



## wwPDB EM Validation Summary Report ⓘ

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 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>.

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

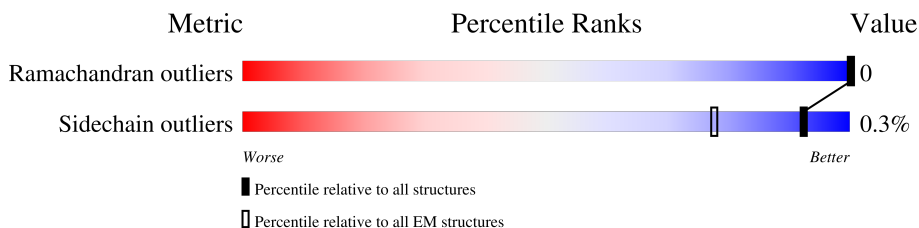
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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.



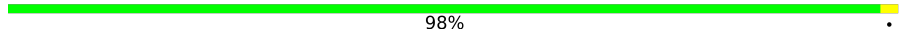
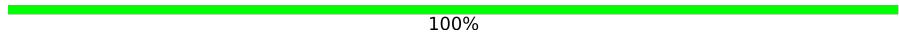
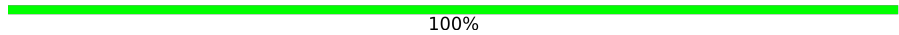




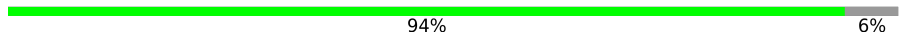

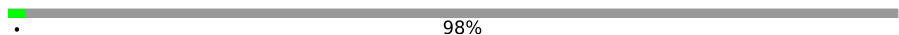
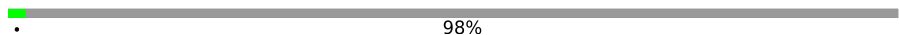


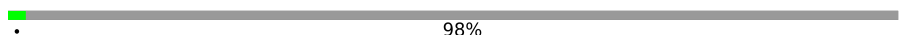
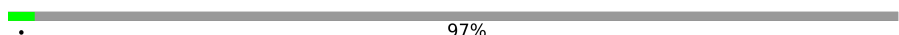

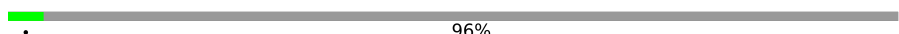

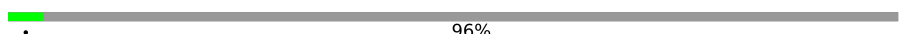
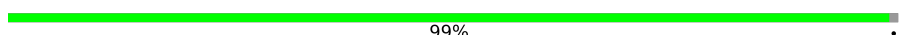
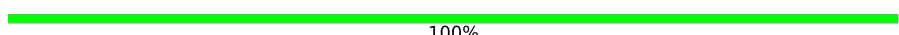
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	806	 9% 81% 18%
1	O	806	 9% 81% 18%
2	B	236	 95% .
2	Q	236	 95% .
3	C	225	 100%
3	S	225	 100%
4	D	230	 98% .
4	T	230	 98% .
5	E	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	H	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	c	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	P	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	657	Total	C	N	O	S	0	0
			5371	3404	917	1027	23		
1	O	657	Total	C	N	O	S	0	0
			5371	3404	917	1027	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
2	Q	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
3	S	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	226	Total	C	N	O	S	0	0
			1805	1151	293	357	4		
4	T	226	Total	C	N	O	S	0	0
			1805	1151	293	357	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	F	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	U	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	V	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	177	Total	C	N	O	S	0	0
			1441	924	230	276	11		
6	H	188	Total	C	N	O	S	0	0
			1516	968	243	292	13		
6	W	174	Total	C	N	O	S	0	0
			1419	913	225	271	10		
6	Z	188	Total	C	N	O	S	0	0
			1516	968	243	292	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	107	Total	C	N	O	S	0	0
			878	560	134	175	9		
7	a	107	Total	C	N	O	S	0	0
			878	560	134	175	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	K	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	L	25	Total	C	N	O	S	0	0
			224	145	37	41	1		
8	b	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	c	19	Total	C	N	O	S	0	0
			170	112	27	30	1		

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

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

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

- Molecule 10 is a protein called Muzzle protein gp44.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	1354	Total	C	N	O	S	0	0
			10925	6948	1815	2137	25		

- Molecule 11 is a protein called Muzzle bound helix.

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

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

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

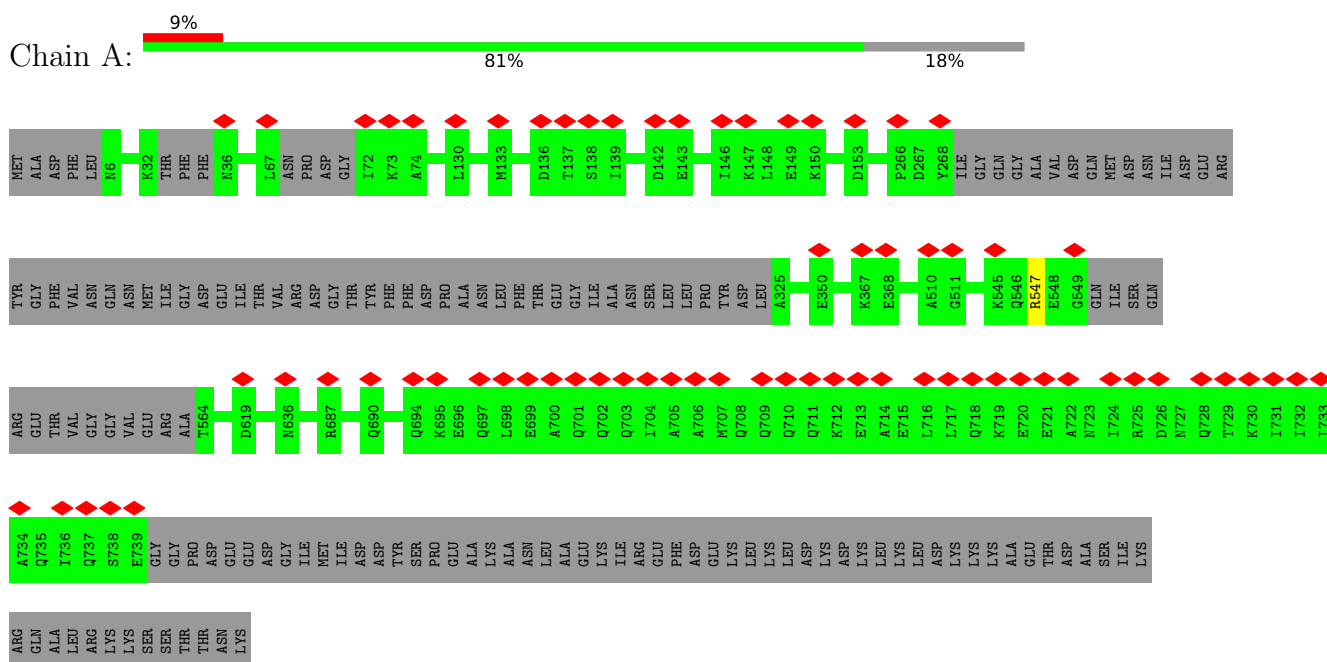
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	O	0
			1	1	
13	O	1	Total	O	0
			1	1	

