



Full wwPDB EM Validation Report ⓘ

Oct 23, 2023 – 04:04 PM JST

PDB ID : 8JOV
EMDB ID : EMD-36463
Title : Portal-tail complex of phage GP4
Authors : Liu, H.; Chen, W.
Deposited on : 2023-06-08
Resolution : 3.80 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:

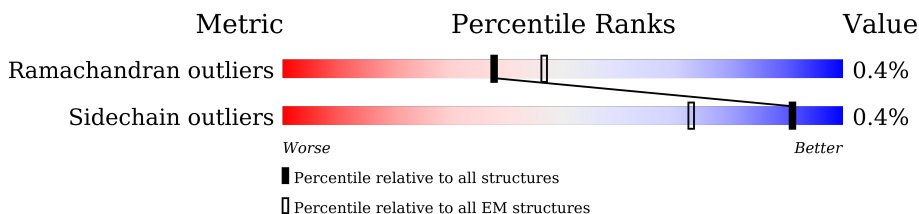
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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 $\leq 5\%$. 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	0	781	
1	3	781	
1	6	781	
1	U	781	
1	Y	781	
1	c	781	
1	g	781	
1	k	781	
1	o	781	

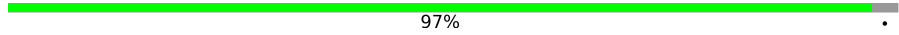
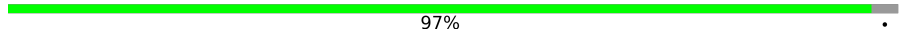
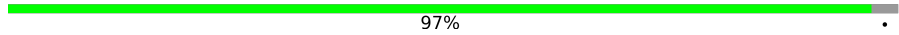
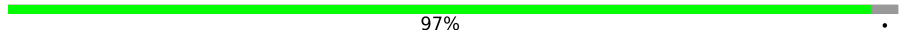
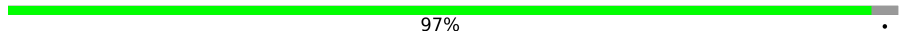
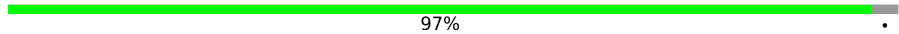
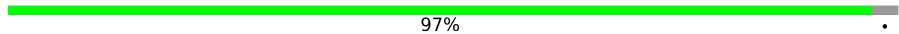
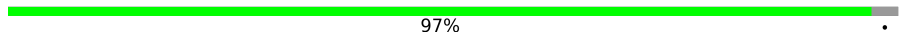







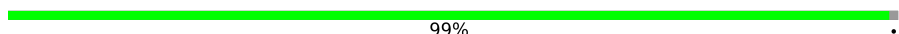
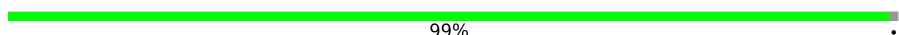
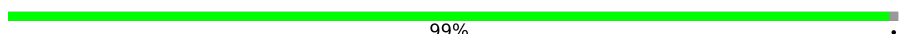
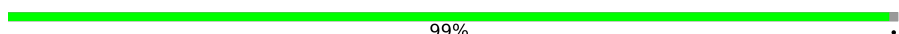
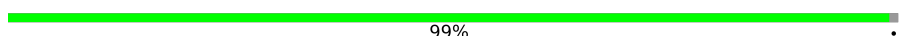
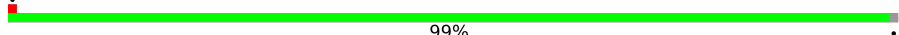
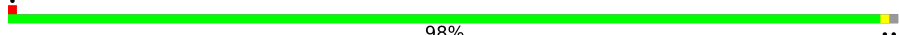
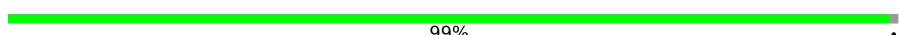
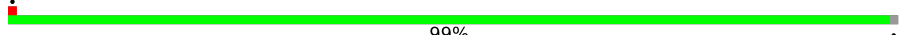
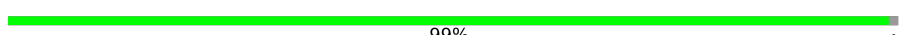
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Mol	Chain	Length	Quality of chain	
1	r	781	69%	30%
1	u	781	70%	30%
1	x	781	69%	30%
2	1	439	26%	74%
2	4	439	26%	74%
2	7	439	26%	74%
2	M	439	26%	74%
2	N	439	26%	74%
2	O	439	26%	74%
2	P	439	26%	74%
2	Q	439	26%	74%
2	R	439	26%	74%
2	V	439	26%	74%
2	Z	439	26%	74%
2	d	439	26%	74%
2	h	439	26%	74%
2	l	439	26%	74%
2	p	439	26%	74%
2	s	439	26%	74%
2	v	439	26%	74%
2	y	439	26%	74%
3	2	220	97%	.
3	5	220	97%	.
3	T	220	97%	.
3	X	220	97%	.

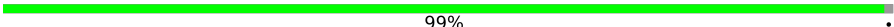
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Mol	Chain	Length	Quality of chain
3	b	220	 97%
3	f	220	 97%
3	j	220	 97%
3	n	220	 97%
3	q	220	 97%
3	t	220	 97%
3	w	220	 97%
3	z	220	 97%
4	A	577	 89% .. 10%
4	B	577	 89% .. 10%
4	C	577	 88% .. 10%
4	D	577	 89% .. 10%
4	E	577	 89% .. 10%
4	F	577	 88% .. 10%
5	G	206	 99%
5	H	206	 99%
5	I	206	 99%
5	J	206	 99%
5	K	206	 99%
5	L	206	 99%
5	S	206	 99%
5	W	206	 98% ..
5	a	206	 99%
5	e	206	 99%
5	i	206	 99%

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Mol	Chain	Length	Quality of chain
5	m	206	 99%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 128070 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	547	4297	2681	780	816	20	0	0
1	3	547	4297	2681	780	816	20	0	0
1	6	547	4297	2681	780	816	20	0	0
1	U	547	4297	2681	780	816	20	0	0
1	Y	547	4297	2681	780	816	20	0	0
1	c	547	4297	2681	780	816	20	0	0
1	g	547	4297	2681	780	816	20	0	0
1	k	547	4297	2681	780	816	20	0	0
1	o	547	4297	2681	780	816	20	0	0
1	r	547	4297	2681	780	816	20	0	0
1	u	547	4297	2681	780	816	20	0	0
1	x	547	4297	2681	780	816	20	0	0

- Molecule 2 is a protein called Putative tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	116	829	507	150	170	2	0	0
2	4	116	829	507	150	170	2	0	0
2	7	116	829	507	150	170	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	N	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	O	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	P	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	Q	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	R	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	V	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	Z	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	d	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	h	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	l	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	p	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	s	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	v	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	y	116	Total	C	N	O	S	0	0
			829	507	150	170	2		

- Molecule 3 is a protein called Virion associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	5	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	T	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	X	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	f	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	j	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	n	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	q	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	t	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	w	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	z	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		

- Molecule 4 is a protein called Virion-associated phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	B	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	C	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	D	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	E	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	F	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		

- Molecule 5 is a protein called gp81 of phage GP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	H	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	I	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		

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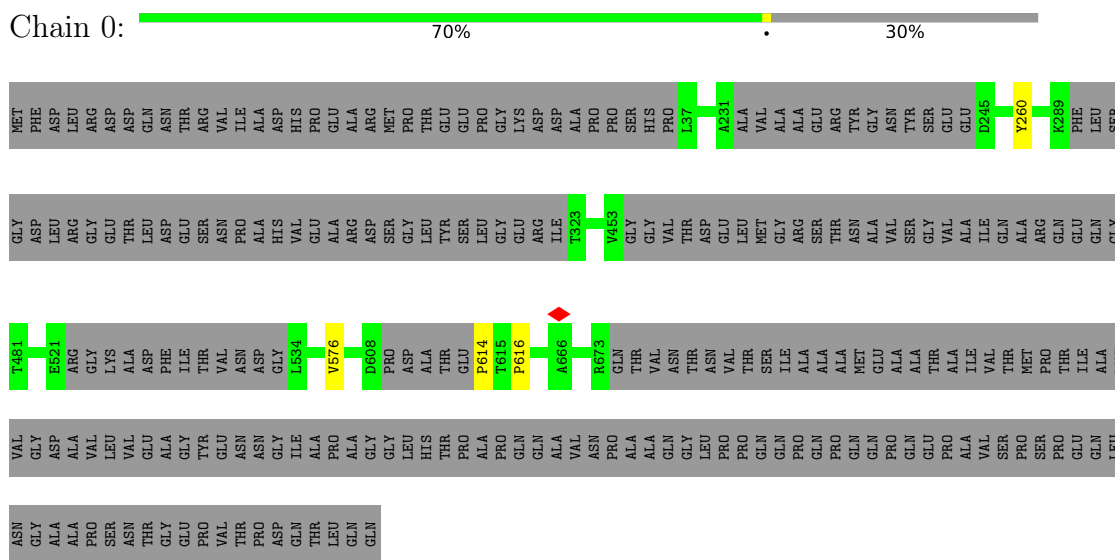
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	K	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	L	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	S	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	W	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	a	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	e	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	i	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	m	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		

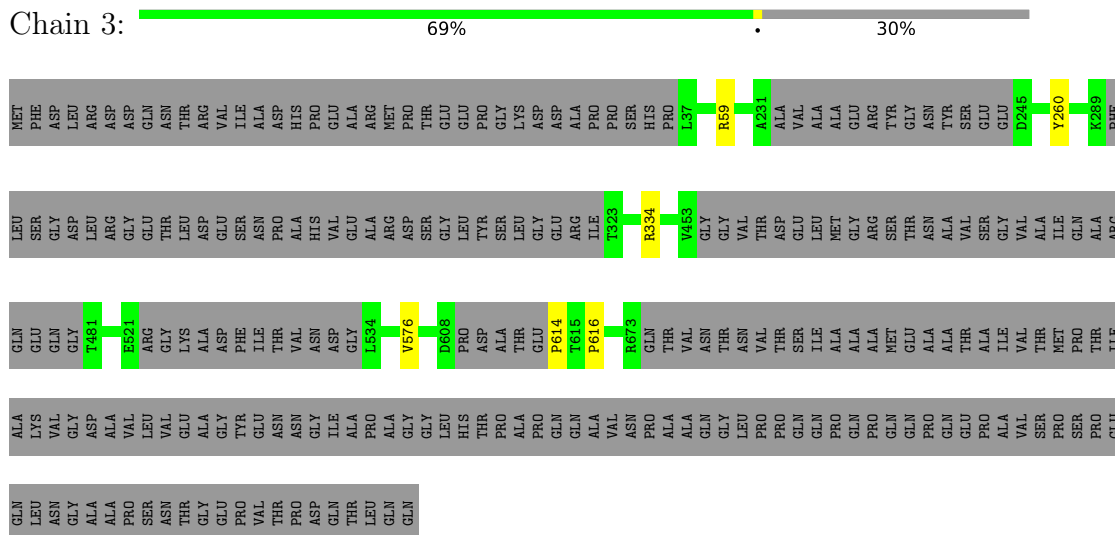
3 Residue-property plots i

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.

