Peptide
1	p	594	THR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/570 (100%)	531 (94%)	34 (6%)	3 (0%)	29	67
1	B	568/570 (100%)	531 (94%)	36 (6%)	1 (0%)	47	80
1	C	568/570 (100%)	526 (93%)	40 (7%)	2 (0%)	34	71
1	D	568/570 (100%)	530 (93%)	38 (7%)	0	100	100
1	E	568/570 (100%)	529 (93%)	37 (6%)	2 (0%)	34	71
1	F	568/570 (100%)	526 (93%)	40 (7%)	2 (0%)	34	71
1	G	568/570 (100%)	534 (94%)	34 (6%)	0	100	100
1	H	568/570 (100%)	533 (94%)	32 (6%)	3 (0%)	29	67
1	I	568/570 (100%)	525 (92%)	43 (8%)	0	100	100
1	J	568/570 (100%)	525 (92%)	40 (7%)	3 (0%)	29	67
1	K	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	568/570 (100%)	539 (95%)	28 (5%)	1 (0%)	47	80
1	M	568/570 (100%)	532 (94%)	35 (6%)	1 (0%)	47	80
1	N	568/570 (100%)	526 (93%)	41 (7%)	1 (0%)	47	80
1	O	568/570 (100%)	528 (93%)	38 (7%)	2 (0%)	34	71
1	P	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34	71
1	Q	568/570 (100%)	537 (94%)	29 (5%)	2 (0%)	34	71
1	R	568/570 (100%)	539 (95%)	28 (5%)	1 (0%)	47	80
1	S	568/570 (100%)	533 (94%)	34 (6%)	1 (0%)	47	80
1	T	568/570 (100%)	532 (94%)	34 (6%)	2 (0%)	34	71
1	U	568/570 (100%)	518 (91%)	47 (8%)	3 (0%)	29	67
1	V	568/570 (100%)	539 (95%)	28 (5%)	1 (0%)	47	80
1	W	568/570 (100%)	530 (93%)	38 (7%)	0	100	100
1	X	568/570 (100%)	532 (94%)	35 (6%)	1 (0%)	47	80
1	Y	568/570 (100%)	529 (93%)	38 (7%)	1 (0%)	47	80
1	Z	568/570 (100%)	528 (93%)	40 (7%)	0	100	100
1	a	568/570 (100%)	528 (93%)	38 (7%)	2 (0%)	34	71
1	b	568/570 (100%)	537 (94%)	31 (6%)	0	100	100
1	c	568/570 (100%)	531 (94%)	35 (6%)	2 (0%)	34	71
1	d	568/570 (100%)	533 (94%)	35 (6%)	0	100	100
1	e	568/570 (100%)	524 (92%)	43 (8%)	1 (0%)	47	80
1	f	568/570 (100%)	524 (92%)	42 (7%)	2 (0%)	34	71
1	g	568/570 (100%)	529 (93%)	39 (7%)	0	100	100
1	h	568/570 (100%)	527 (93%)	37 (6%)	4 (1%)	22	60
1	i	568/570 (100%)	533 (94%)	35 (6%)	0	100	100
1	j	568/570 (100%)	521 (92%)	44 (8%)	3 (0%)	29	67
1	k	568/570 (100%)	527 (93%)	36 (6%)	5 (1%)	17	54
1	l	568/570 (100%)	523 (92%)	44 (8%)	1 (0%)	47	80
1	m	568/570 (100%)	533 (94%)	33 (6%)	2 (0%)	34	71
1	n	568/570 (100%)	535 (94%)	31 (6%)	2 (0%)	34	71
1	o	568/570 (100%)	525 (92%)	41 (7%)	2 (0%)	34	71
1	p	568/570 (100%)	520 (92%)	48 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	23856/23940 (100%)	22242 (93%)	1551 (6%)	63 (0%)	44	75

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	165	ARG
1	E	43	ASP
1	H	159	THR
1	J	202	TYR
1	J	596	ALA
1	K	311	GLN
1	K	484	ILE
1	R	202	TYR
1	V	596	ALA
1	h	88	GLU
1	h	342	MET
1	j	311	GLN
1	j	587	ASP
1	j	588	VAL
1	l	201	GLU
1	A	202	TYR
1	A	311	GLN
1	L	72	ILE
1	O	311	GLN
1	e	311	GLN
1	f	63	GLU
1	E	394	ASN
1	J	311	GLN
1	T	546	ASN
1	c	394	ASN
1	Q	88	GLU
1	Q	311	GLN
1	S	344	GLU
1	U	586	LEU
1	Y	489	ARG
1	h	311	GLN
1	k	490	THR
1	m	156	MET
1	o	88	GLU
1	C	202	TYR
1	C	227	ALA
1	F	489	ARG

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Mol	Chain	Res	Type
1	H	68	GLU
1	H	586	LEU
1	P	311	GLN
1	P	586	LEU
1	T	586	LEU
1	a	70	GLN
1	c	311	GLN
1	k	88	GLU
1	k	311	GLN
1	k	586	LEU
1	m	70	GLN
1	n	520	GLU
1	n	586	LEU
1	F	586	LEU
1	M	202	TYR
1	N	63	GLU
1	O	70	GLN
1	U	137	GLU
1	U	489	ARG
1	X	311	GLN
1	a	394	ASN
1	k	71	GLU
1	o	489	ARG
1	A	595	PRO
1	f	484	ILE
1	h	350	PRO

### 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	492/492 (100%)	489 (99%)	3 (1%)	86 92
1	B	492/492 (100%)	488 (99%)	4 (1%)	81 88
1	C	492/492 (100%)	490 (100%)	2 (0%)	91 94
1	D	492/492 (100%)	491 (100%)	1 (0%)	93 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	F	492/492 (100%)	492 (100%)	0	100	100
1	G	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	H	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	I	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	J	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	K	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	L	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	M	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	N	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	O	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	P	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	Q	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	R	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	S	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	T	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	U	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	V	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	W	492/492 (100%)	487 (99%)	5 (1%)	76	85
1	X	492/492 (100%)	492 (100%)	0	100	100
1	Y	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	Z	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	a	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	b	492/492 (100%)	487 (99%)	5 (1%)	76	85
1	c	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	d	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	e	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	f	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	g	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	h	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	i	492/492 (100%)	489 (99%)	3 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	k	492/492 (100%)	492 (100%)	0	100	100
1	l	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	m	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	n	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	o	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	p	492/492 (100%)	489 (99%)	3 (1%)	86	92
All	All	20664/20664 (100%)	20568 (100%)	96 (0%)	89	93

