



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:54 AM UTC

PDB ID : 7QOJ / pdb_00007qoj
EMDB ID : EMD-14092
Title : Tail barrel assembly of the phicrAss001 virion with C12 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 : 3.21 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

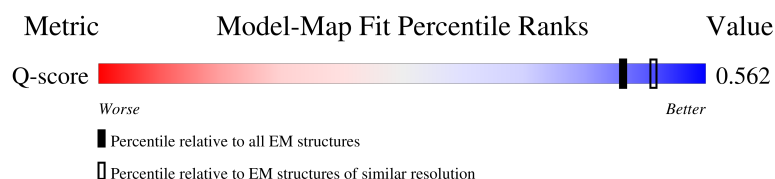
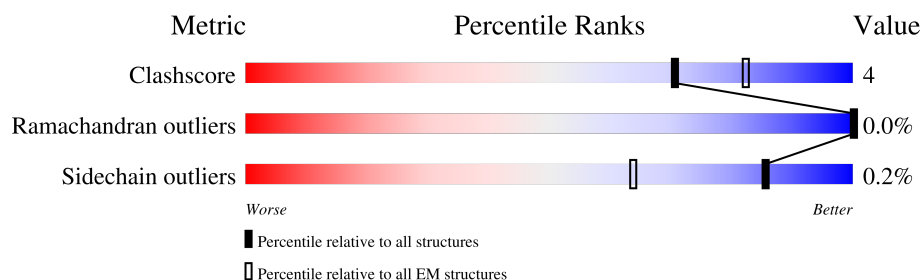
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.21 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.



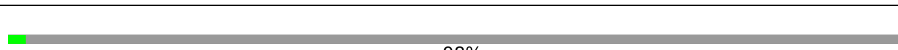
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

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

Mol	Chain	Length	Quality of chain
1	A	806	5% 72% 9% 18%
2	B	236	87% 9% .
3	C	225	92% 8%
4	D	230	90% 9% .

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Mol	Chain	Length	Quality of chain
5	E	238	 90%10%
5	F	238	 88%10%
6	G	215	 75%7%18%
6	H	215	 6%79%9%13%
7	I	114	 81%13%6%
8	J	832	 98%
8	K	832	 98%
8	L	832	 97%
9	M	842	 13%85%
9	N	842	 96%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20218 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
1	A	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
2	B	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
3	C	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
4	D	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	232	Total	C	N	O	S	0	0
			1843	1165	305	369	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		

- 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		

- 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		

- 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		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

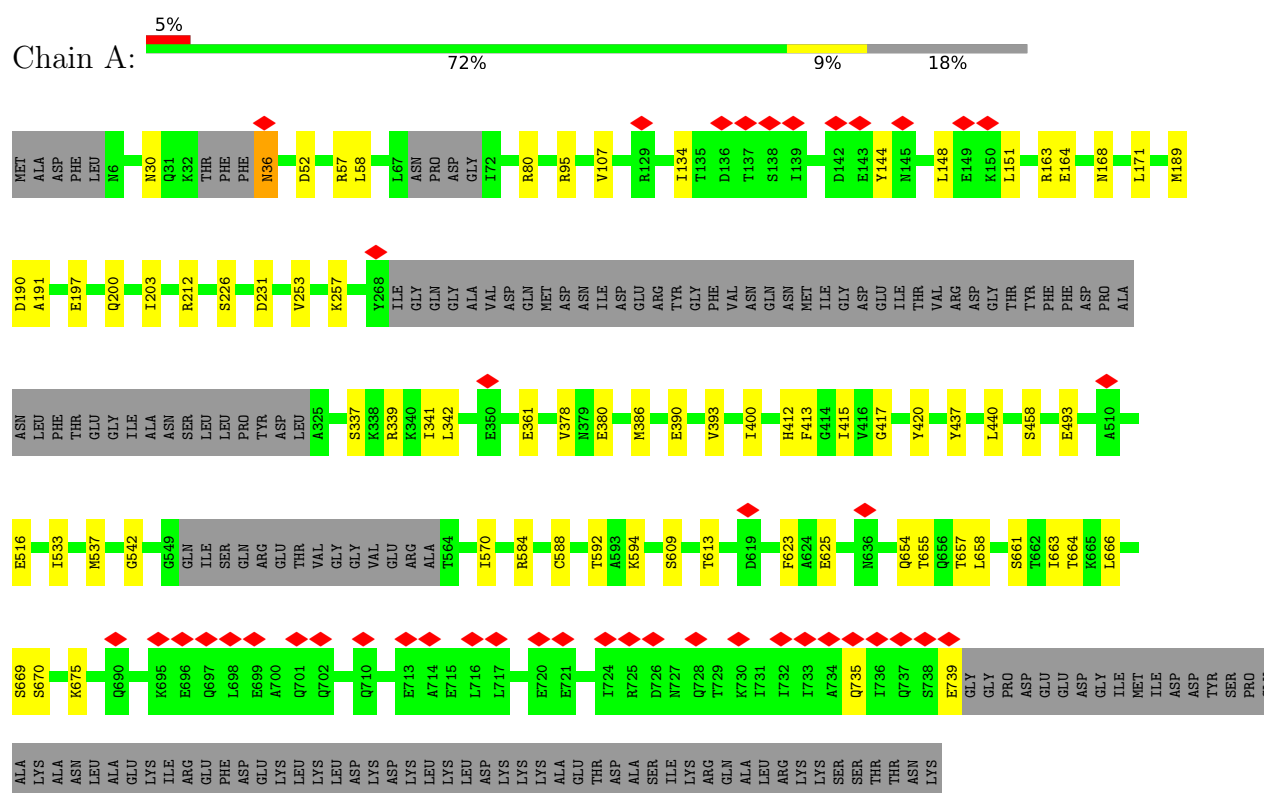
- Molecule 11 is water.