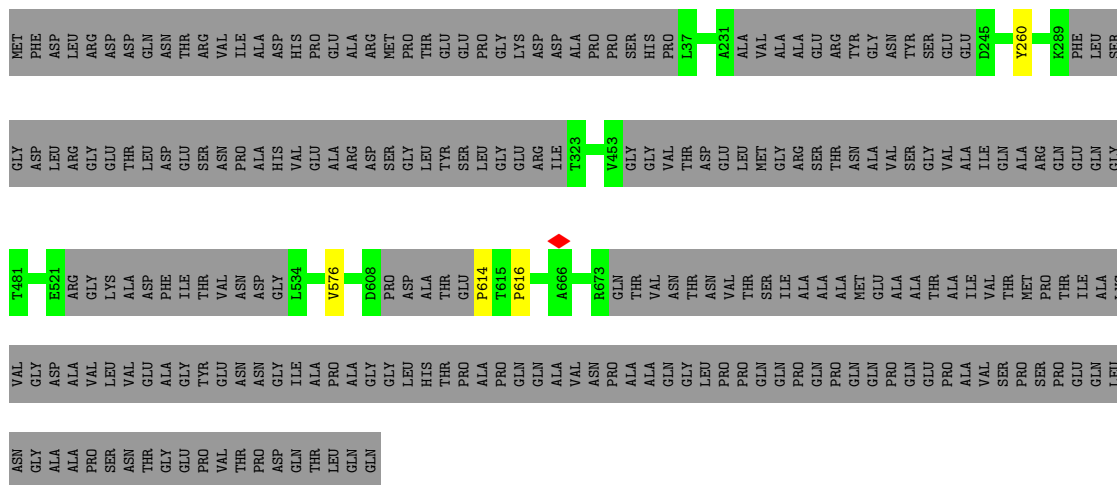
- Molecule 1: Portal protein



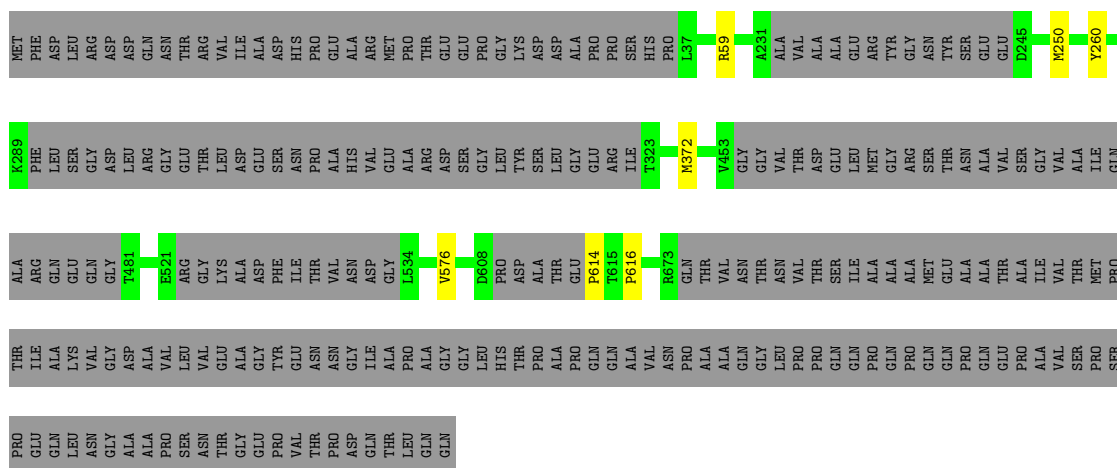
- Molecule 1: Portal protein



- Molecule 1: Portal protein

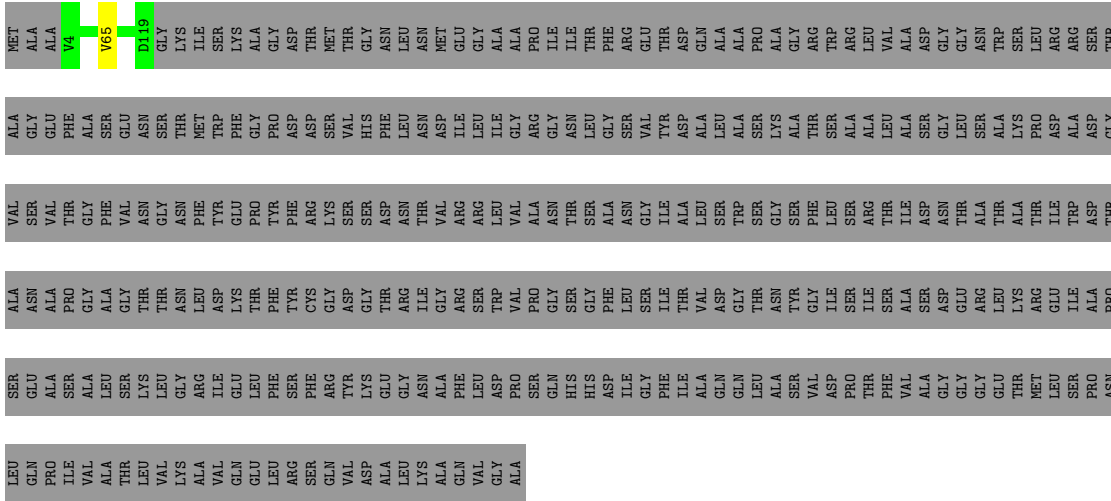


● Molecule 1: Portal protein

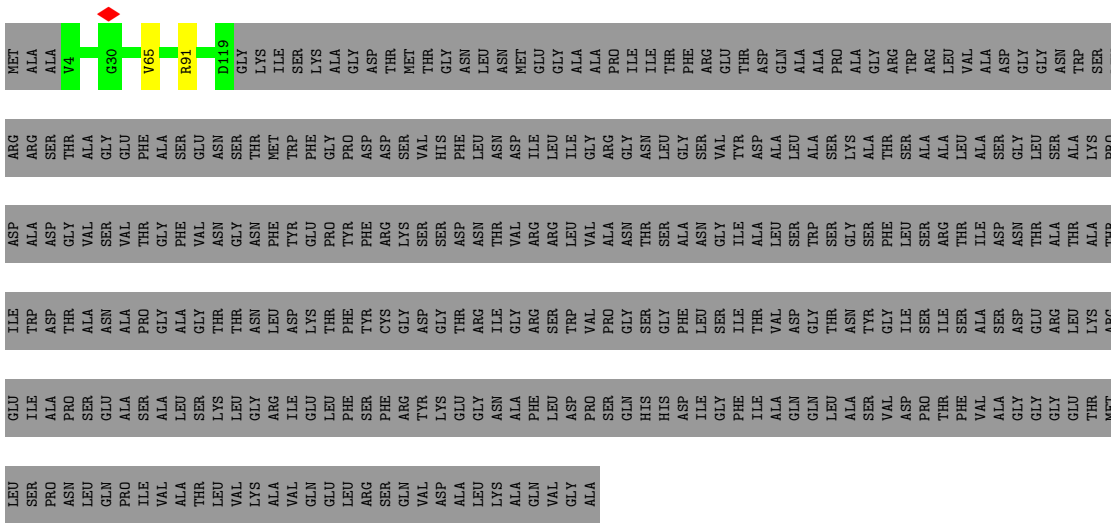


● Molecule 2: Putative tail fiber protein

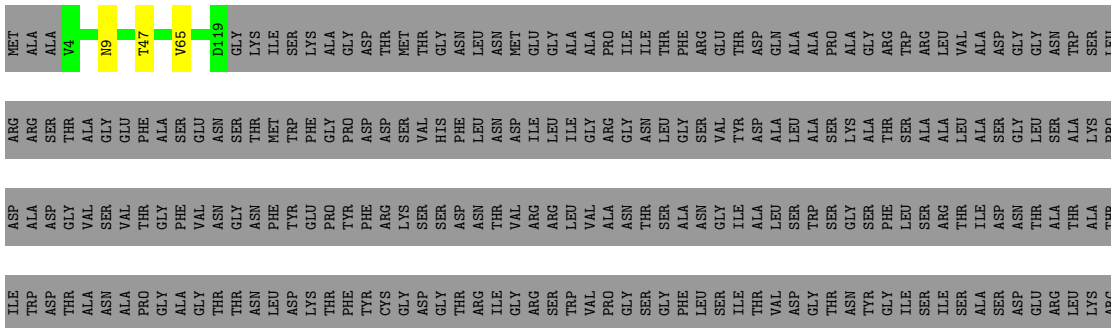


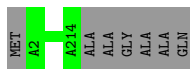


• Molecule 2: Putative tail fiber protein

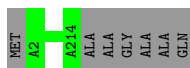


• Molecule 2: Putative tail fiber protein





• Molecule 3: Virion associated protein



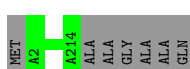
• Molecule 3: Virion associated protein



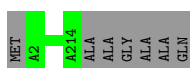
• Molecule 3: Virion associated protein



• Molecule 3: Virion associated protein



• Molecule 3: Virion associated protein

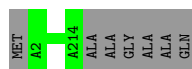


• Molecule 3: Virion associated protein

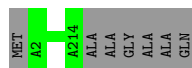


• Molecule 3: Virion associated protein





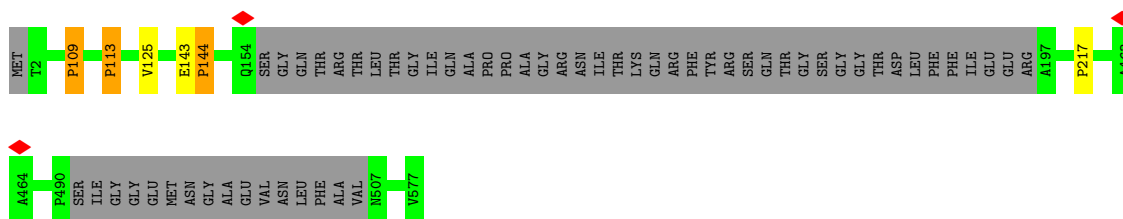
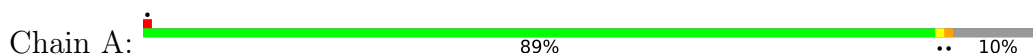
• Molecule 3: Virion associated protein



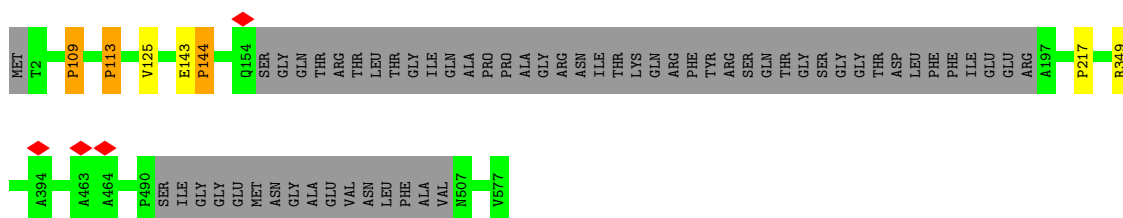
• Molecule 3: Virion associated protein



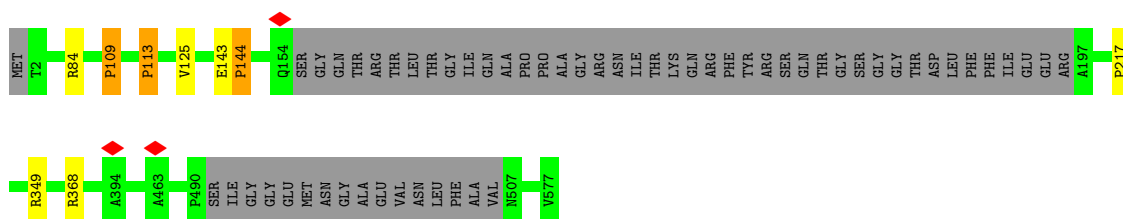
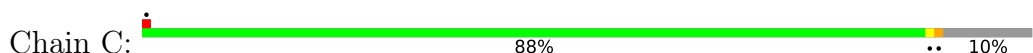
• Molecule 4: Virion-associated phage protein