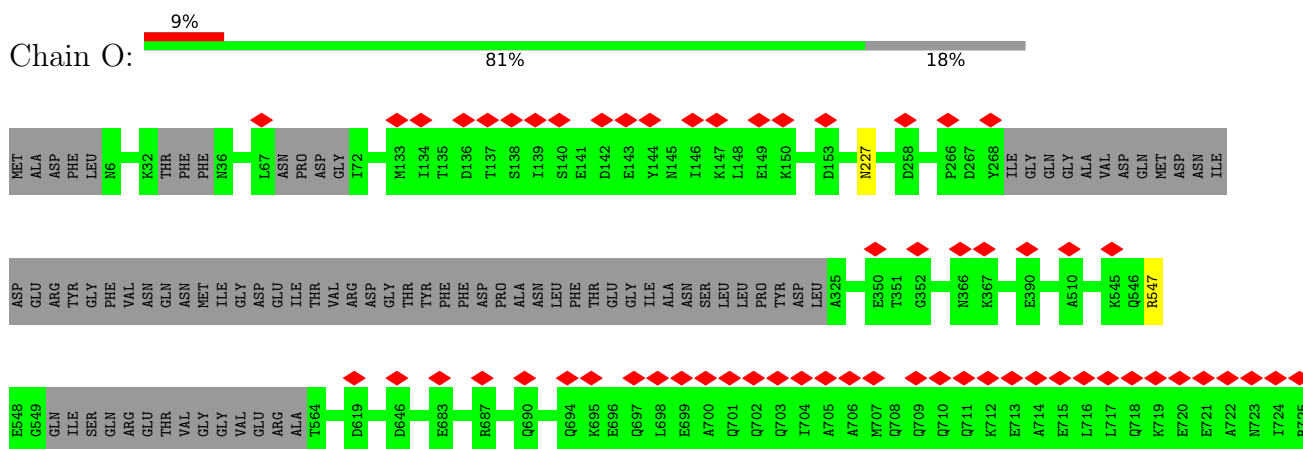
### 3 Residue-property plots

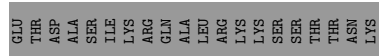
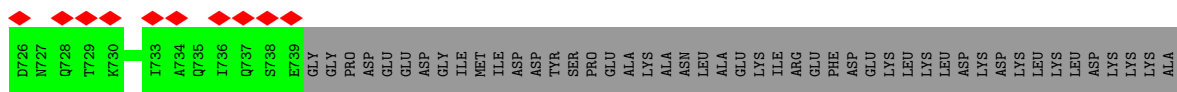
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

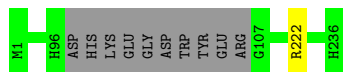


- Molecule 1: Portal protein gp20

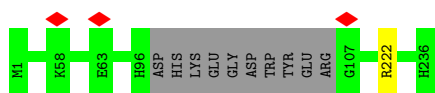




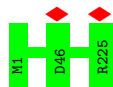
- Molecule 2: Ring protein 1 gp43



- Molecule 2: Ring protein 1 gp43



- Molecule 3: Ring protein 2 gp40



- Molecule 3: Ring protein 2 gp40



- Molecule 4: Ring protein 3 gp35



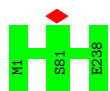
- Molecule 4: Ring protein 3 gp35





• Molecule 5: Ring protein 4/5 gp34

Chain E:  100%



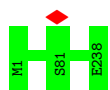
• Molecule 5: Ring protein 4/5 gp34

Chain F:  98%



• Molecule 5: Ring protein 4/5 gp34

Chain U:  100%





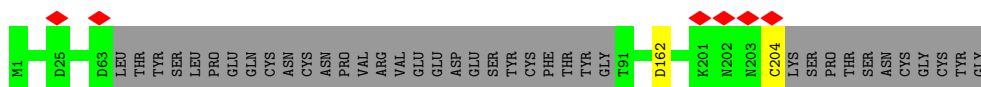
• Molecule 5: Ring protein 4/5 gp34

Chain V:  100%



There are no outlier residues recorded for this chain.

