

# Full wwPDB EM Validation Report (i)

#### May 13, 2023 – 02:22 pm BST

PDB ID : 7QOL

EMDB ID : EMD-14094

Title: Tail assembly of the phicrAss001 virion with C6 symmetry imposed

Authors: Bayfield, O.W.; Shkoporov, A.N.; Yutin, N.; Khokhlova, E.V.; Smith, J.L.R.;

Hawkins, D.E.D.P.; Koonin, E.V.; Hill, C.; Antson, A.A.

Deposited on : 2021-12-24

Resolution : 3.33 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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50

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)

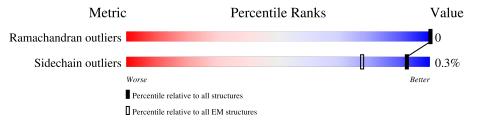
Validation Pipeline (wwPDB-VP) : 2.32.2

## 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 3.33 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	${ m EM\ structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain	
1	A	806	9% 81% 18%	-
1	О	806	81% 18%	-
2	В	236	95%	-
2	Q	236	95%	-
3	С	225	100%	_
3	S	225	100%	_
4	D	230	98%	<del>.</del>
4	Т	230	98%	<del>-</del>
5	Е	238	100%	_

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Mol	Chain	Length	Quality of chain	
5	F	238	98%	•
5	U	238	100%	
5	V	238	100%	
6	G	215	81%	18%
6	Н	215	87%	13%
6	W	215	81%	19%
6	Z	215	87%	13%
7	I	114	94%	6%
7	a	114	90%	• 6%
8	J	832	• 98%	
8	K	832	• 98%	
8	L	832	• 97%	
8	b	832	• 98%	
8	С	832	• 98%	
8	d	832	• 97%	
9	M	842	15% 85%	
9	N	842	• 96%	
9	e	842	15% 85%	
9	f	842	• 96%	
10	Р	1371	99%	
11	R	14	100%	



## 2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 51479 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 gp20.

$\mathbf{Mol}$	Chain	Residues		$\mathbf{A}^{1}$	AltConf	Trace				
1	A	657	10001	C 3404	- '	O 1027	S 23	0	0	
1	О	657		C 3404		O 1027	S 23	0	0	

• Molecule 2 is a protein called Ring protein 1 gp43.

Mol	Chain	Residues		Ato	AltConf	Trace			
2	В	226	Total 1841	C 1188	- '	O 336	S 9	0	0
2	Q	226	Total 1841	C 1188		O 336	S 9	0	0

• Molecule 3 is a protein called Ring protein 2 gp40.

Mol	Chain	Residues		At	AltConf	Trace			
2	С	225	Total	С	N	О	S	0	0
3		225	1841	1180	292	357	12	U	0
2	C	225	Total	С	N	О	S	0	0
3	B	229	1841	1180	292	357	12	0	U

• Molecule 4 is a protein called Ring protein 3 gp35.

Mol	Chain	Residues		$\mathbf{At}$	oms		AltConf	Trace	
4	D	226		C 1151		_	S 4	0	0
4	Т	226	Total 1805	C 1151		_		0	0

• Molecule 5 is a protein called Ring protein 4/5 gp34.



Mol	Chain	Residues		Ato		AltConf	Trace		
5	Е	238	Total	С	N	О	S	0	0
9	l Li	230	1878	1185	312	377	4		0
5	F	238	Total	С	N	О	S	0	0
9	I.	230	1878	1185	312	377	4		U
5	II	238	Total	С	N	О	S	0	0
9		230	1878	1185	312	377	4		0
5	V	238	Total	С	N	О	S	0	0
	v	230	1878	1185	312	377	4		U

• Molecule 6 is a protein called Tail hub protein A gp38.

Mol	Chain	Residues		A	toms		AltConf	Trace	
6	G	177	Total	С	N	О	S	0	0
0	G	111	1441	924	230	276	11	0	U
6	Н	188	Total	С	N	О	S	0	0
0	11	100	1516	968	243	292	13	0	U
6	W	174	Total	С	N	О	S	0	0
0	V V	174	1419	913	225	271	10	0	0
6	7.	188	Total	С	N	О	S	0	0
		100	1516	968	243	292	13		U

• Molecule 7 is a protein called Tail hub protein B gp39.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
7	Т	107	Total	С	N	О	S	0	0
'	1	107	878	560	134	175	9	0	
7		107	Total	С	N	О	S	0	0
1	a	107	878	560	134	175	9	U	U

• Molecule 8 is a protein called Tail fiber protein gp22.

Mol	Chain	Residues		Ato	ms		AltConf	Trace	
8	J	19	Total	С	N	О	S	0	0
0	J	19	170	112	27	30	1	0	U
8	K	19	Total	С	N	О	S	0	0
0	IX	19	170	112	27	30	1	U 	U
8	т	25	Total	С	N	О	S	0	0
0	ь	2.0	224	145	37	41	1	0	0
8	b	19	Total	С	N	О	S	0	0
0	Ь	19	170	112	27	30	1	0	U
8	0	19	Total	С	N	О	S	0	0
	c	19	170	112	27	30	1		U

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Mol	Chain	Residues		Ato	ms	AltConf	Trace		
8	d	25	Total 224	C 145	N 37	O 41	S 1	0	0

• Molecule 9 is a protein called Cargo protein 1 gp45.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	M	126	Total C N O S 987 605 179 201 2	0	0
9	N	32	Total C N O S 251 157 44 49 1	0	0
9	e	126	Total C N O S 987 605 179 201 2	0	0
9	f	32	Total C N O S 251 157 44 49 1	0	0

• Molecule 10 is a protein called Muzzle protein gp44.