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

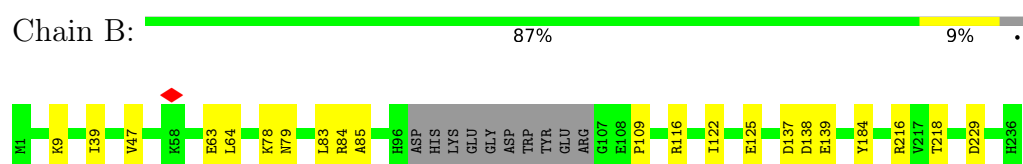
3 Residue-property plots

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 2: Ring protein 1 gp43

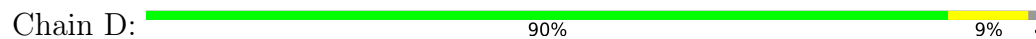


- Molecule 3: Ring protein 2 gp40





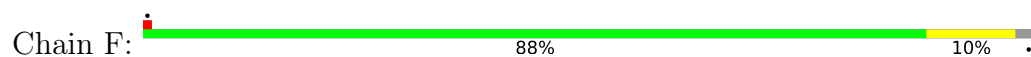
- Molecule 4: Ring protein 3 gp35



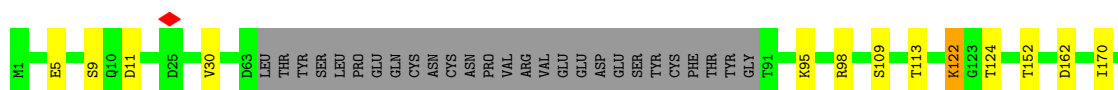
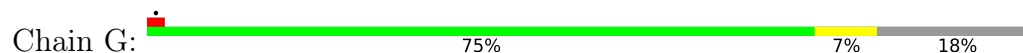
- Molecule 5: Ring protein 4/5 gp34