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	256	ASN
1	A	270	ARG
1	B	69	LYS
1	B	325	GLN
1	B	375	ARG
1	B	489	ARG
1	C	464	ARG
1	C	480	GLN
1	D	502	ILE
1	E	436	ILE
1	G	165	ARG
1	G	324	LYS
1	G	351	ARG
1	H	324	LYS
1	H	467	LYS
1	I	200	ARG
1	I	367	ASN
1	I	558	ARG
1	J	267	ARG
1	J	367	ASN
1	J	489	ARG
1	J	506	ARG
1	K	270	ARG
1	K	489	ARG
1	L	325	GLN
1	M	449	GLN
1	N	285	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	351	ARG
1	N	545	ARG
1	N	560	ARG
1	O	337	ILE
1	O	464	ARG
1	O	472	ILE
1	P	52	ARG
1	P	152	LYS
1	Q	324	LYS
1	Q	351	ARG
1	Q	506	ARG
1	R	270	ARG
1	R	351	ARG
1	R	363	GLN
1	R	422	ASN
1	S	519	ASN
1	T	270	ARG
1	T	464	ARG
1	U	52	ARG
1	U	119	LYS
1	U	544	ILE
1	V	501	ARG
1	W	270	ARG
1	W	274	LYS
1	W	324	LYS
1	W	422	ASN
1	W	501	ARG
1	Y	524	HIS
1	Z	422	ASN
1	a	52	ARG
1	a	75	ARG
1	a	270	ARG
1	a	501	ARG
1	b	52	ARG
1	b	233	LYS
1	b	337	ILE
1	b	464	ARG
1	b	506	ARG
1	c	324	LYS
1	d	241	ARG
1	d	270	ARG
1	d	489	ARG

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Mol	Chain	Res	Type
1	e	131	LYS
1	e	270	ARG
1	e	351	ARG
1	e	534	ILE
1	f	52	ARG
1	f	75	ARG
1	g	75	ARG
1	g	464	ARG
1	g	558	ARG
1	h	75	ARG
1	h	152	LYS
1	i	270	ARG
1	i	489	ARG
1	i	516	ILE
1	j	200	ARG
1	j	489	ARG
1	j	567	ILE
1	l	324	LYS
1	m	285	ARG
1	n	52	ARG
1	n	464	ARG
1	n	558	ARG
1	o	285	ARG
1	p	75	ARG
1	p	464	ARG
1	p	506	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	170	GLN
1	A	212	HIS
1	A	362	GLN
1	A	410	ASN
1	A	433	GLN
1	B	208	GLN
1	B	449	GLN
1	B	592	GLN
1	C	140	ASN
1	C	258	ASN
1	C	308	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	310	ASN
1	C	362	GLN
1	C	547	GLN
1	D	146	GLN
1	D	258	ASN
1	E	308	ASN
1	F	140	ASN
1	F	308	ASN
1	F	483	GLN
1	G	256	ASN
1	G	258	ASN
1	G	323	GLN
1	G	325	GLN
1	H	120	GLN
1	H	433	GLN
1	I	120	GLN
1	I	311	GLN
1	J	208	GLN
1	J	366	ASN
1	J	449	GLN
1	J	480	GLN
1	J	547	GLN
1	K	325	GLN
1	K	433	GLN
1	L	208	GLN
1	L	433	GLN
1	M	170	GLN
1	M	308	ASN
1	M	374	ASN
1	M	485	ASN
1	M	524	HIS
1	N	90	ASN
1	N	120	GLN
1	N	325	GLN
1	N	441	ASN
1	N	547	GLN
1	N	575	ASN
1	O	106	GLN
1	O	402	GLN
1	O	429	GLN
1	O	483	GLN
1	O	485	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	P	256	ASN
1	P	422	ASN
1	Q	140	ASN
1	Q	208	GLN
1	Q	212	HIS
1	Q	308	ASN
1	Q	310	ASN
1	Q	311	GLN
1	Q	363	GLN
1	Q	422	ASN
1	Q	592	GLN
1	R	189	ASN
1	R	592	GLN
1	S	70	GLN
1	S	325	GLN
1	U	146	GLN
1	U	170	GLN
1	U	208	GLN
1	U	410	ASN
1	U	469	HIS
1	V	146	GLN
1	V	208	GLN
1	V	310	ASN
1	V	389	HIS
1	V	394	ASN
1	V	592	GLN
1	W	441	ASN
1	W	483	GLN
1	W	592	GLN
1	X	527	GLN
1	X	528	HIS
1	Y	374	ASN
1	Z	79	GLN
1	Z	120	GLN
1	Z	421	ASN
1	Z	592	GLN
1	a	99	GLN
1	a	103	ASN
1	a	258	ASN
1	a	310	ASN
1	a	421	ASN
1	a	422	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	b	363	GLN
1	b	402	GLN
1	c	99	GLN
1	c	394	ASN
1	c	483	GLN
1	c	485	ASN
1	d	212	HIS
1	d	256	ASN
1	d	258	ASN
1	d	563	ASN
1	e	70	GLN
1	f	128	ASN
1	f	310	ASN
1	g	28	HIS
1	g	48	GLN
1	g	90	ASN
1	g	120	GLN
1	h	99	GLN
1	h	208	GLN
1	h	325	GLN
1	h	422	ASN
1	j	103	ASN
1	j	192	GLN
1	k	308	ASN
1	k	310	ASN
1	k	449	GLN
1	l	308	ASN
1	l	325	GLN
1	l	402	GLN
1	l	483	GLN
1	m	140	ASN
1	m	374	ASN
1	m	422	ASN
1	n	120	GLN
1	n	310	ASN
1	n	311	GLN
1	n	325	GLN
1	o	483	GLN
1	o	485	ASN
1	o	547	GLN
1	p	441	ASN
1	p	546	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

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.

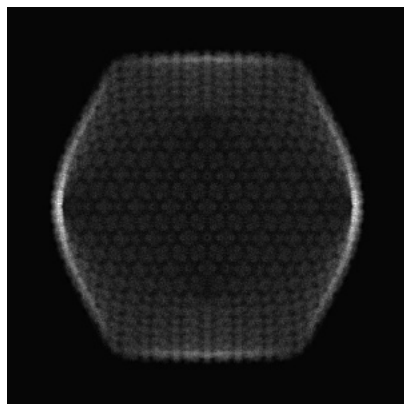
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13862. These allow visual inspection of the internal detail of the map and identification of artifacts.