Mol	Chain	Residues		A	toms			AltConf	Trace
10	Р	1354	Total 10925	C 6948	N 1815	O 2137	S 25	0	0

• Molecule 11 is a protein called Muzzle bound helix.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
11	R	14	Total 70	C 42	N 14	O 14	0	0

• Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Mg 1 1	0
12	О	1	Total Mg 1 1	0

• Molecule 13 is water.

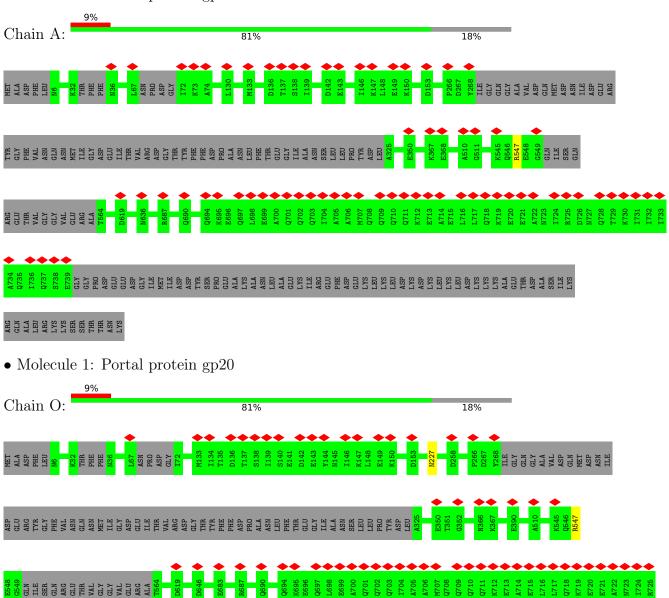
$\mathbf{Mol}$	Chain	Residues	Atoms	AltConf
13	A	1	Total O 1 1	0
13	О	1	Total O 1 1	0



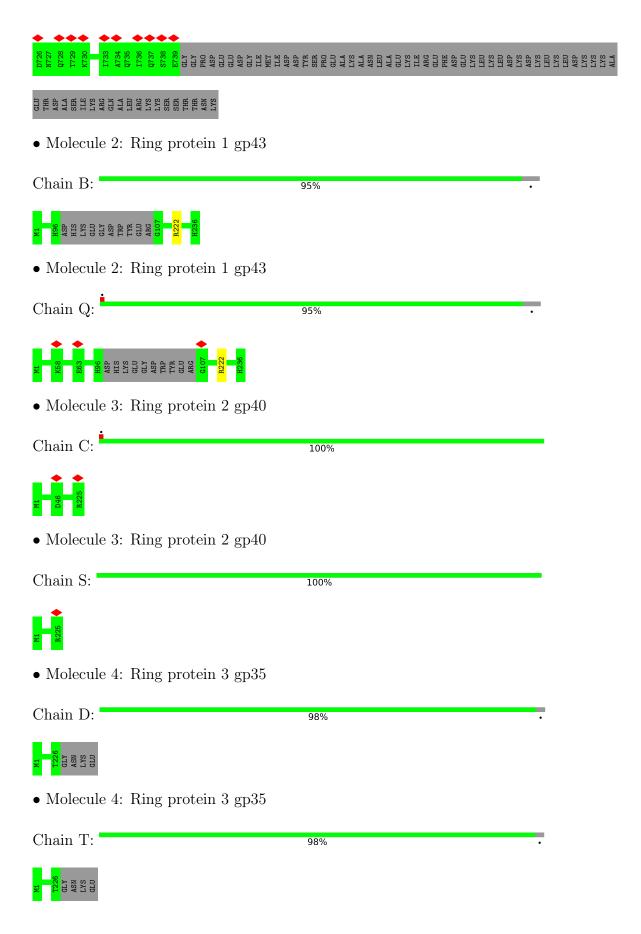
## 3 Residue-property plots (i)