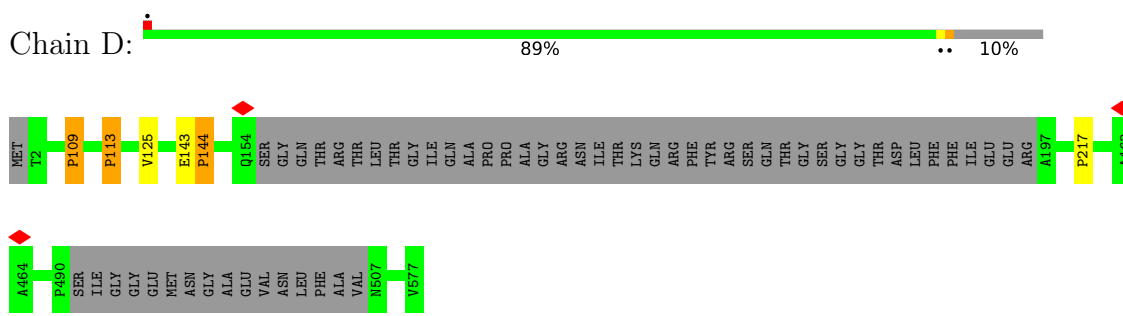
• Molecule 4: Virion-associated phage protein



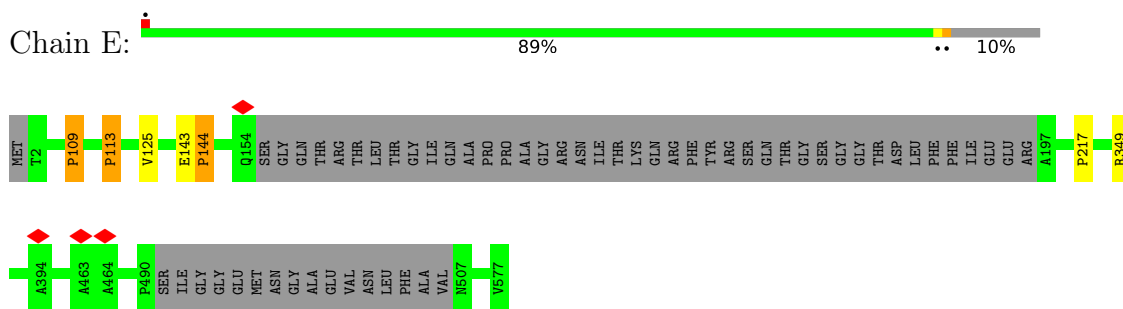
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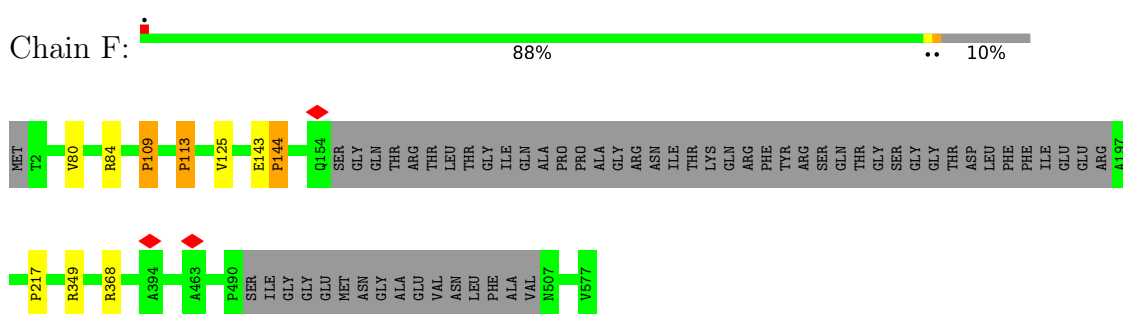
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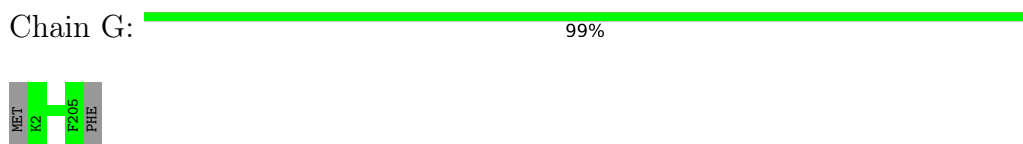
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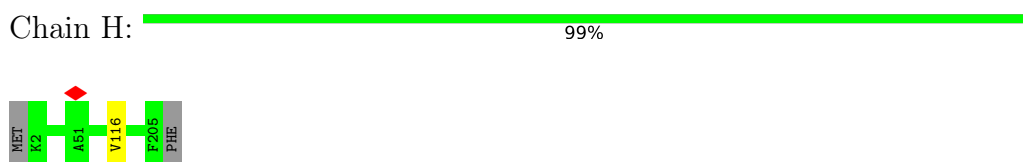
- Molecule 4: Virion-associated phage protein



- Molecule 5: gp81 of phage GP4



- Molecule 5: gp81 of phage GP4



- Molecule 5: gp81 of phage GP4

Chain I:  99%



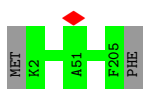
- Molecule 5: gp81 of phage GP4

Chain J:  99%



- Molecule 5: gp81 of phage GP4

Chain K:  99%



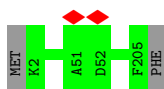
- Molecule 5: gp81 of phage GP4

Chain L:  99%



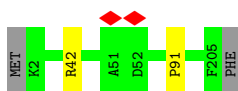
- Molecule 5: gp81 of phage GP4

Chain S:  99%



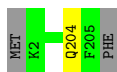
- Molecule 5: gp81 of phage GP4

Chain W:  98%



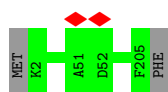
- Molecule 5: gp81 of phage GP4

Chain a:  99%



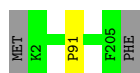
- Molecule 5: gp81 of phage GP4

Chain e:  99%



- Molecule 5: gp81 of phage GP4

Chain i:  99%



- Molecule 5: gp81 of phage GP4

Chain m:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39883	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	31.901	Depositor
Minimum map value	-13.810	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.650	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	508.0, 508.0, 508.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.27, 1.27, 1.27	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	0	0.26	0/4368	0.54	2/5900 (0.0%)
1	3	0.25	0/4368	0.53	2/5900 (0.0%)
1	6	0.26	0/4368	0.54	2/5900 (0.0%)
1	U	0.25	0/4368	0.52	2/5900 (0.0%)
1	Y	0.27	0/4368	0.54	2/5900 (0.0%)
1	c	0.26	0/4368	0.52	2/5900 (0.0%)
1	g	0.26	0/4368	0.54	2/5900 (0.0%)
1	k	0.25	0/4368	0.52	2/5900 (0.0%)
1	o	0.27	0/4368	0.54	2/5900 (0.0%)
1	r	0.26	0/4368	0.52	2/5900 (0.0%)
1	u	0.27	0/4368	0.55	2/5900 (0.0%)
1	x	0.25	0/4368	0.53	3/5900 (0.1%)
2	1	0.25	0/840	0.54	0/1141
2	4	0.27	0/840	0.61	1/1141 (0.1%)
2	7	0.27	0/840	0.61	0/1141
2	M	0.26	0/840	0.56	0/1141
2	N	0.27	0/840	0.57	0/1141
2	O	0.26	0/840	0.58	0/1141
2	P	0.25	0/840	0.55	0/1141
2	Q	0.25	0/840	0.55	0/1141
2	R	0.26	0/840	0.57	0/1141
2	V	0.25	0/840	0.54	0/1141
2	Z	0.28	0/840	0.61	1/1141 (0.1%)
2	d	0.27	0/840	0.61	0/1141
2	h	0.26	0/840	0.56	0/1141
2	l	0.27	0/840	0.57	0/1141
2	p	0.26	0/840	0.57	0/1141
2	s	0.24	0/840	0.56	0/1141
2	v	0.27	0/840	0.62	1/1141 (0.1%)
2	y	0.26	0/840	0.57	0/1141
3	2	0.27	0/1653	0.51	0/2265
3	5	0.26	0/1653	0.52	0/2265
3	T	0.27	0/1653	0.54	0/2265
3	X	0.27	0/1653	0.53	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	b	0.27	0/1653	0.54	0/2265
3	f	0.27	0/1653	0.55	0/2265
3	j	0.28	0/1653	0.53	0/2265
3	n	0.28	0/1653	0.55	0/2265
3	q	0.27	0/1653	0.50	0/2265
3	t	0.27	0/1653	0.51	0/2265
3	w	0.27	0/1653	0.50	0/2265
3	z	0.26	0/1653	0.51	0/2265
4	A	0.26	0/3893	0.55	4/5306 (0.1%)
4	B	0.26	0/3893	0.55	4/5306 (0.1%)
4	C	0.26	0/3893	0.55	4/5306 (0.1%)
4	D	0.26	0/3893	0.55	4/5306 (0.1%)
4	E	0.26	0/3893	0.55	4/5306 (0.1%)
4	F	0.26	0/3893	0.56	4/5306 (0.1%)
5	G	0.27	0/1648	0.54	0/2241
5	H	0.28	0/1648	0.56	0/2241
5	I	0.28	0/1648	0.55	0/2241
5	J	0.28	0/1648	0.55	0/2241
5	K	0.27	0/1648	0.56	0/2241
5	L	0.28	0/1648	0.55	0/2241
5	S	0.27	0/1648	0.54	0/2241
5	W	0.28	0/1648	0.57	1/2241 (0.0%)
5	a	0.27	0/1648	0.53	0/2241
5	e	0.27	0/1648	0.54	0/2241
5	i	0.29	0/1648	0.56	1/2241 (0.0%)
5	m	0.28	0/1648	0.54	0/2241
All	All	0.26	0/130506	0.54	54/177246 (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	r	0	1
4	F	0	1
5	H	0	1
All	All	0	3

