Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 04:13 pm GMT

PDB ID	:	8BFP
EMDB ID	:	EMD-13862
Title	:	Jumbo Phage phi-kp24 empty capsid pentamer 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

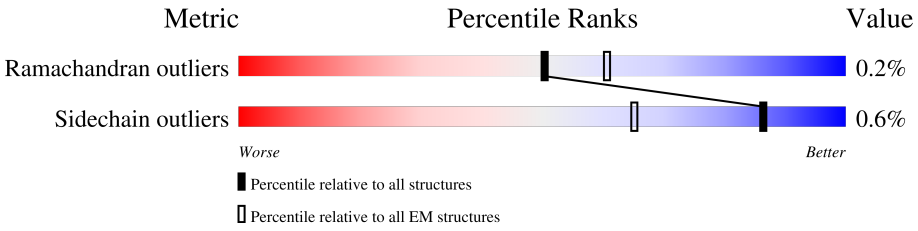
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 >=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 <=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	26% 100%
1	B	570	22% 100%
1	C	570	24% 99%
1	D	570	24% 99%
1	E	570	24% 99%
1	G	570	11% 98%
1	H	570	13% 99%
1	I	570	9% 99%
1	J	570	14% 99%

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Mol	Chain	Length	Quality of chain
1	K	570	16% 99%
1	L	570	12% 99%
1	M	570	11% 99%
1	N	570	11% 99%
1	O	570	12% 100%
1	P	570	15% 99%
1	Q	570	11% 99%
1	R	570	15% 98%
1	S	570	12% 99%
1	T	570	14% 99%
1	U	570	14% 99%
1	V	570	11% 99%
1	W	570	11% 99%
1	X	570	11% 99%
1	Y	570	14% 98%
1	Z	570	14% 99%
1	a	570	10% 99%
1	b	570	9% 99%
1	c	570	11% 99%
1	d	570	10% 99%
1	e	570	14% 99%
1	f	570	9% 99%
1	g	570	11% 99%
1	h	570	9% 99%
1	i	570	13% 99%

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Mol	Chain	Length	Quality of chain
1	j	570	9% 99%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 156905 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
1	A	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	B	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	C	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	D	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	E	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	G	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	H	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	I	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	J	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	K	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	L	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	M	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	N	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	O	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	P	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	Q	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		
1	R	570	Total	C	N	O	S	0	0
			4483	2835	761	873	14		

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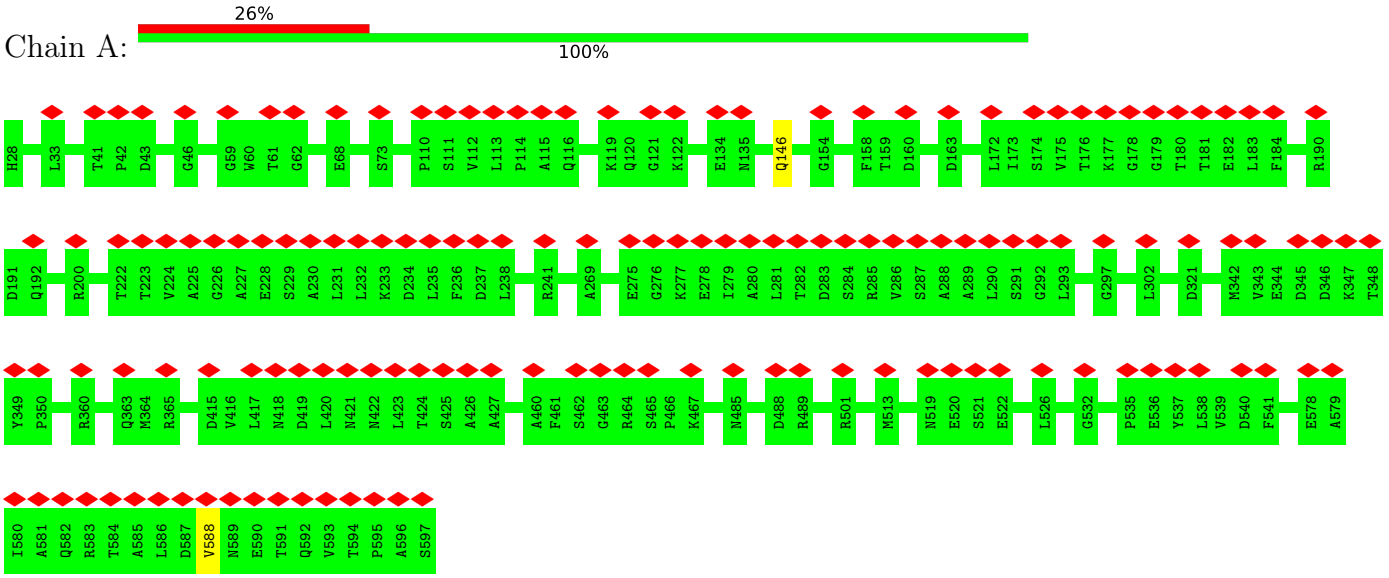
Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	T	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	U	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	V	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	W	570	Total 4483	C 2835	N 761	O 873	S 14	0	0
1	X	570	Total 4483	C 2835	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

3 Residue-property plots (i)

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

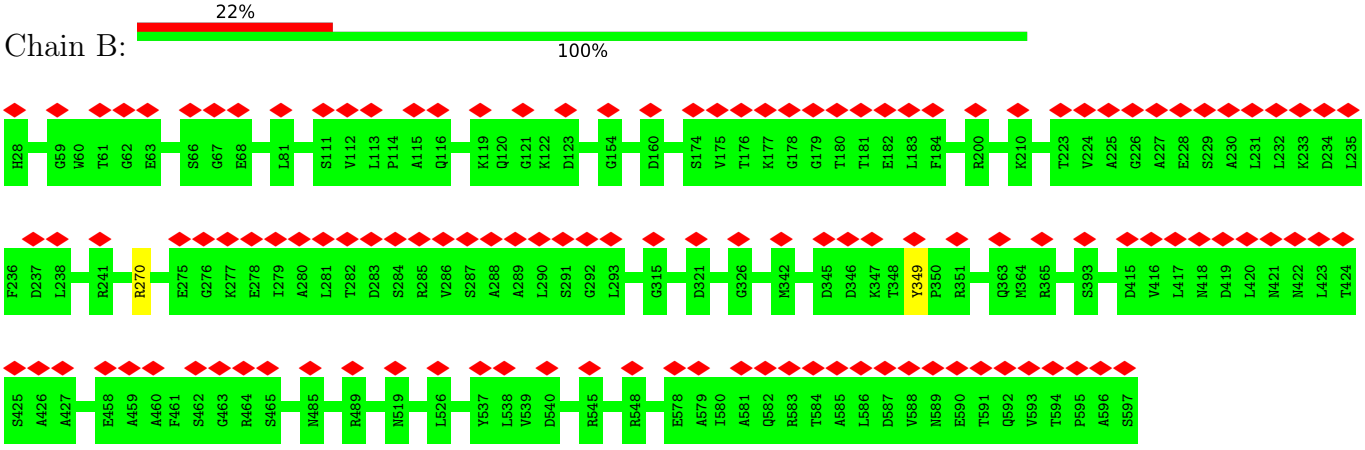
• Molecule 1: Major head protein

Chain A:



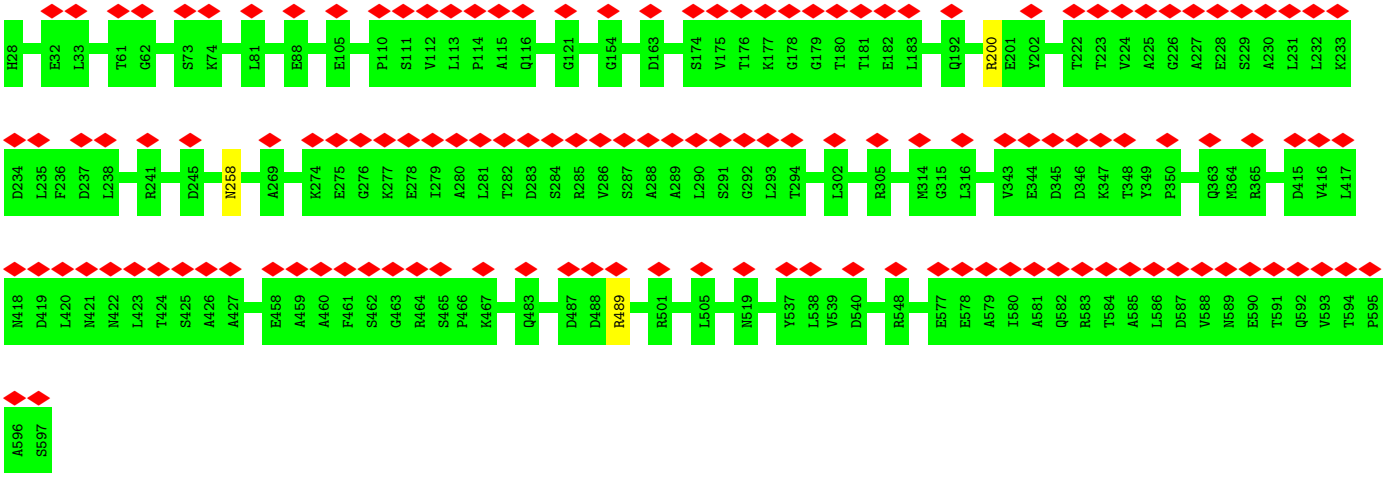
• Molecule 1: Major head protein

Chain B:



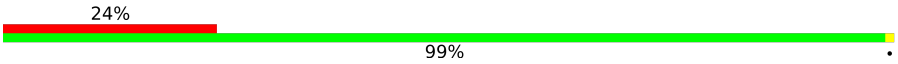
• Molecule 1: Major head protein

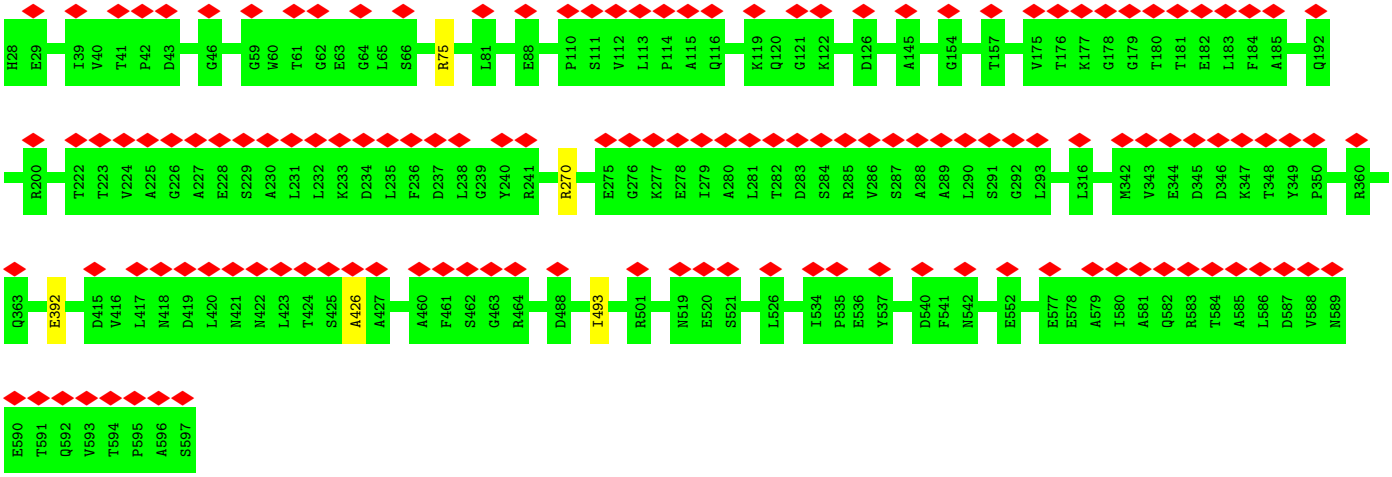
Chain C:



• Molecule 1: Major head protein

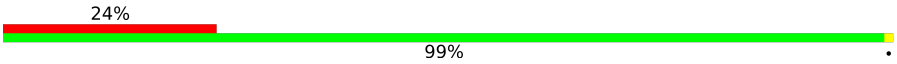
Chain D:

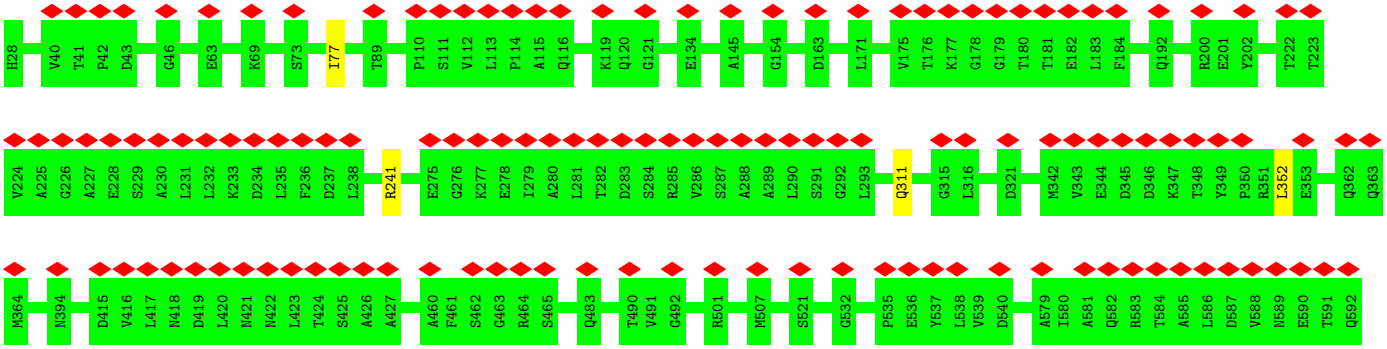


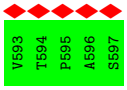


• Molecule 1: Major head protein

Chain E:

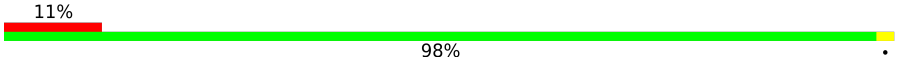


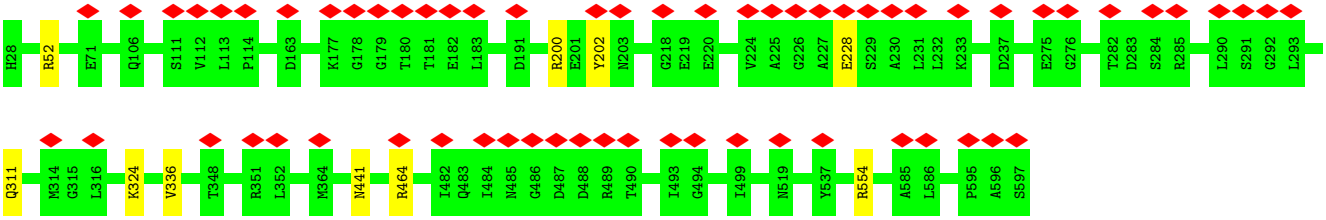




• Molecule 1: Major head protein

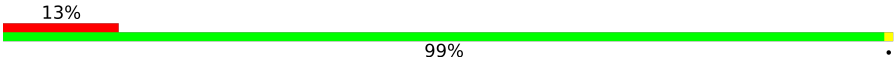
Chain G:

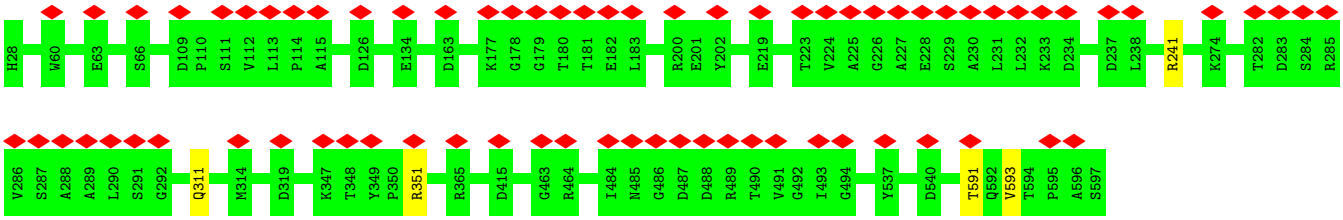




• Molecule 1: Major head protein

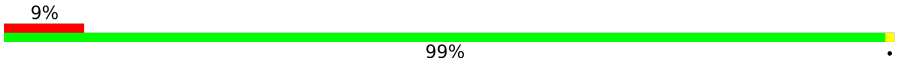
Chain H:

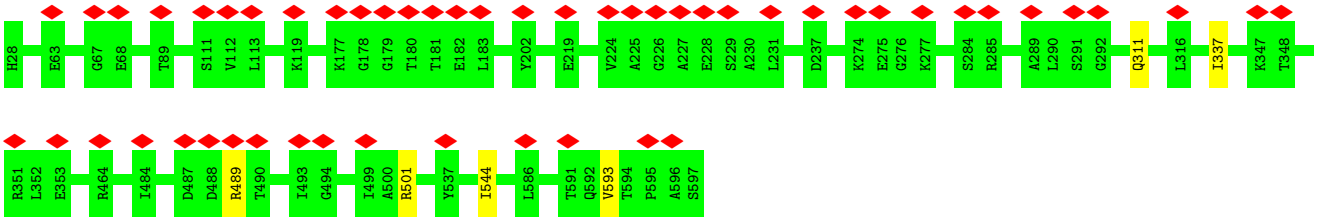




• Molecule 1: Major head protein

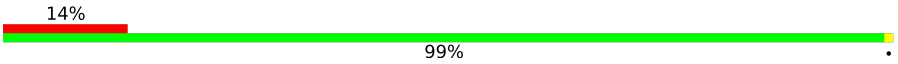
Chain I:

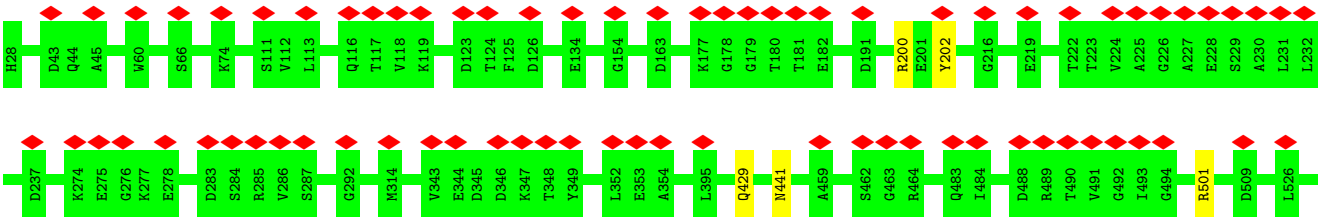


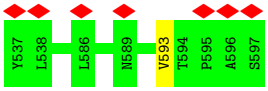


• Molecule 1: Major head protein

Chain J:

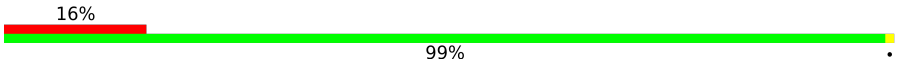


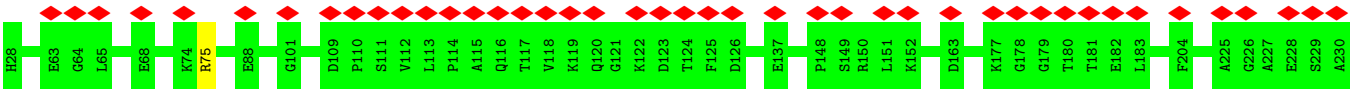


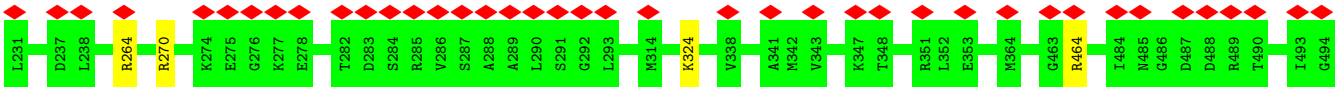


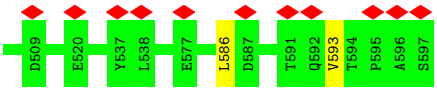
• Molecule 1: Major head protein

Chain K:



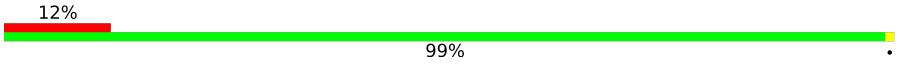


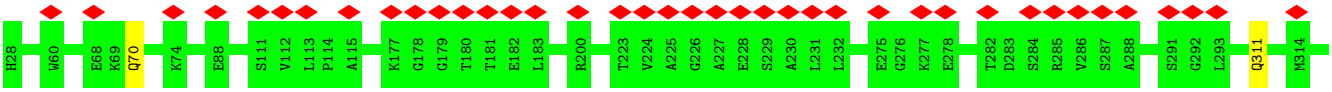


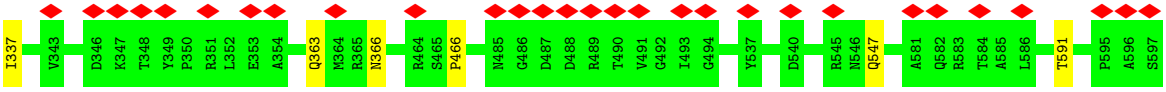


• Molecule 1: Major head protein

Chain L:

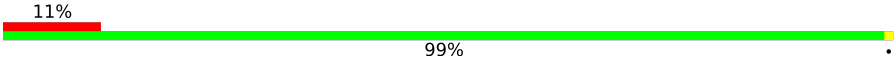


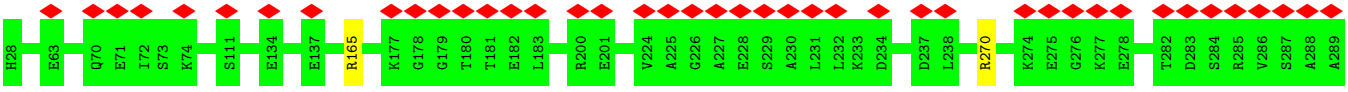


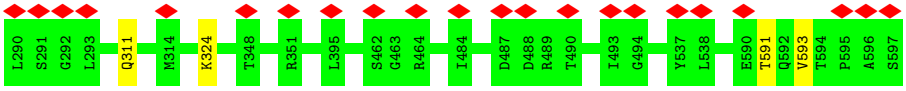


• Molecule 1: Major head protein

Chain M:

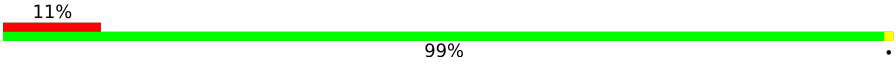


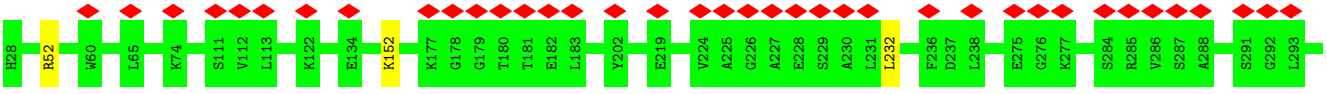


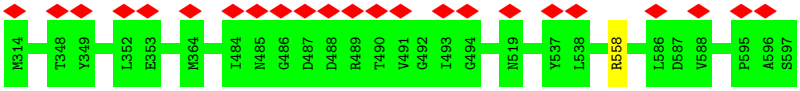


• Molecule 1: Major head protein

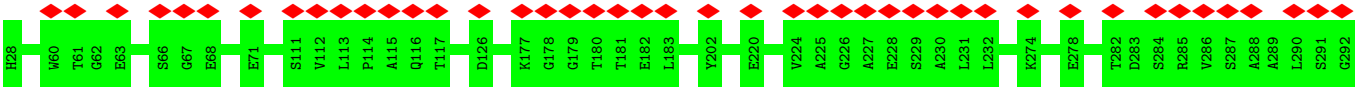
Chain N:

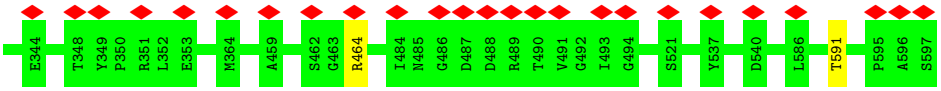




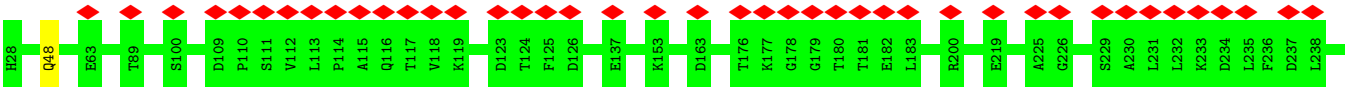


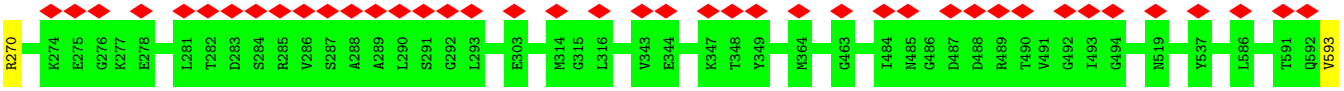
• Molecule 1: Major head protein



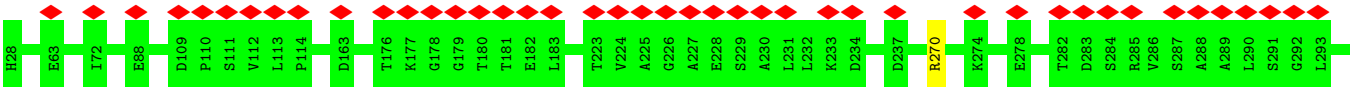


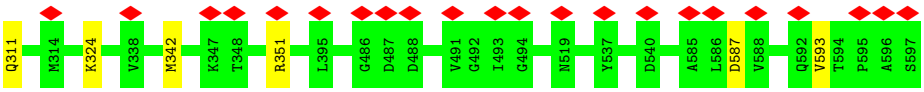
• Molecule 1: Major head protein



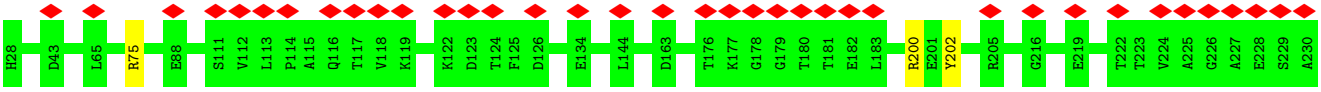


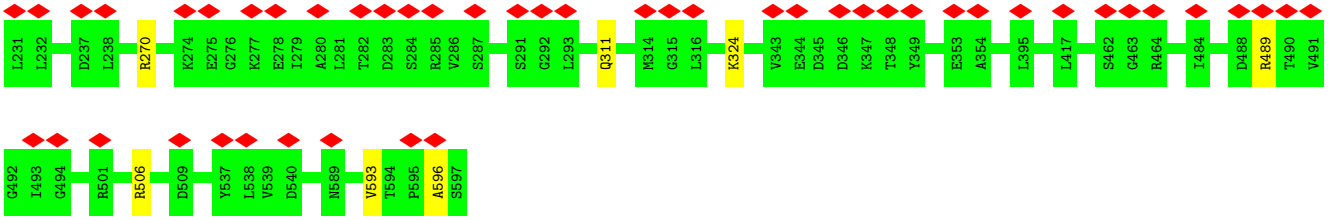
• Molecule 1: Major head protein





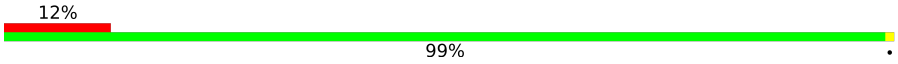
• Molecule 1: Major head protein

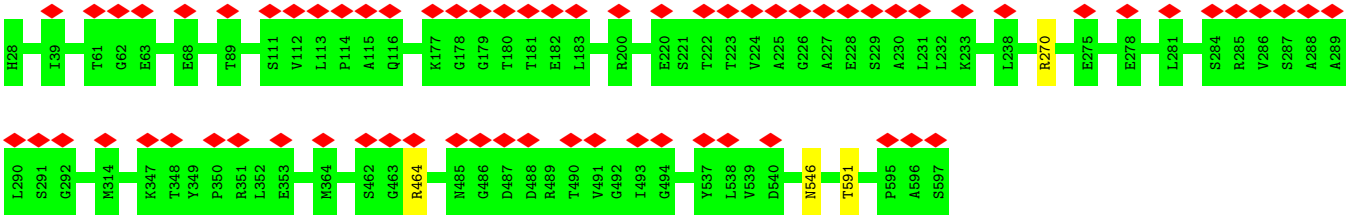




• Molecule 1: Major head protein

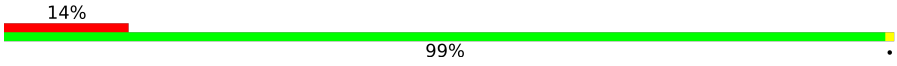
Chain S:

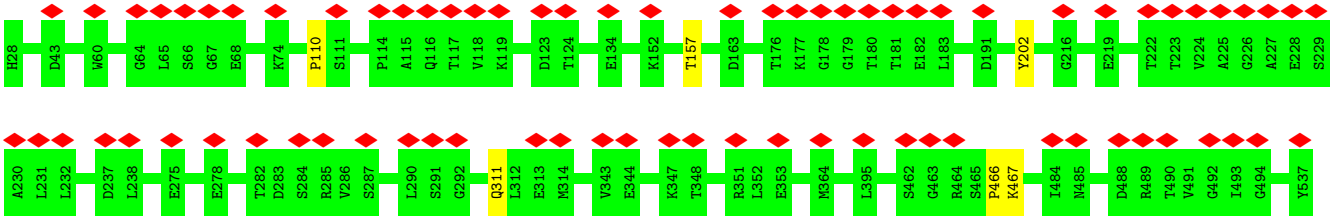




• Molecule 1: Major head protein

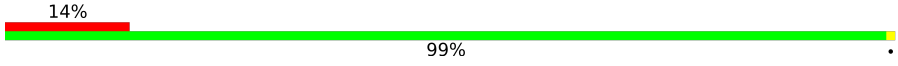
Chain T:

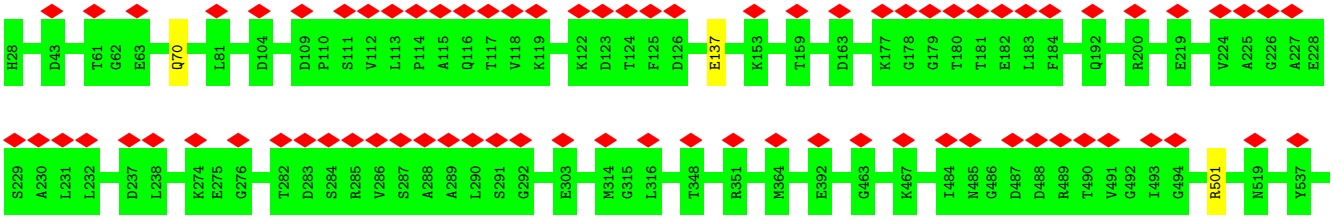




• Molecule 1: Major head protein

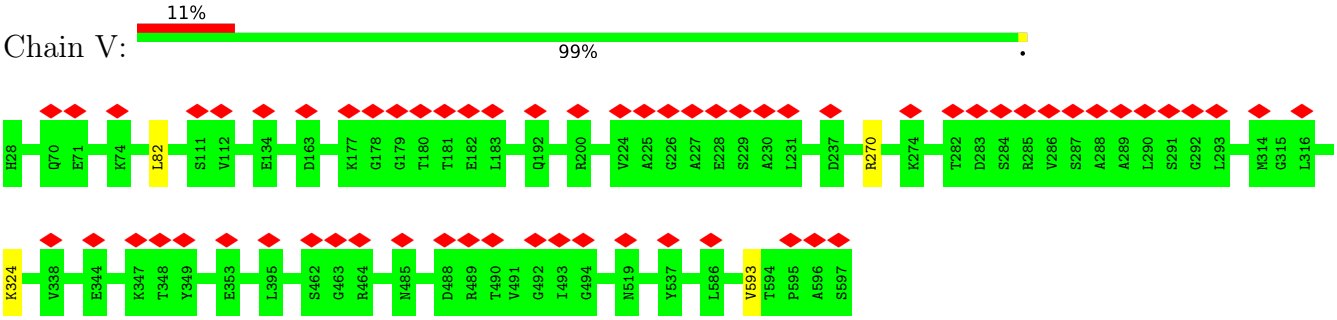
Chain U:





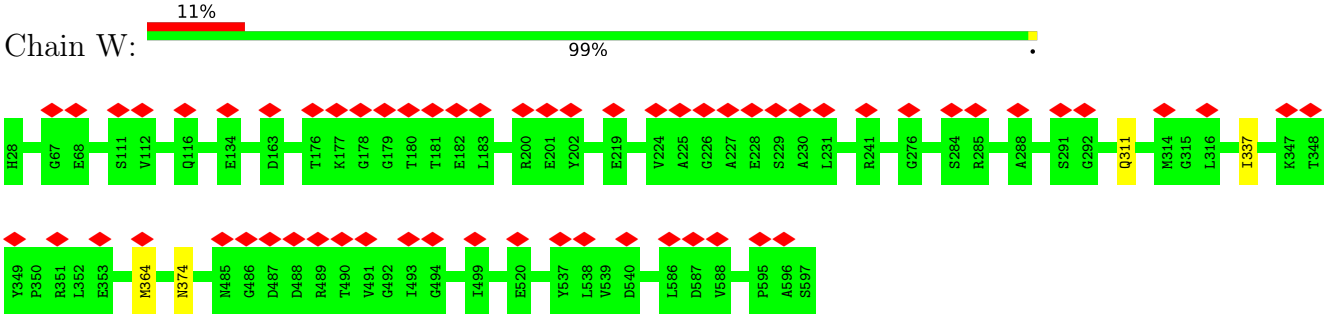
• Molecule 1: Major head protein

Chain V:



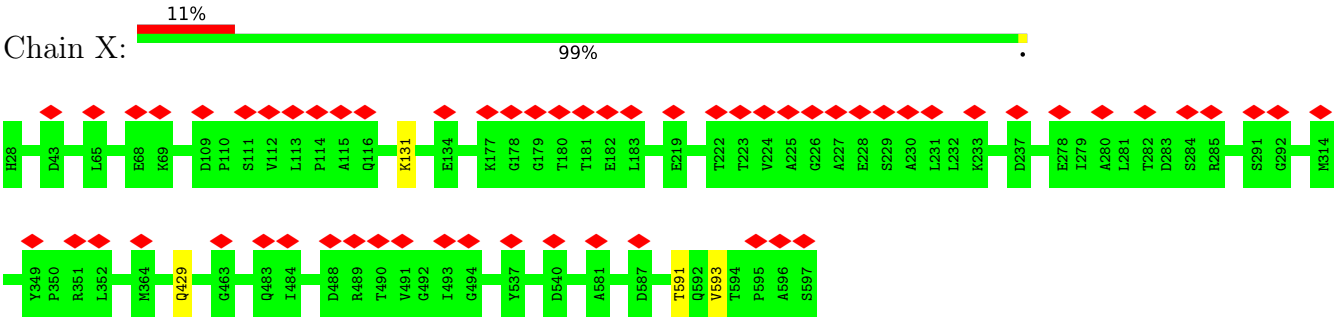
• Molecule 1: Major head protein

Chain W:



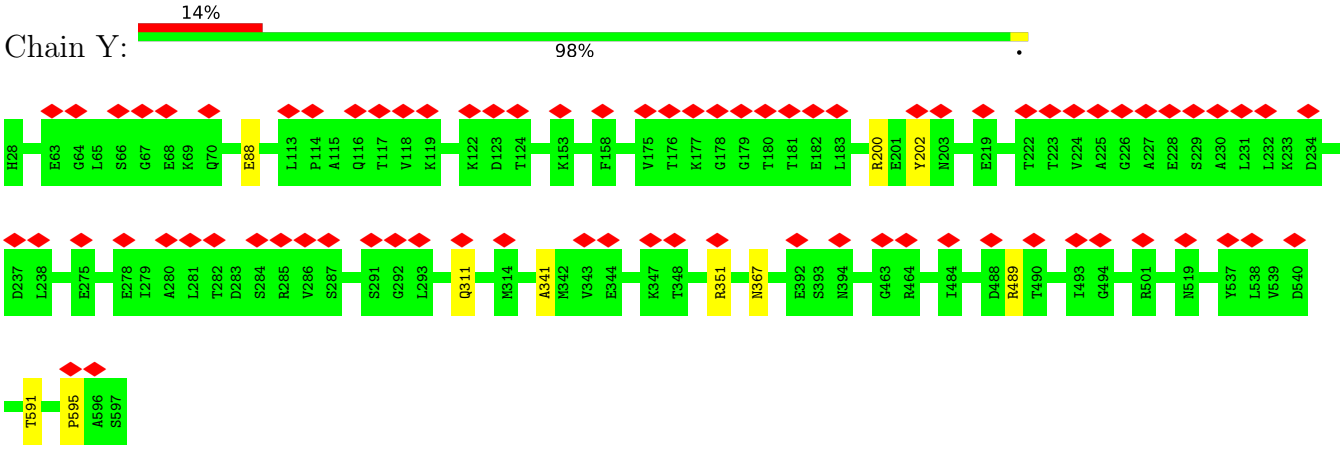
• Molecule 1: Major head protein

Chain X:



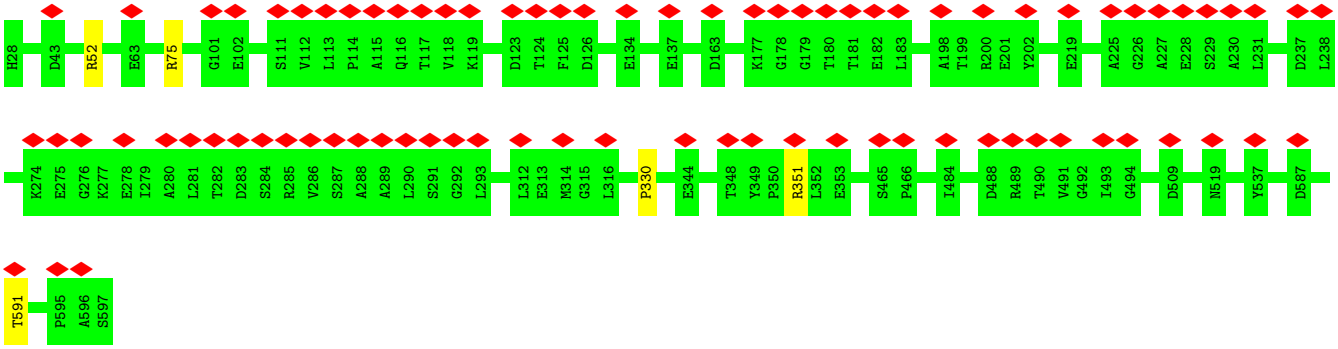
• Molecule 1: Major head protein

Chain Y:

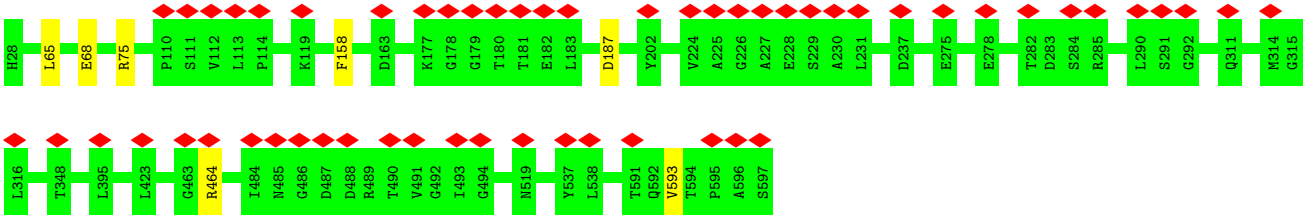


• Molecule 1: Major head protein

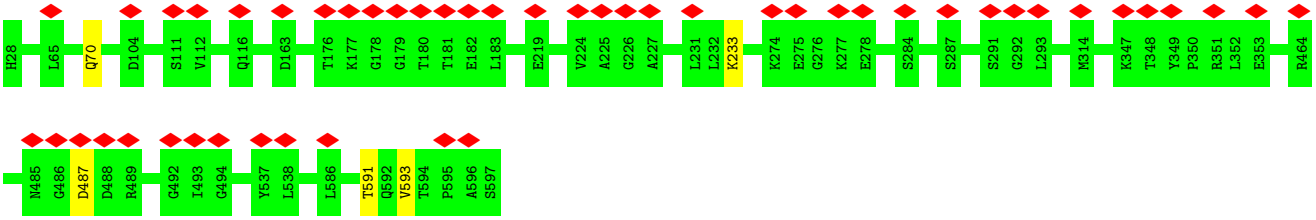
Chain Z:



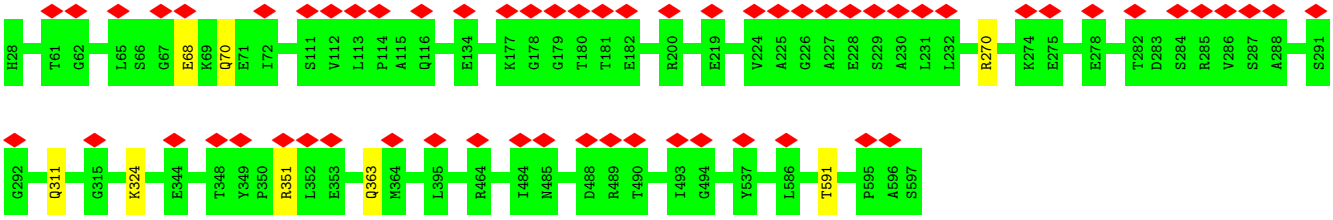
• Molecule 1: Major head protein



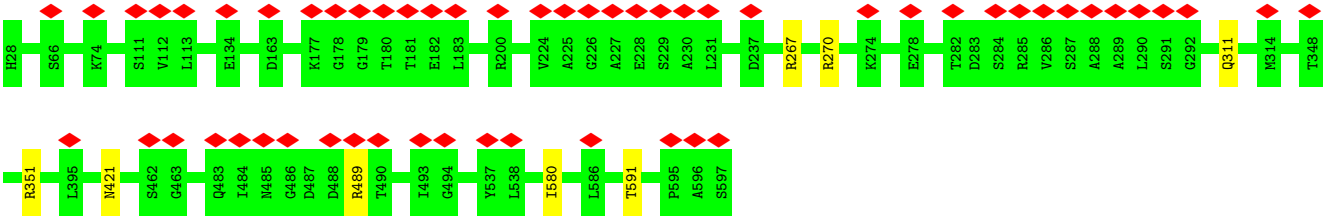
• Molecule 1: Major head protein



• Molecule 1: Major head protein

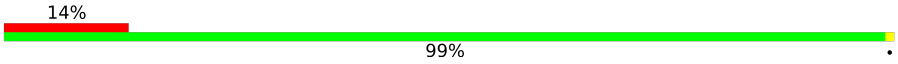


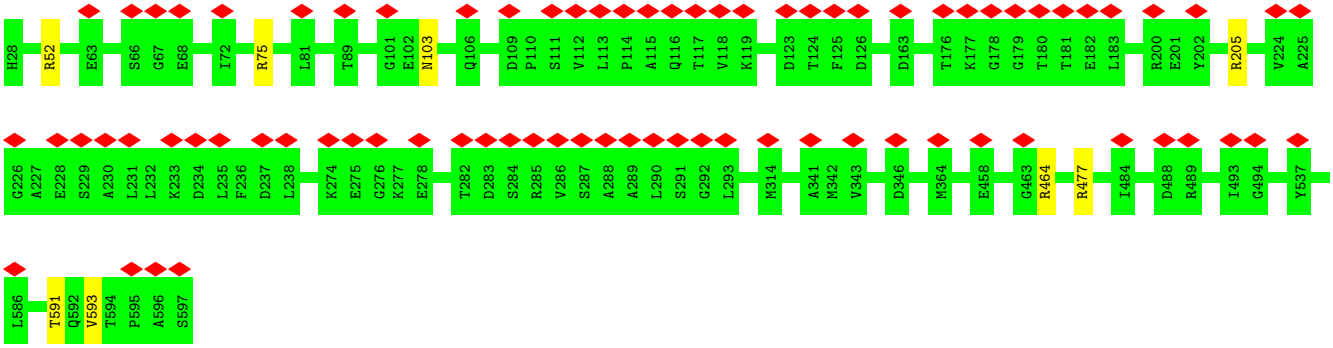
• Molecule 1: Major head protein



• Molecule 1: Major head protein

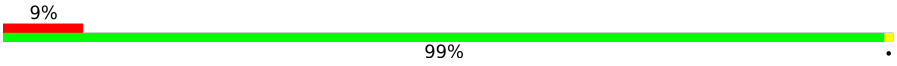
Chain e:

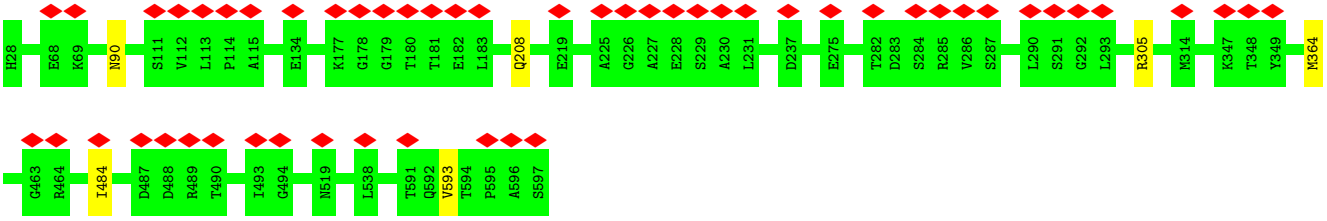




• Molecule 1: Major head protein

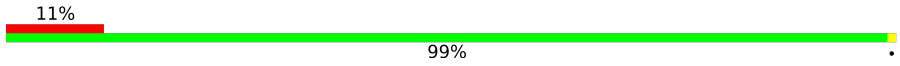
Chain f:

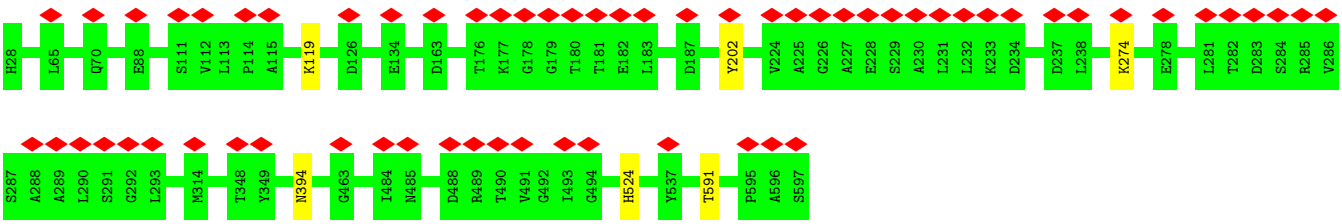




• Molecule 1: Major head protein

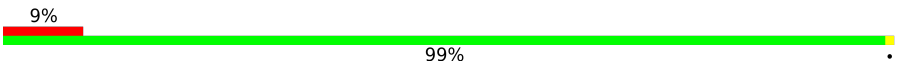
Chain g:

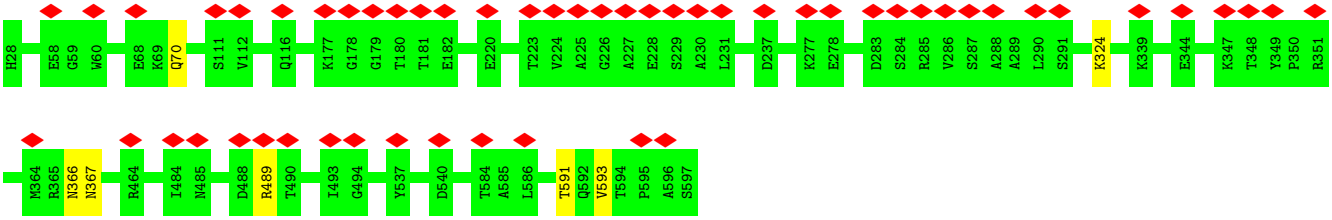




• Molecule 1: Major head protein

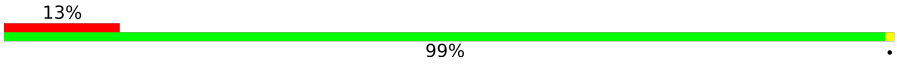
Chain h:

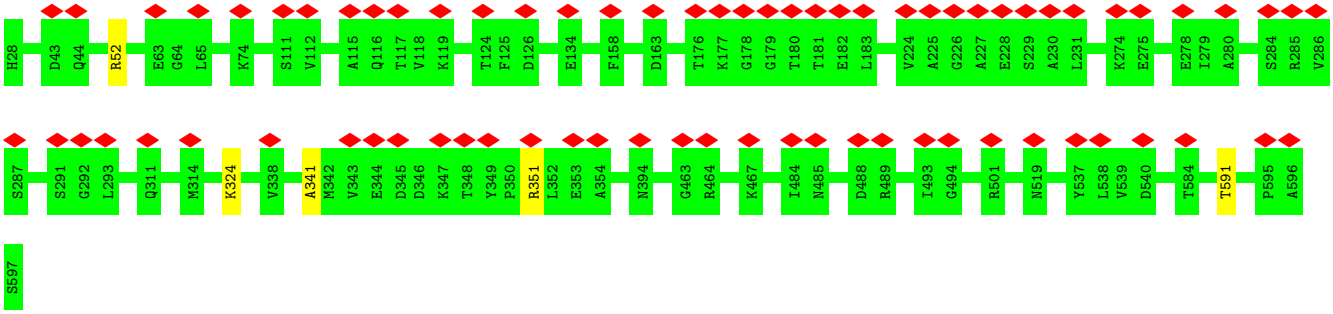




• Molecule 1: Major head protein

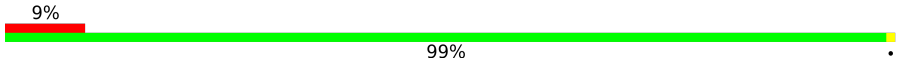
Chain i:

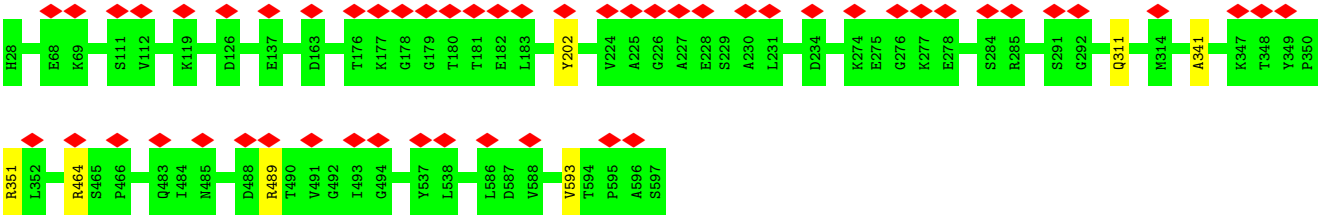




• Molecule 1: Major head protein

Chain j:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19193	Depositor
Resolution determination method	FSC 0.33 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.55	0/6184
1	B	0.29	0/4559	0.55	0/6184
1	C	0.29	0/4559	0.56	0/6184
1	D	0.29	0/4559	0.55	0/6184
1	E	0.29	0/4559	0.53	0/6184
1	G	0.29	0/4559	0.56	0/6184
1	H	0.30	1/4559 (0.0%)	0.55	0/6184
1	I	0.28	0/4559	0.54	1/6184 (0.0%)
1	J	0.29	0/4559	0.57	1/6184 (0.0%)
1	K	0.29	0/4559	0.58	1/6184 (0.0%)
1	L	0.29	0/4559	0.55	1/6184 (0.0%)
1	M	0.30	0/4559	0.56	1/6184 (0.0%)
1	N	0.28	0/4559	0.55	1/6184 (0.0%)
1	O	0.30	0/4559	0.55	0/6184
1	P	0.28	0/4559	0.55	1/6184 (0.0%)
1	Q	0.29	0/4559	0.56	2/6184 (0.0%)
1	R	0.30	0/4559	0.57	1/6184 (0.0%)
1	S	0.29	0/4559	0.54	0/6184
1	T	0.30	1/4559 (0.0%)	0.56	1/6184 (0.0%)
1	U	0.29	0/4559	0.55	1/6184 (0.0%)
1	V	0.28	0/4559	0.55	2/6184 (0.0%)
1	W	0.29	0/4559	0.56	1/6184 (0.0%)
1	X	0.28	0/4559	0.55	1/6184 (0.0%)
1	Y	0.28	0/4559	0.55	0/6184
1	Z	0.34	1/4559 (0.0%)	0.59	3/6184 (0.0%)
1	a	0.30	0/4559	0.57	3/6184 (0.0%)
1	b	0.28	0/4559	0.56	1/6184 (0.0%)
1	c	0.29	0/4559	0.56	0/6184
1	d	0.29	0/4559	0.54	0/6184
1	e	0.29	0/4559	0.56	1/6184 (0.0%)
1	f	0.29	0/4559	0.57	2/6184 (0.0%)
1	g	0.29	0/4559	0.55	0/6184
1	h	0.29	0/4559	0.56	1/6184 (0.0%)
1	i	0.29	0/4559	0.54	0/6184

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	j	0.29	0/4559	0.58	1/6184 (0.0%)
All	All	0.29	3/159565 (0.0%)	0.56	28/216440 (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	G	0	2
1	H	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	O	0	1
1	S	0	1
1	T	0	2
1	X	0	1
1	Y	0	2
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	g	0	1
1	h	0	1
1	i	0	2
1	j	0	1
All	All	0	24

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	330	PRO	CG-CD	-11.91	1.11	1.50
1	H	593	VAL	C-N	-5.73	1.20	1.34
1	T	466	PRO	C-N	-5.71	1.21	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	j	593	VAL	C-N-CA	16.53	163.02	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	330	PRO	N-CD-CG	-14.30	81.75	103.20
1	e	593	VAL	C-N-CA	11.52	150.51	121.70
1	h	593	VAL	C-N-CA	10.61	148.22	121.70
1	K	593	VAL	C-N-CA	8.81	143.73	121.70
1	U	593	VAL	C-N-CA	8.66	143.34	121.70
1	Z	330	PRO	CA-N-CD	-8.51	99.59	111.50
1	M	593	VAL	C-N-CA	7.76	141.11	121.70
1	J	593	VAL	C-N-CA	7.71	140.97	121.70
1	Z	330	PRO	CA-CB-CG	-7.35	90.04	104.00
1	X	593	VAL	C-N-CA	6.95	139.09	121.70
1	R	593	VAL	C-N-CA	6.62	138.26	121.70
1	f	593	VAL	C-N-CA	6.52	137.99	121.70
1	a	187	ASP	CB-CG-OD1	6.30	123.97	118.30
1	V	593	VAL	C-N-CA	6.13	137.04	121.70
1	b	593	VAL	C-N-CA	6.13	137.03	121.70
1	I	593	VAL	C-N-CA	5.92	136.49	121.70
1	N	232	LEU	CA-CB-CG	5.85	128.75	115.30
1	L	466	PRO	C-N-CA	-5.84	107.10	121.70
1	a	65	LEU	CA-CB-CG	5.63	128.25	115.30
1	T	110	PRO	CA-N-CD	-5.55	103.73	111.50
1	a	593	VAL	C-N-CA	5.53	135.52	121.70
1	Q	342	MET	CA-CB-CG	5.51	122.67	113.30
1	V	82	LEU	CA-CB-CG	5.32	127.54	115.30
1	P	593	VAL	C-N-CA	5.29	134.92	121.70
1	W	364	MET	CG-SD-CE	-5.28	91.75	100.20
1	Q	593	VAL	C-N-CA	5.20	134.69	121.70
1	f	364	MET	CA-CB-CG	5.07	121.91	113.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	336	VAL	Peptide
1	G	554	ARG	Sidechain
1	H	591	THR	Peptide
1	K	586	LEU	Peptide
1	L	591	THR	Peptide
1	M	591	THR	Peptide
1	O	591	THR	Peptide
1	S	591	THR	Peptide
1	T	157	THR	Peptide
1	T	591	THR	Peptide

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Mol	Chain	Res	Type	Group
1	X	591	THR	Peptide
1	Y	341	ALA	Peptide
1	Y	591	THR	Peptide
1	Z	591	THR	Peptide
1	a	158	PHE	Peptide
1	b	591	THR	Peptide
1	c	591	THR	Peptide
1	d	591	THR	Peptide
1	e	591	THR	Peptide
1	g	591	THR	Peptide
1	h	591	THR	Peptide
1	i	341	ALA	Peptide
1	i	591	THR	Peptide
1	j	341	ALA	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/570 (100%)	543 (96%)	23 (4%)	2 (0%)	34	71
1	B	568/570 (100%)	541 (95%)	26 (5%)	1 (0%)	47	80
1	C	568/570 (100%)	538 (95%)	30 (5%)	0	100	100
1	D	568/570 (100%)	537 (94%)	29 (5%)	2 (0%)	34	71
1	E	568/570 (100%)	541 (95%)	25 (4%)	2 (0%)	34	71
1	G	568/570 (100%)	525 (92%)	40 (7%)	3 (0%)	29	67
1	H	568/570 (100%)	532 (94%)	35 (6%)	1 (0%)	47	80
1	I	568/570 (100%)	526 (93%)	40 (7%)	2 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	568/570 (100%)	535 (94%)	32 (6%)	1 (0%)	47 80
1	K	568/570 (100%)	532 (94%)	36 (6%)	0	100 100
1	L	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34 71
1	M	568/570 (100%)	525 (92%)	42 (7%)	1 (0%)	47 80
1	N	568/570 (100%)	536 (94%)	32 (6%)	0	100 100
1	O	568/570 (100%)	524 (92%)	44 (8%)	0	100 100
1	P	568/570 (100%)	526 (93%)	42 (7%)	0	100 100
1	Q	568/570 (100%)	526 (93%)	40 (7%)	2 (0%)	34 71
1	R	568/570 (100%)	524 (92%)	41 (7%)	3 (0%)	29 67
1	S	568/570 (100%)	526 (93%)	42 (7%)	0	100 100
1	T	568/570 (100%)	521 (92%)	45 (8%)	2 (0%)	34 71
1	U	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34 71
1	V	568/570 (100%)	528 (93%)	40 (7%)	0	100 100
1	W	568/570 (100%)	524 (92%)	43 (8%)	1 (0%)	47 80
1	X	568/570 (100%)	531 (94%)	37 (6%)	0	100 100
1	Y	568/570 (100%)	524 (92%)	40 (7%)	4 (1%)	22 60
1	Z	568/570 (100%)	531 (94%)	37 (6%)	0	100 100
1	a	568/570 (100%)	529 (93%)	38 (7%)	1 (0%)	47 80
1	b	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34 71
1	c	568/570 (100%)	527 (93%)	38 (7%)	3 (0%)	29 67
1	d	568/570 (100%)	519 (91%)	48 (8%)	1 (0%)	47 80
1	e	568/570 (100%)	538 (95%)	29 (5%)	1 (0%)	47 80
1	f	568/570 (100%)	528 (93%)	40 (7%)	0	100 100
1	g	568/570 (100%)	532 (94%)	34 (6%)	2 (0%)	34 71
1	h	568/570 (100%)	530 (93%)	36 (6%)	2 (0%)	34 71
1	i	568/570 (100%)	538 (95%)	30 (5%)	0	100 100
1	j	568/570 (100%)	522 (92%)	44 (8%)	2 (0%)	34 71
All	All	19880/19950 (100%)	18549 (93%)	1286 (6%)	45 (0%)	50 80

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	588	VAL

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Mol	Chain	Res	Type
1	R	202	TYR
1	R	596	ALA
1	W	311	GLN
1	e	477	ARG
1	A	146	GLN
1	D	426	ALA
1	U	70	GLN
1	a	68	GLU
1	c	311	GLN
1	E	311	GLN
1	J	202	TYR
1	T	202	TYR
1	Y	88	GLU
1	Y	311	GLN
1	g	202	TYR
1	j	202	TYR
1	G	202	TYR
1	G	311	GLN
1	I	311	GLN
1	I	489	ARG
1	L	311	GLN
1	U	137	GLU
1	Y	202	TYR
1	d	311	GLN
1	g	394	ASN
1	h	489	ARG
1	j	311	GLN
1	D	392	GLU
1	Q	311	GLN
1	R	311	GLN
1	b	70	GLN
1	h	70	GLN
1	E	352	LEU
1	G	228	GLU
1	H	311	GLN
1	L	70	GLN
1	M	311	GLN
1	Q	587	ASP
1	T	311	GLN
1	b	487	ASP
1	c	68	GLU
1	c	70	GLN

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Mol	Chain	Res	Type
1	B	349	TYR
1	Y	595	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%)	492 (100%)	0	100	100
1	B	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	C	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	D	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	E	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	G	492/492 (100%)	487 (99%)	5 (1%)	76	85
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%)	487 (99%)	5 (1%)	76	85
1	L	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	M	492/492 (100%)	489 (99%)	3 (1%)	86	92
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%)	490 (100%)	2 (0%)	91	94
1	Q	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	R	492/492 (100%)	486 (99%)	6 (1%)	71	83
1	S	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	T	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	U	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	V	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	W	492/492 (100%)	490 (100%)	2 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	Y	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	Z	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	a	492/492 (100%)	490 (100%)	2 (0%)	91	94
1	b	492/492 (100%)	491 (100%)	1 (0%)	93	96
1	c	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	d	492/492 (100%)	486 (99%)	6 (1%)	71	83
1	e	492/492 (100%)	487 (99%)	5 (1%)	76	85
1	f	492/492 (100%)	488 (99%)	4 (1%)	81	88
1	g	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	h	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	i	492/492 (100%)	489 (99%)	3 (1%)	86	92
1	j	492/492 (100%)	489 (99%)	3 (1%)	86	92
All	All	17220/17220 (100%)	17118 (99%)	102 (1%)	86	92

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	270	ARG
1	C	200	ARG
1	C	258	ASN
1	C	489	ARG
1	D	75	ARG
1	D	270	ARG
1	D	493	ILE
1	E	77	ILE
1	E	241	ARG
1	G	52	ARG
1	G	200	ARG
1	G	324	LYS
1	G	441	ASN
1	G	464	ARG
1	H	241	ARG
1	H	351	ARG
1	I	337	ILE
1	I	501	ARG
1	I	544	ILE

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Mol	Chain	Res	Type
1	J	200	ARG
1	J	429	GLN
1	J	441	ASN
1	J	501	ARG
1	K	75	ARG
1	K	264	ARG
1	K	270	ARG
1	K	324	LYS
1	K	464	ARG
1	L	337	ILE
1	L	363	GLN
1	L	366	ASN
1	L	547	GLN
1	M	165	ARG
1	M	270	ARG
1	M	324	LYS
1	N	52	ARG
1	N	152	LYS
1	N	558	ARG
1	O	464	ARG
1	P	48	GLN
1	P	270	ARG
1	Q	270	ARG
1	Q	324	LYS
1	Q	351	ARG
1	R	75	ARG
1	R	200	ARG
1	R	270	ARG
1	R	324	LYS
1	R	489	ARG
1	R	506	ARG
1	S	270	ARG
1	S	464	ARG
1	S	546	ASN
1	T	467	LYS
1	U	501	ARG
1	V	270	ARG
1	V	324	LYS
1	W	337	ILE
1	W	374	ASN
1	X	131	LYS
1	X	429	GLN