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

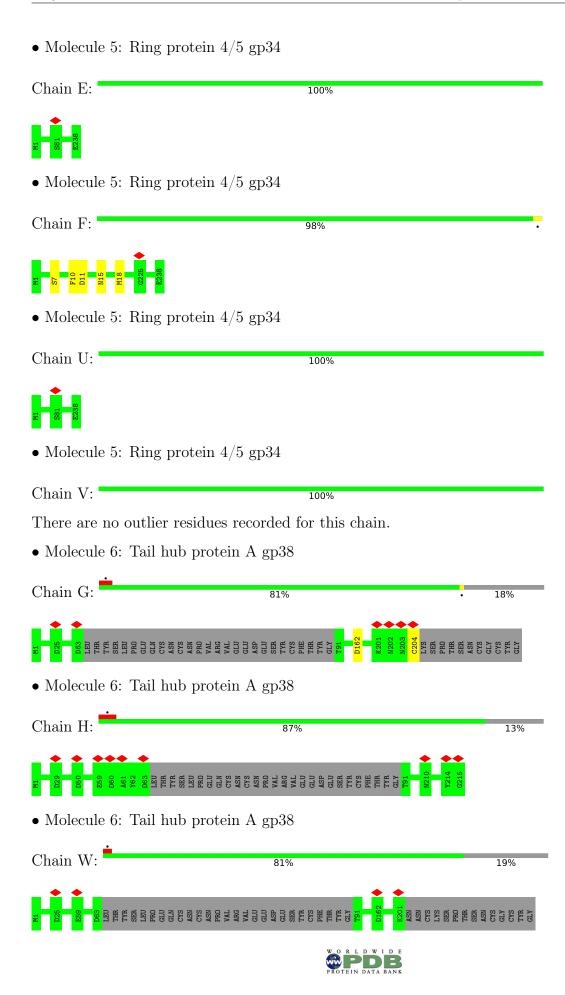
• Molecule 1: Portal protein gp20

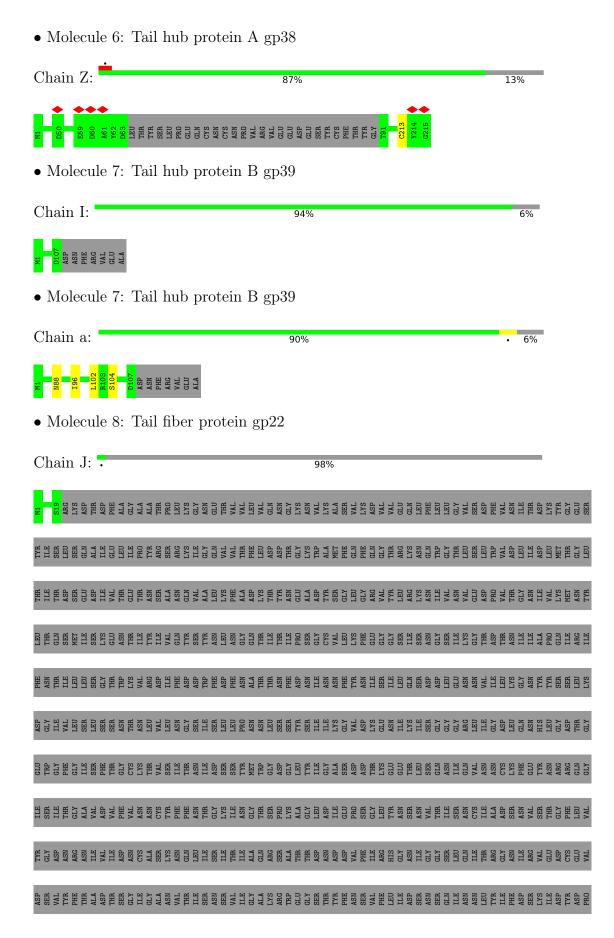










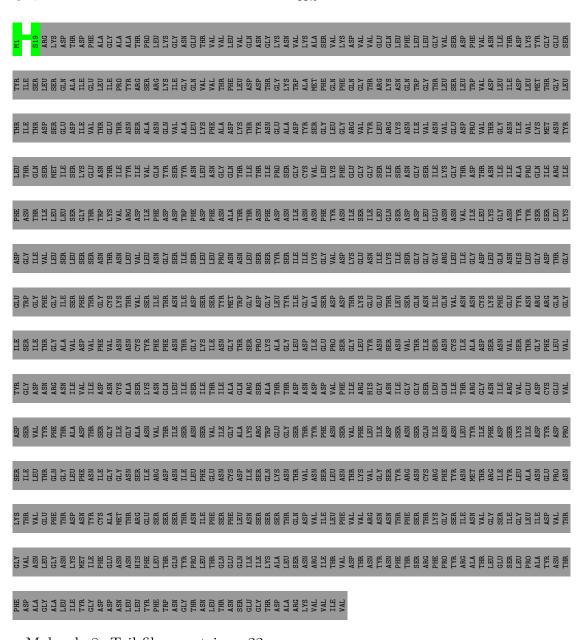




SER	ILE	THE	GLN	GLY	PHE	ASN	GLY	GLY	ASN	TIE	ARG	ASP	ASN	ILE	LEU	PHE	ASN	CYS	ASP	ILE	GLN	LYS	ASN	THR	ASN	SER	LEU	ASN	LYS	VAL	GLY	TYR	ARG	ASN	ARG	PHE	TYR	ASN	THE	ARG	ILE	TYR.	ALA	ASN	PRO	ASN
LYS	THR	di.u	PHE	ASP	ASN	CYS	ALA	MET	THR	GLII	SER	SER	SER	THR	ASN	ILE	SER	PHE	LEU	ASN	SER	SER	THR	GEN	VAL	ILE	LEU	PHE	VAL	ARG	ASN	THR	PHE	SER	I.YS	GLY	SER	ILE	VAT.	GLY	SER	HE GI.Y	LEU	ILE	VAL	THR
GLY	VAL	LEU	GLY	ASN	MET	TLE	GLU	ASN	ASN	PHE	LEU	THE	GLN	TYR	PRO	LEU	GLN	CLU	GLN	ILE	LYS	ALA	LEU	SER	ARG	ILE	THR :::	VAL	THR	ASN	TYR	PHE	THR	SER	PHE	PRO	TYR	ARG	THR	LEU	GLU	SER	PRO	ALA	ASN	THE
PHE	ASP	GLY	ALA	LEU	TYR	GLY	ASP	ASN	LEU	TVB	PHE	TRP	ASN	GLY	THR	ASN	THE	ASN	SER	GLU	THR	ASP	ALA	ARG	VAL	VAL	ILE	VAL																		

• Molecule 8: Tail fiber protein gp22

Chain K: 98%



• Molecule 8: Tail fiber protein gp22

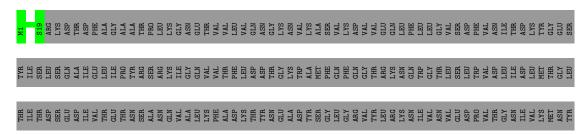


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• Molecule 8: Tail fiber protein gp22