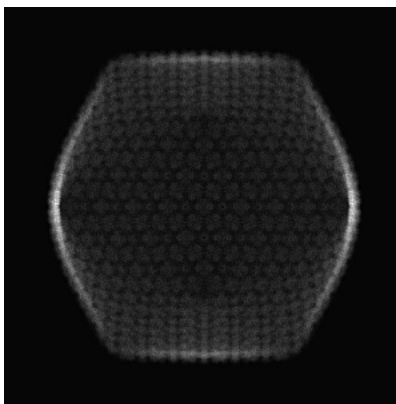
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

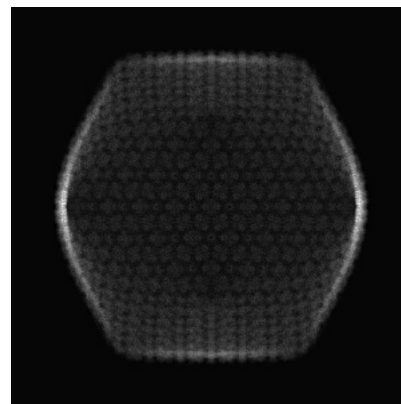
#### 6.1.1 Primary map



X

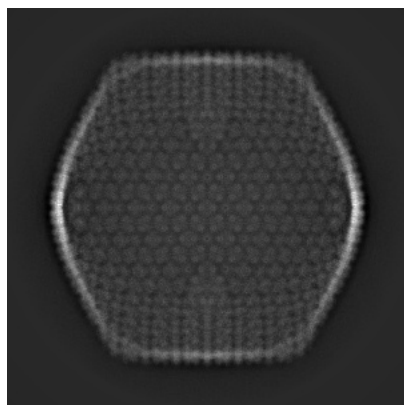


Y

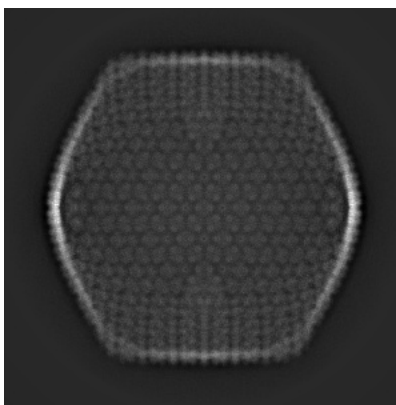


Z

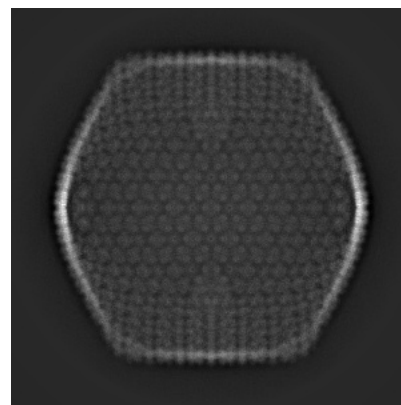
#### 6.1.2 Raw map



X



Y

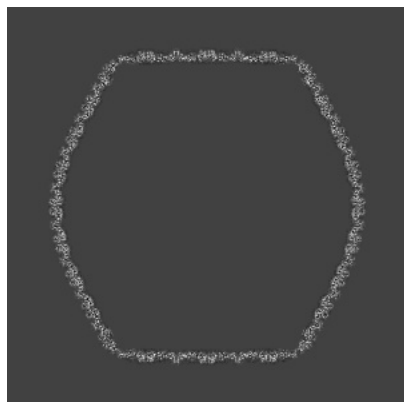


Z

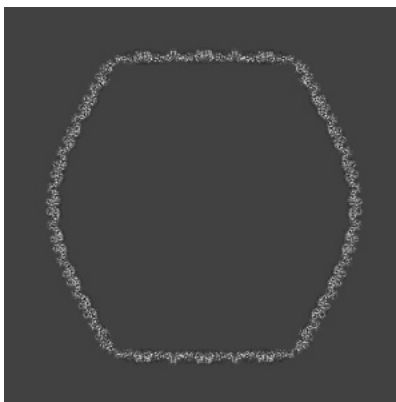
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

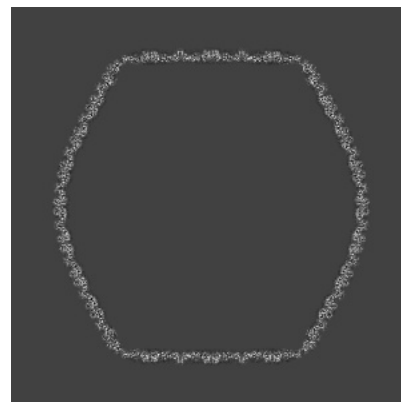
### 6.2.1 Primary map



X Index: 400

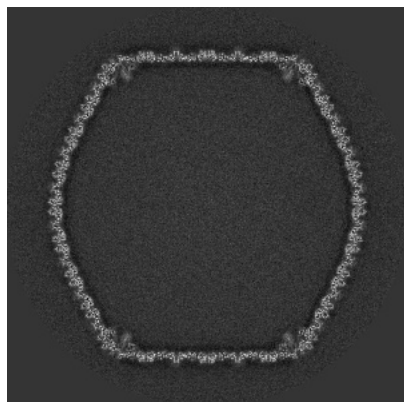


Y Index: 400

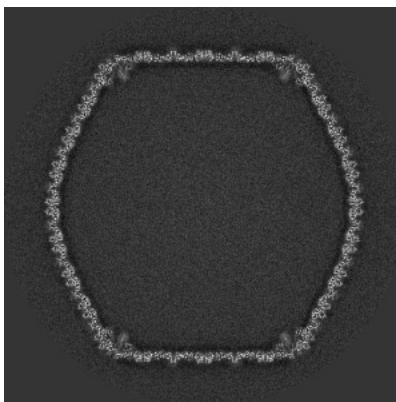


Z Index: 400

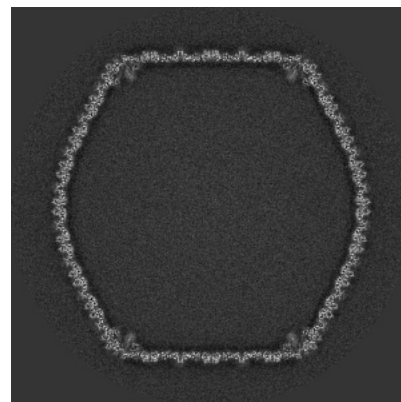
### 6.2.2 Raw map



X Index: 400



Y Index: 400

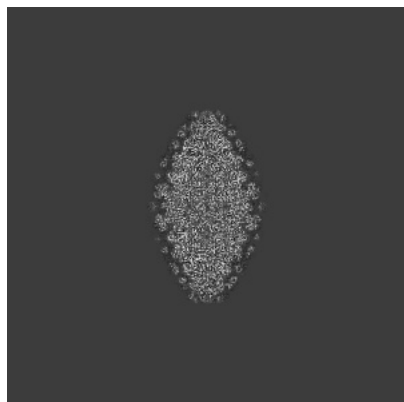


Z Index: 400

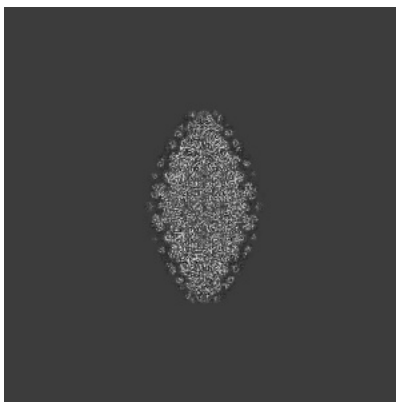
The images above show central slices of the map in three orthogonal directions.