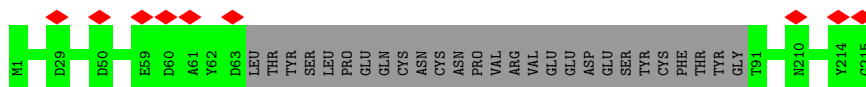
• Molecule 6: Tail hub protein A gp38

Chain G:  81%  18%





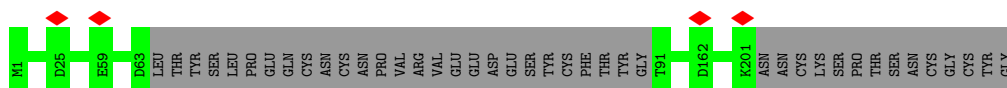
• Molecule 6: Tail hub protein A gp38

Chain H:  87%  13%



• Molecule 6: Tail hub protein A gp38

Chain W:  81%  19%





```

SER ILE THR VAL GLU PHE GLY LEU ASP THR ASN ASN ILE LEU ASP THR VAL
LYS THR VAL GLU PHE THR ASP THR ASN TYR ASN MET MET THR THR VAL VAL
GLY VAL ASN LEU GLY ASP ASN LYS MET ILE TYR ILE ASP THR ASN ASN THR
PHE ASP ALA GLY ALA LEU LEU LEU ASP ASP ALA ASP ASN ASN ASN HIS THR
  
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● Molecule 8: Tail fiber protein gp22

Chain K:  98%

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MET ASP MET ASP MET ASP MET ASP MET ASP MET ASP MET ASP MET ASP MET ASP
S19 LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
LYS ASP LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
PHE LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
LYS ASP LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
PHE ASP LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
ASP LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
GLY THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
TRP THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE
THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
PHE THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ASP THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
GLY THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
TRP THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE
SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER
TYR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ASP THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
SER THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE ILE
LYS THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR
GLY VAL ASN VAL THR THR THR THR THR THR THR THR THR THR THR THR THR
PHE ASP ALA GLY ALA LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
  
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● Molecule 8: Tail fiber protein gp22



















## 4 Experimental information

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 CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/5468	0.55	0/7374
1	O	0.28	0/5468	0.54	0/7374
2	B	0.28	0/1881	0.52	0/2548
2	Q	0.28	0/1881	0.53	0/2548
3	C	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	T	0.28	0/1837	0.56	0/2491
5	E	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	H	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	c	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	e	0.27	0/1003	0.62	0/1347
9	f	0.28	0/255	0.57	0/342
10	P	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 mainchain group or atoms of a sidechain that are expected to be planar.

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	Observed(°)	Ideal(°)
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:

Mol	Chain	Res	Type	Group
10	P	1061	ASP	Mainchain
10	P	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	Percentiles	
1	O	647/806 (80%)	632 (98%)	15 (2%)	0	100	100
2	B	222/236 (94%)	216 (97%)	6 (3%)	0	100	100
2	Q	222/236 (94%)	216 (97%)	6 (3%)	0	100	100
3	C	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	T	224/230 (97%)	217 (97%)	7 (3%)	0	100	100
5	E	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	H	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	c	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	e	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
9	f	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
10	P	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	Percentiles	
1	A	588/714 (82%)	587 (100%)	1 (0%)	93	97
1	O	588/714 (82%)	586 (100%)	2 (0%)	92	96
2	B	206/215 (96%)	205 (100%)	1 (0%)	88	93
2	Q	206/215 (96%)	205 (100%)	1 (0%)	88	93