Chain b: 598%

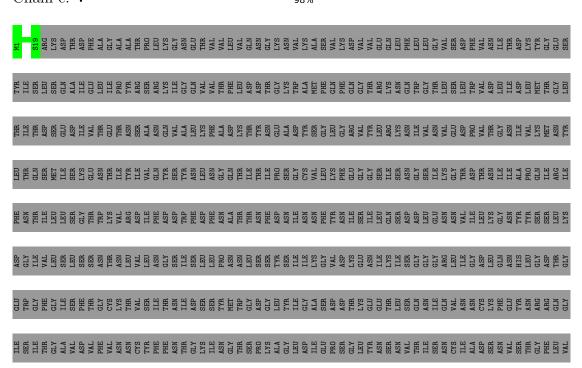




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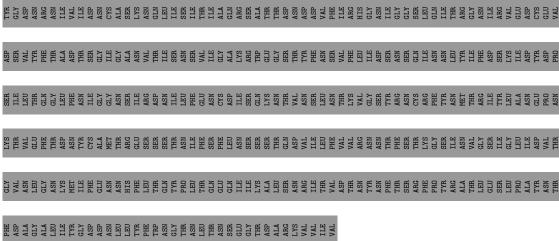
• Molecule 8: Tail fiber protein gp22

Chain c: . 98%

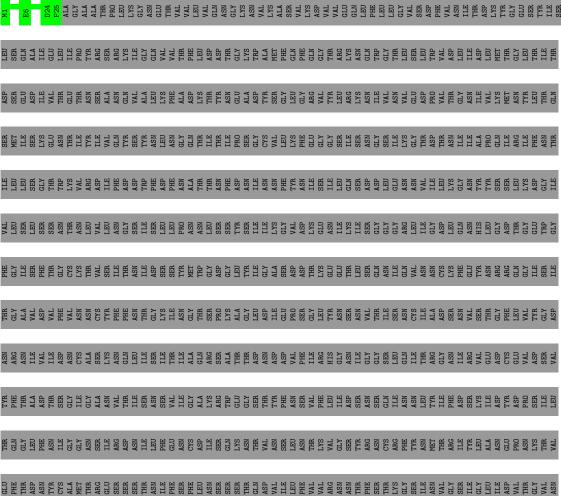




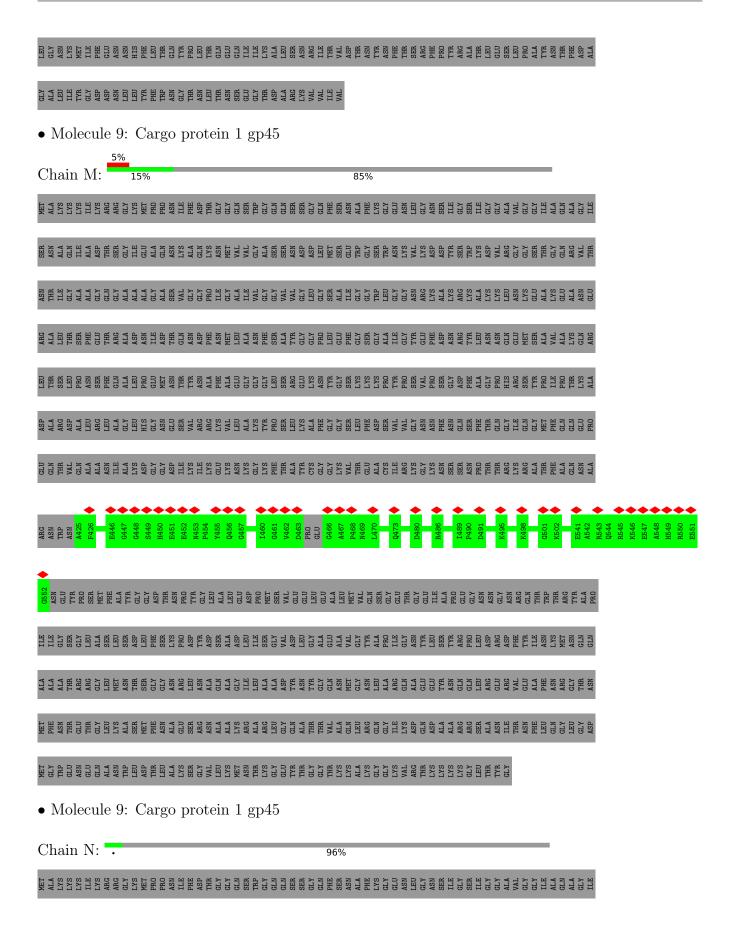
Chain d:



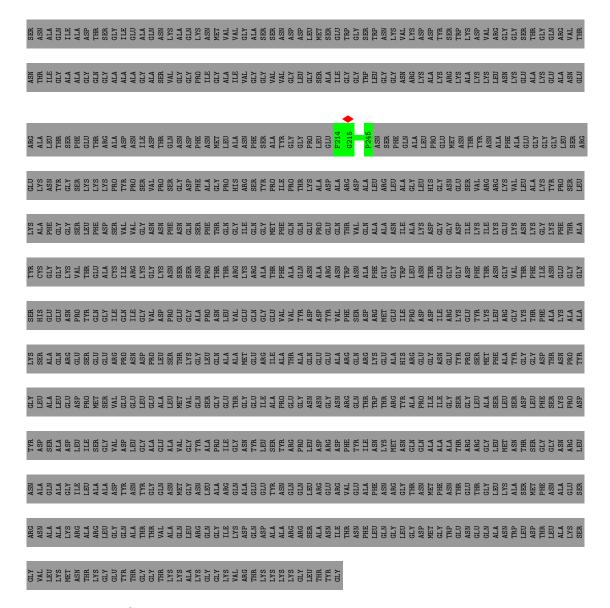
• Molecule 8: Tail fiber protein gp22





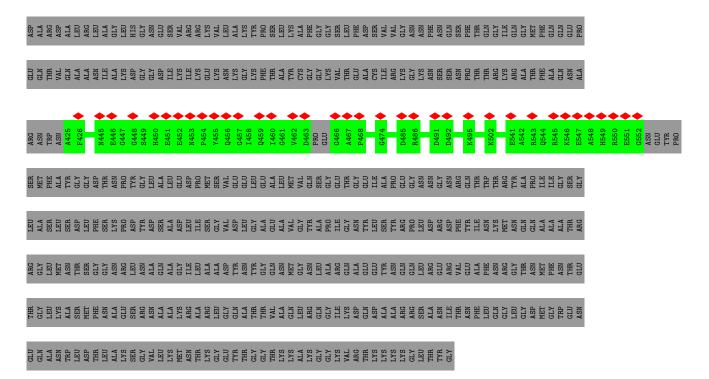






• Molecule 9: Cargo protein 1 gp45





• Molecule 9: Cargo protein 1 gp45

Chain f:

- 96%

- 96%

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- 96%

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- 96%

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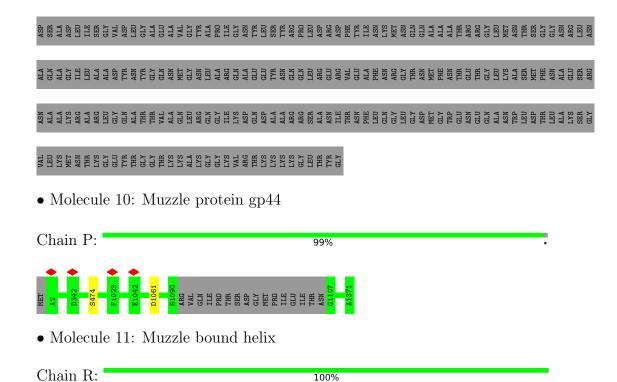
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There are no outlier residues recorded for this chain.



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	46280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	51	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.290	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	892.2228, 892.2228, 892.2228	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.394098, 1.394098, 1.394098	Depositor



## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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).

N (f = 1	Cl :-	Во	nd lengths	Вс	ond angles
Mol	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	0.28	0/5468	0.55	0/7374
1	О	0.28	0/5468	0.54	0/7374
2	В	0.28	0/1881	0.52	0/2548
2	Q	0.28	0/1881	0.53	0/2548
3	С	0.31	0/1886	0.54	0/2552
3	S	0.30	0/1886	0.54	0/2552
4	D	0.28	0/1837	0.56	0/2491
4	Т	0.28	0/1837	0.56	0/2491
5	Е	0.29	0/1910	0.52	0/2594
5	F	0.41	1/1910 (0.1%)	0.62	0/2594
5	U	0.29	0/1910	0.53	0/2594
5	V	0.30	0/1910	0.55	0/2594
6	G	0.31	0/1469	0.56	1/1989 (0.1%)
6	Н	0.32	0/1546	0.56	0/2093
6	W	0.28	0/1447	0.54	0/1959
6	Z	0.28	0/1546	0.53	0/2093
7	I	0.29	0/895	0.57	0/1208
7	a	0.33	0/895	0.59	0/1208
8	J	0.31	0/174	0.61	0/232
8	K	0.33	0/174	0.57	0/232
8	L	0.36	0/229	0.61	0/305
8	b	0.33	0/174	0.59	0/232
8	С	0.31	0/174	0.52	0/232
8	d	0.32	0/229	0.64	0/305
9	M	0.27	0/1003	0.59	0/1347
9	N	0.30	0/255	0.56	0/342
9	е	0.27	0/1003	0.62	0/1347
9	f	0.28	0/255	0.57	0/342
10	Р	0.27	0/11197	0.53	0/15227
All	All	0.29	1/52449~(0.0%)	0.55	1/70999 (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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	Р	0	2

#### All (1) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
5	F	7	SER	CA-CB	-5.58	1.44	1.52

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
6	G	162	ASP	CB-CG-OD1	6.07	123.77	118.30

There are no chirality outliers.

#### All (2) planarity outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type	Group
10	Р	1061	ASP	Mainchain
10	Р	474	SER	Peptide