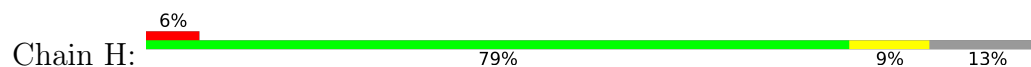
- Molecule 5: Ring protein 4/5 gp34



- Molecule 6: Tail hub protein A gp38



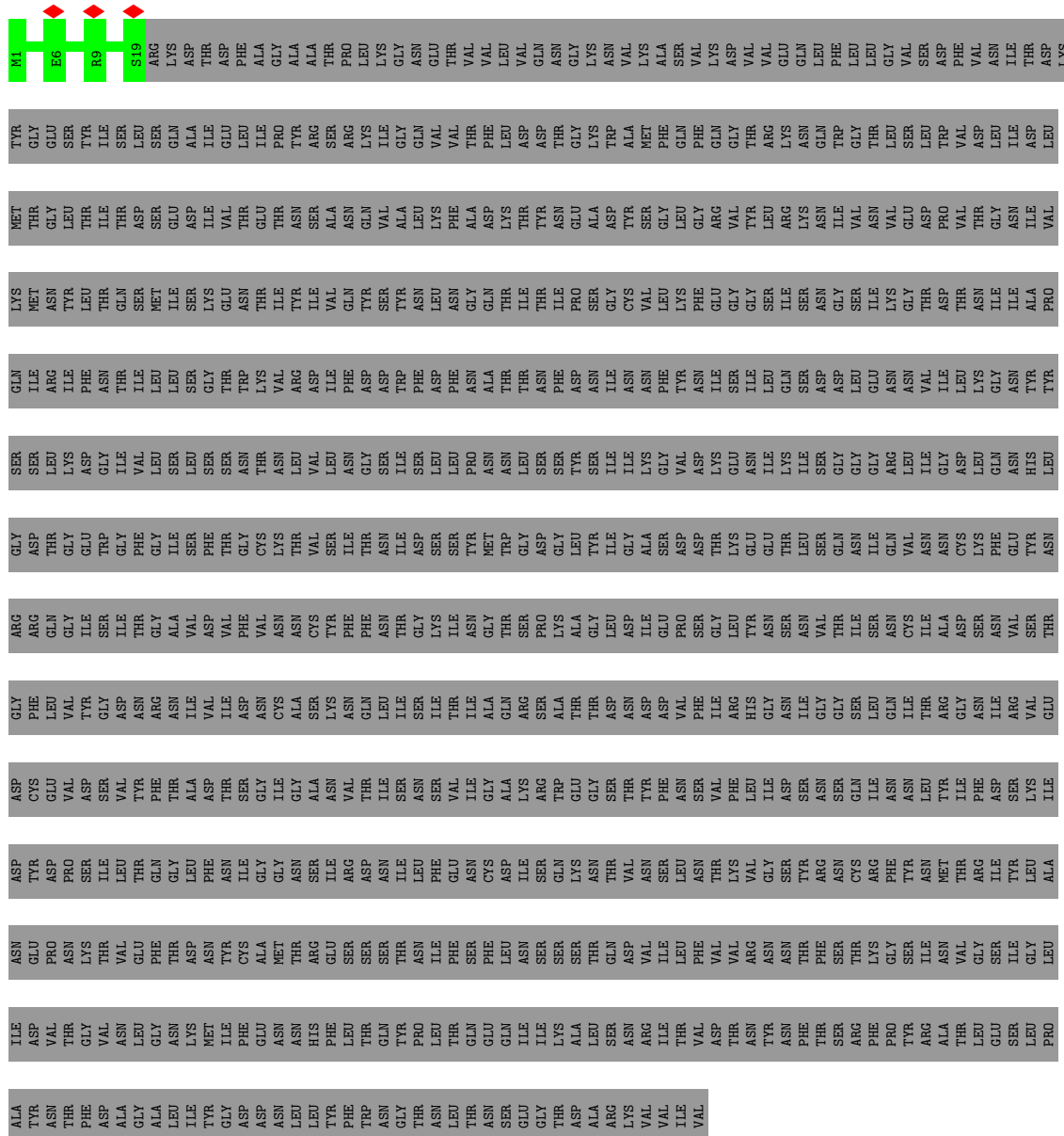
- Molecule 6: Tail hub protein A gp38



- Molecule 7: Tail hub protein B gp39



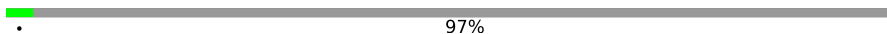
Chain J: 98%



Chain K: 98%

[illegible]

- Molecule 8: Tail fiber protein gp22

Chain L: [illegible]