3	C	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	T	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	H	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	I	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	c	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	Percentiles	
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

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	a	102	LEU
7	a	96	ILE
1	O	227	ASN
7	a	88	ASN
8	L	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
10	P	1273	ASN
10	P	1181	ASN
6	Z	190	GLN
6	H	210	ASN
10	P	155	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.

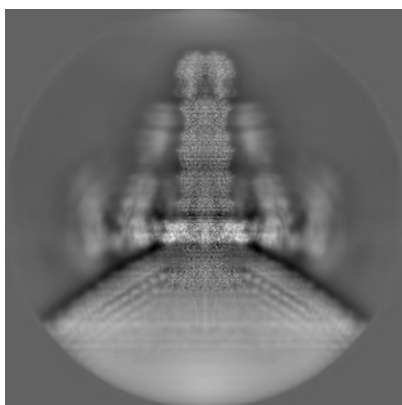
## 6 Map visualisation [i](#)

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.

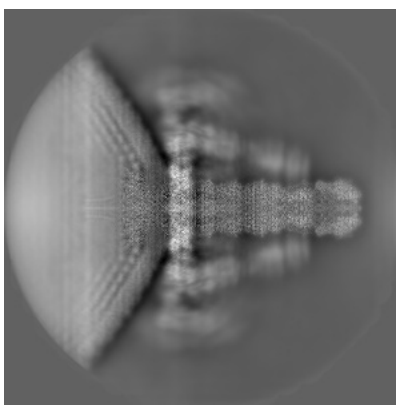
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

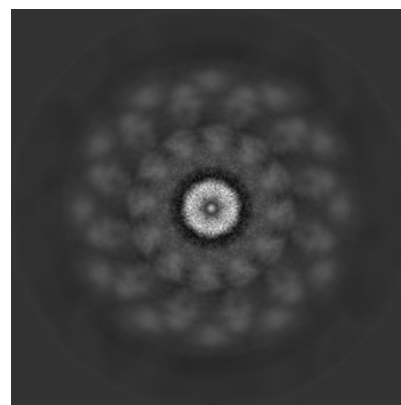
#### 6.1.1 Primary map



X



Y

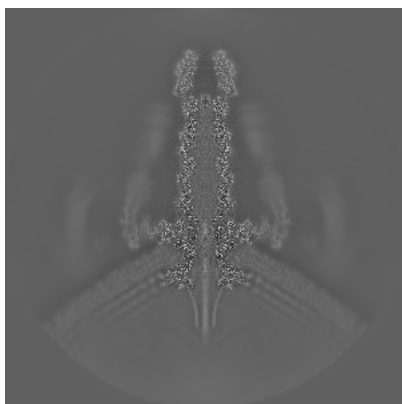


Z

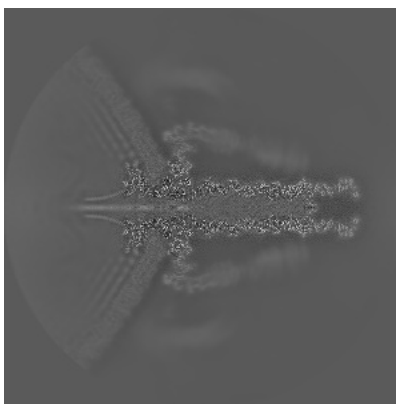
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

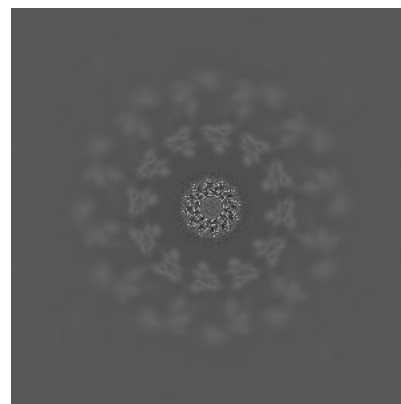
#### 6.2.1 Primary map



X Index: 320



Y Index: 320

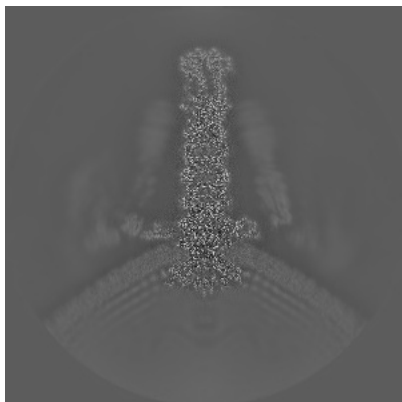


Z Index: 320

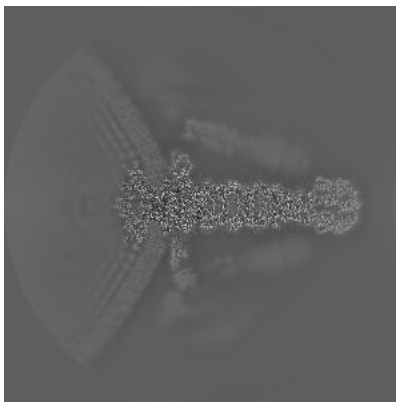