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	84	PRO	CA-N-CD	-7.34	101.22	111.50
2	Z	84	PRO	CA-N-CD	-7.14	101.50	111.50
4	A	113	PRO	N-CA-CB	6.92	111.60	103.30
4	E	113	PRO	N-CA-CB	6.90	111.58	103.30
4	B	113	PRO	N-CA-CB	6.88	111.55	103.30
4	C	113	PRO	N-CA-CB	6.86	111.53	103.30
4	D	113	PRO	N-CA-CB	6.85	111.52	103.30
4	F	113	PRO	N-CA-CB	6.85	111.52	103.30
4	D	109	PRO	N-CA-CB	6.77	111.43	103.30
4	B	109	PRO	N-CA-CB	6.77	111.42	103.30
4	F	109	PRO	N-CA-CB	6.76	111.41	103.30
4	A	109	PRO	N-CA-CB	6.75	111.40	103.30
4	E	109	PRO	N-CA-CB	6.74	111.39	103.30
4	C	109	PRO	N-CA-CB	6.71	111.36	103.30
2	v	84	PRO	CA-N-CD	-6.36	102.60	111.50
4	B	144	PRO	N-CA-CB	6.18	110.72	103.30
4	A	144	PRO	N-CA-CB	6.17	110.70	103.30
4	D	144	PRO	N-CA-CB	6.16	110.69	103.30
4	F	144	PRO	N-CA-CB	6.16	110.69	103.30
4	E	144	PRO	N-CA-CB	6.15	110.68	103.30
4	C	144	PRO	N-CA-CB	6.14	110.67	103.30
1	c	614	PRO	N-CA-CB	5.95	110.44	103.30
1	o	614	PRO	N-CA-CB	5.95	110.44	103.30
1	6	614	PRO	N-CA-CB	5.95	110.44	103.30
1	g	614	PRO	N-CA-CB	5.95	110.44	103.30
1	3	614	PRO	N-CA-CB	5.94	110.43	103.30
1	0	614	PRO	N-CA-CB	5.94	110.42	103.30
1	U	614	PRO	N-CA-CB	5.93	110.42	103.30
1	x	614	PRO	N-CA-CB	5.93	110.41	103.30
1	u	614	PRO	N-CA-CB	5.93	110.41	103.30
1	Y	614	PRO	N-CA-CB	5.92	110.41	103.30
1	r	614	PRO	N-CA-CB	5.92	110.41	103.30
1	k	614	PRO	N-CA-CB	5.91	110.39	103.30
5	W	91	PRO	CA-N-CD	-5.88	103.26	111.50
5	i	91	PRO	CA-N-CD	-5.85	103.31	111.50
4	C	217	PRO	N-CA-CB	5.77	110.22	103.30
4	D	217	PRO	N-CA-CB	5.77	110.22	103.30
4	F	217	PRO	N-CA-CB	5.77	110.22	103.30
4	A	217	PRO	N-CA-CB	5.76	110.22	103.30
4	B	217	PRO	N-CA-CB	5.71	110.16	103.30
4	E	217	PRO	N-CA-CB	5.70	110.14	103.30
1	g	616	PRO	N-CA-CB	5.67	110.10	103.30
1	r	616	PRO	N-CA-CB	5.66	110.09	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	616	PRO	N-CA-CB	5.65	110.08	103.30
1	u	616	PRO	N-CA-CB	5.65	110.08	103.30
1	3	616	PRO	N-CA-CB	5.64	110.07	103.30
1	c	616	PRO	N-CA-CB	5.64	110.07	103.30
1	0	616	PRO	N-CA-CB	5.64	110.06	103.30
1	6	616	PRO	N-CA-CB	5.63	110.06	103.30
1	o	616	PRO	N-CA-CB	5.63	110.06	103.30
1	U	616	PRO	N-CA-CB	5.61	110.04	103.30
1	k	616	PRO	N-CA-CB	5.61	110.03	103.30
1	x	616	PRO	N-CA-CB	5.59	110.01	103.30
1	x	372	MET	CA-CB-CG	5.12	122.00	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	80	VAL	Peptide
5	H	116	VAL	Peptide
1	r	558	ARG	Sidechain

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	0	535/781 (68%)	516 (96%)	17 (3%)	2 (0%)	34 70
1	3	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	34 70
1	6	535/781 (68%)	516 (96%)	17 (3%)	2 (0%)	34 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	535/781 (68%)	517 (97%)	16 (3%)	2 (0%)	34	70
1	Y	535/781 (68%)	523 (98%)	10 (2%)	2 (0%)	34	70
1	c	535/781 (68%)	519 (97%)	14 (3%)	2 (0%)	34	70
1	g	535/781 (68%)	518 (97%)	15 (3%)	2 (0%)	34	70
1	k	535/781 (68%)	518 (97%)	15 (3%)	2 (0%)	34	70
1	o	535/781 (68%)	519 (97%)	14 (3%)	2 (0%)	34	70
1	r	535/781 (68%)	517 (97%)	16 (3%)	2 (0%)	34	70
1	u	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	34	70
1	x	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	34	70
2	1	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	17	54
2	4	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	7	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	17	54
2	M	114/439 (26%)	108 (95%)	5 (4%)	1 (1%)	17	54
2	N	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	17	54
2	O	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	17	54
2	P	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	Q	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	17	54
2	R	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	17	54
2	V	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	17	54
2	Z	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	d	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	17	54
2	h	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	l	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	17	54
2	p	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	s	114/439 (26%)	108 (95%)	5 (4%)	1 (1%)	17	54
2	v	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	17	54
2	y	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	17	54
3	2	211/220 (96%)	200 (95%)	11 (5%)	0	100	100
3	5	211/220 (96%)	202 (96%)	9 (4%)	0	100	100
3	T	211/220 (96%)	196 (93%)	15 (7%)	0	100	100
3	X	211/220 (96%)	198 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	b	211/220 (96%)	196 (93%)	15 (7%)	0	100	100
3	f	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
3	j	211/220 (96%)	197 (93%)	14 (7%)	0	100	100
3	n	211/220 (96%)	193 (92%)	18 (8%)	0	100	100
3	q	211/220 (96%)	203 (96%)	8 (4%)	0	100	100
3	t	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
3	w	211/220 (96%)	201 (95%)	10 (5%)	0	100	100
3	z	211/220 (96%)	202 (96%)	9 (4%)	0	100	100
4	A	512/577 (89%)	483 (94%)	24 (5%)	5 (1%)	15	52
4	B	512/577 (89%)	480 (94%)	27 (5%)	5 (1%)	15	52
4	C	512/577 (89%)	477 (93%)	30 (6%)	5 (1%)	15	52
4	D	512/577 (89%)	480 (94%)	27 (5%)	5 (1%)	15	52
4	E	512/577 (89%)	481 (94%)	26 (5%)	5 (1%)	15	52
4	F	512/577 (89%)	479 (94%)	28 (6%)	5 (1%)	15	52
5	G	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	H	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	I	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	J	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	K	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
5	L	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	S	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	W	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	a	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	e	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	i	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	m	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	16500/25848 (64%)	15768 (96%)	660 (4%)	72 (0%)	38	70

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	576	VAL
1	3	576	VAL

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Mol	Chain	Res	Type
1	6	576	VAL
4	A	109	PRO
4	A	113	PRO
4	A	144	PRO
4	B	109	PRO
4	B	113	PRO
4	B	144	PRO
4	C	109	PRO
4	C	113	PRO
4	C	144	PRO
4	D	109	PRO
4	D	113	PRO
4	D	144	PRO
4	E	109	PRO
4	E	113	PRO
4	E	144	PRO
4	F	109	PRO
4	F	113	PRO
4	F	144	PRO
1	U	576	VAL
1	Y	576	VAL
1	c	576	VAL
1	g	576	VAL
1	k	576	VAL
1	o	576	VAL
1	r	576	VAL
1	u	576	VAL
1	x	576	VAL
4	A	143	GLU
4	B	143	GLU
4	C	143	GLU
4	D	143	GLU
4	E	143	GLU
4	F	143	GLU
2	1	65	VAL
2	4	65	VAL
2	M	65	VAL
2	N	65	VAL
2	P	65	VAL
2	Q	65	VAL
2	V	65	VAL
2	Z	65	VAL

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Mol	Chain	Res	Type
2	h	65	VAL
2	l	65	VAL
2	s	65	VAL
2	v	65	VAL
2	y	65	VAL
1	3	260	TYR
2	7	65	VAL
4	A	125	VAL
4	B	125	VAL
4	C	125	VAL
4	D	125	VAL
4	E	125	VAL
4	F	125	VAL
2	O	65	VAL
2	R	65	VAL
1	U	260	TYR
1	c	260	TYR
2	d	65	VAL
1	k	260	TYR
2	p	65	VAL
1	x	260	TYR
1	6	260	TYR
1	o	260	TYR
1	r	260	TYR
1	0	260	TYR
1	Y	260	TYR
1	g	260	TYR
1	u	260	TYR

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	0	432/657 (66%)	432 (100%)	0	100	100
1	3	432/657 (66%)	430 (100%)	2 (0%)	88	94
1	6	432/657 (66%)	430 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	432/657 (66%)	429 (99%)	3 (1%)	84	91
1	Y	432/657 (66%)	430 (100%)	2 (0%)	88	94
1	c	432/657 (66%)	430 (100%)	2 (0%)	88	94
1	g	432/657 (66%)	431 (100%)	1 (0%)	93	97
1	k	432/657 (66%)	431 (100%)	1 (0%)	93	97
1	o	432/657 (66%)	431 (100%)	1 (0%)	93	97
1	r	432/657 (66%)	430 (100%)	2 (0%)	88	94
1	u	432/657 (66%)	432 (100%)	0	100	100
1	x	432/657 (66%)	430 (100%)	2 (0%)	88	94
2	1	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	4	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	7	84/333 (25%)	84 (100%)	0	100	100
2	M	84/333 (25%)	83 (99%)	1 (1%)	71	84
2	N	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	O	84/333 (25%)	84 (100%)	0	100	100
2	P	84/333 (25%)	83 (99%)	1 (1%)	71	84
2	Q	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	R	84/333 (25%)	84 (100%)	0	100	100
2	V	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	Z	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	d	84/333 (25%)	84 (100%)	0	100	100
2	h	84/333 (25%)	83 (99%)	1 (1%)	71	84
2	l	84/333 (25%)	82 (98%)	2 (2%)	49	71
2	p	84/333 (25%)	84 (100%)	0	100	100
2	s	84/333 (25%)	84 (100%)	0	100	100
2	v	84/333 (25%)	83 (99%)	1 (1%)	71	84
2	y	84/333 (25%)	84 (100%)	0	100	100
3	2	167/169 (99%)	167 (100%)	0	100	100
3	5	167/169 (99%)	167 (100%)	0	100	100
3	T	167/169 (99%)	167 (100%)	0	100	100
3	X	167/169 (99%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	167/169 (99%)	167 (100%)	0	100	100
3	f	167/169 (99%)	167 (100%)	0	100	100
3	j	167/169 (99%)	167 (100%)	0	100	100
3	n	167/169 (99%)	167 (100%)	0	100	100
3	q	167/169 (99%)	167 (100%)	0	100	100
3	t	167/169 (99%)	167 (100%)	0	100	100
3	w	167/169 (99%)	167 (100%)	0	100	100
3	z	167/169 (99%)	167 (100%)	0	100	100
4	A	366/464 (79%)	366 (100%)	0	100	100
4	B	366/464 (79%)	365 (100%)	1 (0%)	92	96
4	C	366/464 (79%)	363 (99%)	3 (1%)	81	89
4	D	366/464 (79%)	366 (100%)	0	100	100
4	E	366/464 (79%)	365 (100%)	1 (0%)	92	96
4	F	366/464 (79%)	363 (99%)	3 (1%)	81	89
5	G	170/172 (99%)	170 (100%)	0	100	100
5	H	170/172 (99%)	170 (100%)	0	100	100
5	I	170/172 (99%)	170 (100%)	0	100	100
5	J	170/172 (99%)	170 (100%)	0	100	100
5	K	170/172 (99%)	170 (100%)	0	100	100
5	L	170/172 (99%)	170 (100%)	0	100	100
5	S	170/172 (99%)	170 (100%)	0	100	100
5	W	170/172 (99%)	169 (99%)	1 (1%)	86	92
5	a	170/172 (99%)	169 (99%)	1 (1%)	86	92
5	e	170/172 (99%)	170 (100%)	0	100	100
5	i	170/172 (99%)	170 (100%)	0	100	100
5	m	170/172 (99%)	169 (99%)	1 (1%)	86	92
All	All	12936/20754 (62%)	12889 (100%)	47 (0%)	91	95