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

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

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	647/806 (80%)	632 (98%)	15 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	О	647/806~(80%)	632 (98%)	15 (2%)	0	100	100
2	В	222/236~(94%)	216 (97%)	6 (3%)	0	100	100
2	Q	222/236 (94%)	216 (97%)	6 (3%)	0	100	100
3	С	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
3	S	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
4	D	224/230 (97%)	218 (97%)	6 (3%)	0	100	100
4	Т	224/230 (97%)	217 (97%)	7 (3%)	0	100	100
5	Е	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
5	F	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
5	U	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
5	V	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
6	G	173/215 (80%)	169 (98%)	4 (2%)	0	100	100
6	Н	184/215 (86%)	180 (98%)	4 (2%)	0	100	100
6	W	170/215 (79%)	167 (98%)	3 (2%)	0	100	100
6	Z	184/215 (86%)	180 (98%)	4 (2%)	0	100	100
7	I	105/114 (92%)	101 (96%)	4 (4%)	0	100	100
7	a	105/114 (92%)	100 (95%)	5 (5%)	0	100	100
8	J	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	K	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	L	23/832 (3%)	23 (100%)	0	0	100	100
8	b	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	С	17/832 (2%)	17 (100%)	0	0	100	100
8	d	23/832 (3%)	23 (100%)	0	0	100	100
9	M	122/842 (14%)	117 (96%)	5 (4%)	0	100	100
9	N	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
9	е	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
9	f	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
10	Р	1350/1371 (98%)	1297 (96%)	53 (4%)	0	100	100
All	All	6265/14765 (42%)	6059 (97%)	206 (3%)	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	Outliers   Percent	
1	A	588/714~(82%)	587 (100%)	1 (0%)	93	97
1	О	588/714 (82%)	586 (100%)	2 (0%)	92	96
2	В	206/215 (96%)	205 (100%)	1 (0%)	88	93
2	Q	$206/215\ (96\%)$	205 (100%)	1 (0%)	88	93
3	С	$208/208\ (100\%)$	208 (100%)	0	100	100
3	S	$208/208\ (100\%)$	208 (100%)	0	100	100
4	D	$207/210\ (99\%)$	207 (100%)	0	100	100
4	Т	$207/210\ (99\%)$	207 (100%)	0	100	100
5	E	211/211 (100%)	211 (100%)	0	100	100
5	F	211/211 (100%)	207 (98%)	4 (2%)	57	79
5	U	211/211 (100%)	211 (100%)	0	100	100
5	V	211/211 (100%)	211 (100%)	0	100	100
6	G	168/203 (83%)	167 (99%)	1 (1%)	86	92
6	Н	177/203~(87%)	177 (100%)	0	100	100
6	W	$165/203\ (81\%)$	165 (100%)	0	100	100
6	Z	177/203~(87%)	176 (99%)	1 (1%)	86	92
7	Ι	$100/106\ (94\%)$	100 (100%)	0	100	100
7	a	100/106~(94%)	96 (96%)	4 (4%)	31	63
8	J	18/736 (2%)	18 (100%)	0	100	100
8	K	18/736 (2%)	18 (100%)	0	100	100
8	L	24/736 (3%)	23 (96%)	1 (4%)	30	62
8	b	18/736 (2%)	18 (100%)	0	100	100
8	С	18/736 (2%)	18 (100%)	0	100	100
8	d	24/736 (3%)	24 (100%)	0	100	100
9	M	100/644 (16%)	100 (100%)	0	100	100
9	N	26/644 (4%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
9	e	100/644 (16%)	100 (100%)	0	100	100
9	f	26/644 (4%)	26 (100%)	0	100	100
10	P	1210/1226 (99%)	1210 (100%)	0	100	100
All	All	5731/12780 (45%)	5715 (100%)	16 (0%)	92	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	ARG
2	В	222	ARG
5	F	10	PHE
5	F	11	ASP
5	F	15	ASN
5	F	18	MET
6	G	204	CYS
8	L	20	ARG
1	О	227	ASN
1	О	547	ARG
2	Q	222	ARG
6	Z	213	CYS
7	a	88	ASN
7	a	96	ILE
7	a	102	LEU
7	a	104	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such side chains are listed below:

Mol	Chain	Res	Type
5	F	4	ASN
5	F	15	ASN
6	Н	190	GLN
6	Н	210	ASN
6	Z	190	GLN
10	Р	155	ASN
10	Р	1181	ASN
10	Р	1273	ASN



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.



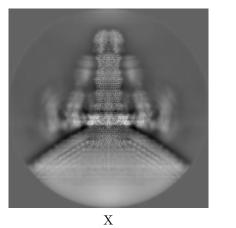
## 6 Map visualisation (i)

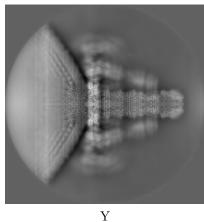
This section contains visualisations of the EMDB entry EMD-14094. These allow visual inspection of the internal detail of the map and identification of artifacts.

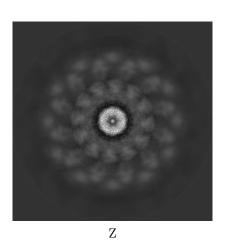
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map







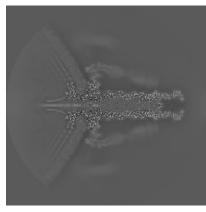
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

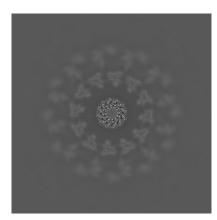
#### 6.2.1 Primary map







Y Index: 320



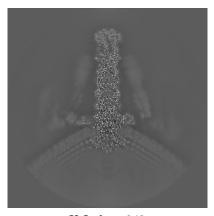
Z Index: 320

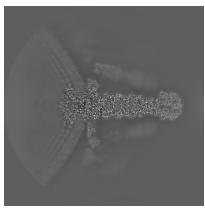


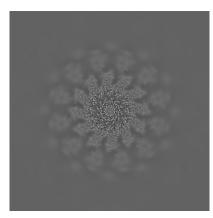
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map







X Index: 342

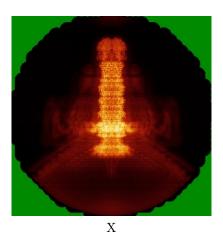
Y Index: 298

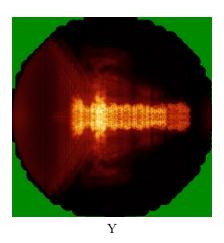
Z Index: 274

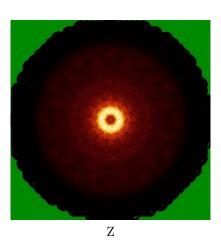
The images above show the largest variance slices of the map in three orthogonal directions.