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Mol	Chain	Res	Type
1	Y	200	ARG
1	Y	351	ARG
1	Y	367	ASN
1	Y	489	ARG
1	Z	52	ARG
1	Z	75	ARG
1	Z	351	ARG
1	a	75	ARG
1	a	464	ARG
1	b	233	LYS
1	c	270	ARG
1	c	324	LYS
1	c	351	ARG
1	c	363	GLN
1	d	267	ARG
1	d	270	ARG
1	d	351	ARG
1	d	421	ASN
1	d	489	ARG
1	d	580	ILE
1	e	52	ARG
1	e	75	ARG
1	e	103	ASN
1	e	205	ARG
1	e	464	ARG
1	f	90	ASN
1	f	208	GLN
1	f	305	ARG
1	f	484	ILE
1	g	119	LYS
1	g	274	LYS
1	g	524	HIS
1	h	324	LYS
1	h	366	ASN
1	h	367	ASN
1	i	52	ARG
1	i	324	LYS
1	i	351	ARG
1	j	351	ARG
1	j	464	ARG
1	j	489	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	B	140	ASN
1	B	362	GLN
1	B	363	GLN
1	C	103	ASN
1	D	140	ASN
1	D	429	GLN
1	E	70	GLN
1	E	120	GLN
1	E	433	GLN
1	E	449	GLN
1	G	192	GLN
1	G	310	ASN
1	H	192	GLN
1	H	311	GLN
1	I	120	GLN
1	I	394	ASN
1	I	592	GLN
1	J	70	GLN
1	J	363	GLN
1	K	28	HIS
1	K	527	GLN
1	L	311	GLN
1	L	483	GLN
1	L	485	ASN
1	L	547	GLN
1	L	592	GLN
1	M	103	ASN
1	M	308	ASN
1	M	394	ASN
1	N	106	GLN
1	N	363	GLN
1	N	402	GLN
1	N	441	ASN
1	N	589	ASN
1	O	394	ASN
1	O	524	HIS
1	P	106	GLN
1	P	212	HIS
1	P	402	GLN
1	P	592	GLN
1	Q	480	GLN

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Mol	Chain	Res	Type
1	Q	575	ASN
1	R	48	GLN
1	R	310	ASN
1	R	410	ASN
1	S	483	GLN
1	S	546	ASN
1	T	99	GLN
1	T	116	GLN
1	T	140	ASN
1	T	389	HIS
1	T	589	ASN
1	U	70	GLN
1	V	192	GLN
1	V	323	GLN
1	V	422	ASN
1	V	483	GLN
1	W	99	GLN
1	W	363	GLN
1	X	212	HIS
1	Y	48	GLN
1	Y	389	HIS
1	Y	483	GLN
1	Z	483	GLN
1	Z	485	ASN
1	b	433	GLN
1	b	592	GLN
1	c	48	GLN
1	c	429	GLN
1	c	433	GLN
1	d	429	GLN
1	d	449	GLN
1	e	70	GLN
1	e	140	ASN
1	e	208	GLN
1	e	212	HIS
1	e	433	GLN
1	e	485	ASN
1	f	308	ASN
1	f	433	GLN
1	g	422	ASN
1	g	527	GLN
1	g	592	GLN

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Mol	Chain	Res	Type
1	h	70	GLN
1	h	402	GLN
1	i	99	GLN
1	i	258	ASN
1	i	469	HIS
1	j	362	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 monosaccharides 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.

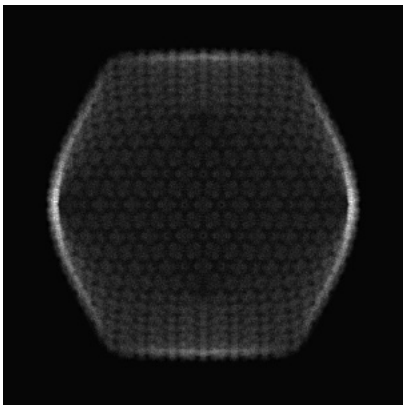
6 Map visualisation

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.

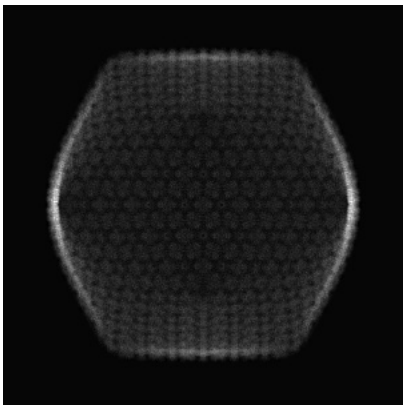
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

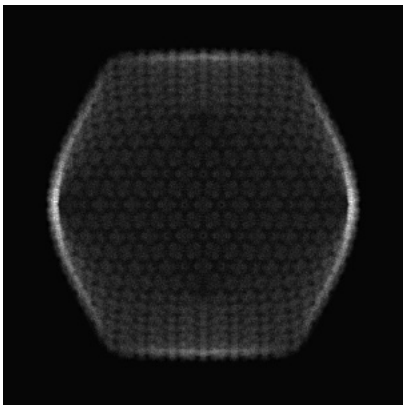
6.1.1 Primary map



X

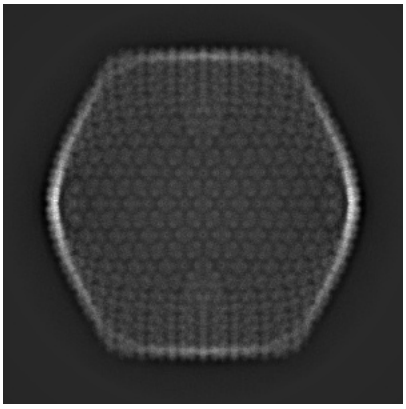


Y

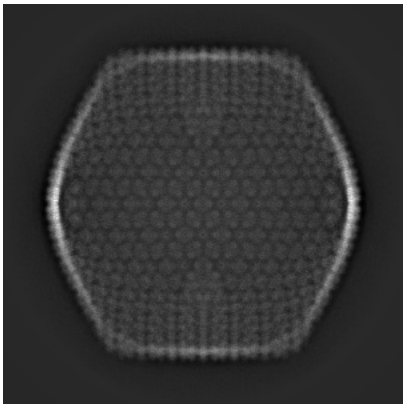


Z

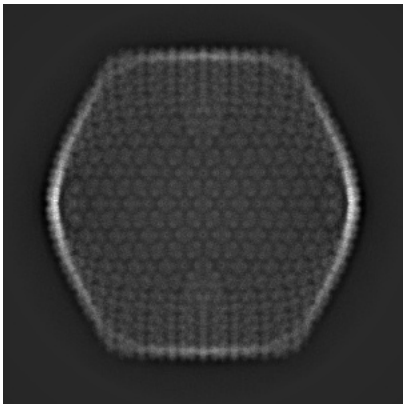
6.1.2 Raw map



X



Y

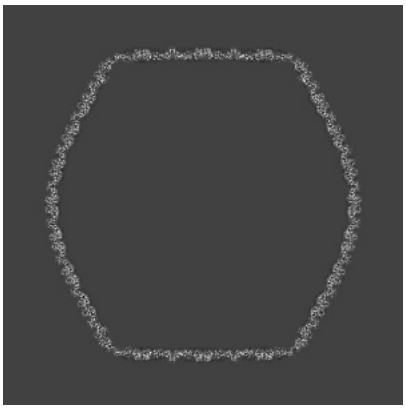


Z

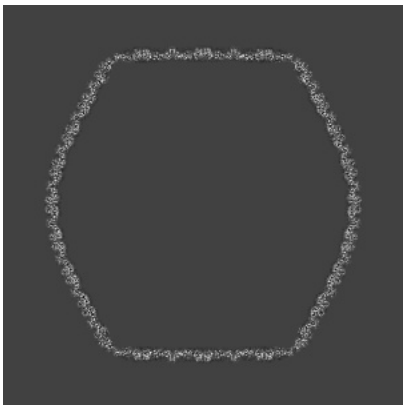
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

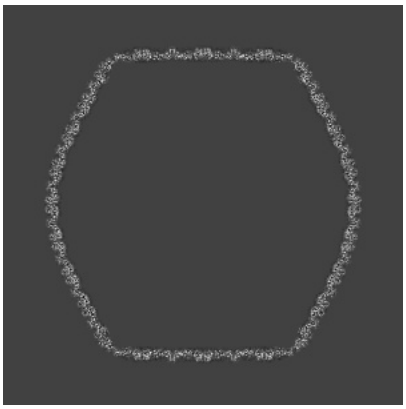
6.2.1 Primary map



X Index: 400

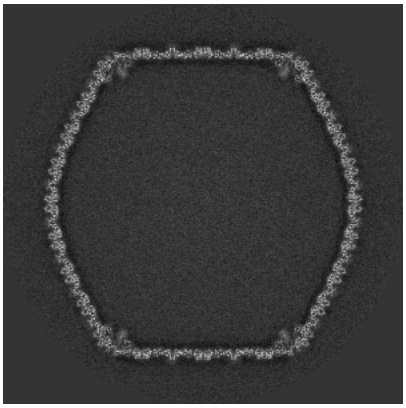


Y Index: 400

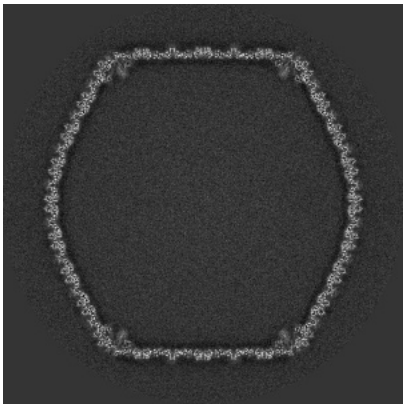


Z Index: 400

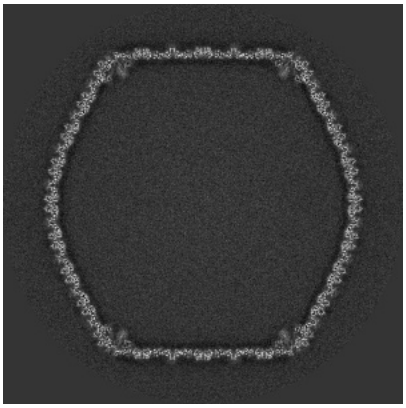
6.2.2 Raw map



X Index: 400



Y Index: 400

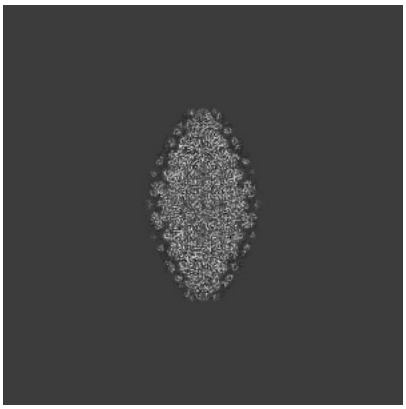


Z Index: 400

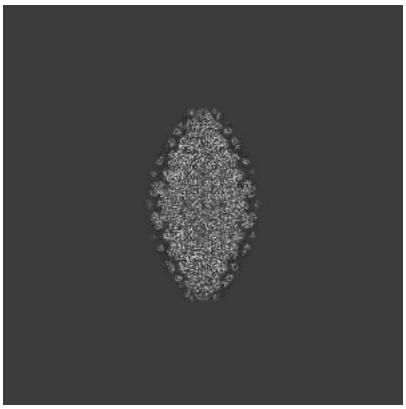
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

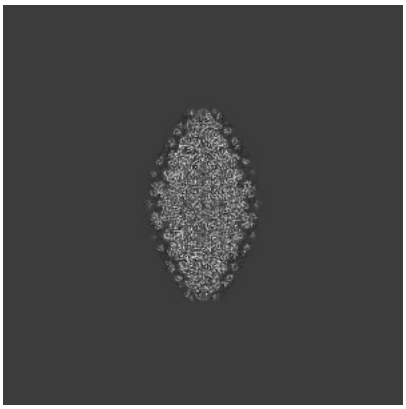
6.3.1 Primary map



X Index: 693

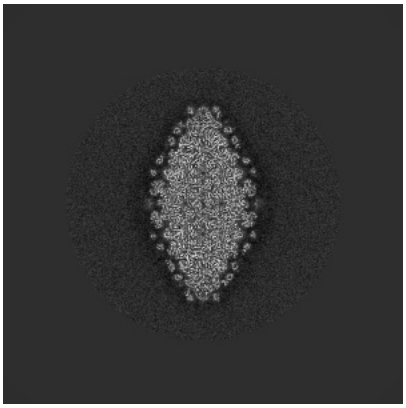


Y Index: 693

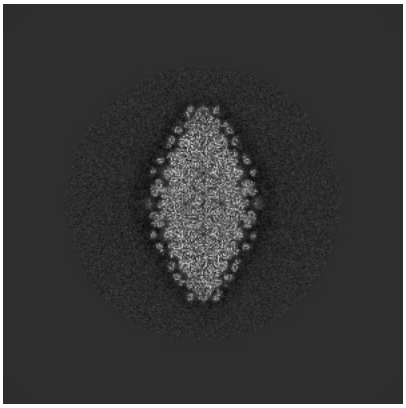


Z Index: 693

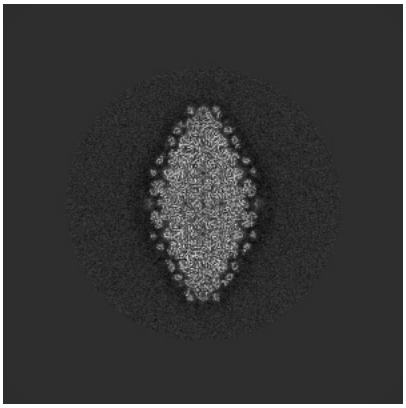
6.3.2 Raw map



X Index: 693



Y Index: 107



Z Index: 693

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

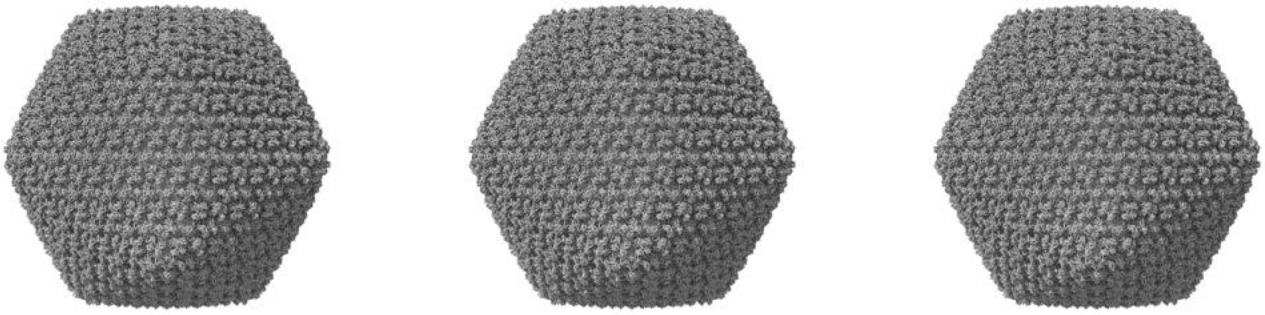
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

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



X Y Z

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.

