



## wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 11:42 am BST

PDB ID : 8B3O  
EMDB ID : EMD-15831  
Title : CryoEM structure of the pointy tip (proteins pIII/pVI/pVIII) from the filamentous bacteriophage  
Authors : Conners, R.; McLaren, M.; Gold, V.A.M.  
Deposited on : 2022-09-16  
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

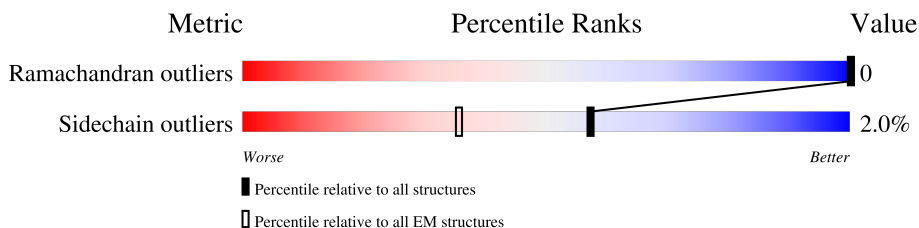
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 2.97 Å.

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










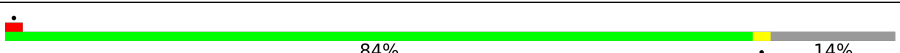
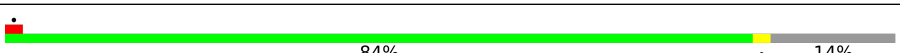
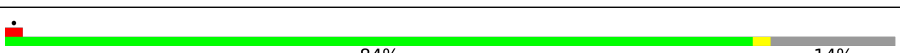
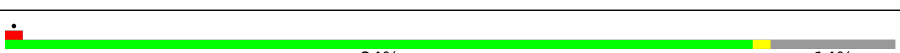
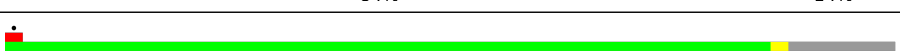

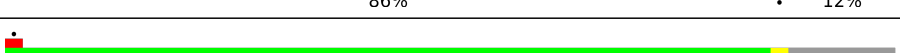
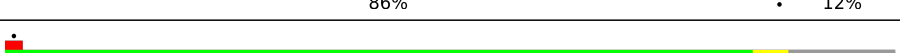

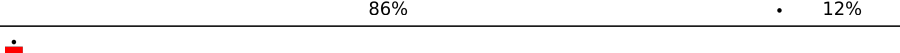
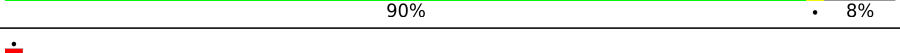
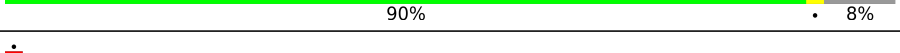
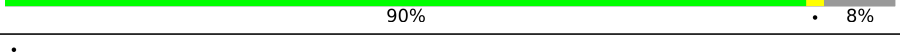


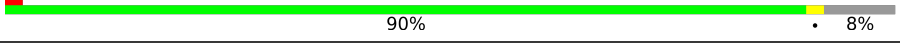
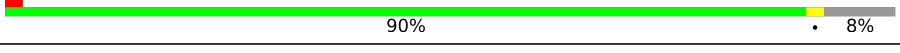
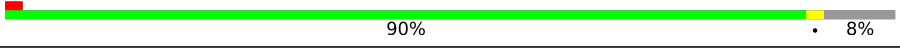
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	KKK	50	70% 30%
1	LLL	50	70% 30%
1	MMM	50	70% 30%
1	NNN	50	70% 30%
1	OOO	50	68% 30%
1	PPP	50	48% 52%
1	QQQ	50	48% 52%
1	RRR	50	48% 52%
1	SSS	50	48% 52%

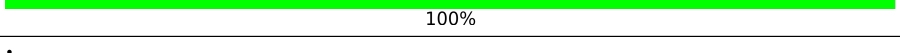
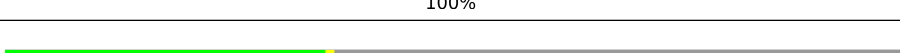

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	TTT	50	 48% 52%
1	UUU	50	 90% 8%
1	VVV	50	 90% 8%
1	WWW	50	 90% 8%
1	XXX	50	 90% 8%
1	YYY	50	 90% 8%
1	ZZZ	50	 84% 14%
1	aaa	50	 84% 14%
1	bbb	50	 84% 14%
1	ccc	50	 84% 14%
1	ddd	50	 84% 14%
1	eee	50	 86% 12%
1	fff	50	 86% 12%
1	ggg	50	 86% 12%
1	hhh	50	 84% 12%
1	iii	50	 86% 12%
1	jjj	50	 90% 8%
1	kkk	50	 90% 8%
1	lll	50	 90% 8%
1	mmm	50	 90% 8%
1	nnn	50	 90% 8%
1	ooo	50	 90% 8%
1	ppp	50	 90% 8%
1	qqq	50	 90% 8%
1	rrr	50	 90% 8%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	sss	50	 90% 8%
2	AAA	112	 100%
2	BBB	112	 100%
2	CCC	112	 100%
2	DDD	112	 100%
2	EEE	112	 100%
3	FFF	406	 36% 64%
3	GGG	406	 36% 64%
3	HHH	406	 36% 64%
3	III	406	 36% 64%
3	JJJ	406	 36% 64%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20475 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 Capsid protein G8P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	KKK	35	258	172	40	44	2	0	0
1	PPP	24	175	118	28	28	1	0	0
1	UUU	46	339	223	53	61	2	0	0
1	ZZZ	43	319	211	50	56	2	0	0
1	eee	44	328	217	51	58	2	0	0
1	jjj	46	339	223	53	61	2	0	0
1	ooo	46	339	223	53	61	2	0	0
1	LLL	35	258	172	40	44	2	0	0
1	QQQ	24	175	118	28	28	1	0	0
1	VVV	46	339	223	53	61	2	0	0
1	aaa	43	319	211	50	56	2	0	0
1	fff	44	328	217	51	58	2	0	0
1	kkk	46	339	223	53	61	2	0	0
1	ppp	46	339	223	53	61	2	0	0
1	MMM	35	258	172	40	44	2	0	0
1	RRR	24	175	118	28	28	1	0	0
1	WWW	46	339	223	53	61	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	bbb	43	Total	C	N	O	S	0	0
			319	211	50	56	2		
1	ggg	44	Total	C	N	O	S	0	0
			328	217	51	58	2		
1	lll	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	qqq	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	NNN	35	Total	C	N	O	S	0	0
			258	172	40	44	2		
1	SSS	24	Total	C	N	O	S	0	0
			175	118	28	28	1		
1	XXX	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	ccc	43	Total	C	N	O	S	0	0
			319	211	50	56	2		
1	hhh	44	Total	C	N	O	S	0	0
			328	217	51	58	2		
1	mmm	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	rrr	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	OOO	35	Total	C	N	O	S	0	0
			258	172	40	44	2		
1	TTT	24	Total	C	N	O	S	0	0
			175	118	28	28	1		
1	YYY	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	ddd	43	Total	C	N	O	S	0	0
			319	211	50	56	2		
1	iii	44	Total	C	N	O	S	0	0
			328	217	51	58	2		
1	nnn	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
1	sss	46	Total	C	N	O	S	0	0
			339	223	53	61	2		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
KKK	21	MET	TYR	engineered mutation	UNP P69540
PPP	21	MET	TYR	engineered mutation	UNP P69540
UUU	21	MET	TYR	engineered mutation	UNP P69540

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
ZZZ	21	MET	TYR	engineered mutation	UNP P69540
eee	21	MET	TYR	engineered mutation	UNP P69540
jjj	21	MET	TYR	engineered mutation	UNP P69540
ooo	21	MET	TYR	engineered mutation	UNP P69540
LLL	21	MET	TYR	engineered mutation	UNP P69540
QQQ	21	MET	TYR	engineered mutation	UNP P69540
VVV	21	MET	TYR	engineered mutation	UNP P69540
aaa	21	MET	TYR	engineered mutation	UNP P69540
fff	21	MET	TYR	engineered mutation	UNP P69540
kkk	21	MET	TYR	engineered mutation	UNP P69540
ppp	21	MET	TYR	engineered mutation	UNP P69540
MMM	21	MET	TYR	engineered mutation	UNP P69540
RRR	21	MET	TYR	engineered mutation	UNP P69540
WWW	21	MET	TYR	engineered mutation	UNP P69540
bbb	21	MET	TYR	engineered mutation	UNP P69540
ggg	21	MET	TYR	engineered mutation	UNP P69540
lll	21	MET	TYR	engineered mutation	UNP P69540
qqq	21	MET	TYR	engineered mutation	UNP P69540
NNN	21	MET	TYR	engineered mutation	UNP P69540
SSS	21	MET	TYR	engineered mutation	UNP P69540
XXX	21	MET	TYR	engineered mutation	UNP P69540
ccc	21	MET	TYR	engineered mutation	UNP P69540
hhh	21	MET	TYR	engineered mutation	UNP P69540
mmm	21	MET	TYR	engineered mutation	UNP P69540
rrr	21	MET	TYR	engineered mutation	UNP P69540
OOO	21	MET	TYR	engineered mutation	UNP P69540
TTT	21	MET	TYR	engineered mutation	UNP P69540
YYY	21	MET	TYR	engineered mutation	UNP P69540
ddd	21	MET	TYR	engineered mutation	UNP P69540
iii	21	MET	TYR	engineered mutation	UNP P69540
nnn	21	MET	TYR	engineered mutation	UNP P69540
sss	21	MET	TYR	engineered mutation	UNP P69540

- Molecule 2 is a protein called Head virion protein G6P.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AAA	112	Total	C	N	O	S	0	0
			875	602	129	142	2		
2	BBB	112	Total	C	N	O	S	0	0
			875	602	129	142	2		
2	CCC	112	Total	C	N	O	S	0	0
			875	602	129	142	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DDD	112	Total	C	N	O	S	0	0
			875	602	129	142	2		
2	EEE	112	Total	C	N	O	S	0	0
			875	602	129	142	2		

- Molecule 3 is a protein called Attachment protein G3P.