The images above show central slices of the map in three orthogonal directions.

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

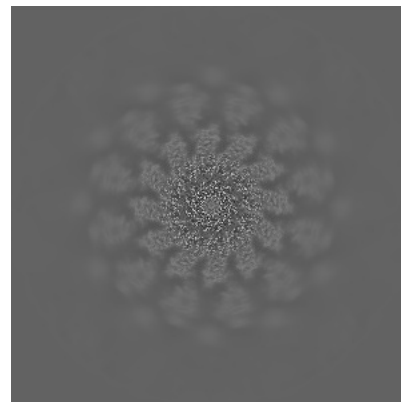
### 6.3.1 Primary map



X Index: 342



Y Index: 298

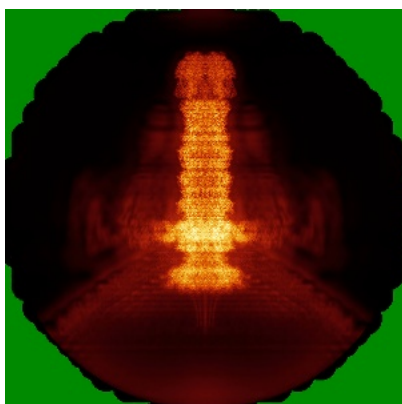


Z Index: 274

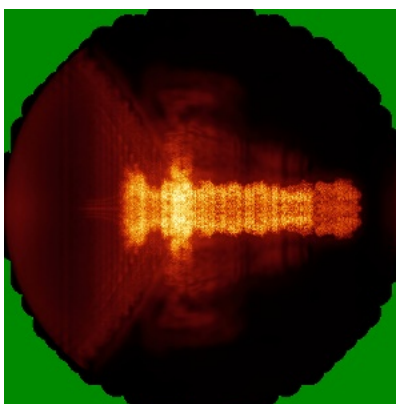
The images above show the largest variance slices of the map in three orthogonal directions.

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

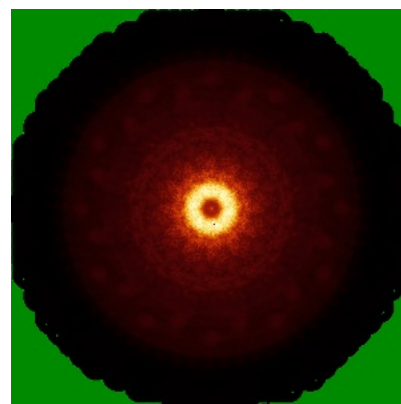
### 6.4.1 Primary map



X



Y

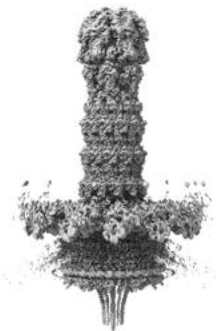


Z

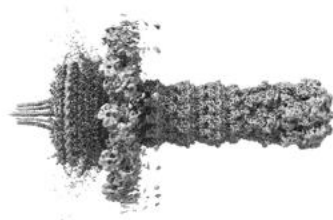
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

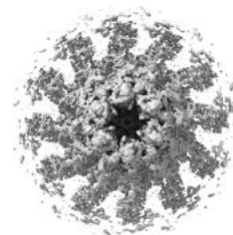
### 6.5.1 Primary map



X



Y



Z

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.

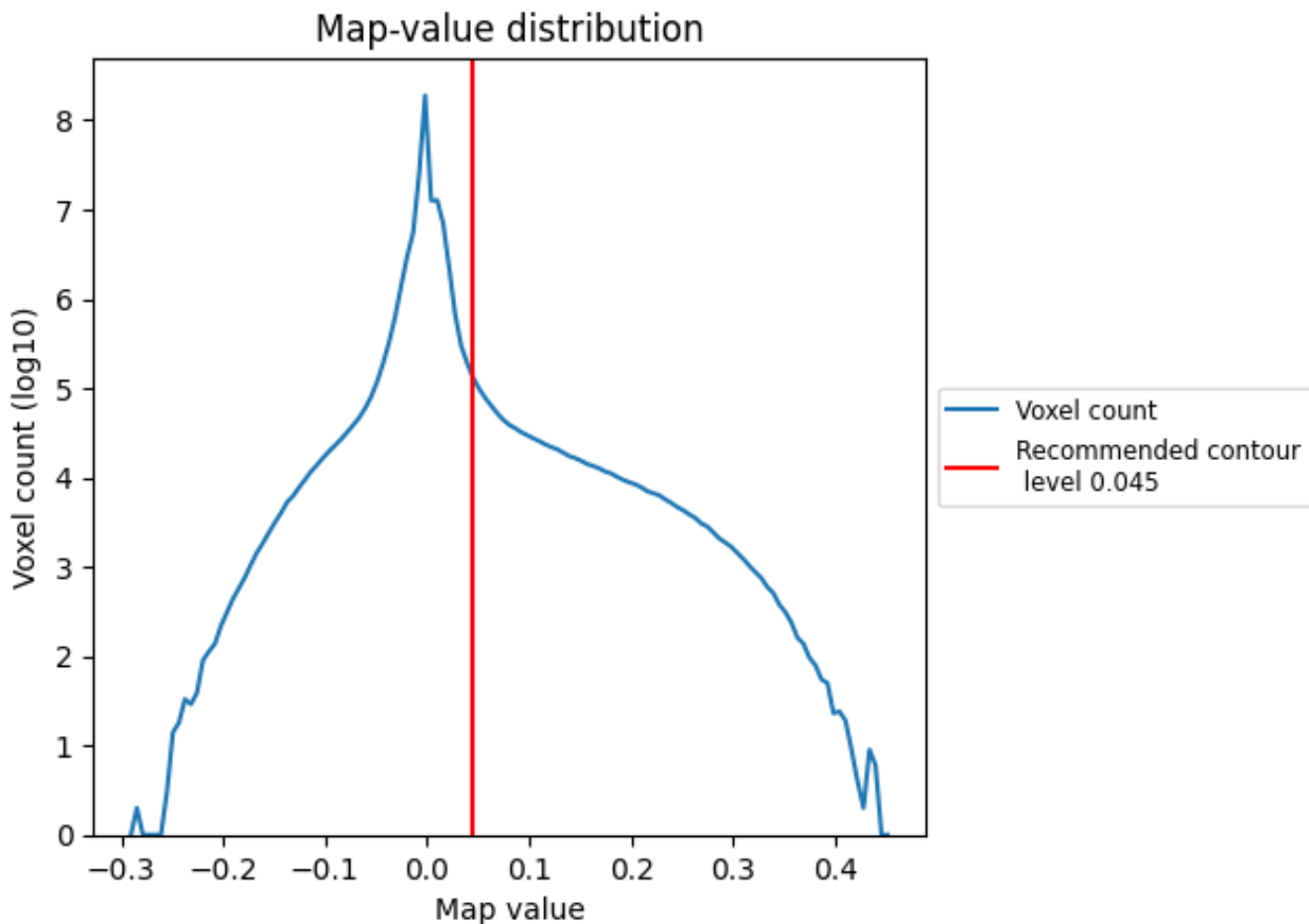
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

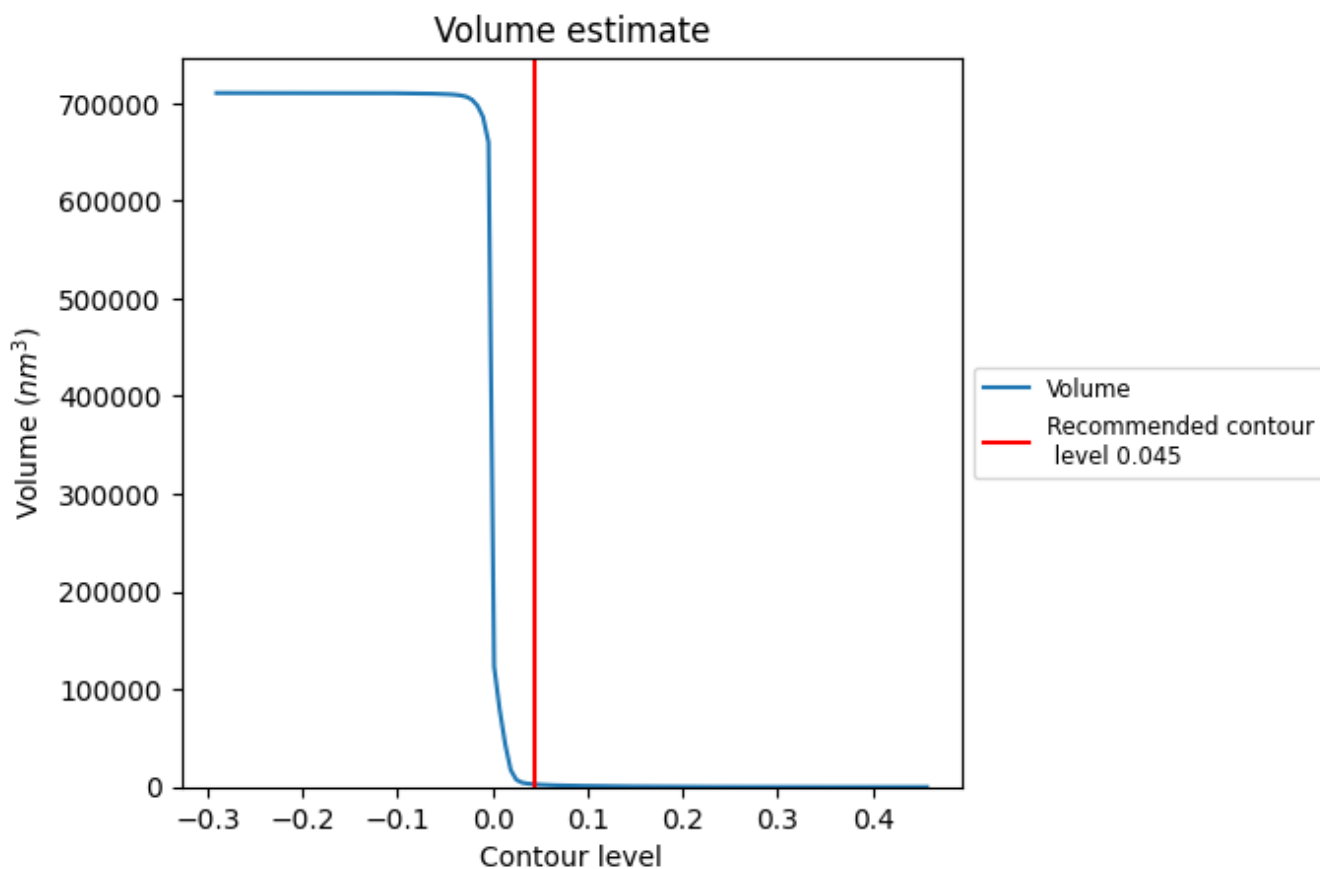
This section contains the results of statistical analysis of the map.

### 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.

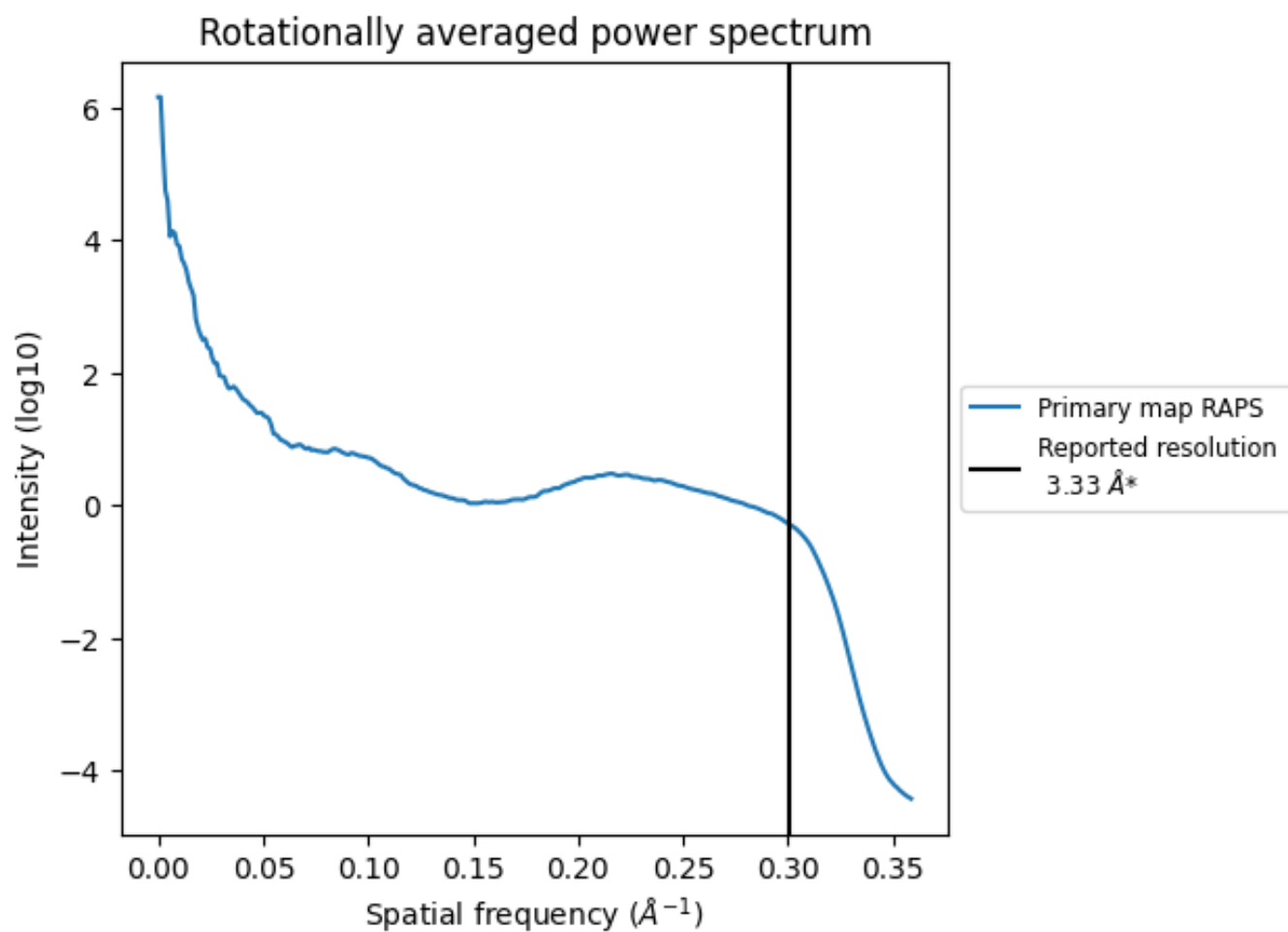
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2647 nm<sup>3</sup>; this corresponds to an approximate mass of 2391 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](#)