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

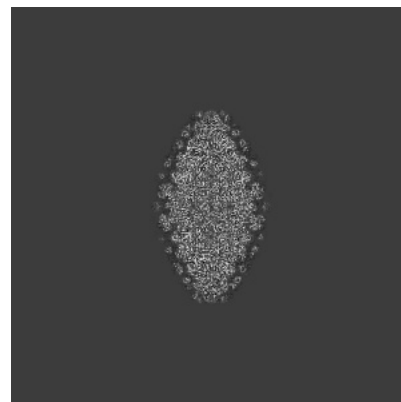
### 6.3.1 Primary map



X Index: 693

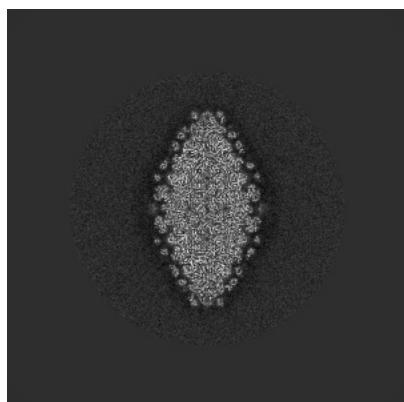


Y Index: 693

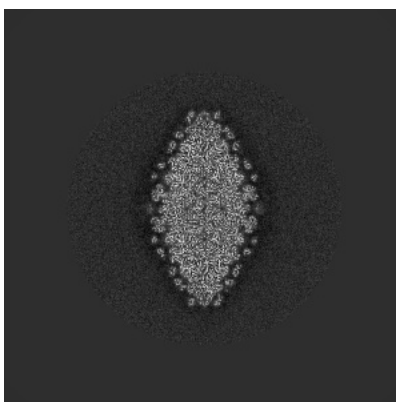


Z Index: 693

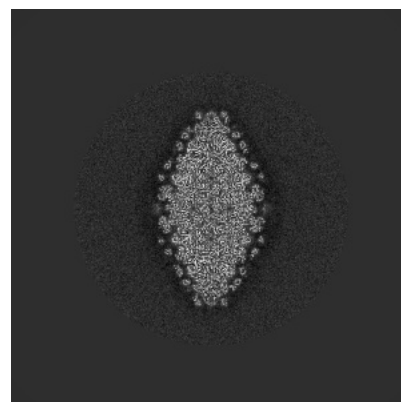
### 6.3.2 Raw map



X Index: 693



Y Index: 107

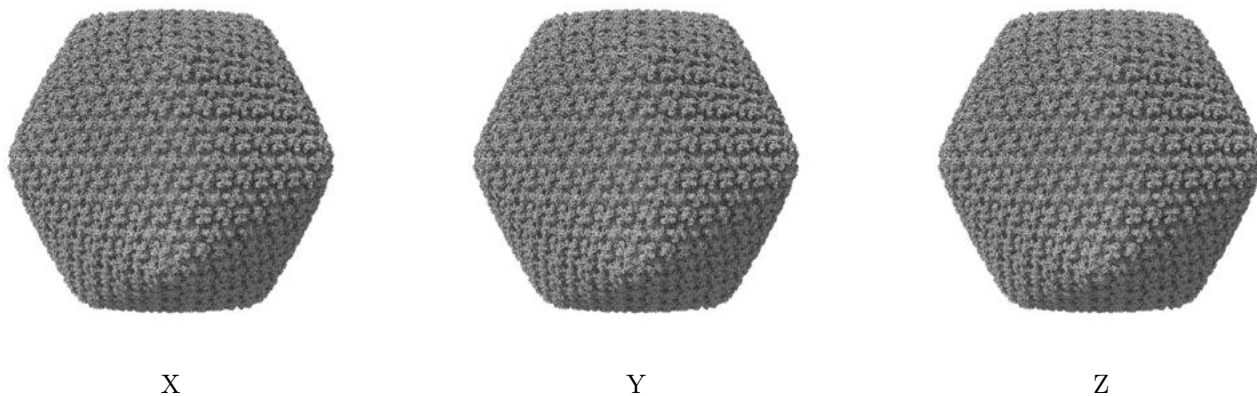


Z Index: 693

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

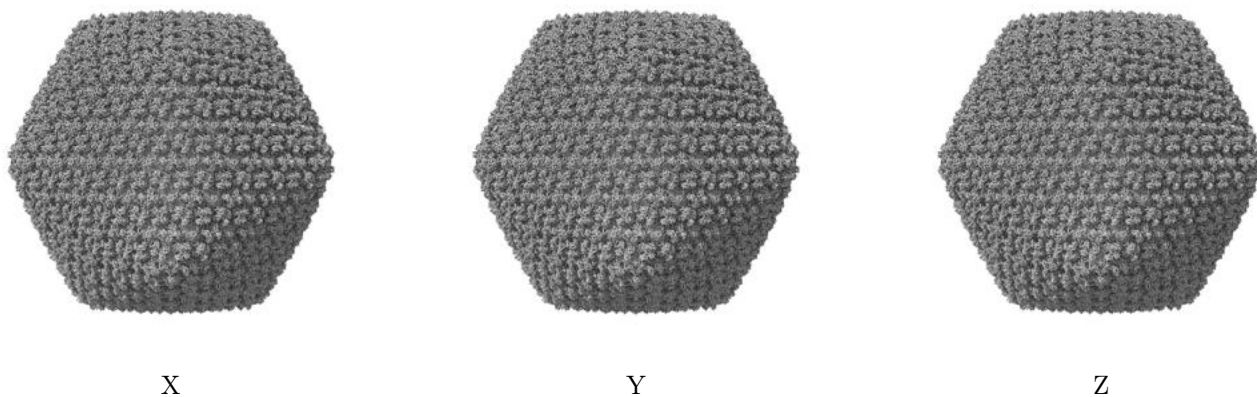
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