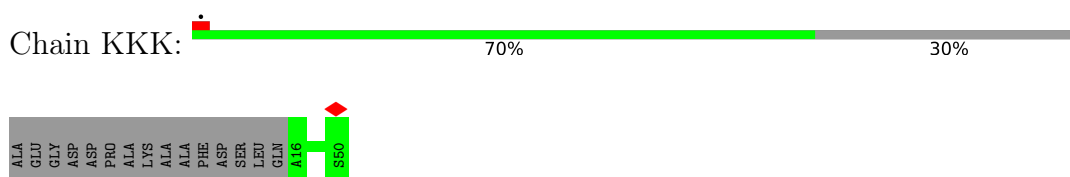
Mol	Chain	Residues	Atoms					AltConf	Trace
3	FFF	148	Total	C	N	O	S	0	0
			1123	708	185	223	7		
3	GGG	148	Total	C	N	O	S	0	0
			1123	708	185	223	7		
3	HHH	148	Total	C	N	O	S	0	0
			1123	708	185	223	7		
3	III	148	Total	C	N	O	S	0	0
			1123	708	185	223	7		
3	JJJ	148	Total	C	N	O	S	0	0
			1123	708	185	223	7		



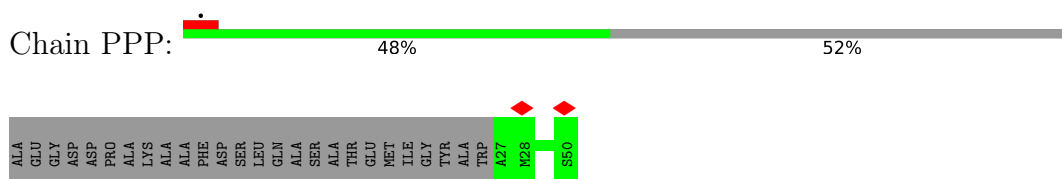
### 3 Residue-property plots [i](#)

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.

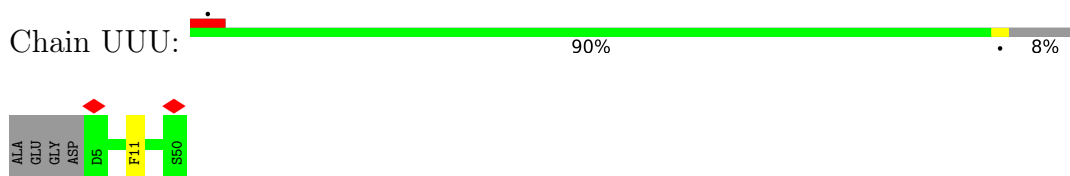
- Molecule 1: Capsid protein G8P



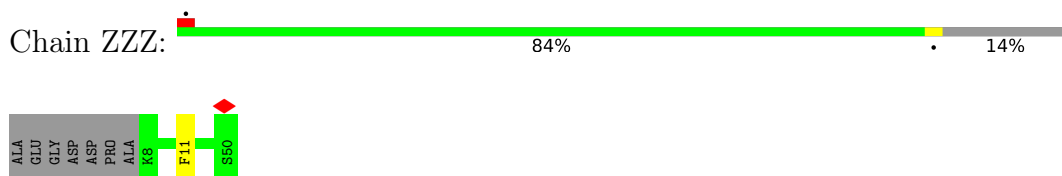
- Molecule 1: Capsid protein G8P



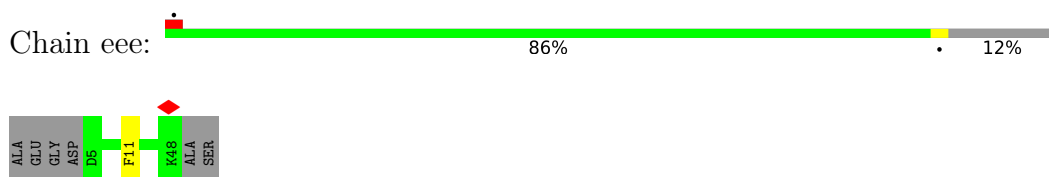
- Molecule 1: Capsid protein G8P



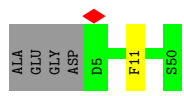
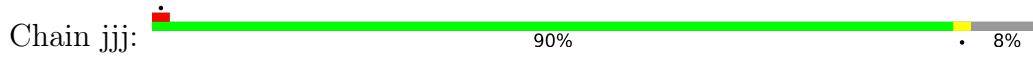
- Molecule 1: Capsid protein G8P



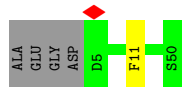
- Molecule 1: Capsid protein G8P



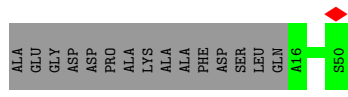
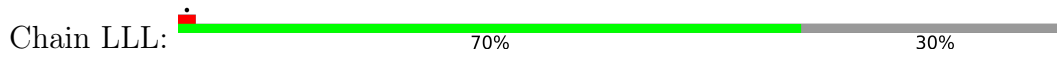
• Molecule 1: Capsid protein G8P



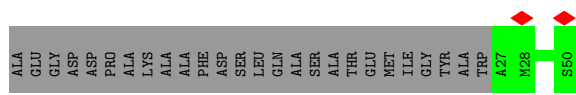
• Molecule 1: Capsid protein G8P



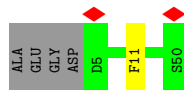
• Molecule 1: Capsid protein G8P



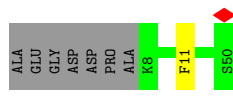
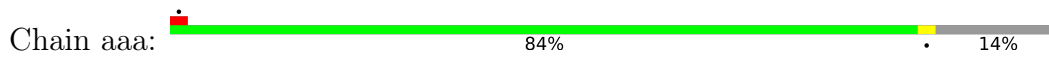
• Molecule 1: Capsid protein G8P



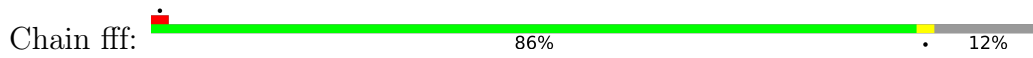
• Molecule 1: Capsid protein G8P

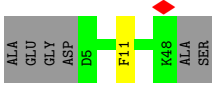


• Molecule 1: Capsid protein G8P

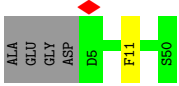


• Molecule 1: Capsid protein G8P

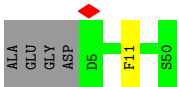




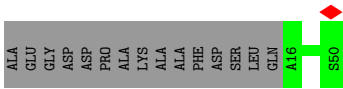
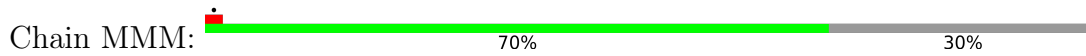
- Molecule 1: Capsid protein G8P



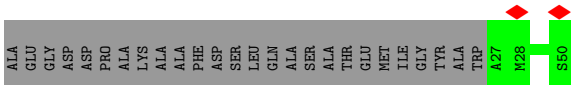
- Molecule 1: Capsid protein G8P



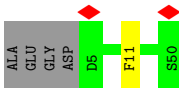
- Molecule 1: Capsid protein G8P



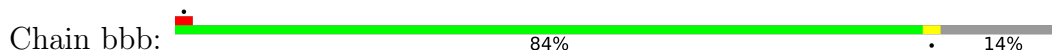
- Molecule 1: Capsid protein G8P



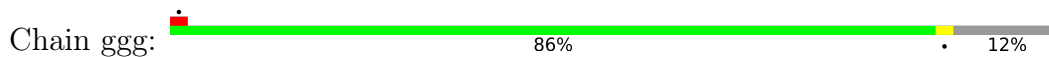
- Molecule 1: Capsid protein G8P



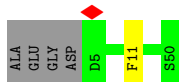
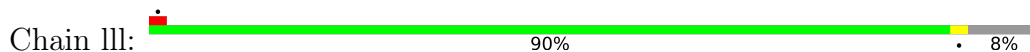
- Molecule 1: Capsid protein G8P



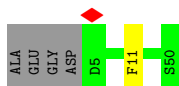
- Molecule 1: Capsid protein G8P



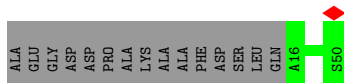
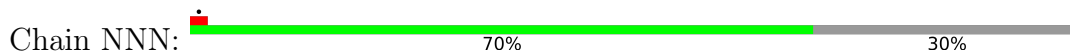
• Molecule 1: Capsid protein G8P