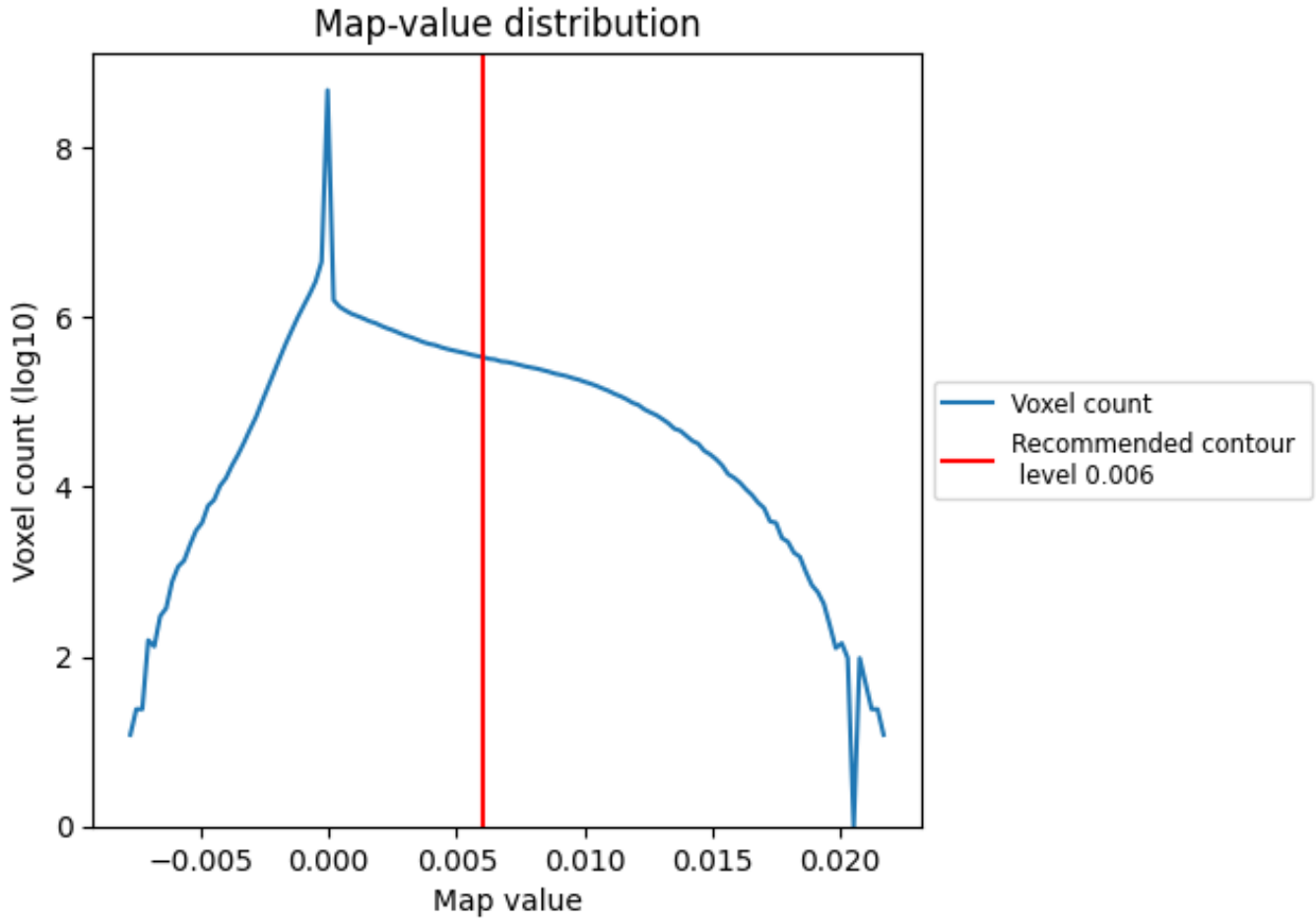
6.5 Mask visualisation (i)

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

7 Map analysis

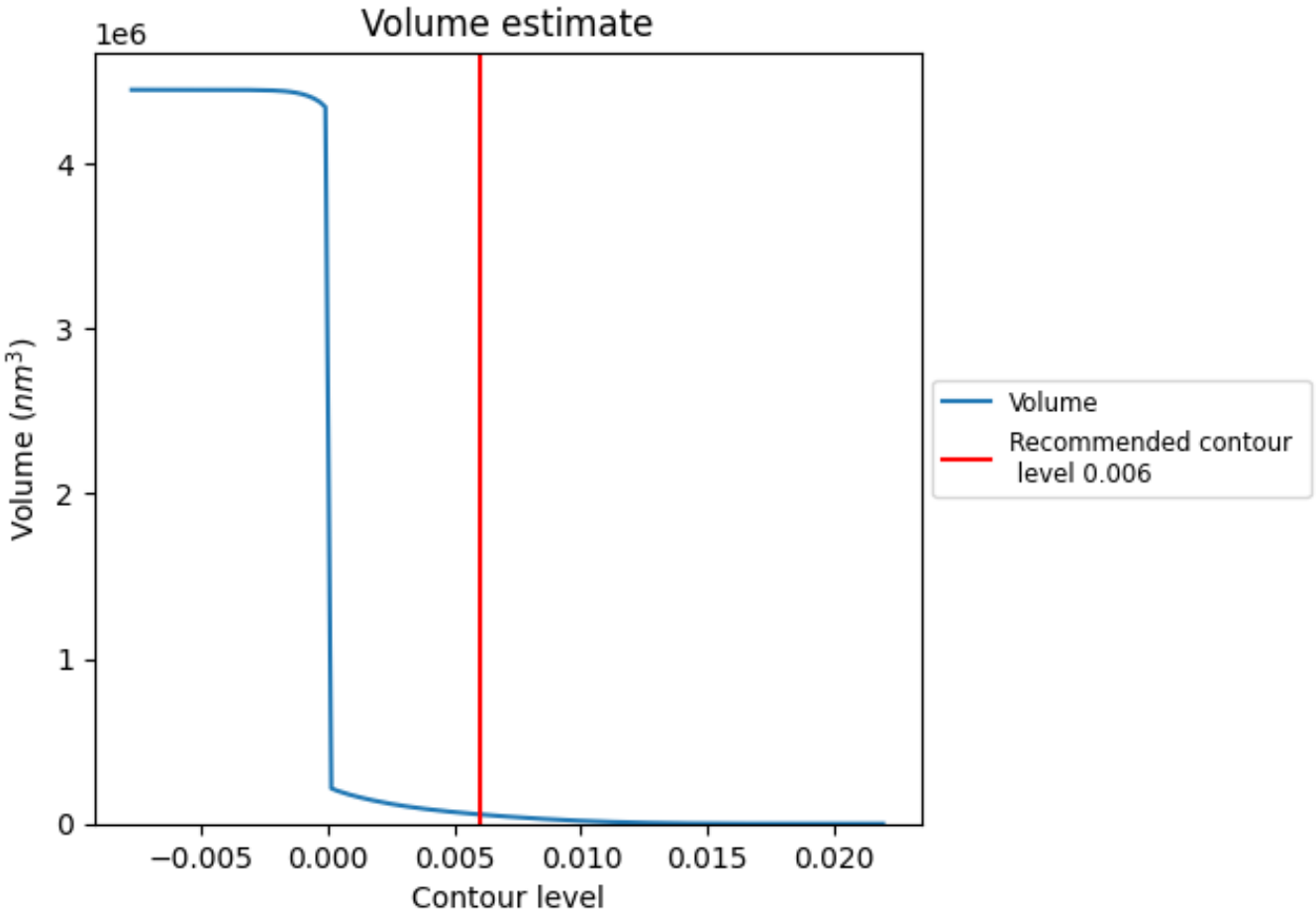
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

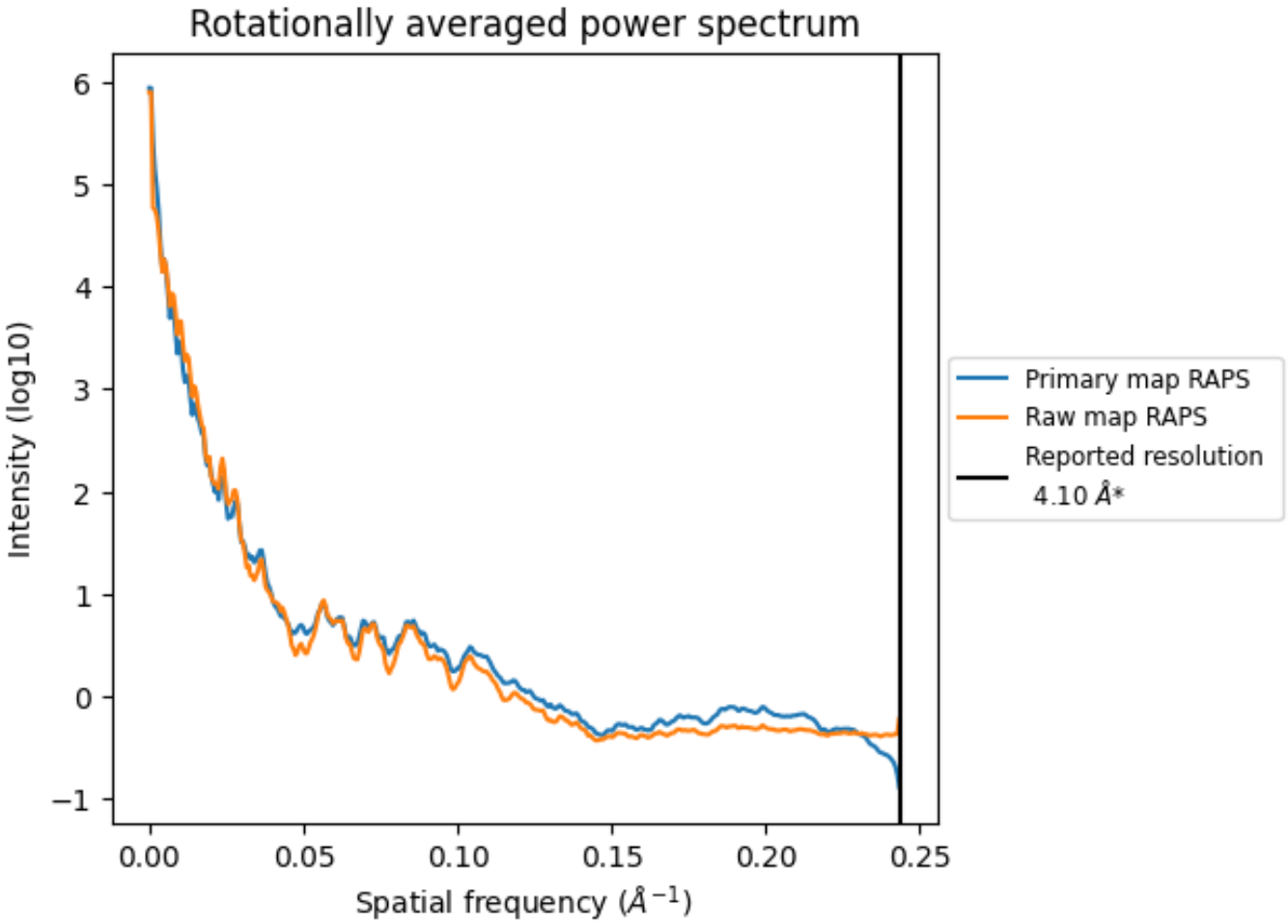
7.2 Volume estimate



The volume at the recommended contour level is 56255 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)