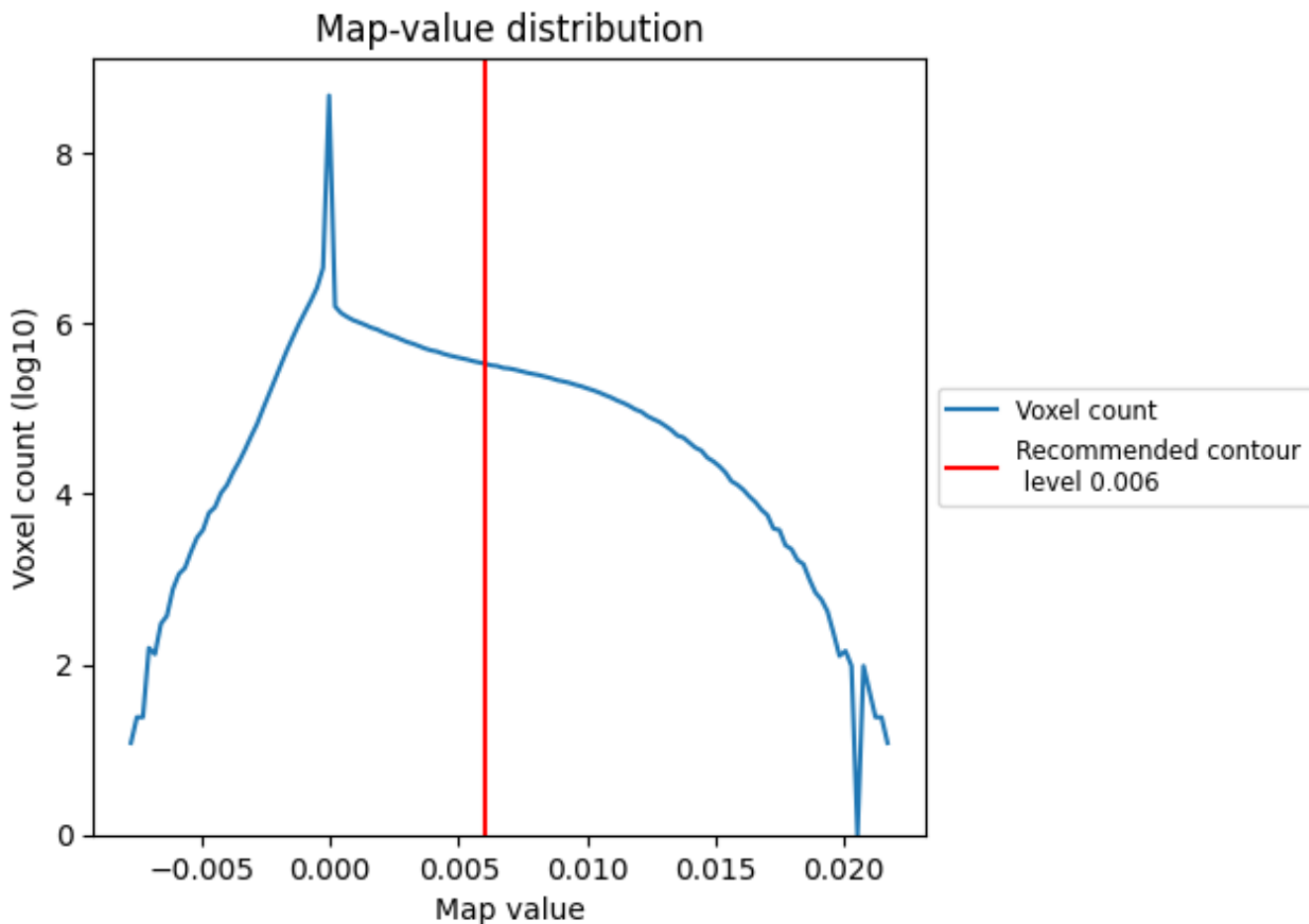
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

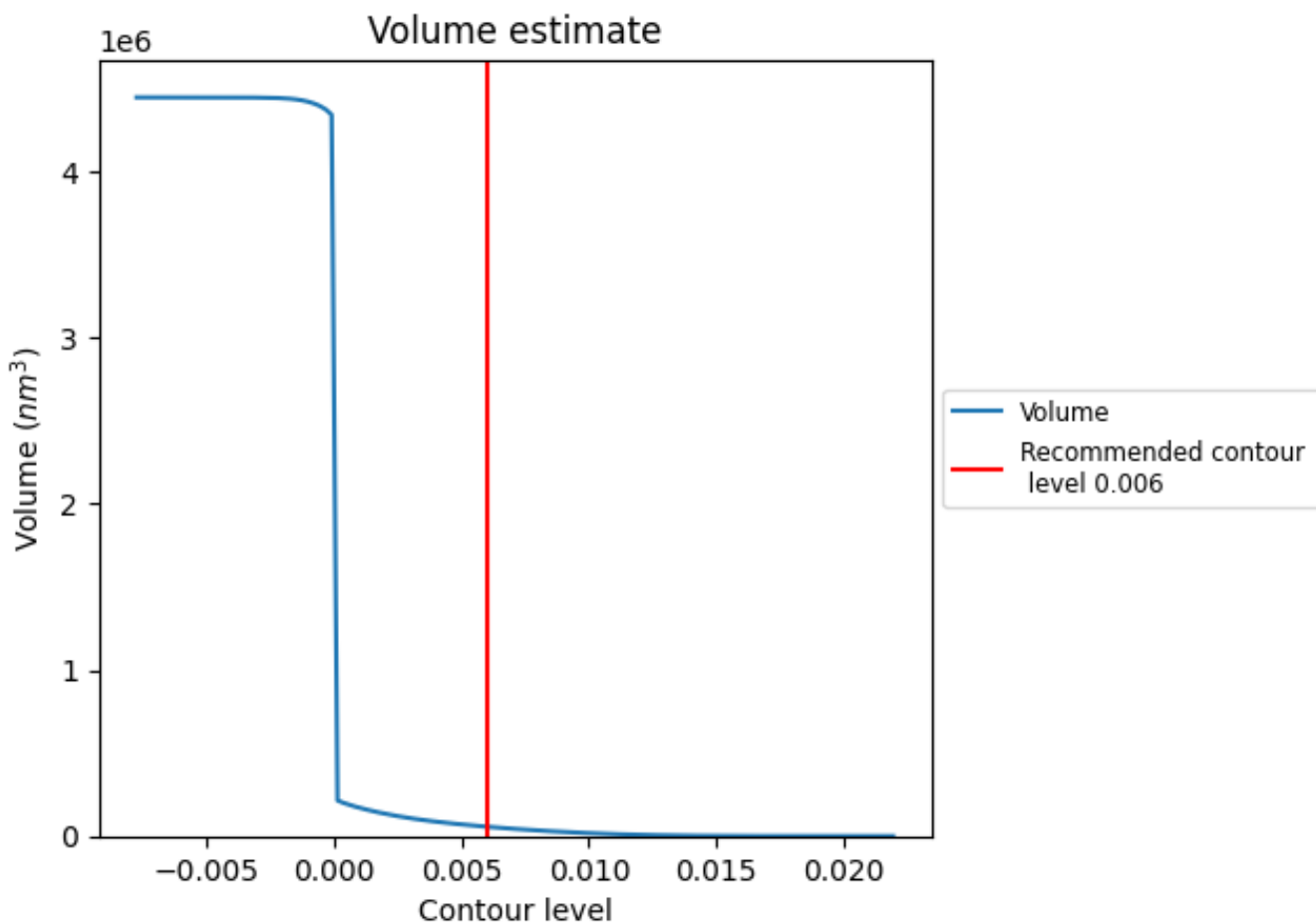
This section contains the results of statistical analysis of the map.