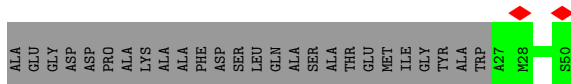
• Molecule 1: Capsid protein G8P



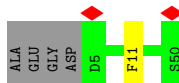
• Molecule 1: Capsid protein G8P



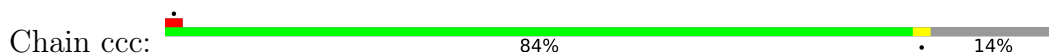
• Molecule 1: Capsid protein G8P

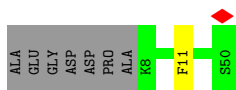


• Molecule 1: Capsid protein G8P

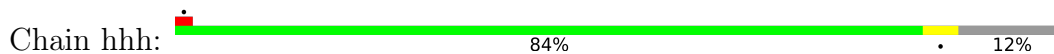


• Molecule 1: Capsid protein G8P

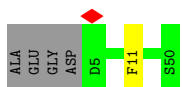




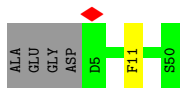
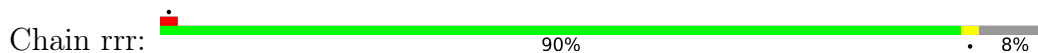
• Molecule 1: Capsid protein G8P



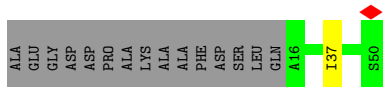
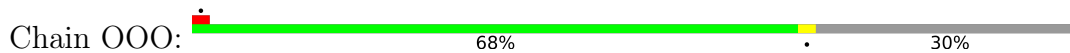
• Molecule 1: Capsid protein G8P



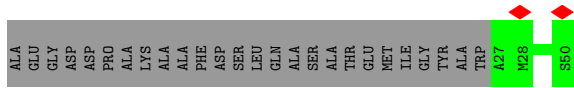
• Molecule 1: Capsid protein G8P



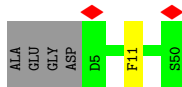
• Molecule 1: Capsid protein G8P



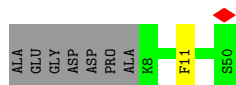
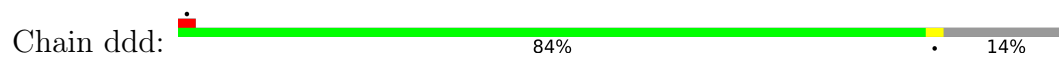
• Molecule 1: Capsid protein G8P



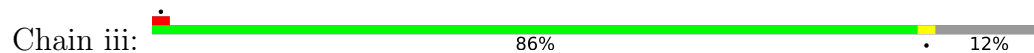
• Molecule 1: Capsid protein G8P



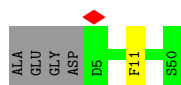
• Molecule 1: Capsid protein G8P



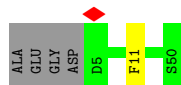
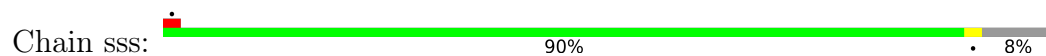
- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 1: Capsid protein G8P



- Molecule 2: Head virion protein G6P



- Molecule 2: Head virion protein G6P



- Molecule 2: Head virion protein G6P









GLY	GLY	GLY	SER	GLU	GLY	GLY	SER	GLY	GLY	SER	GLY	SER	GLY	D2957	L3445	F367	L376	R404	GLU	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	------	------	------	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	86242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.889	Depositor
Minimum map value	-0.228	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.222	Depositor
Map size ( $\text{\AA}$ )	422.86078, 422.86078, 422.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1012, 1.1012, 1.1012	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	KKK	0.30	0/262	0.53	0/352
1	LLL	0.30	0/262	0.53	0/352
1	MMM	0.30	0/262	0.53	0/352
1	NNN	0.30	0/262	0.53	0/352
1	OOO	0.30	0/262	0.53	0/352
1	PPP	0.30	0/176	0.53	0/234
1	QQQ	0.30	0/176	0.53	0/234
1	RRR	0.30	0/176	0.53	0/234
1	SSS	0.30	0/176	0.53	0/234
1	TTT	0.30	0/176	0.53	0/234
1	UUU	0.29	0/345	0.53	0/465
1	VVV	0.29	0/345	0.53	0/465
1	WWW	0.29	0/345	0.53	0/465
1	XXX	0.29	0/345	0.53	0/465
1	YYY	0.29	0/345	0.53	0/465
1	ZZZ	0.30	0/324	0.54	0/435
1	aaa	0.30	0/324	0.54	0/435
1	bbb	0.30	0/324	0.54	0/435
1	ccc	0.30	0/324	0.54	0/435
1	ddd	0.30	0/324	0.54	0/435
1	eee	0.29	0/334	0.64	0/450
1	fff	0.29	0/334	0.64	0/450
1	ggg	0.29	0/334	0.64	0/450
1	hhh	0.29	0/334	0.64	0/450
1	iii	0.29	0/334	0.64	0/450
1	jjj	0.28	0/345	0.60	0/465
1	kkk	0.28	0/345	0.60	0/465
1	lll	0.28	0/345	0.61	0/465
1	mmm	0.28	0/345	0.61	0/465
1	nnn	0.28	0/345	0.61	0/465
1	ooo	0.29	0/345	0.54	0/465
1	ppp	0.29	0/345	0.54	0/465
1	qqq	0.29	0/345	0.54	0/465
1	rrr	0.29	0/345	0.54	0/465

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	sss	0.29	0/345	0.54	0/465
2	AAA	0.29	0/895	0.58	0/1216
2	BBB	0.29	0/895	0.58	0/1216
2	CCC	0.29	0/895	0.58	0/1216
2	DDD	0.29	0/895	0.58	0/1216
2	EEE	0.29	0/895	0.58	0/1216
3	FFF	0.29	0/1146	0.58	0/1547
3	GGG	0.29	0/1146	0.57	0/1547
3	HHH	0.29	0/1146	0.57	0/1547
3	III	0.29	0/1146	0.57	0/1547
3	JJJ	0.29	0/1146	0.57	0/1547
All	All	0.29	0/20860	0.57	0/28145

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	KKK	33/50 (66%)	33 (100%)	0	0	100	100
1	LLL	33/50 (66%)	33 (100%)	0	0	100	100
1	MMM	33/50 (66%)	33 (100%)	0	0	100	100
1	NNN	33/50 (66%)	33 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OOO	33/50 (66%)	33 (100%)	0	0	100	100
1	PPP	22/50 (44%)	22 (100%)	0	0	100	100
1	QQQ	22/50 (44%)	22 (100%)	0	0	100	100
1	RRR	22/50 (44%)	22 (100%)	0	0	100	100
1	SSS	22/50 (44%)	22 (100%)	0	0	100	100
1	TTT	22/50 (44%)	22 (100%)	0	0	100	100
1	UUU	44/50 (88%)	44 (100%)	0	0	100	100
1	VVV	44/50 (88%)	44 (100%)	0	0	100	100
1	WWW	44/50 (88%)	44 (100%)	0	0	100	100
1	XXX	44/50 (88%)	44 (100%)	0	0	100	100
1	YYY	44/50 (88%)	44 (100%)	0	0	100	100
1	ZZZ	41/50 (82%)	41 (100%)	0	0	100	100
1	aaa	41/50 (82%)	41 (100%)	0	0	100	100
1	bbb	41/50 (82%)	41 (100%)	0	0	100	100
1	ccc	41/50 (82%)	41 (100%)	0	0	100	100
1	ddd	41/50 (82%)	41 (100%)	0	0	100	100
1	eee	42/50 (84%)	42 (100%)	0	0	100	100
1	fff	42/50 (84%)	42 (100%)	0	0	100	100
1	ggg	42/50 (84%)	42 (100%)	0	0	100	100
1	hhh	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
1	iii	42/50 (84%)	42 (100%)	0	0	100	100
1	jjj	44/50 (88%)	44 (100%)	0	0	100	100
1	kkk	44/50 (88%)	44 (100%)	0	0	100	100
1	lll	44/50 (88%)	44 (100%)	0	0	100	100
1	mmm	44/50 (88%)	44 (100%)	0	0	100	100
1	nnn	44/50 (88%)	44 (100%)	0	0	100	100
1	ooo	44/50 (88%)	44 (100%)	0	0	100	100
1	ppp	44/50 (88%)	44 (100%)	0	0	100	100
1	qqq	44/50 (88%)	44 (100%)	0	0	100	100
1	rrr	44/50 (88%)	44 (100%)	0	0	100	100
1	sss	44/50 (88%)	44 (100%)	0	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AAA	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
2	BBB	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
2	CCC	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
2	DDD	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
2	EEE	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
3	FFF	146/406 (36%)	132 (90%)	14 (10%)	0	100	100
3	GGG	146/406 (36%)	133 (91%)	13 (9%)	0	100	100
3	HHH	146/406 (36%)	133 (91%)	13 (9%)	0	100	100
3	III	146/406 (36%)	133 (91%)	13 (9%)	0	100	100
3	JJJ	146/406 (36%)	132 (90%)	14 (10%)	0	100	100
All	All	2630/4340 (61%)	2522 (96%)	108 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	KKK	26/36 (72%)	26 (100%)	0	100	100
1	LLL	26/36 (72%)	26 (100%)	0	100	100
1	MMM	26/36 (72%)	26 (100%)	0	100	100
1	NNN	26/36 (72%)	26 (100%)	0	100	100
1	OOO	26/36 (72%)	25 (96%)	1 (4%)	33	67
1	PPP	19/36 (53%)	19 (100%)	0	100	100
1	QQQ	19/36 (53%)	19 (100%)	0	100	100
1	RRR	19/36 (53%)	19 (100%)	0	100	100
1	SSS	19/36 (53%)	19 (100%)	0	100	100
1	TTT	19/36 (53%)	19 (100%)	0	100	100
1	UUU	34/36 (94%)	33 (97%)	1 (3%)	42	74