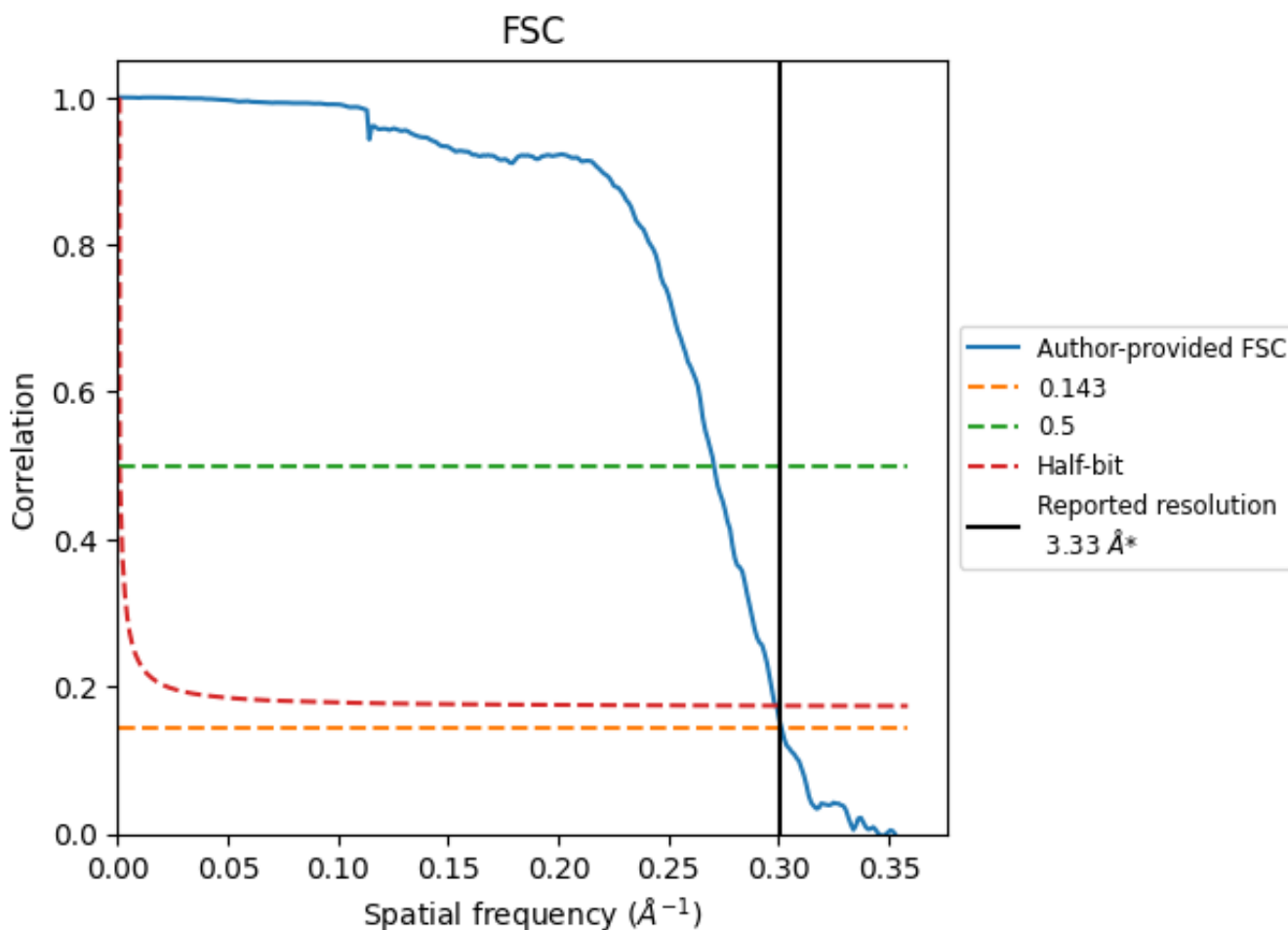


\*Reported resolution corresponds to spatial frequency of 0.300 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

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

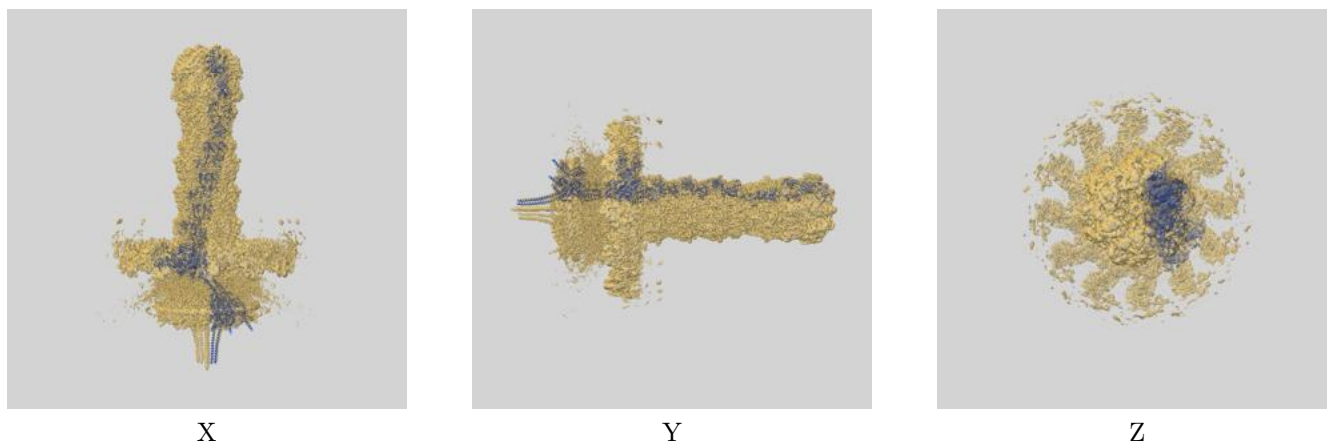
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

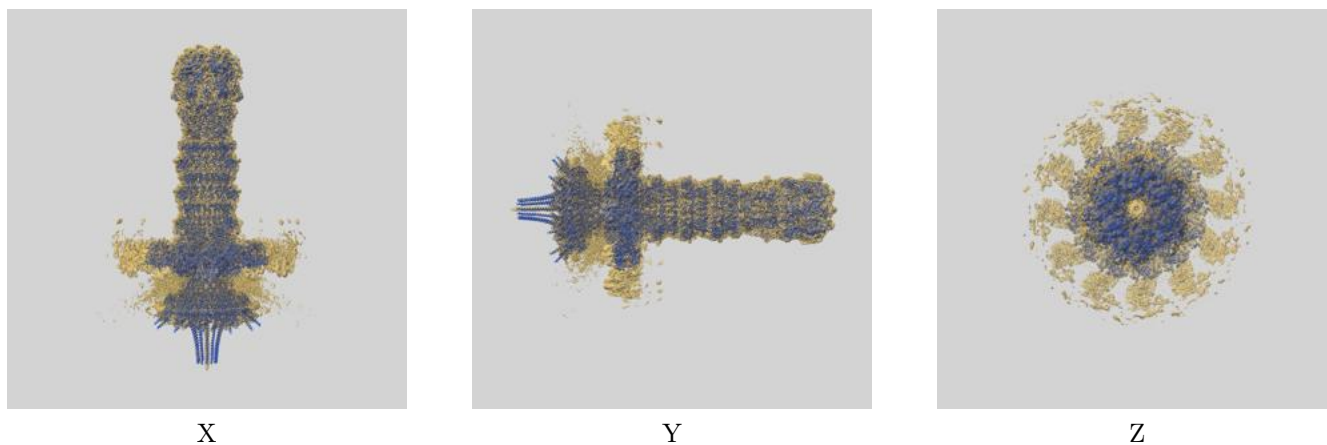
This section contains information regarding the fit between EMDB map EMD-14094 and PDB model 7QOL. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

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

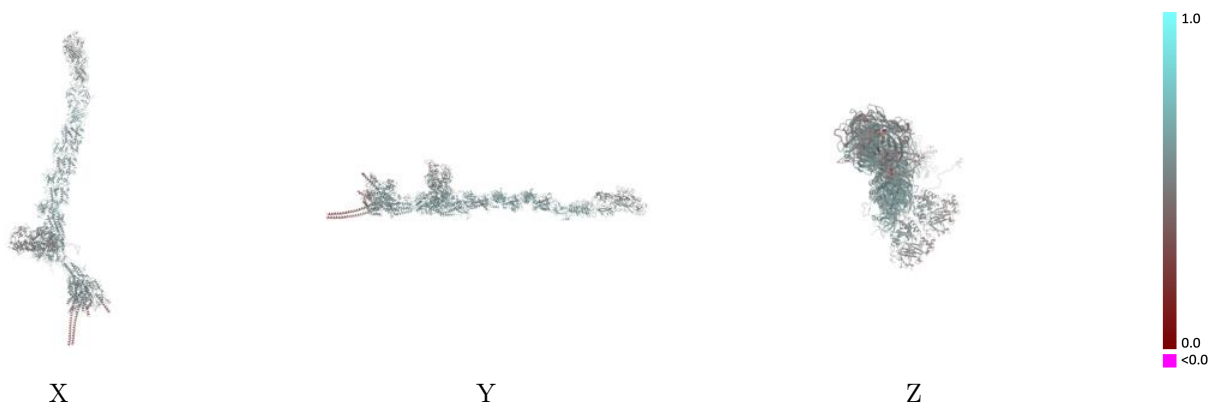


#### 9.1.2 Map-model assembly overlay [i](#)



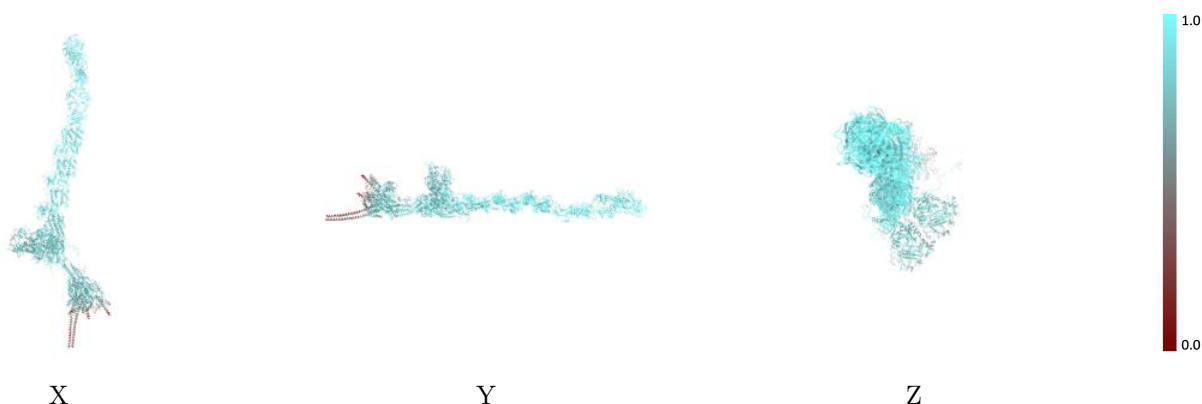
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



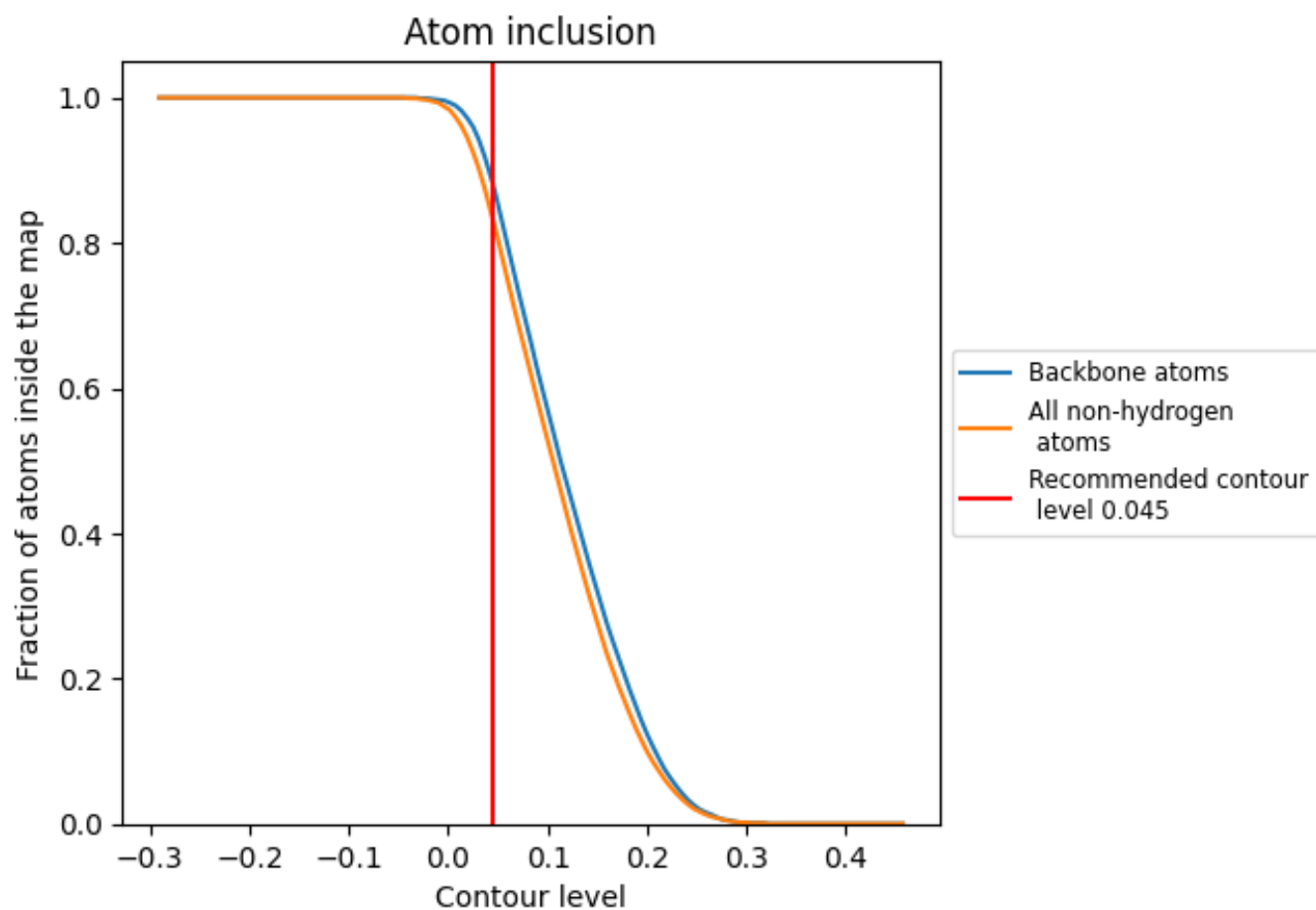
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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
B	 0.8740	 0.5730
C	 0.9030	 0.5730
D	 0.9110	 0.5550
E	 0.9260	 0.5630
F	 0.9200	 0.5540
G	 0.7760	 0.5020
H	 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
O	 0.7320	 0.5110
P	 0.9190	 0.5170
Q	 0.8600	 0.5660
R	 0.8710	 0.5060
S	 0.9050	 0.5730
T	 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