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	68	MET
2	1	91	ARG

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Mol	Chain	Res	Type
1	3	59	ARG
1	3	334	ARG
2	4	9	ASN
2	4	91	ARG
1	6	371	TRP
1	6	430	ASN
4	B	349	ARG
4	C	84	ARG
4	C	349	ARG
4	C	368	ARG
4	E	349	ARG
4	F	84	ARG
4	F	349	ARG
4	F	368	ARG
2	M	91	ARG
2	N	9	ASN
2	N	91	ARG
2	P	91	ARG
2	Q	9	ASN
2	Q	91	ARG
1	U	376	GLN
1	U	485	ASN
1	U	598	LYS
2	V	68	MET
2	V	91	ARG
5	W	42	ARG
1	Y	371	TRP
1	Y	558	ARG
2	Z	9	ASN
2	Z	91	ARG
5	a	204	GLN
1	c	59	ARG
1	c	250	MET
1	g	430	ASN
2	h	91	ARG
1	k	59	ARG
2	l	9	ASN
2	l	47	THR
5	m	200	ARG
1	o	250	MET
1	r	391	SER
1	r	598	LYS

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Mol	Chain	Res	Type
2	v	91	ARG
1	x	59	ARG
1	x	250	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	74	GLN
3	2	145	HIS
1	3	376	GLN
1	3	452	GLN
3	5	145	HIS
4	B	70	GLN
4	C	70	GLN
4	C	486	ASN
4	D	328	HIS
4	E	70	GLN
4	F	328	HIS
4	F	486	ASN
5	J	195	GLN
2	M	74	GLN
2	P	74	GLN
5	S	12	HIS
5	S	194	GLN
2	V	74	GLN
5	W	12	HIS
1	Y	485	ASN
5	a	107	GLN
5	a	194	GLN
5	a	204	GLN
1	c	452	GLN
2	d	9	ASN
5	e	12	HIS
2	h	74	GLN
5	i	12	HIS
1	k	452	GLN
1	k	498	GLN
5	m	194	GLN
1	o	430	ASN
2	p	74	GLN
3	q	145	HIS
1	r	393	ASN

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Mol	Chain	Res	Type
2	s	74	GLN
3	t	145	HIS
2	v	8	ASN
3	w	145	HIS
1	x	452	GLN
1	x	498	GLN
2	y	74	GLN
2	y	108	GLN
3	z	145	HIS

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.

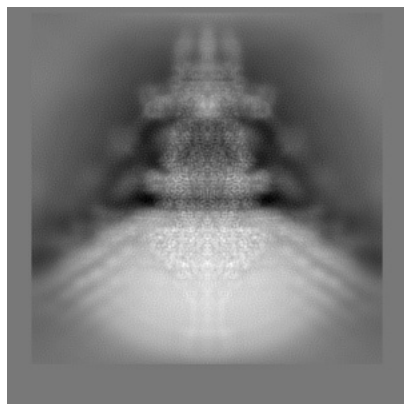
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36463. These allow visual inspection of the internal detail of the map and identification of artifacts.

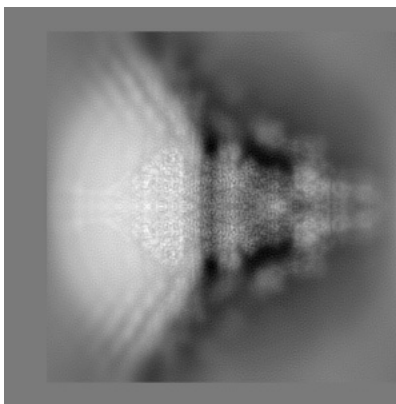
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

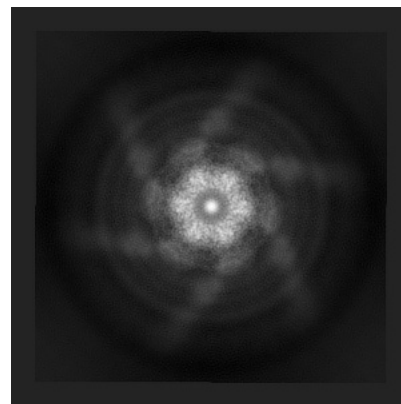
6.1.1 Primary map



X

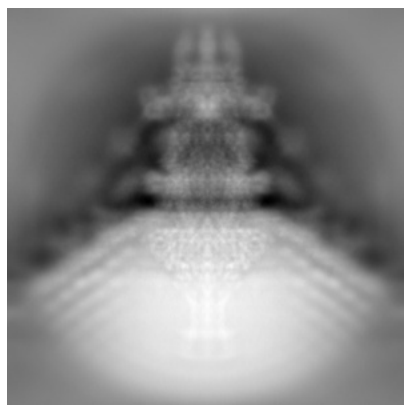


Y

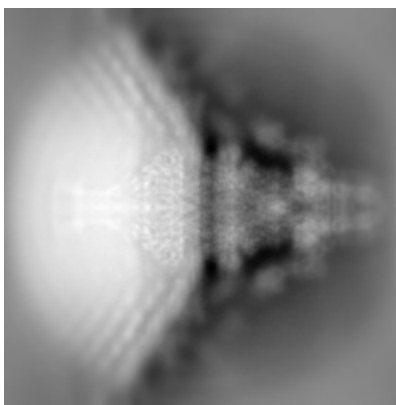


Z

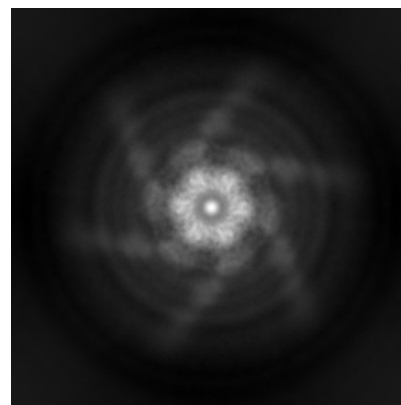
6.1.2 Raw map



X



Y

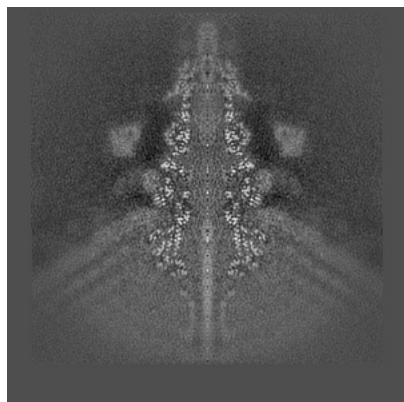


Z

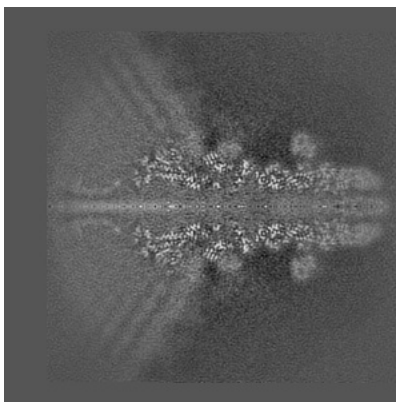
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

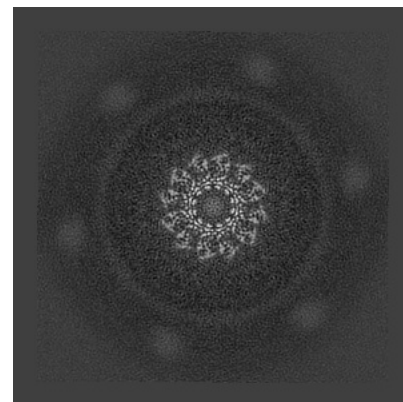
6.2.1 Primary map



X Index: 200

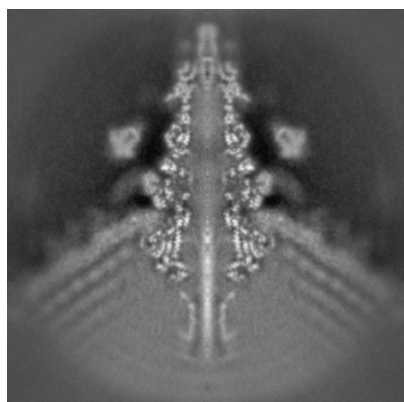


Y Index: 200

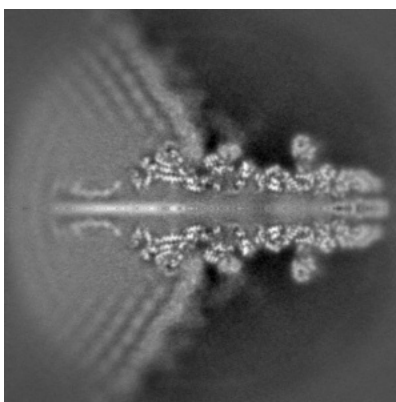


Z Index: 200

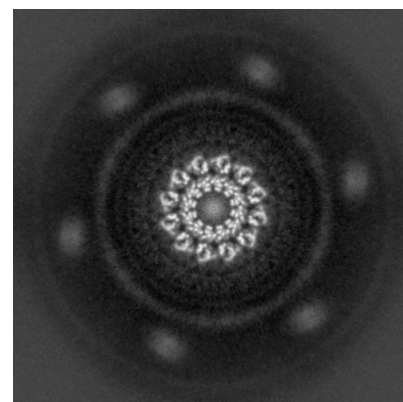
6.2.2 Raw map



X Index: 200



Y Index: 200

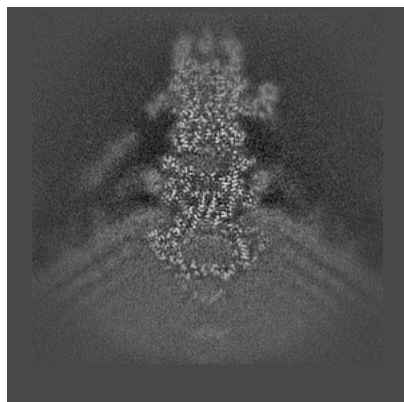


Z Index: 200

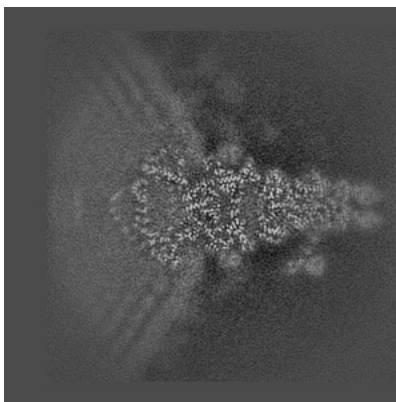
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