### 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](#)

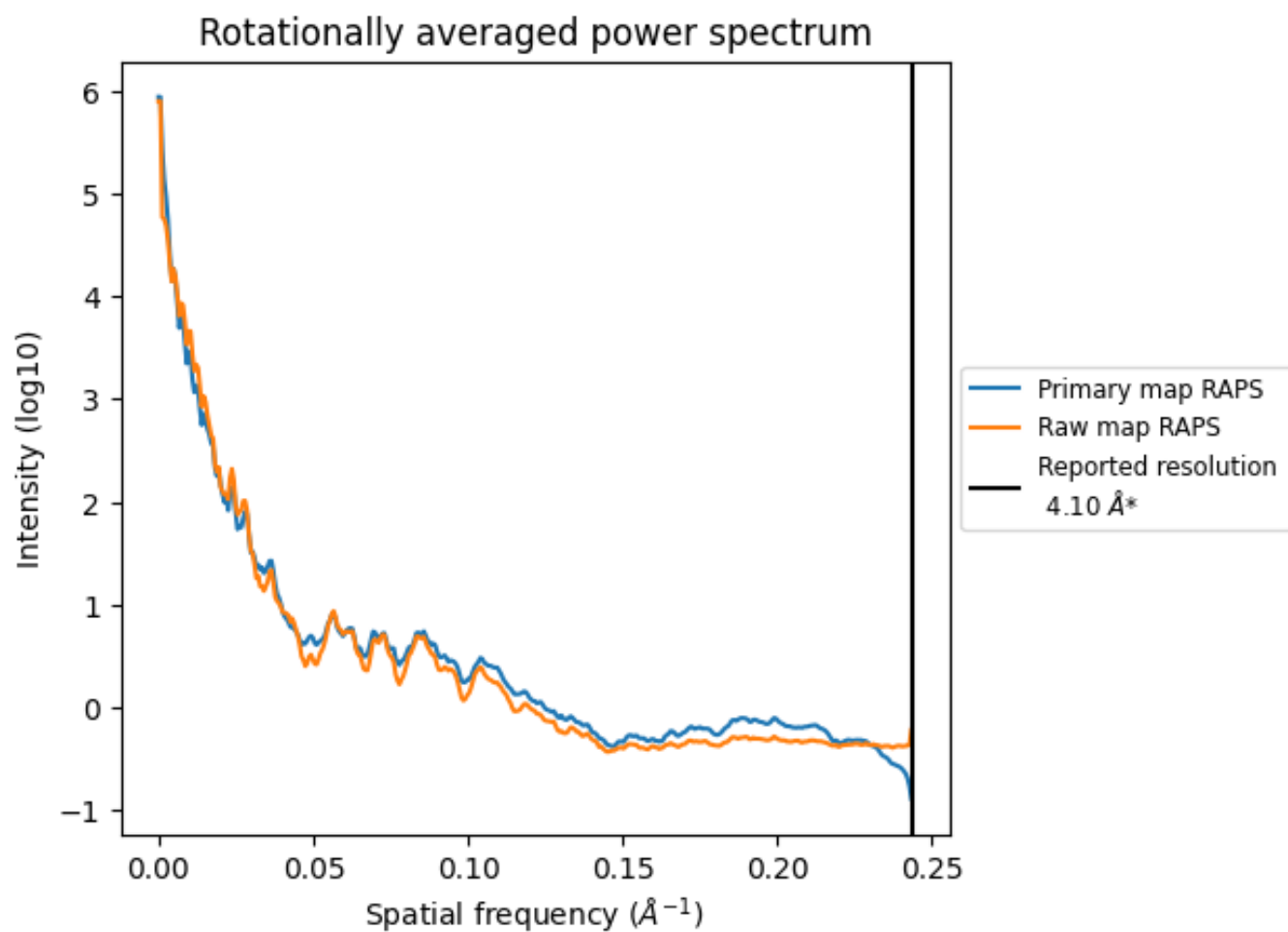


The volume at the recommended contour level is  $56255 \text{ nm}^3$ ; this corresponds to an approximate mass of 50817 kDa.