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

#### 6.4.1 Primary map





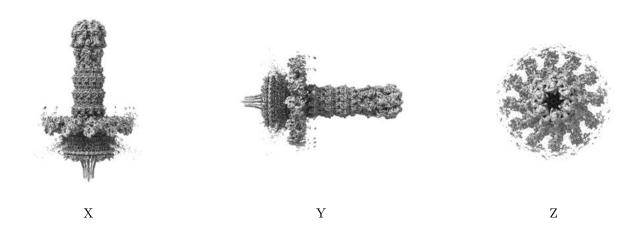


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.6 Mask visualisation (i)

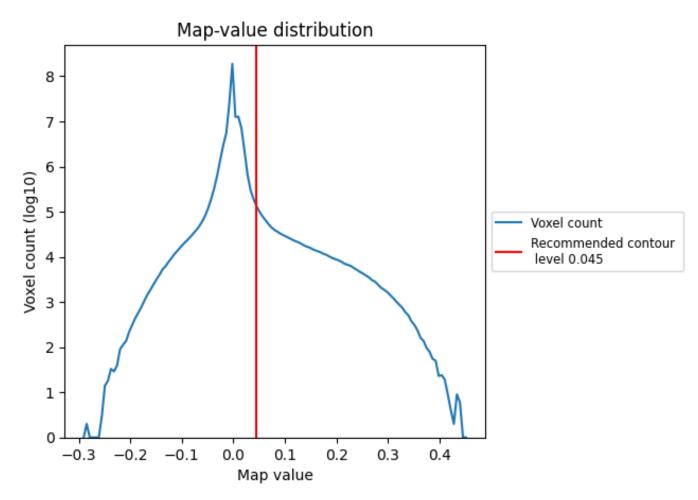
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

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

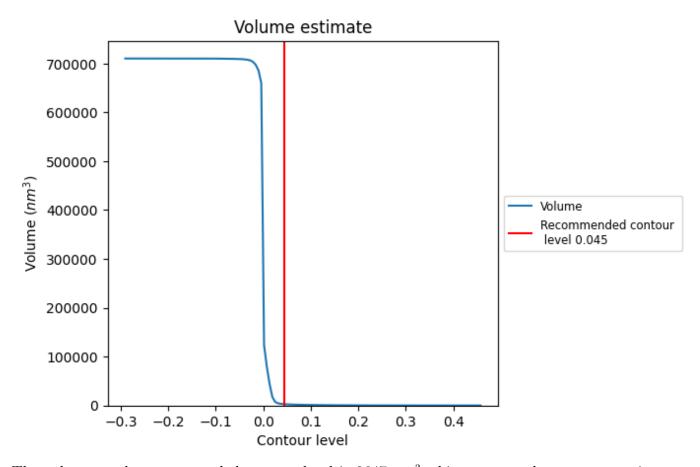
### 7.1 Map-value distribution (i)



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)

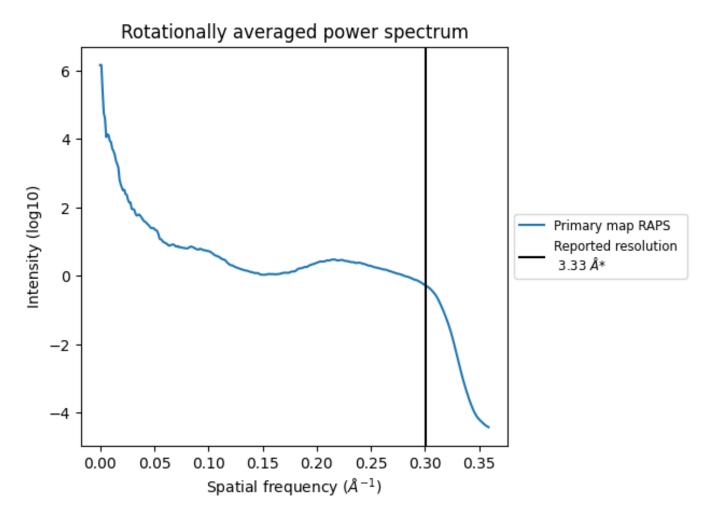


The volume at the recommended contour level is  $2647~\mathrm{nm^3}$ ; this corresponds to an approximate mass of  $2391~\mathrm{kDa}$ .