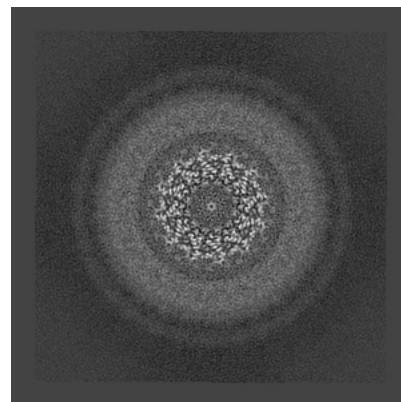
6.3.1 Primary map



X Index: 181

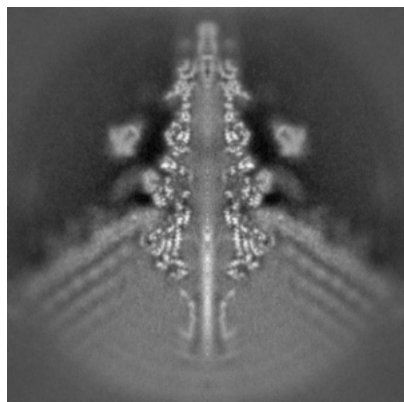


Y Index: 220

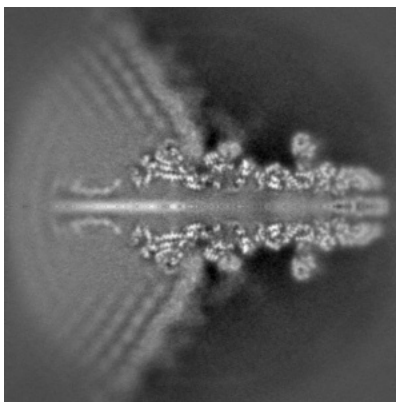


Z Index: 176

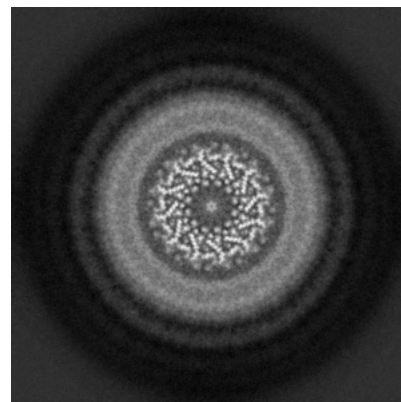
6.3.2 Raw map



X Index: 200



Y Index: 200

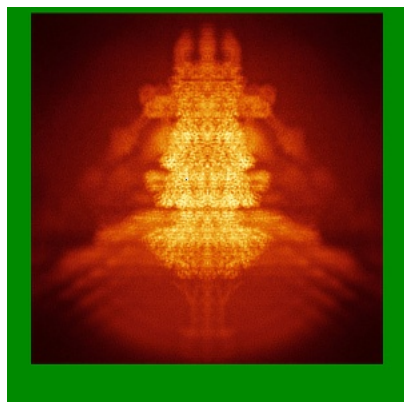


Z Index: 176

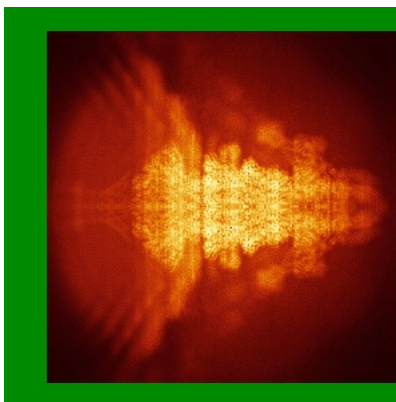
The images above show the largest variance slices of the map in three orthogonal directions.

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

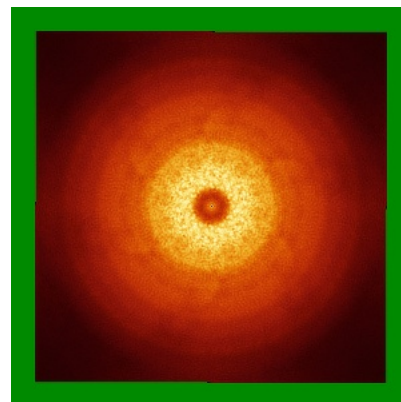
6.4.1 Primary map



X

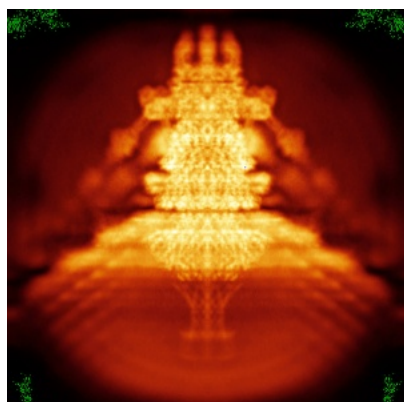


Y

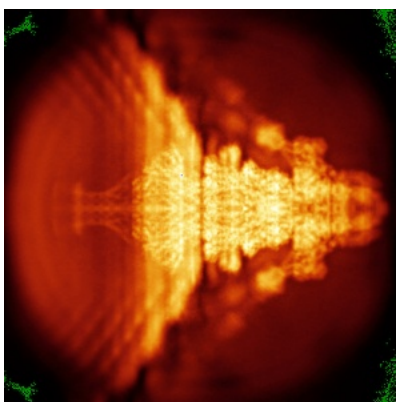


Z

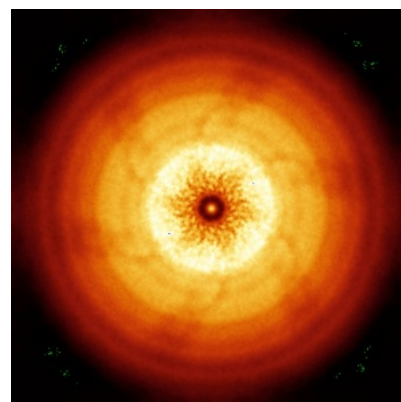
6.4.2 Raw map



X



Y

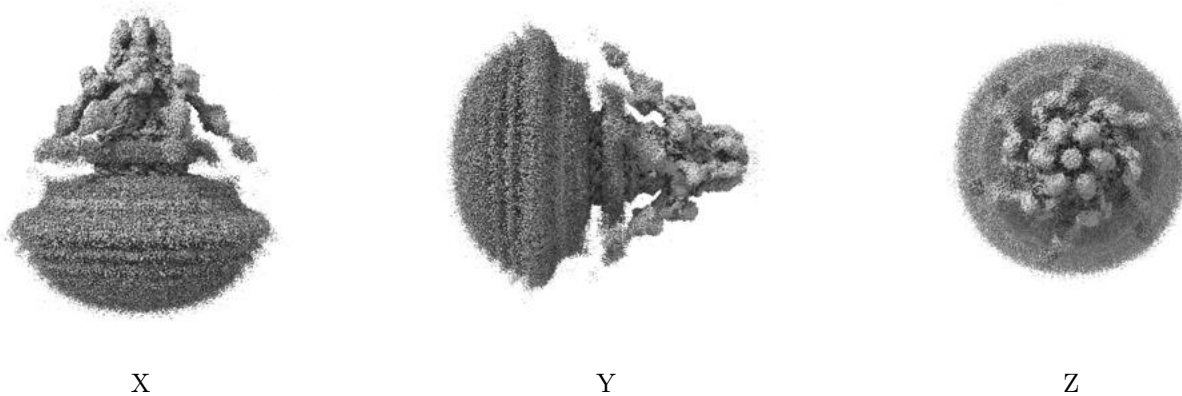


Z

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

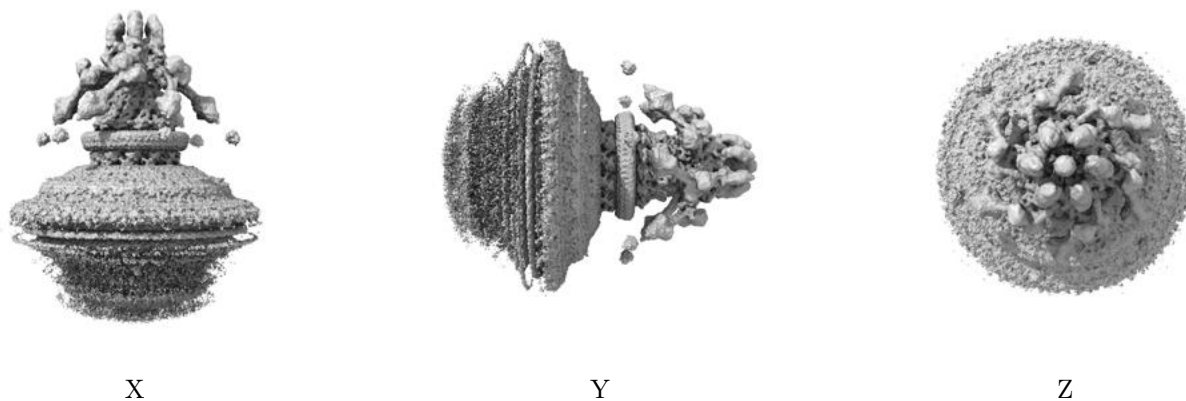
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

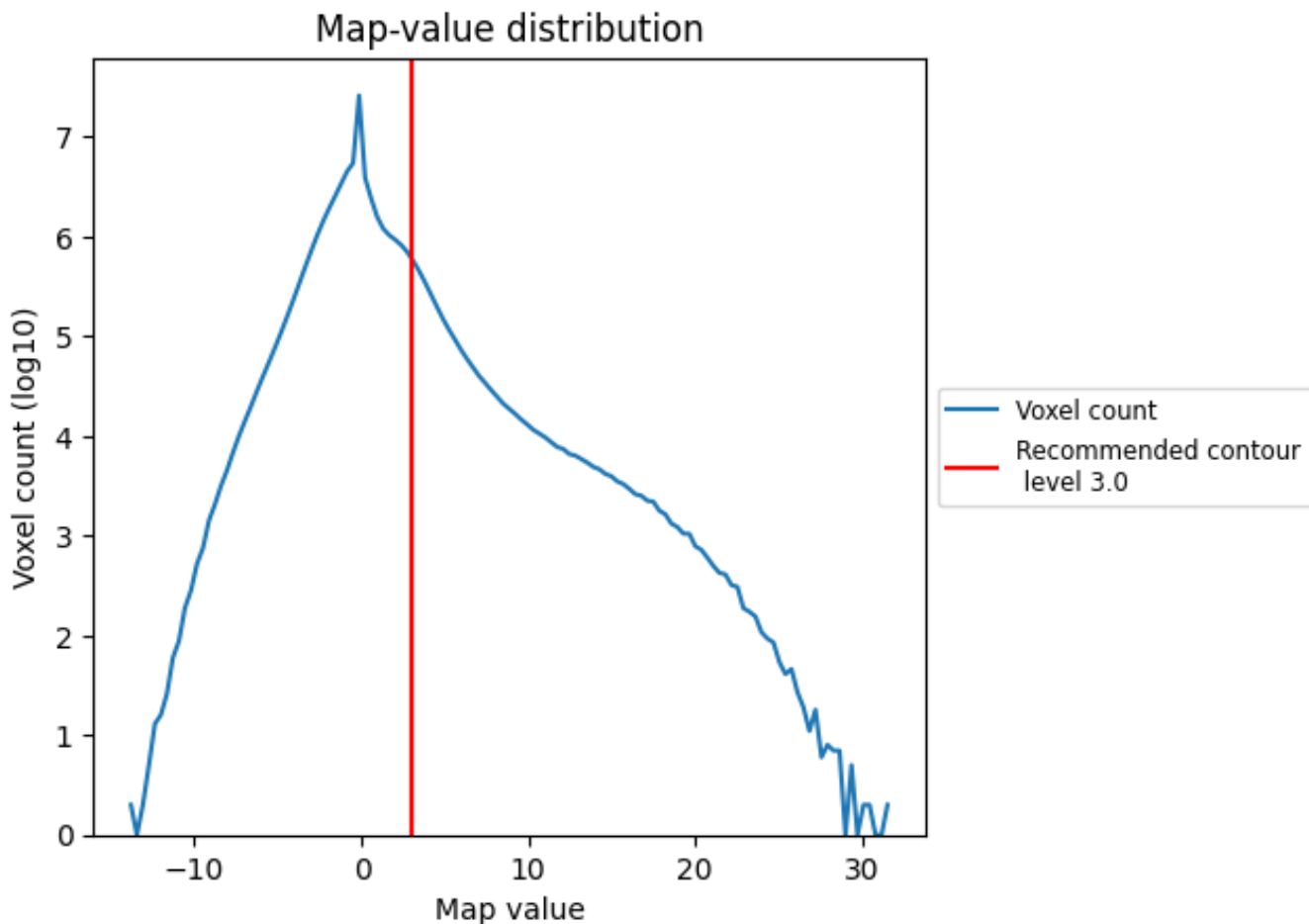
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