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

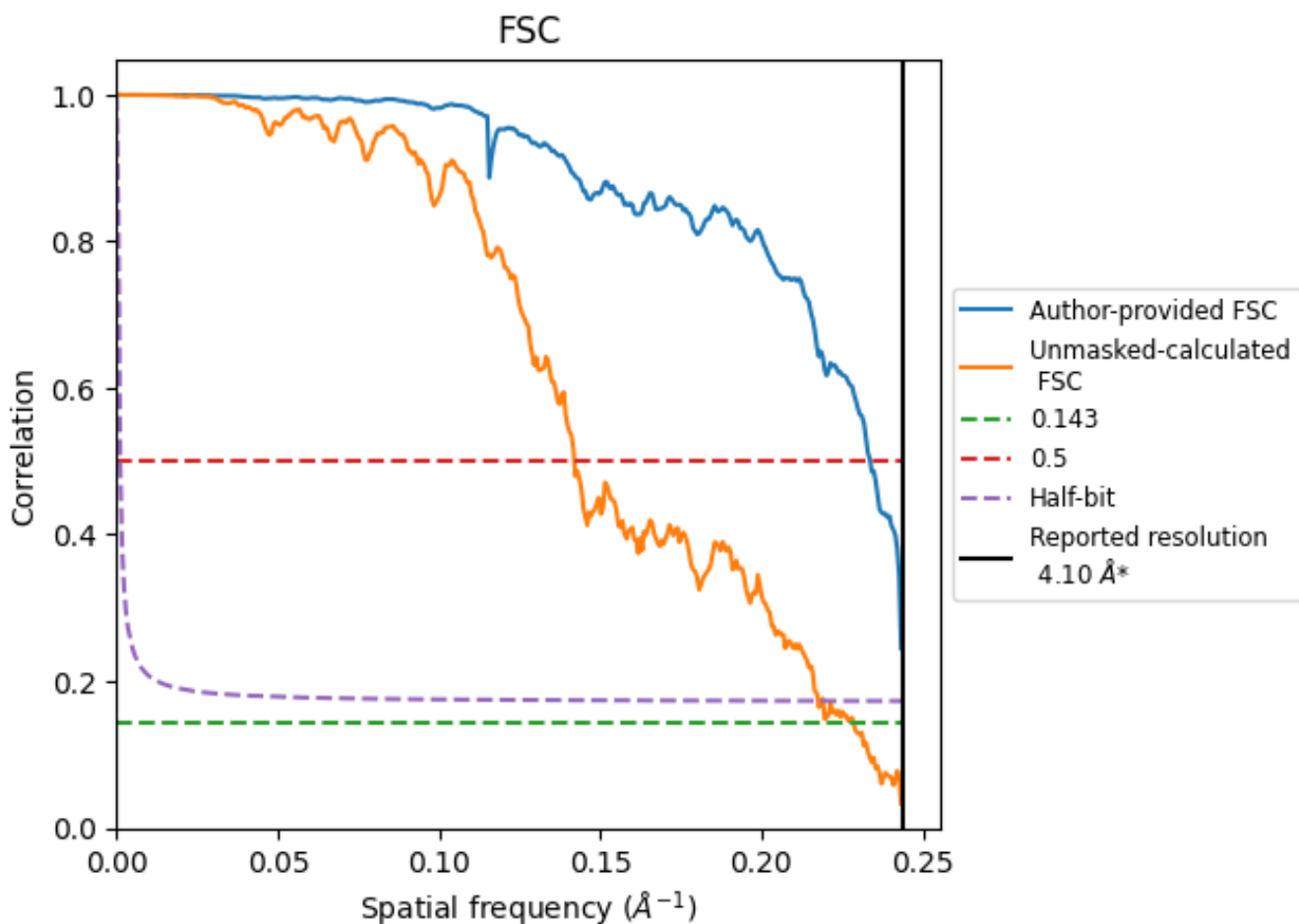


\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$

## 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 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

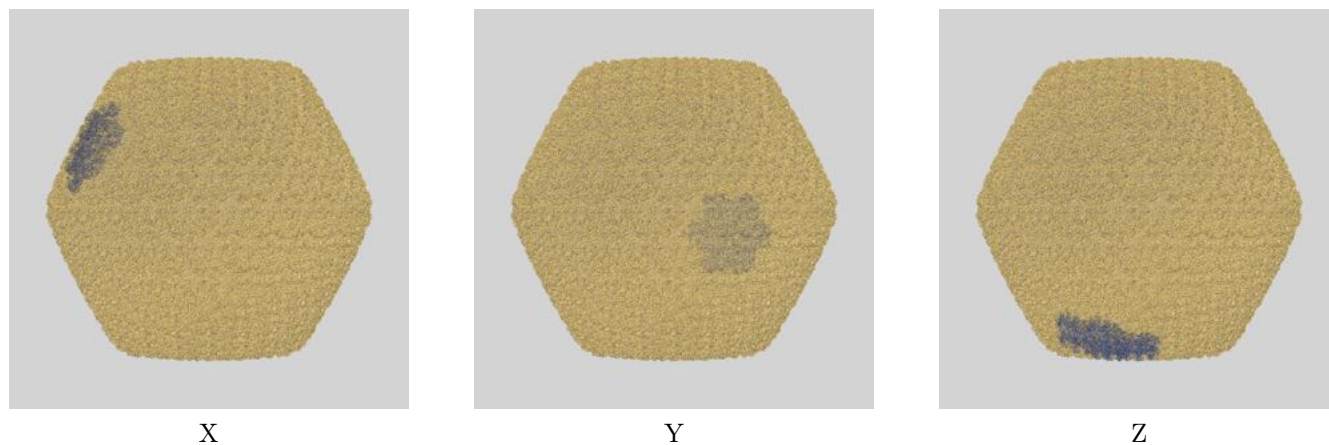
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	4.28	-
Unmasked-calculated*	4.38	7.04	4.60

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

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

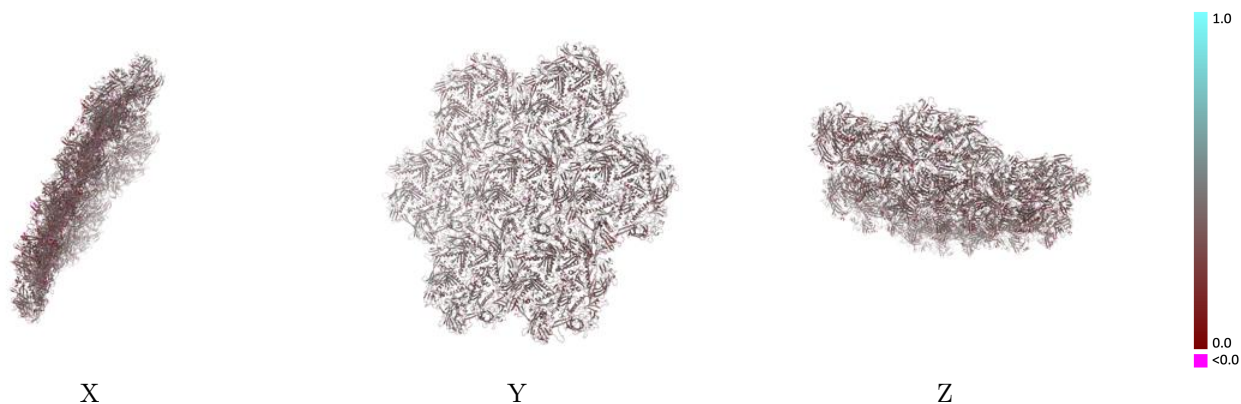
This section contains information regarding the fit between EMDB map EMD-13862 and PDB model 8BFL. Per-residue inclusion information can be found in section 3 on page 8.