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	VVV	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	WWW	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	XXX	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	YYY	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	ZZZ	32/36 (89%)	31 (97%)	1 (3%)	40	73
1	aaa	32/36 (89%)	31 (97%)	1 (3%)	40	73
1	bbb	32/36 (89%)	31 (97%)	1 (3%)	40	73
1	ccc	32/36 (89%)	31 (97%)	1 (3%)	40	73
1	ddd	32/36 (89%)	31 (97%)	1 (3%)	40	73
1	eee	33/36 (92%)	32 (97%)	1 (3%)	41	73
1	fff	33/36 (92%)	32 (97%)	1 (3%)	41	73
1	ggg	33/36 (92%)	32 (97%)	1 (3%)	41	73
1	hhh	33/36 (92%)	31 (94%)	2 (6%)	18	51
1	iii	33/36 (92%)	32 (97%)	1 (3%)	41	73
1	jjj	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	kkk	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	lll	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	mmm	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	nnn	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	ooo	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	ppp	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	qqq	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	rrr	34/36 (94%)	33 (97%)	1 (3%)	42	74
1	sss	34/36 (94%)	33 (97%)	1 (3%)	42	74
2	AAA	97/97 (100%)	97 (100%)	0	100	100
2	BBB	97/97 (100%)	97 (100%)	0	100	100
2	CCC	97/97 (100%)	97 (100%)	0	100	100
2	DDD	97/97 (100%)	97 (100%)	0	100	100
2	EEE	97/97 (100%)	97 (100%)	0	100	100
3	FFF	116/310 (37%)	113 (97%)	3 (3%)	46	76
3	GGG	116/310 (37%)	113 (97%)	3 (3%)	46	76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	HHH	116/310 (37%)	113 (97%)	3 (3%)	46	76
3	III	116/310 (37%)	113 (97%)	3 (3%)	46	76
3	JJJ	116/310 (37%)	113 (97%)	3 (3%)	46	76
All	All	2125/3295 (64%)	2083 (98%)	42 (2%)	57	81

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	III	376	LEU
1	ddd	11	PHE
1	hhh	11	PHE
1	rrr	11	PHE
3	JJJ	367	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

There are no chain breaks in this entry.

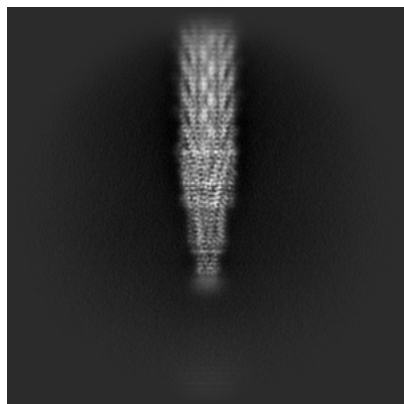
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15831. These allow visual inspection of the internal detail of the map and identification of artifacts.

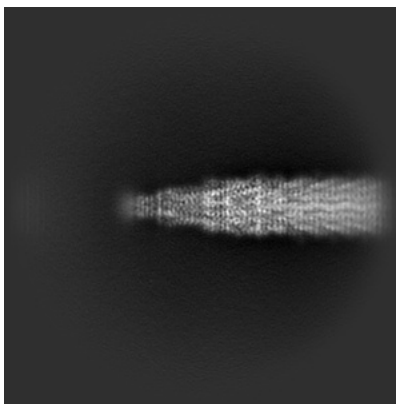
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

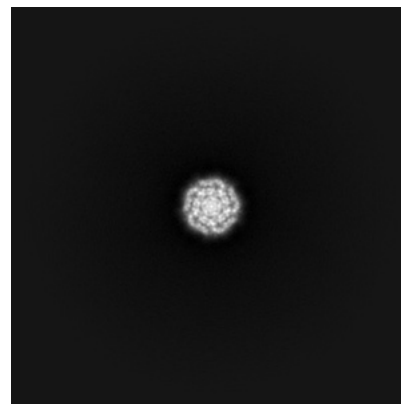
#### 6.1.1 Primary map



X

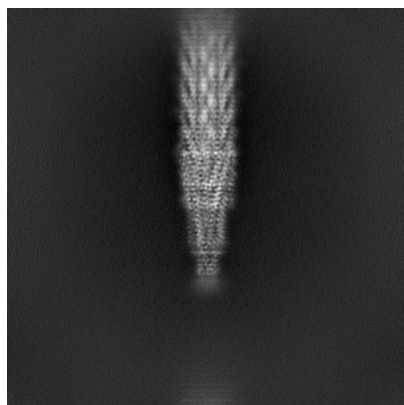


Y

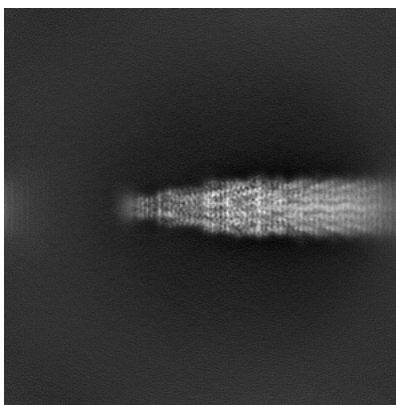


Z

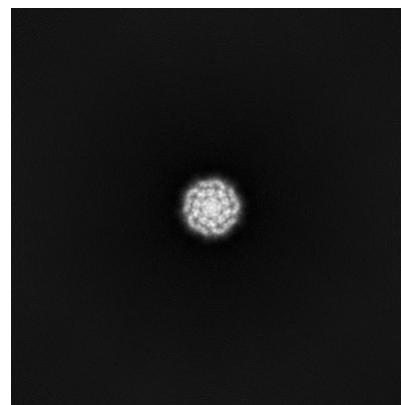
#### 6.1.2 Raw map



X



Y

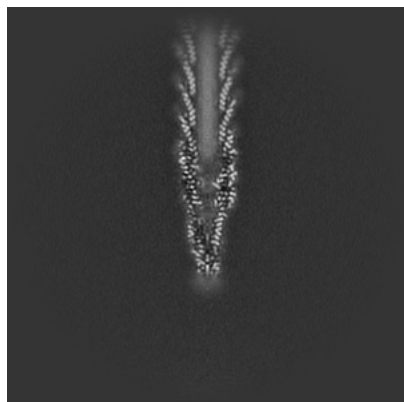


Z

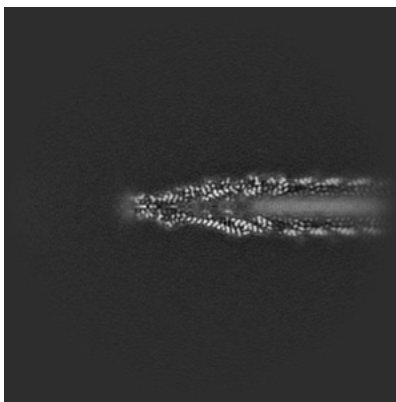
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