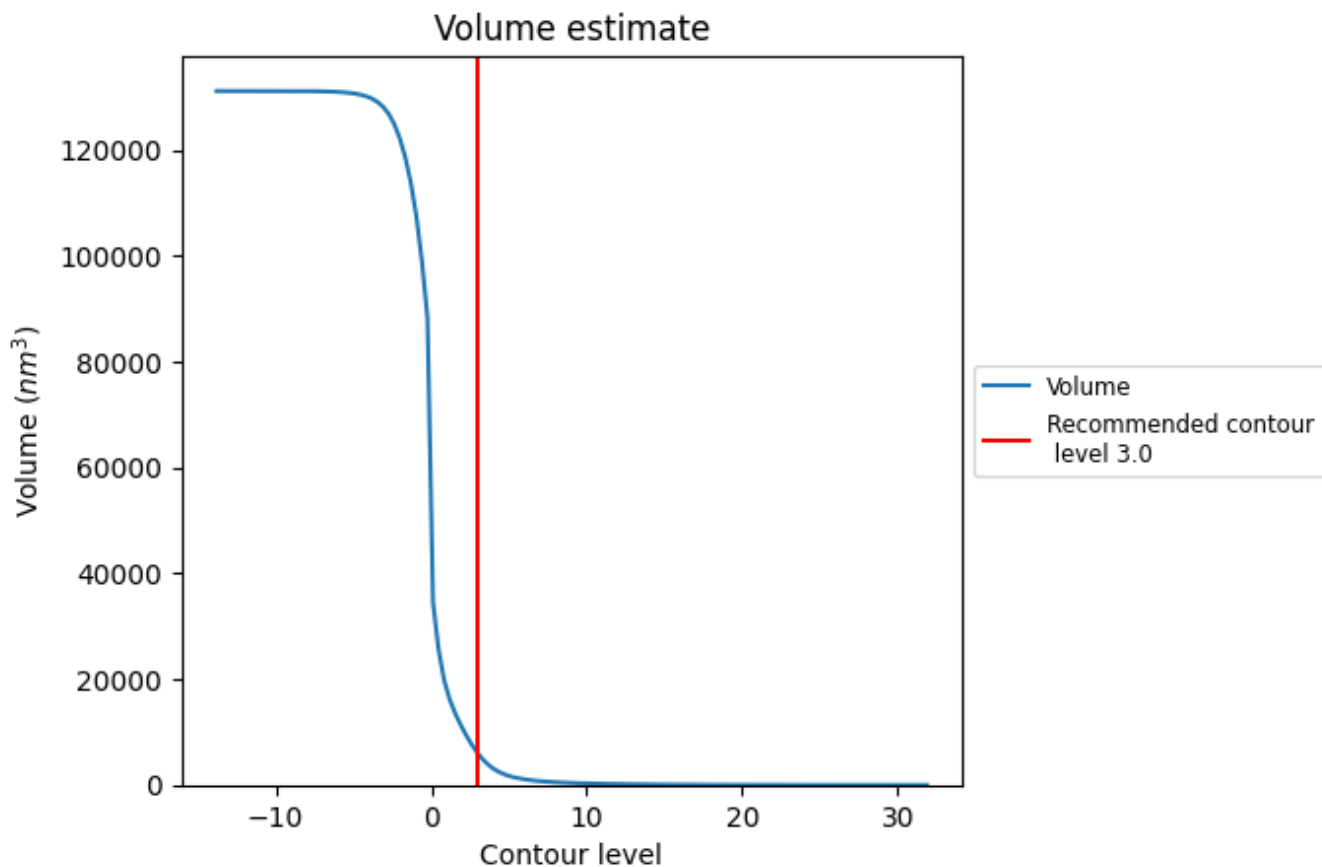
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

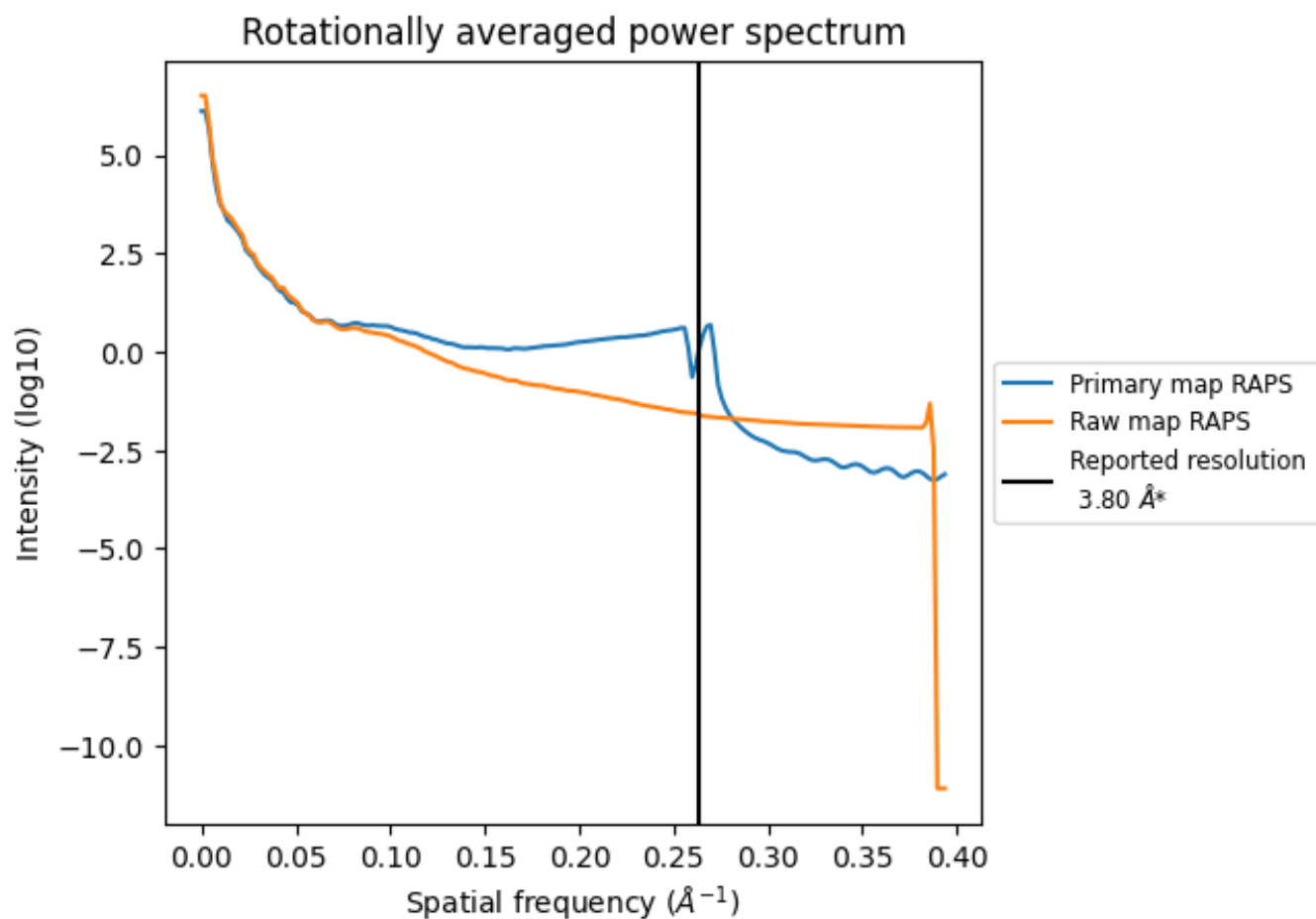
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5957 nm^3 ; this corresponds to an approximate mass of 5381 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