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



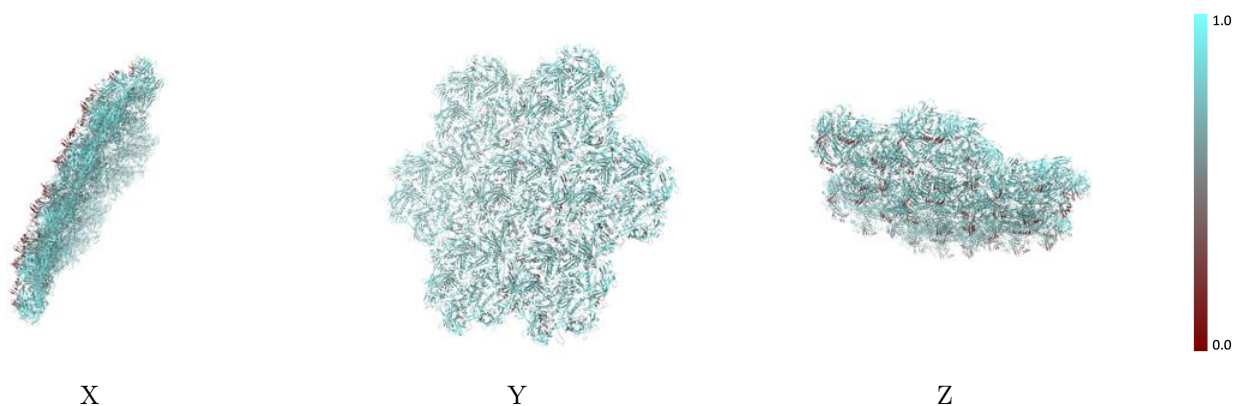
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



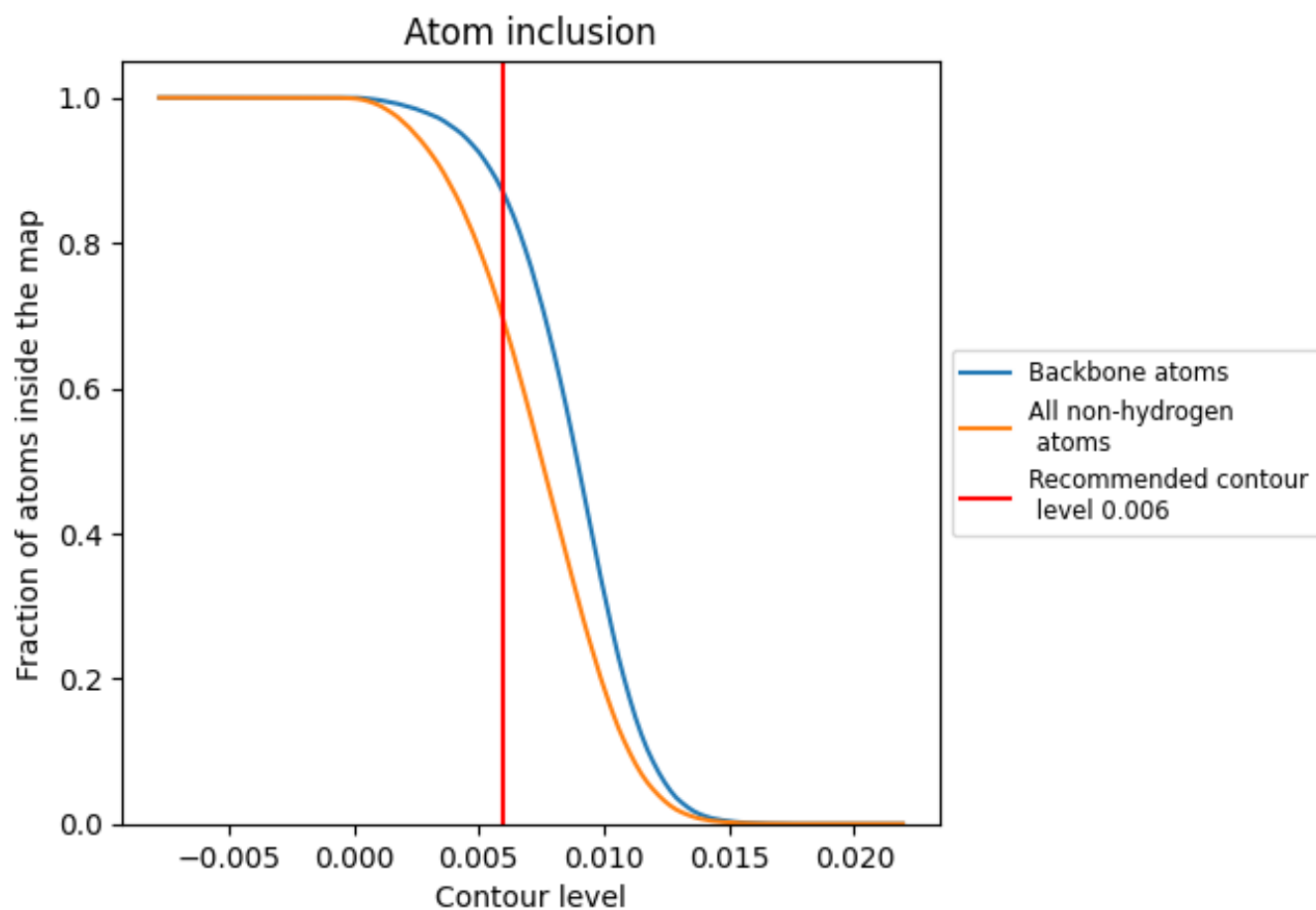
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 69% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6925	 0.3590
A	 0.6734	 0.3500
B	 0.6893	 0.3620
C	 0.6950	 0.3580
D	 0.6746	 0.3450
E	 0.6825	 0.3540
F	 0.6771	 0.3480
G	 0.6893	 0.3620
H	 0.7010	 0.3690
I	 0.7076	 0.3770
J	 0.6898	 0.3640
K	 0.6875	 0.3600
L	 0.7085	 0.3720
M	 0.6857	 0.3580
N	 0.6764	 0.3530
O	 0.6787	 0.3570
P	 0.6971	 0.3640
Q	 0.6714	 0.3510
R	 0.6711	 0.3570
S	 0.7023	 0.3680
T	 0.6982	 0.3680
U	 0.6930	 0.3640
V	 0.7089	 0.3740
W	 0.7073	 0.3740
X	 0.6923	 0.3580
Y	 0.7126	 0.3710
Z	 0.7071	 0.3570
a	 0.6971	 0.3560
b	 0.7117	 0.3720
c	 0.7135	 0.3670
d	 0.6985	 0.3510
e	 0.6893	 0.3500
f	 0.6648	 0.3330
g	 0.6825	 0.3460
h	 0.6873	 0.3450



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Chain	Atom inclusion	Q-score
i	 0.6782	 0.3420
j	 0.6784	 0.3370
k	 0.6955	 0.3600
l	 0.7148	 0.3680
m	 0.7119	 0.3700
n	 0.6880	 0.3520
o	 0.6912	 0.3550
p	 0.7057	 0.3580