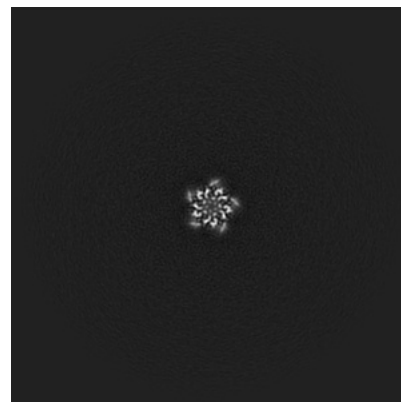
### 6.2.1 Primary map



X Index: 192

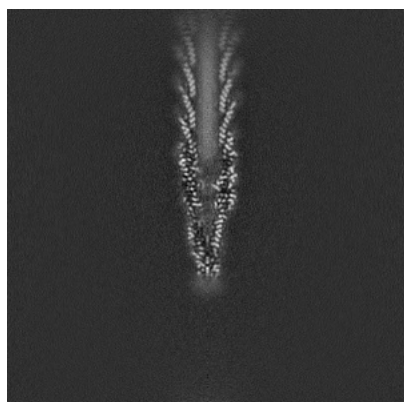


Y Index: 192

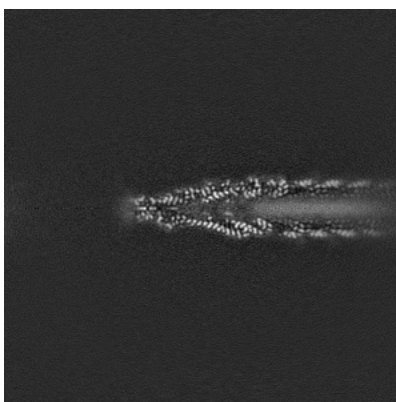


Z Index: 192

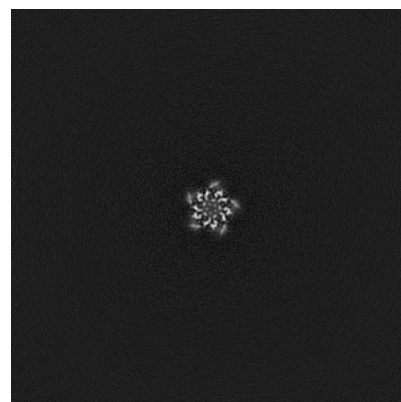
### 6.2.2 Raw map



X Index: 192



Y Index: 192

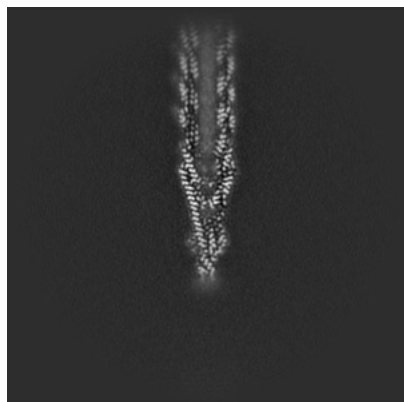


Z Index: 192

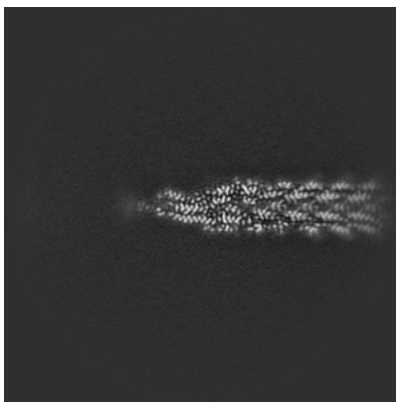
The images above show central slices of the map in three orthogonal directions.

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

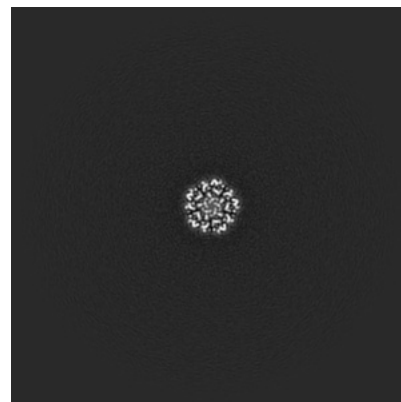
### 6.3.1 Primary map



X Index: 185

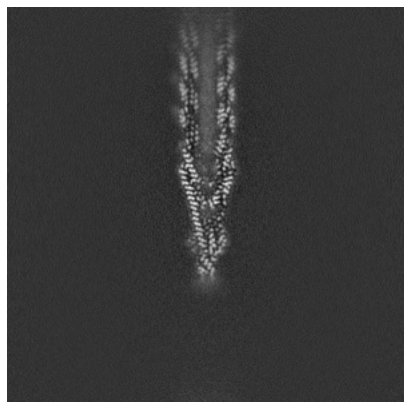


Y Index: 204

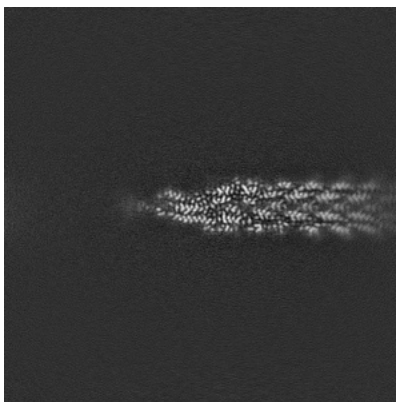


Z Index: 214

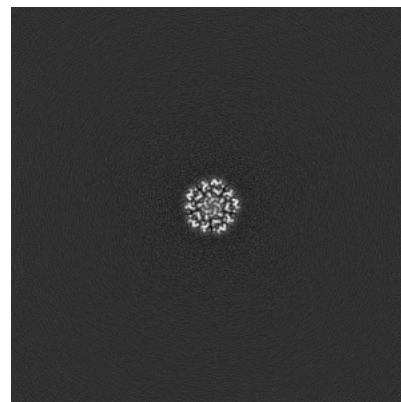
### 6.3.2 Raw map



X Index: 185



Y Index: 204

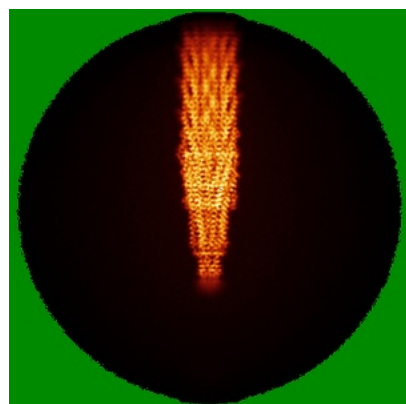


Z Index: 214

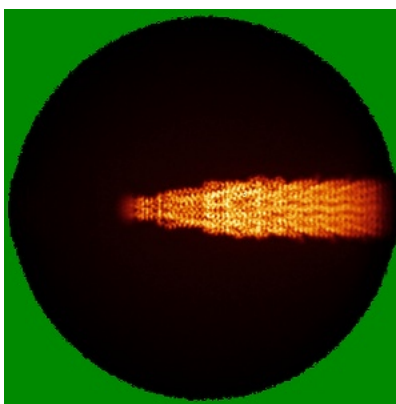
The images above show the largest variance slices of the map in three orthogonal directions.

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

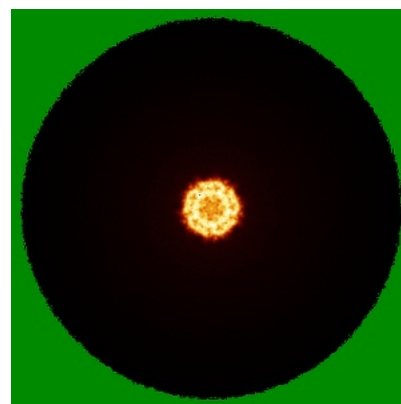
### 6.4.1 Primary map



X

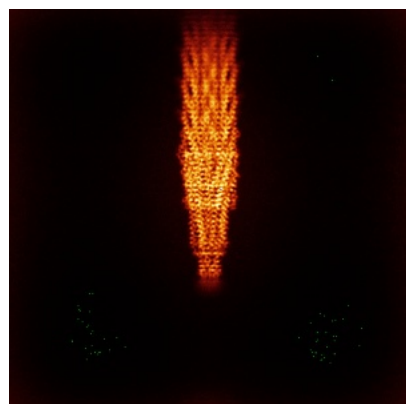


Y

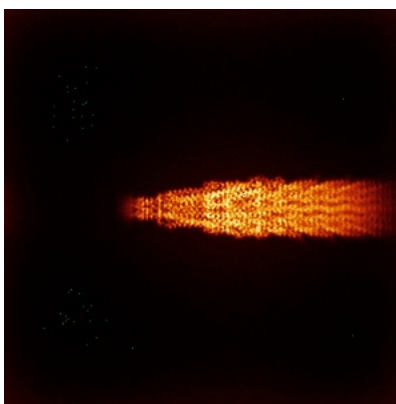


Z

### 6.4.2 Raw map



X



Y

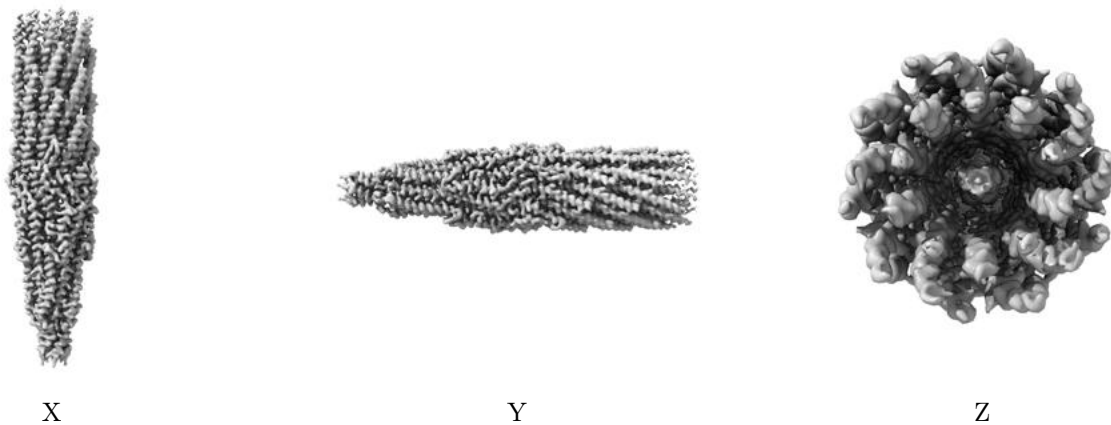


Z

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

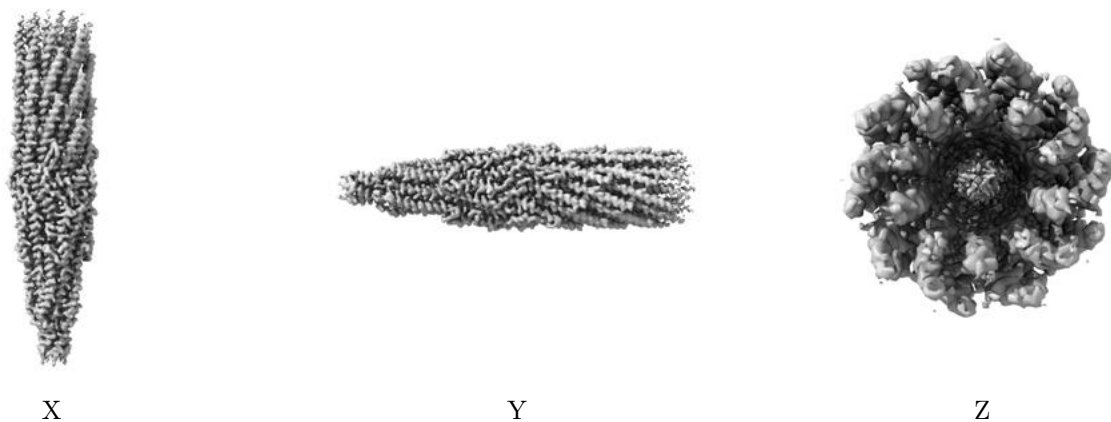
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.222. 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.