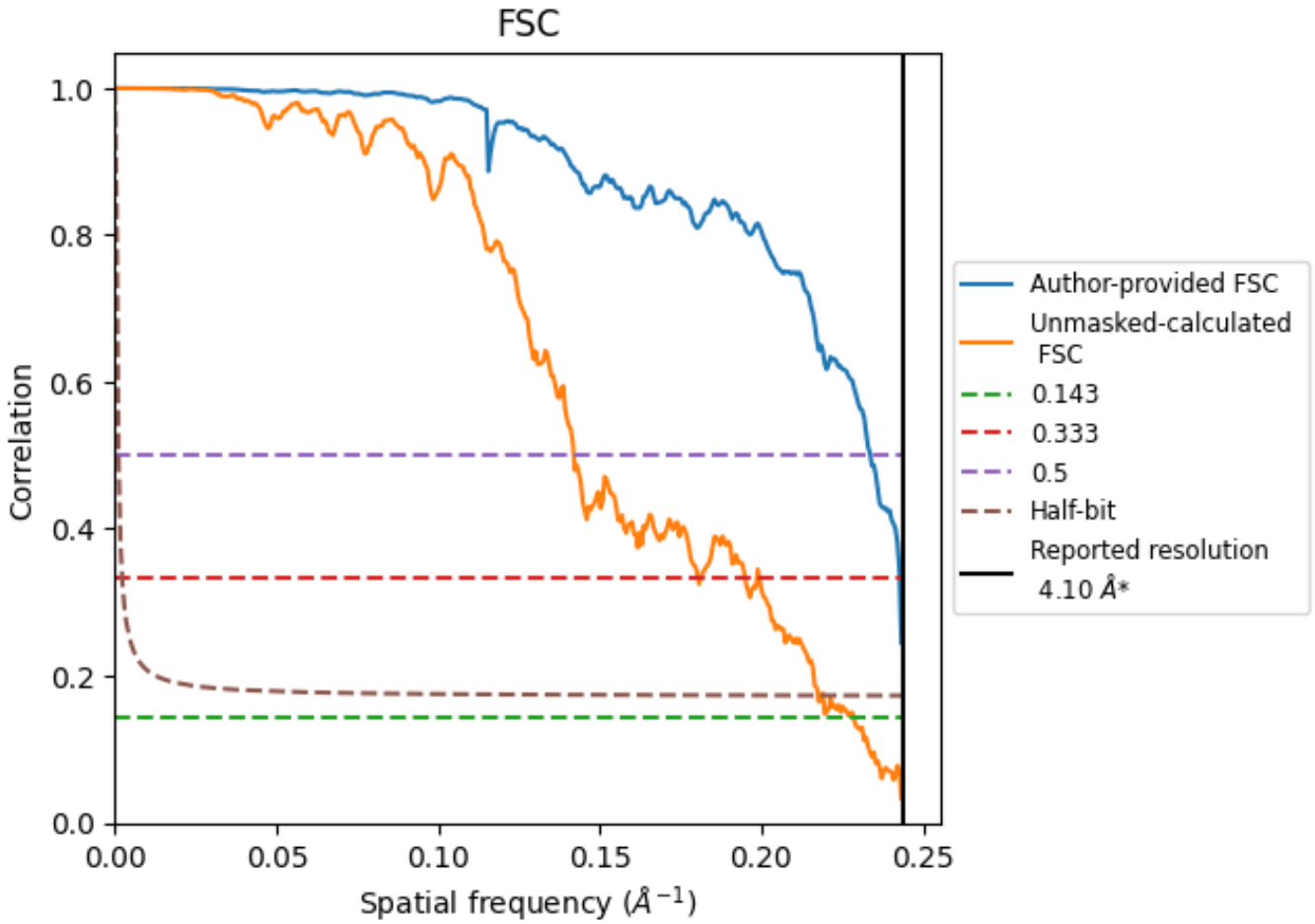


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

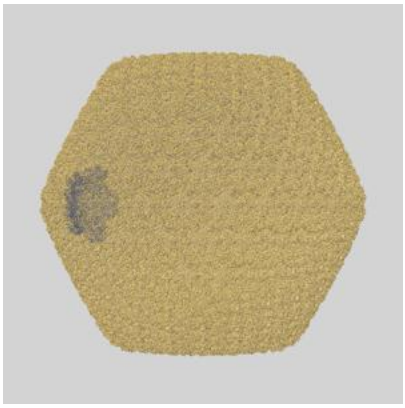
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	0.333
Reported by author	-	-	-	4.10
Author-provided FSC curve	-	4.28	-	4.12
Unmasked-calculated*	4.38	7.04	4.60	5.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.33 CUT-OFF 5.54 differs from the reported value 4.1 by more than 10 %

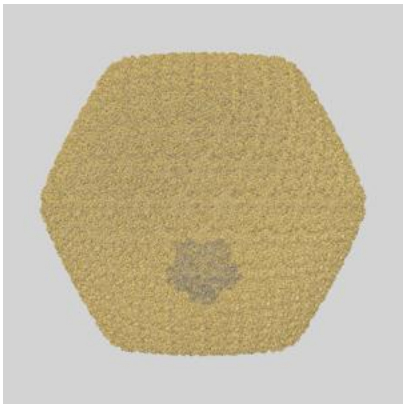
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13862 and PDB model 8BFP. Per-residue inclusion information can be found in section 3 on page 7.

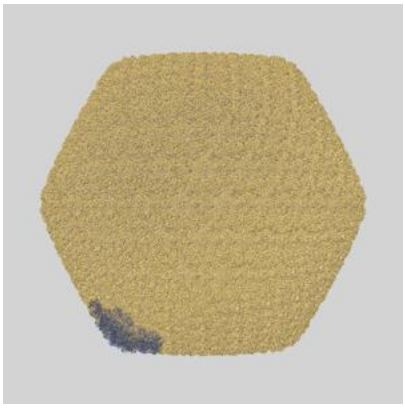
9.1 Map-model overlay



X



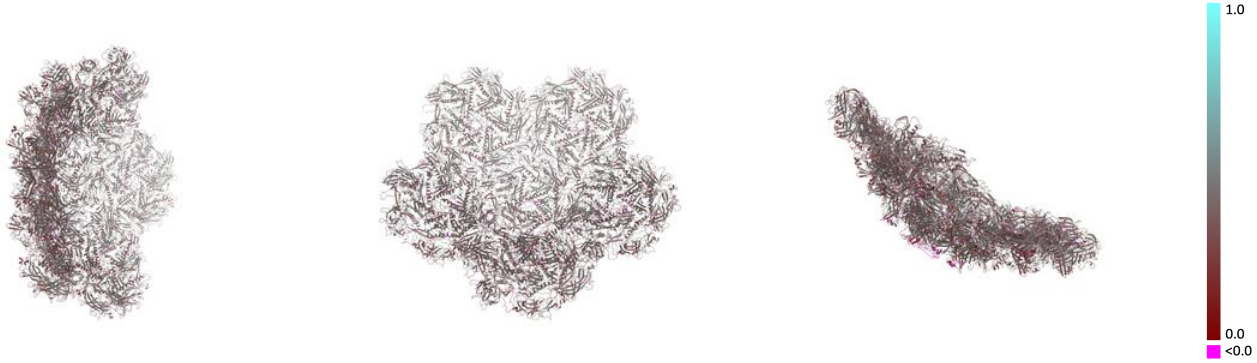
Y



Z

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.

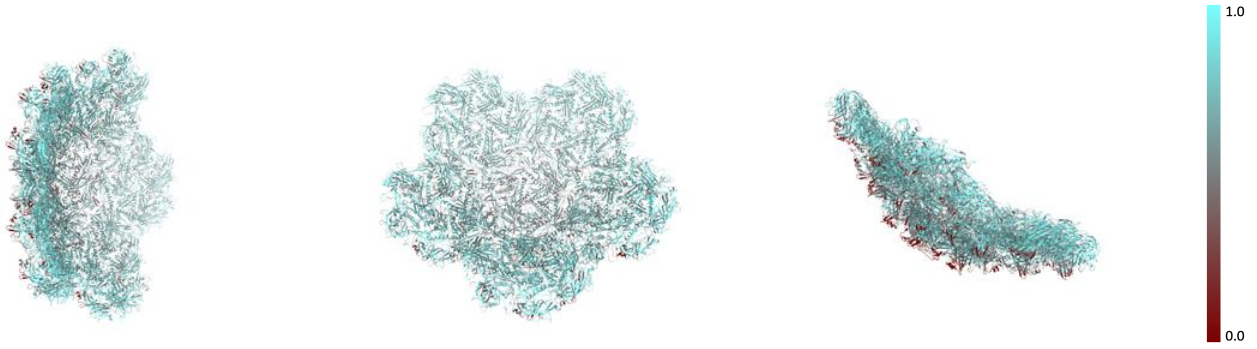
9.2 Q-score mapped to coordinate model



X Y Z

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.

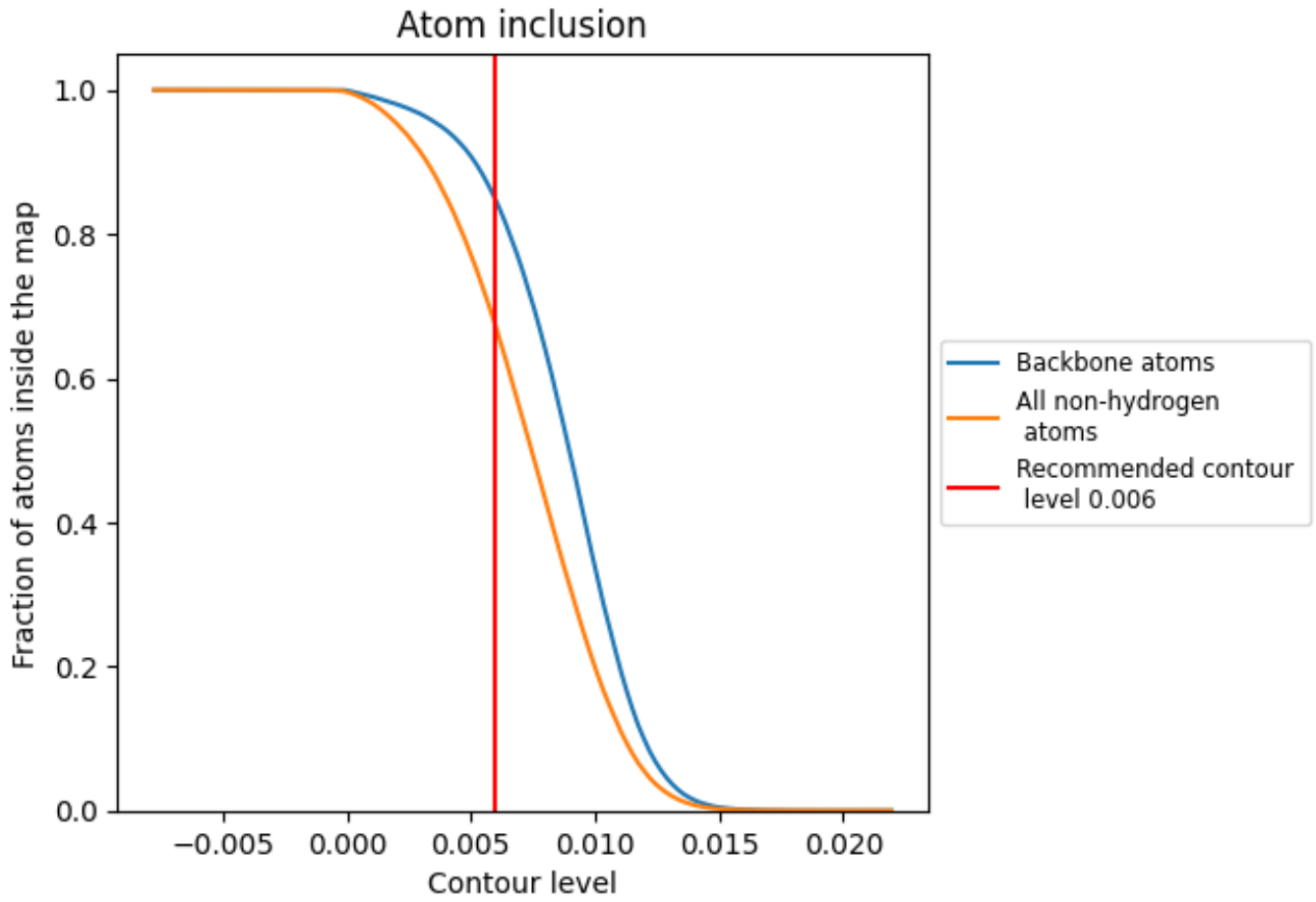
9.3 Atom inclusion mapped to coordinate model



X Y Z

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, 85% of all backbone atoms, 67% 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	0.6721	0.3680
A	0.5467	0.3400
B	0.5749	0.3530
C	0.5710	0.3520
D	0.5583	0.3440
E	0.5626	0.3480
G	0.6975	0.3720
H	0.6923	0.3750
I	0.7171	0.3770
J	0.6582	0.3690
K	0.6493	0.3680
L	0.6880	0.3700
M	0.7155	0.3710
N	0.7132	0.3720
O	0.6866	0.3740
P	0.6573	0.3690
Q	0.6962	0.3690
R	0.6634	0.3630
S	0.6780	0.3660
T	0.6543	0.3620
U	0.6668	0.3710
V	0.7039	0.3760
W	0.7076	0.3750
X	0.6923	0.3780
Y	0.6668	0.3650
Z	0.6675	0.3610
a	0.7205	0.3740
b	0.7294	0.3810
c	0.6864	0.3720
d	0.7146	0.3770
e	0.6623	0.3660
f	0.7044	0.3730
g	0.7117	0.3740
h	0.7091	0.3790
i	0.6655	0.3630
j	0.7342	0.3790