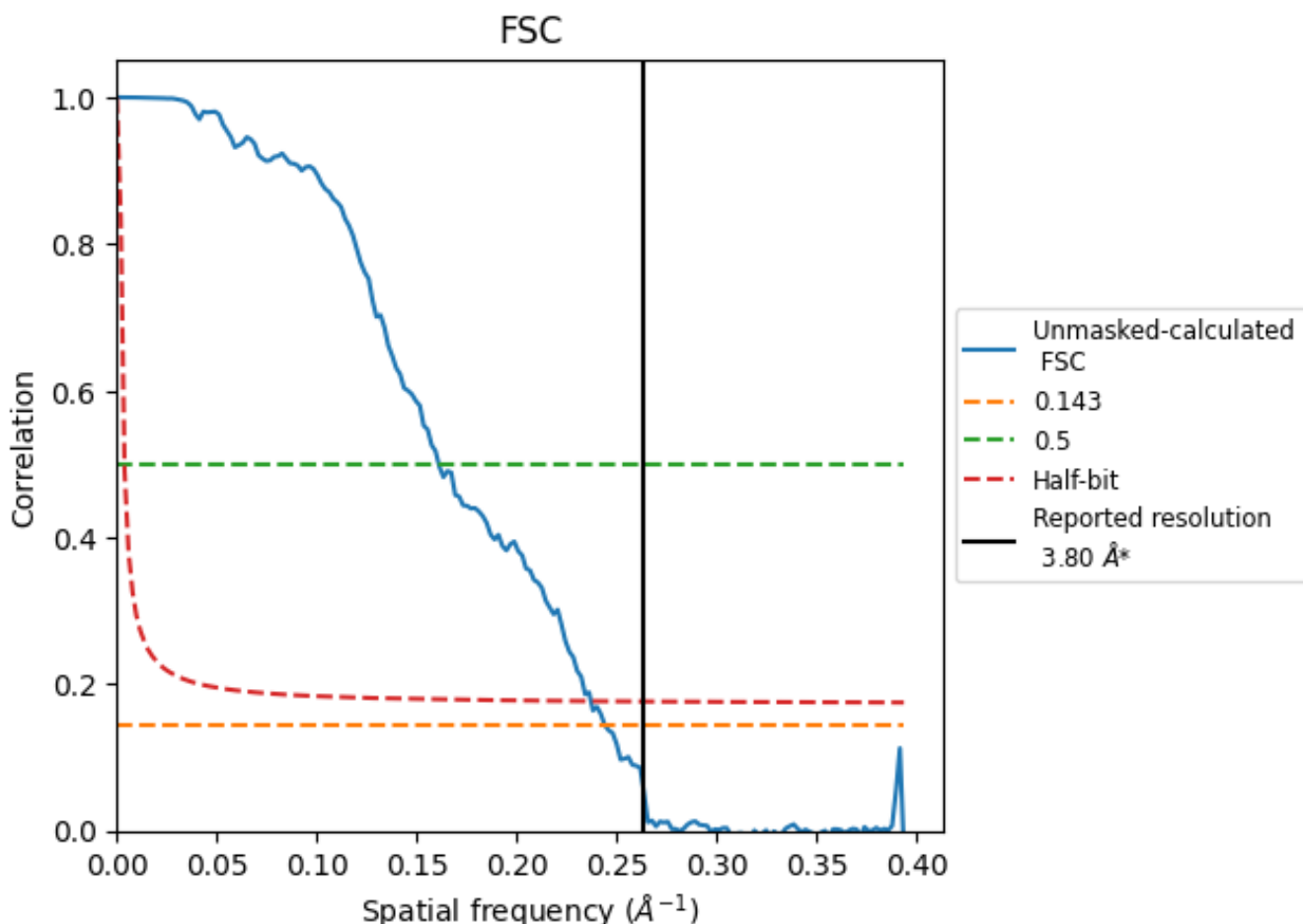


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

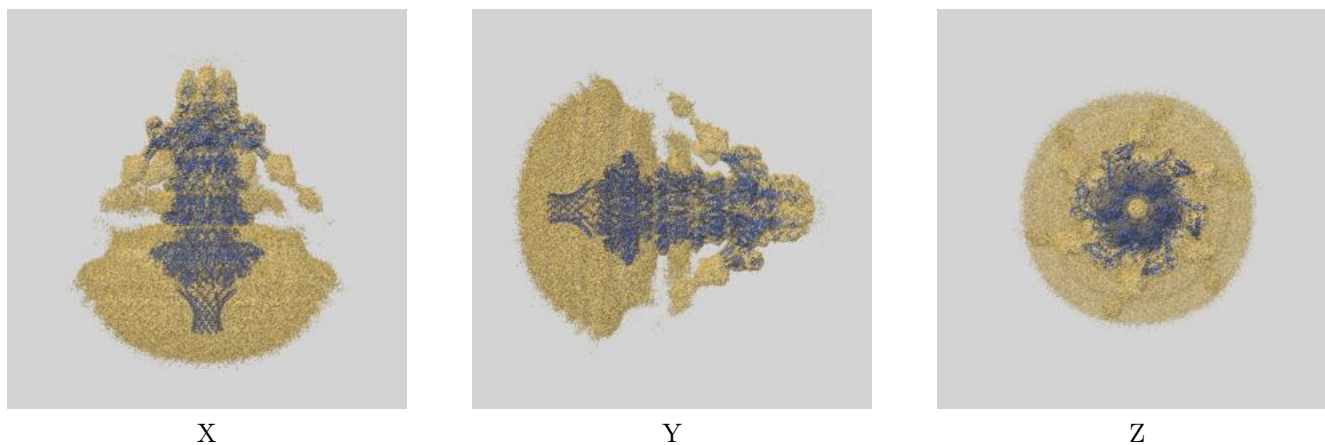
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	6.21	4.22

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

9 Map-model fit [i](#)

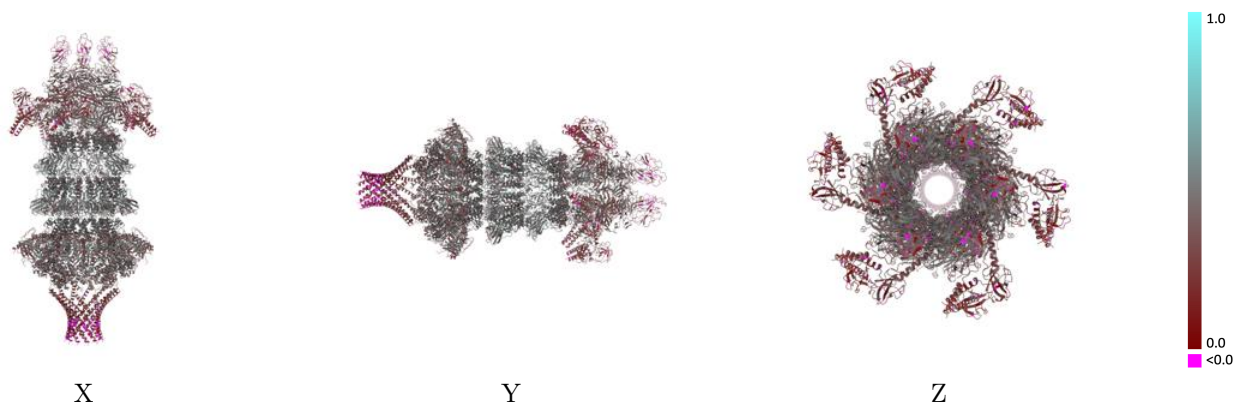
This section contains information regarding the fit between EMDB map EMD-36463 and PDB model 8JOV. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



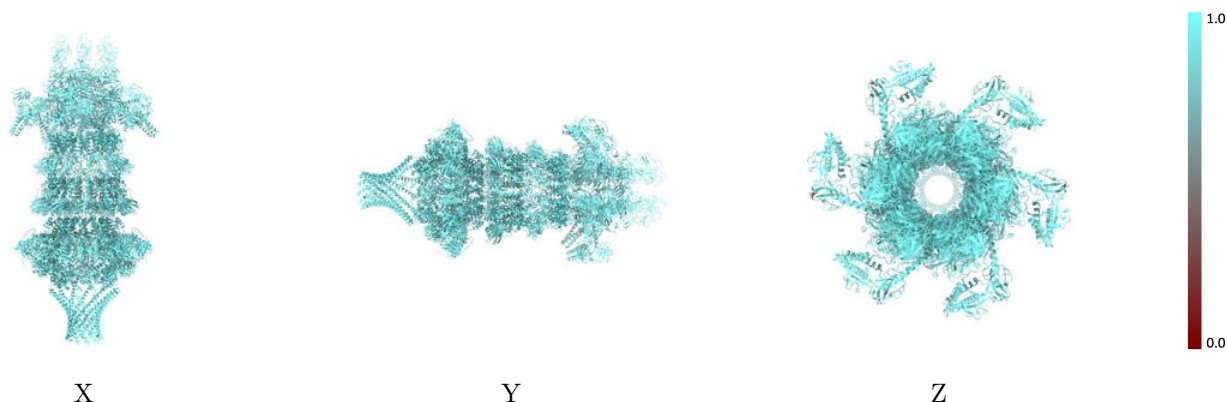
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



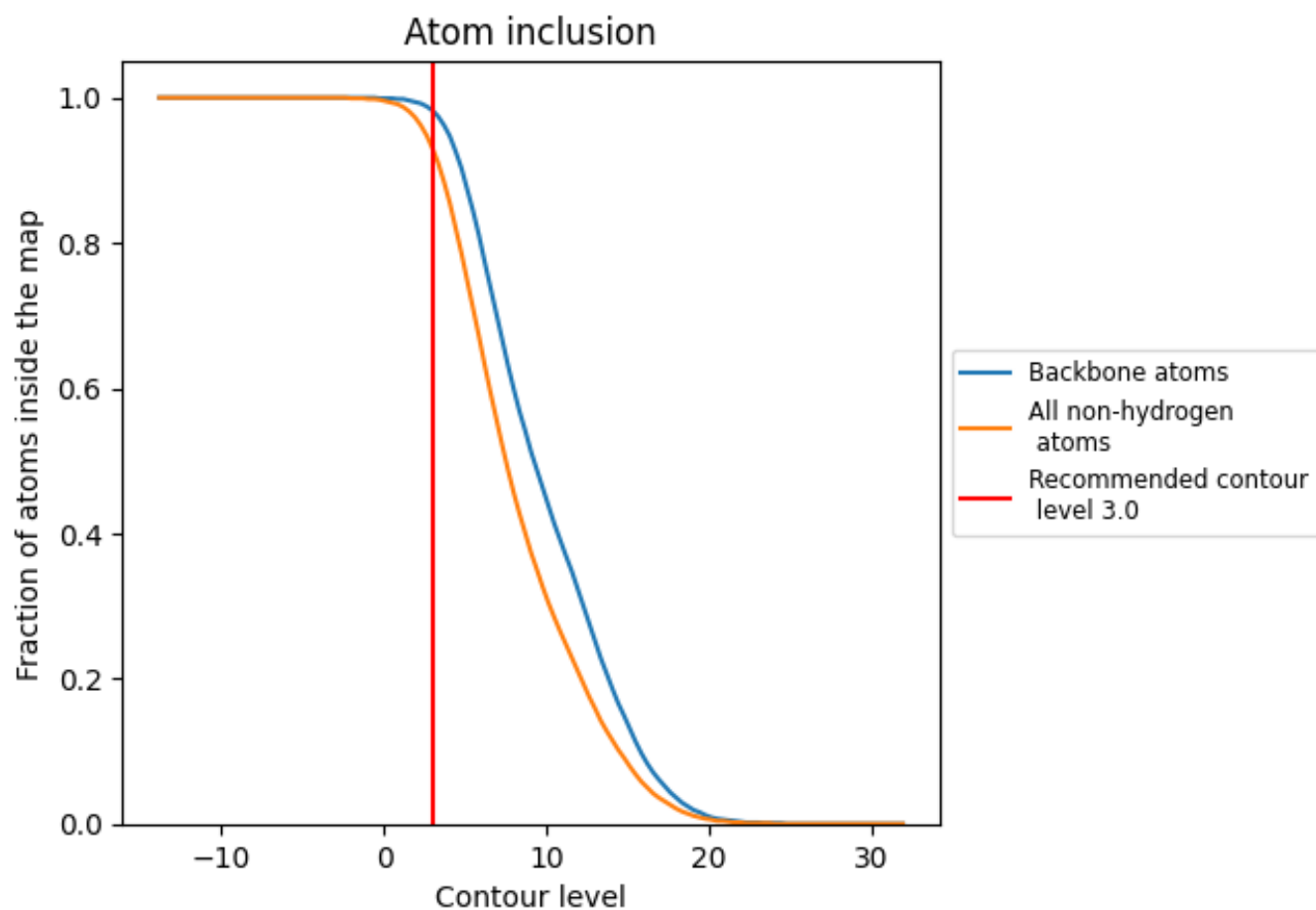
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.4050
0	 0.9310	 0.4100
1	 0.8900	 0.2720
2	 0.9530	 0.4690
3	 0.9280	 0.4080
4	 0.9040	 0.3510
5	 0.9550	 0.4700
6	 0.9260	 0.4120
7	 0.9040	 0.2300
A	 0.9350	 0.3860
B	 0.9390	 0.3850
C	 0.9330	 0.3850
D	 0.9360	 0.3880
E	 0.9400	 0.3870
F	 0.9340	 0.3860
G	 0.9180	 0.4580
H	 0.9190	 0.4520
I	 0.9170	 0.4500
J	 0.9150	 0.4550
K	 0.9190	 0.4530
L	 0.9170	 0.4520
M	 0.9040	 0.2770
N	 0.9100	 0.3410
O	 0.9030	 0.2240
P	 0.8900	 0.2780
Q	 0.9010	 0.3440
R	 0.9040	 0.2240
S	 0.9310	 0.4620
T	 0.9560	 0.4550
U	 0.9270	 0.4060
V	 0.8850	 0.2670
W	 0.9240	 0.4530
X	 0.9580	 0.4570
Y	 0.9280	 0.4100
Z	 0.9080	 0.3480



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Chain	Atom inclusion	Q-score
a	 0.9240	 0.4570
b	 0.9530	 0.4550
c	 0.9280	 0.4070
d	 0.9040	 0.2370
e	 0.9290	 0.4610
f	 0.9570	 0.4560
g	 0.9300	 0.4110
h	 0.8970	 0.2730
i	 0.9210	 0.4530
j	 0.9530	 0.4540
k	 0.9250	 0.4060
l	 0.9050	 0.3390
m	 0.9270	 0.4590
n	 0.9510	 0.4500
o	 0.9260	 0.4110
p	 0.9060	 0.2290
q	 0.9530	 0.4670
r	 0.9310	 0.4080
s	 0.8940	 0.2790
t	 0.9550	 0.4690
u	 0.9250	 0.4090
v	 0.9050	 0.3440
w	 0.9550	 0.4700
x	 0.9260	 0.4080
y	 0.9140	 0.2330
z	 0.9560	 0.4690