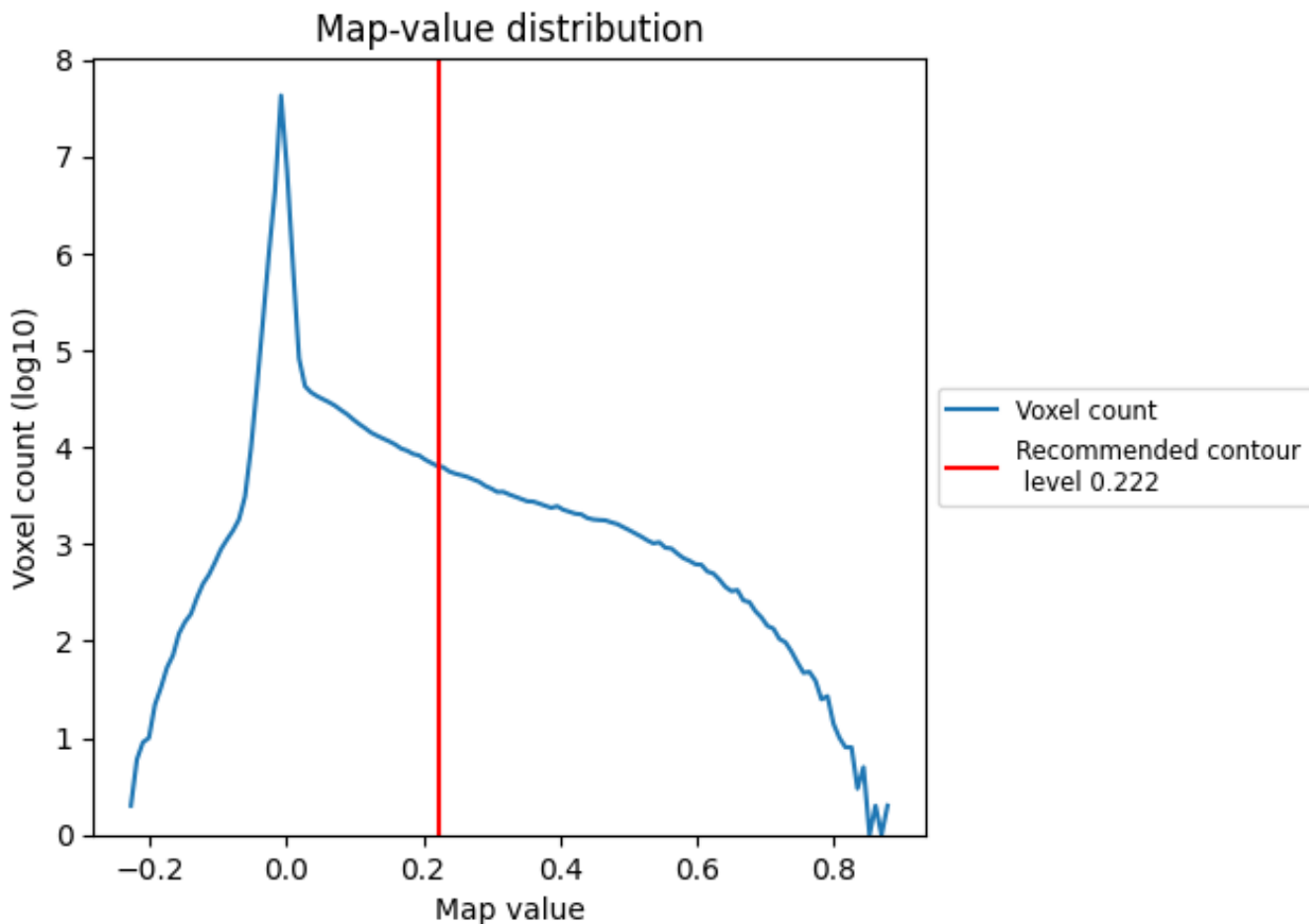
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

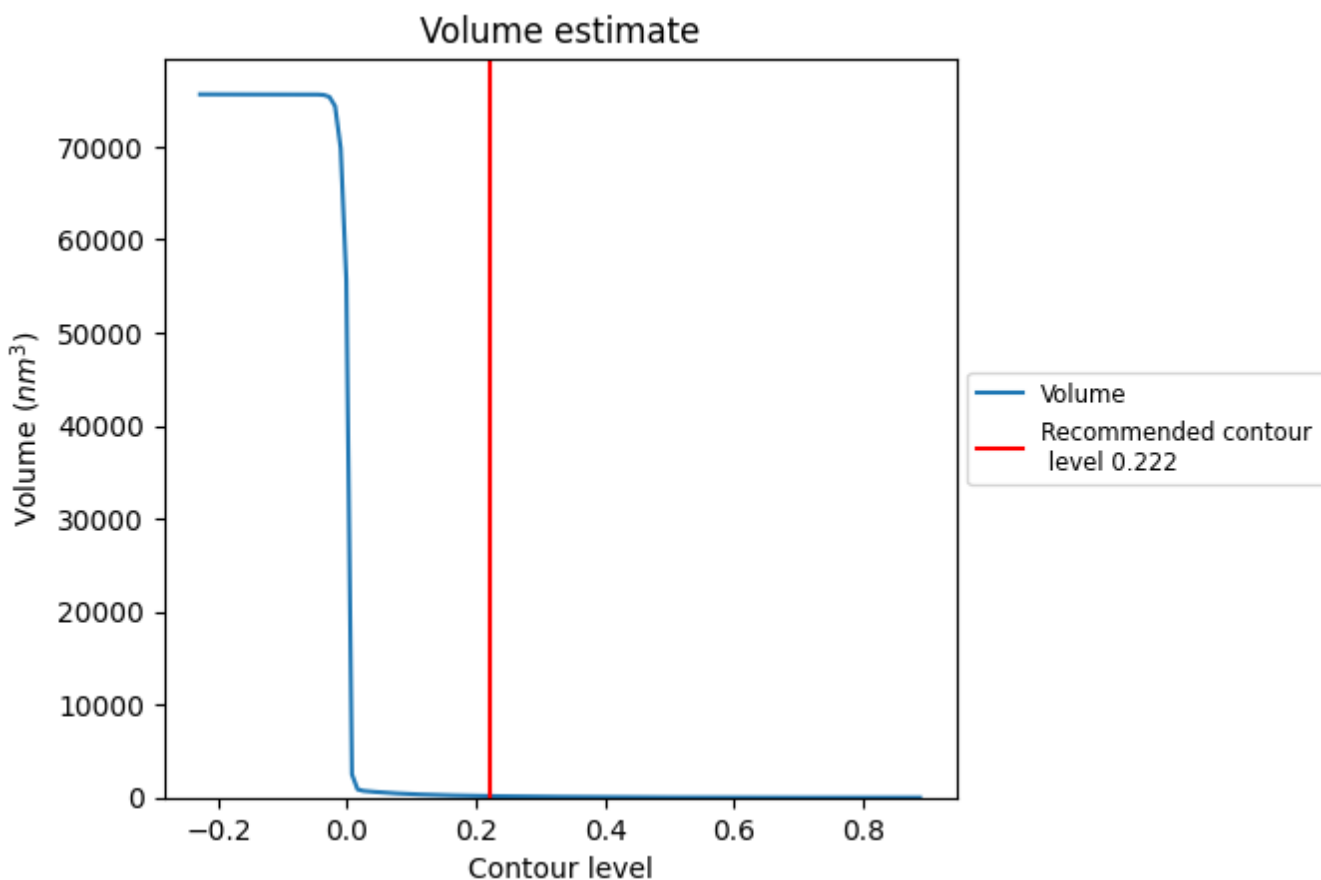
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