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)



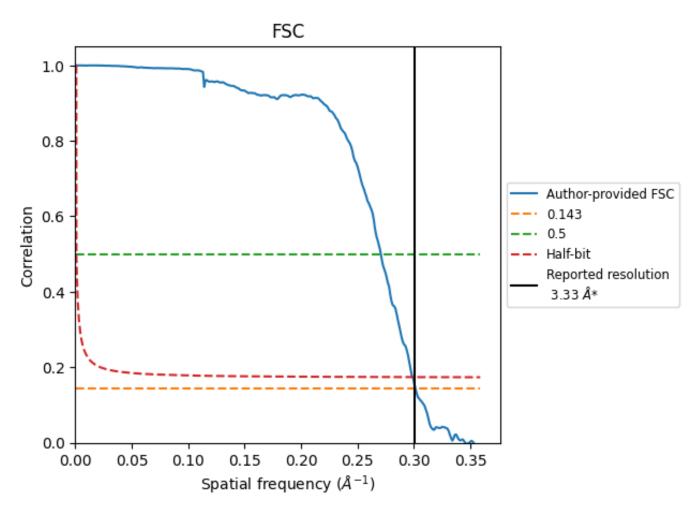
<sup>\*</sup>Reported resolution corresponds to spatial frequency of 0.300  $\rm \AA^{-1}$ 



## 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 0.300  $\rm \AA^{-1}$ 



## 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.33	-	-	
Author-provided FSC curve	3.32	3.69	3.35	
Unmasked-calculated*	-	-	-	

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

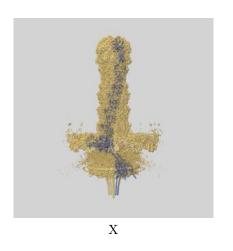


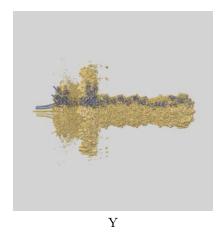
## 9 Map-model fit (i)

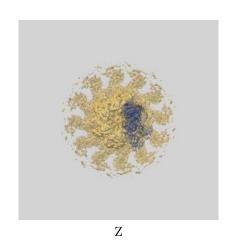
This section contains information regarding the fit between EMDB map EMD-14094 and PDB model 7QOL. Per-residue inclusion information can be found in section 3 on page 7.

#### 9.1 Map-model overlays

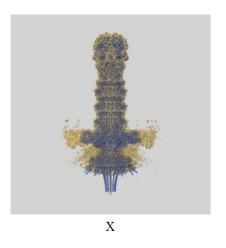
#### 9.1.1 Map-model overlay (i)

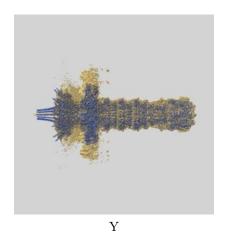


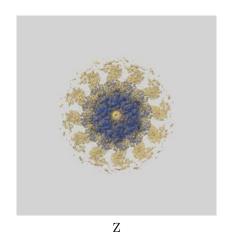




#### 9.1.2 Map-model assembly overlay (i)



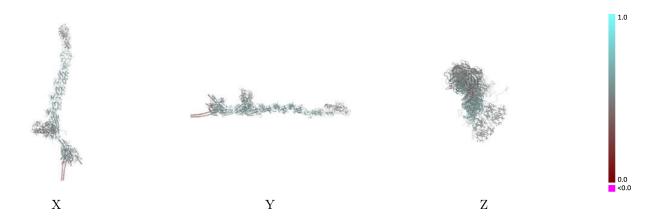




The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

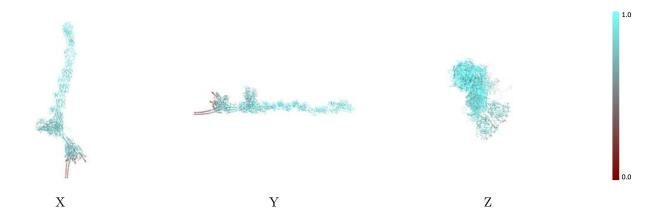


### 9.2 Q-score mapped to coordinate model (i)



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

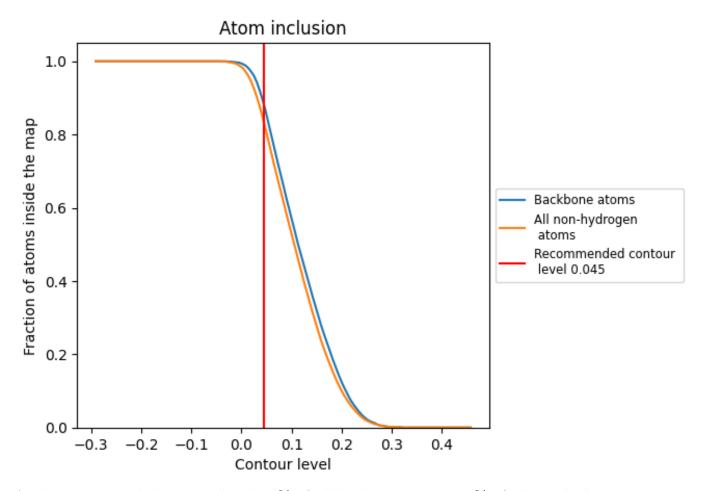
#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).



### 9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.5250
A	0.7260	0.5110
В	0.8740	0.5730
С	0.9030	0.5730
D	0.9110	0.5550
Е	0.9260	0.5630
F	0.9200	0.5540
G	0.7760	0.5020
Н	0.7990	0.4810
I	0.8360	0.5080
J	0.7230	0.4210
K	0.7590	0.4460
L	0.7110	0.4440
M	0.5060	0.4530
N	0.7590	0.5160
О	0.7320	0.5110
P	0.9190	0.5170
Q	0.8600	0.5660
R	0.8710	0.5060
S	0.9050	0.5730
Т	0.9180	0.5600
U	0.9320	0.5610
V	0.9340	0.5610
W	0.7940	0.4950
Z	0.8120	0.4930
a	0.8300	0.5150
b	0.7050	0.4220
c	0.7890	0.4780
d	0.7110	0.4820
e	0.5240	0.4340
f	0.7220	0.5120