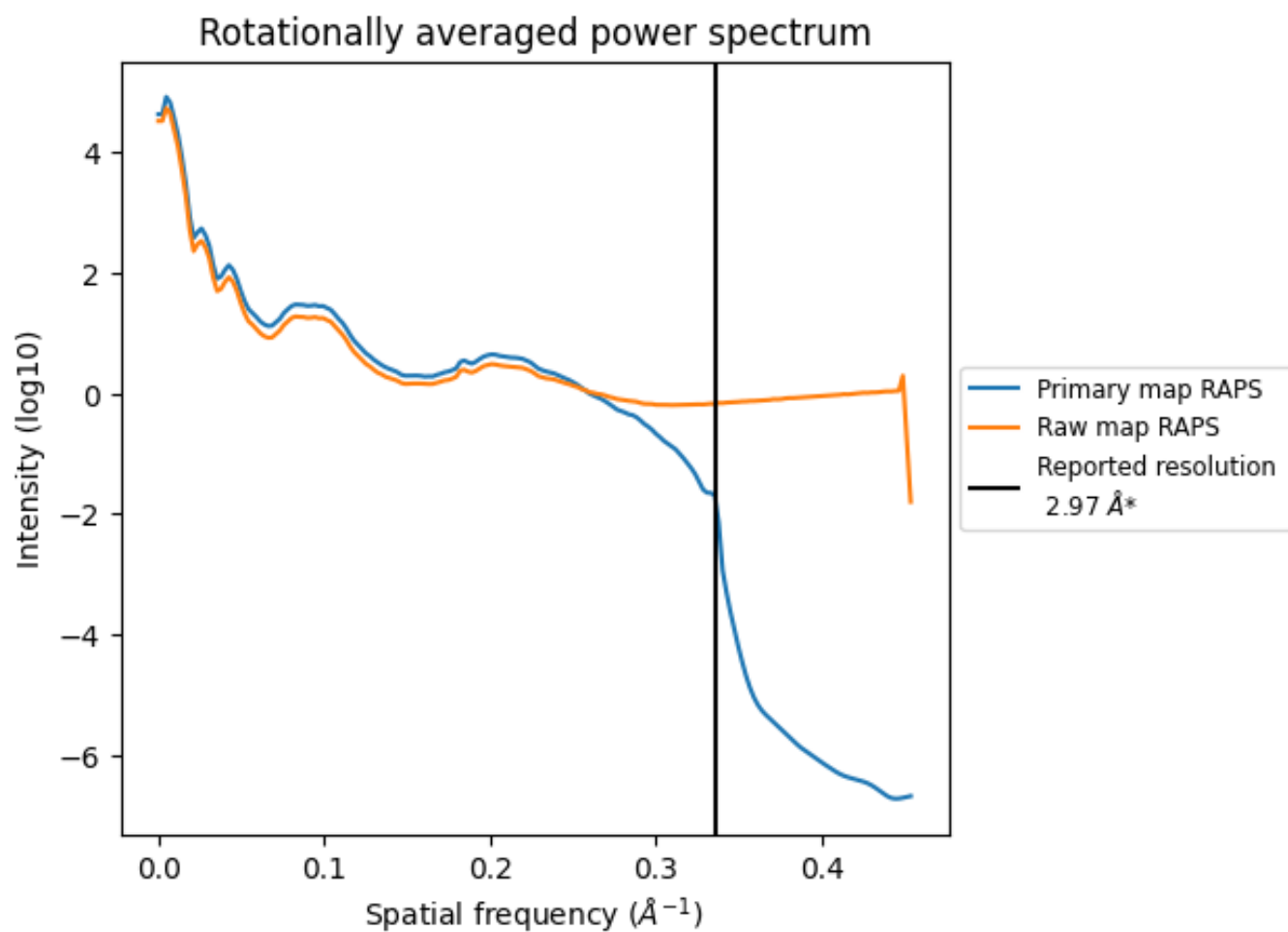


The volume at the recommended contour level is 157 nm<sup>3</sup>; this corresponds to an approximate mass of 142 kDa.

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

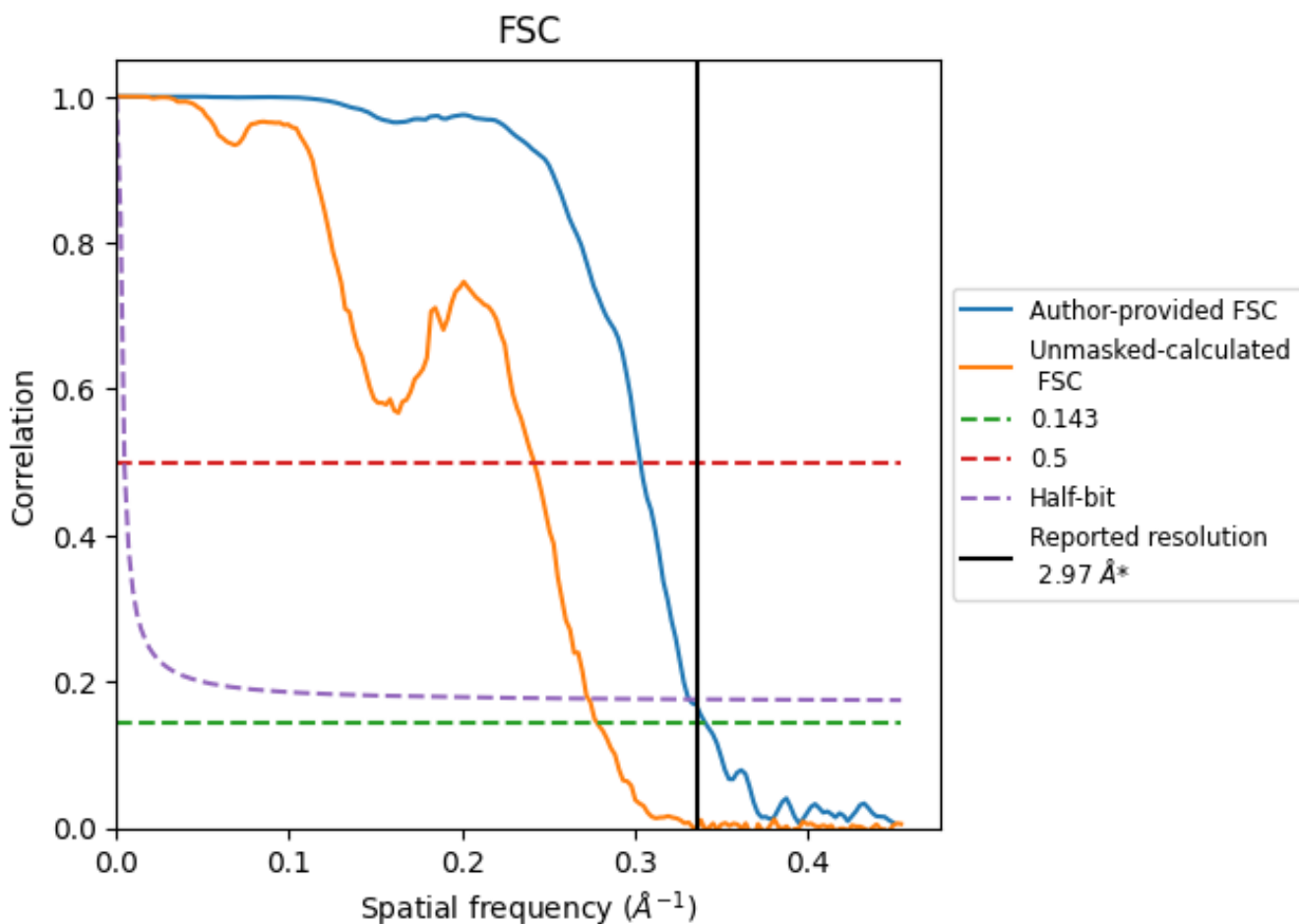


\*Reported resolution corresponds to spatial frequency of  $0.337 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

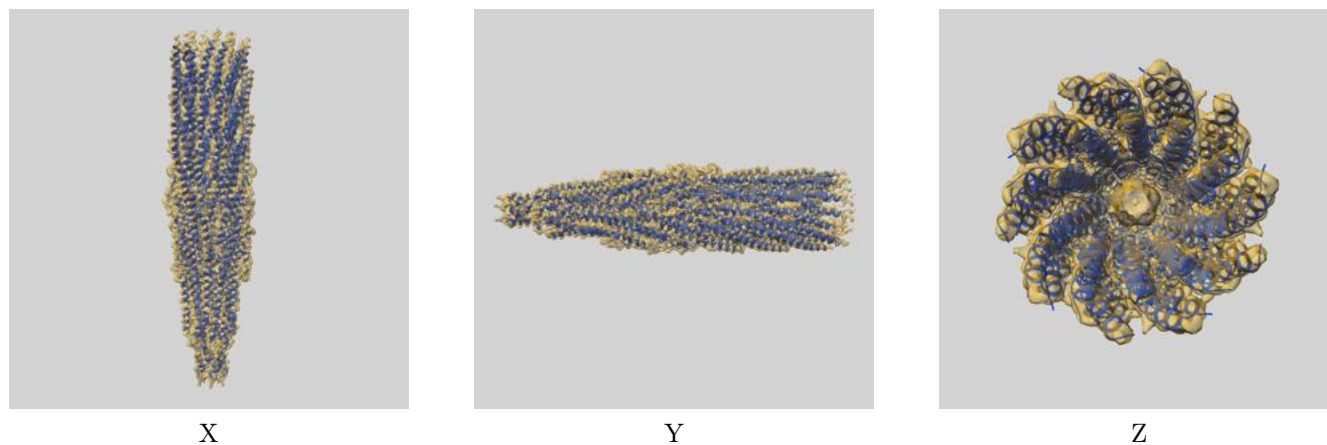
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.93	3.30	3.02
Unmasked-calculated*	3.59	4.14	3.66

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 2.97 by more than 10 %

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

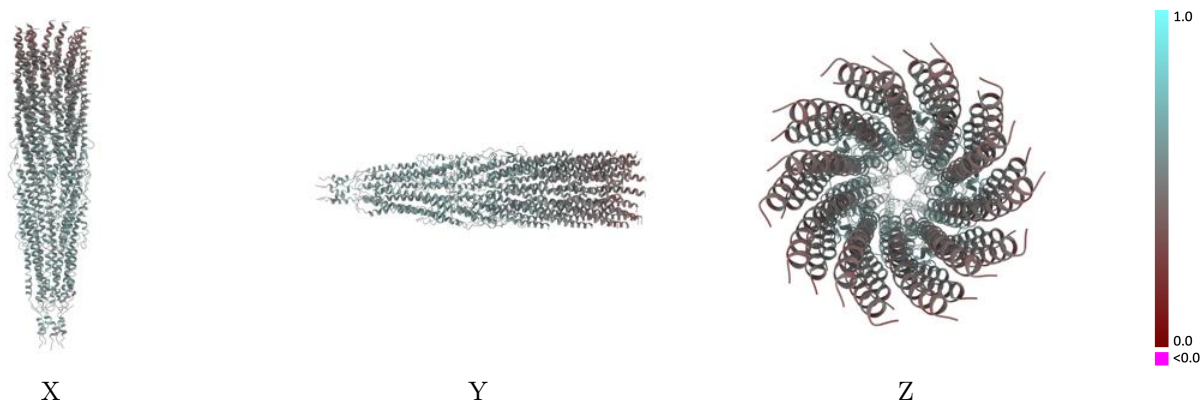
This section contains information regarding the fit between EMDB map EMD-15831 and PDB model 8B3O. Per-residue inclusion information can be found in section 3 on page 9.

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



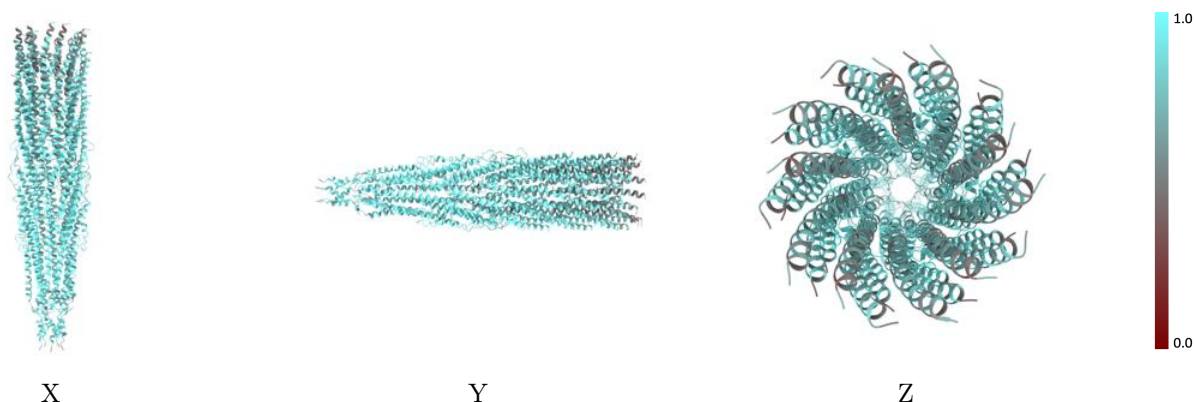
The images above show the 3D surface view of the map at the recommended contour level 0.222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



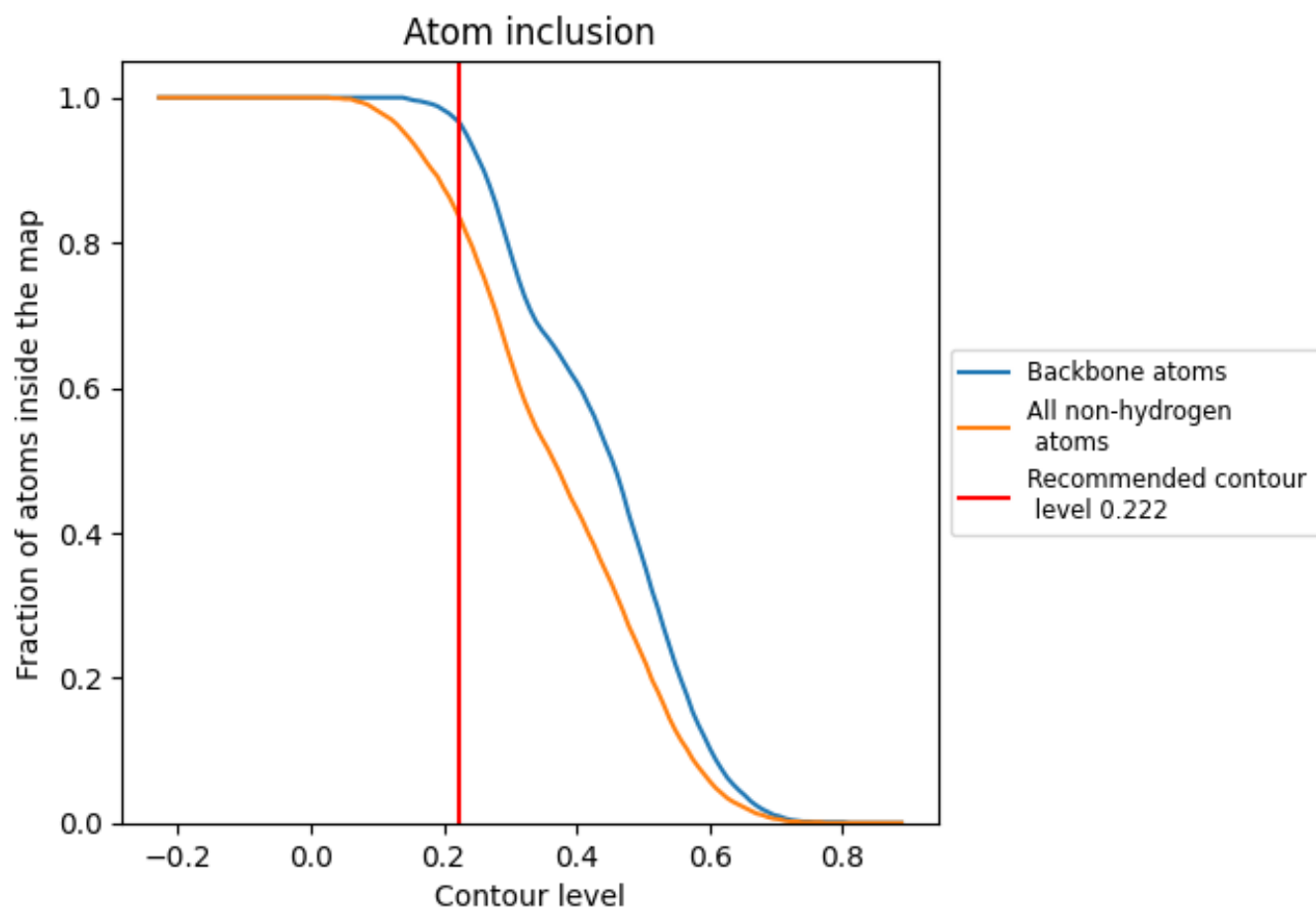
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.222).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 84% 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 (0.222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5160
AAA	 0.9250	 0.5570
BBB	 0.9270	 0.5570
CCC	 0.9240	 0.5570
DDD	 0.9240	 0.5560
EEE	 0.9250	 0.5560
FFF	 0.8810	 0.5470
GGG	 0.8770	 0.5450
HHH	 0.8760	 0.5430
III	 0.8760	 0.5430
JJJ	 0.8750	 0.5450
KKK	 0.6560	 0.4260
LLL	 0.6680	 0.4280
MMM	 0.6680	 0.4310
NNN	 0.6720	 0.4300
OOO	 0.6640	 0.4290
PPP	 0.5540	 0.4180
QQQ	 0.5430	 0.4180
RRR	 0.5490	 0.4230
SSS	 0.5490	 0.4190
TTT	 0.5540	 0.4170
UUU	 0.8010	 0.4800
VVV	 0.8070	 0.4800
WWW	 0.8100	 0.4830
XXX	 0.8070	 0.4800
YYY	 0.8100	 0.4810
ZZZ	 0.7380	 0.4570
aaa	 0.7410	 0.4550
bbb	 0.7380	 0.4560
ccc	 0.7380	 0.4550
ddd	 0.7380	 0.4550
eee	 0.8590	 0.5180
fff	 0.8620	 0.5240
ggg	 0.8590	 0.5250
hhh	 0.8680	 0.5240



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
iii	 0.8590	 0.5230
jjj	 0.8750	 0.5290
kkk	 0.8690	 0.5290
lll	 0.8720	 0.5270
mmm	 0.8720	 0.5270
nnn	 0.8780	 0.5260
ooo	 0.8280	 0.5110
ppp	 0.8400	 0.5100
qqq	 0.8310	 0.5140
rrr	 0.8250	 0.5110
sss	 0.8280	 0.5090