TRP	ASN	ALA	GLY	GLU
THR	THR	THR	SER	TYR
ASN	GLU	ARG	GLY	PRO
ASN	THR	ARG	LEU	SER
GLN	GLY	GLY	ALA	MET
ALA	LEU	MET	SER	PHE
ASN	LYS	ALA	LEU	TYR
TRP	ALA	ASN	SER	ALA
ASP	SER	THR	ASP	GLY
THR	MET	SER	LEU	GLY
LEU	PHE	GLY	PHE	ASP
LEU	ASN	GLY	SER	THR
ALA	ALA	ASN	LYS	ASN
LYS	GLU	ARG	PRO	PRO
SER	SER	LEU	ASP	TYR
GLY	ARG	ASN	TYR	GLY
VAL	ASN	ALA	ASP	LEU
LEU	ALA	GLN	SER	ALA
LYS	ALA	ALA	ALA	LEU
MET	LYS	GLY	ASP	GLU
THR	ALA	ILE	LEU	ASP
THR	ARG	LEU	ILE	PRO
LYS	ARG	ALA	SER	MET
GLY	LEU	ALA	GLY	SER
GLU	GLY	ASP	VAL	VAL
THR	GLN	TYR	ASP	GLU
GLY	ALA	ASN	LEU	GLU
GLY	THR	GLY	GLY	LEU
THR	VAL	GLN	GLU	ALA
LYS	ALA	ASN	ALA	LEU
LYS	GLN	MET	VAL	MET
ALA	LEU	GLY	VAL	GLY
LYS	ARG	ASN	TYR	GLN
GLY	GLN	LEU	ALA	SER
GLY	GLY	ALA	PRO	GLY
LYS	ILE	ARG	ILE	GLU
VAL	LYS	GLN	GLY	THR
ARG	ASP	ALA	ASN	GLY
THR	GLN	GLU	TYR	GLU
LYS	ALA	TYR	LEU	ILE
LYS	ALA	ASN	SER	ALA
LYS	ARG	GLN	TYR	PRO
GLY	ARG	GLN	PRO	GLY
LEU	SER	LEU	LEU	ASN
THR	ALA	ARG	ASP	ASN
TYR	ASN	GLU	ARG	GLY
GLY	ILE	VAL	ASP	ASN
	THR	ASN	PHE	ARG
	ASN	GLU	TYR	GLN
	PHE	ALA	ILE	THR
	LEU	PHE	ASN	TRP
	GLN	ASN	LYS	THR
	GLY	GLY	MET	ARG
	LEU	GLY	ASN	TYR
	LEU	THR	GLN	ALA
	ASP	ASN	PRO	PRO
	MET	MET	ALA	ILE
	GLY	THR	ALA	ILE

- Molecule 9: Cargo protein 1 gp45

Chain N: 96%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	122709	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	0.762	Depositor
Minimum map value	-0.553	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	535.3336, 535.3336, 535.3336	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3940979, 1.3940979, 1.3940979	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	0.25	1/5468 (0.0%)	0.43	1/7374 (0.0%)
2	B	0.29	0/1881	0.51	0/2548
3	C	0.30	0/1886	0.45	0/2552
4	D	0.26	0/1837	0.42	0/2491
5	E	0.25	0/1910	0.38	0/2594
5	F	0.23	0/1873	0.39	0/2541
6	G	0.28	0/1469	0.47	0/1989
6	H	0.20	0/1546	0.39	0/2093
7	I	0.27	0/895	0.46	0/1208
8	J	0.35	0/174	0.59	0/232
8	K	0.27	0/174	0.40	0/232
8	L	0.17	0/229	0.35	0/305
9	M	0.18	0/1003	0.35	0/1347
9	N	0.29	0/255	0.52	0/342
All	All	0.26	1/20600 (0.0%)	0.43	1/27848 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	CYS	C-O	-6.52	1.16	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	CYS	CA-C-O	-6.04	114.14	120.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5371	0	5333	41	0
2	B	1841	0	1863	13	0
3	C	1841	0	1800	12	0
4	D	1805	0	1813	11	0
5	E	1878	0	1870	14	0
5	F	1843	0	1838	13	0
6	G	1441	0	1425	9	0
6	H	1516	0	1493	18	0
7	I	878	0	844	16	0
8	J	170	0	167	0	0
8	K	170	0	167	2	0
8	L	224	0	217	1	0
9	M	987	0	930	7	0
9	N	251	0	239	1	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
All	All	20218	0	19999	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:190:GLN:HE22	7:I:13:THR:HG22	1.06	1.18
6:H:190:GLN:HE22	7:I:13:THR:CG2	1.61	1.13
6:H:190:GLN:NE2	7:I:13:THR:HG22	1.76	1.01
2:B:116:ARG:NH1	6:H:163:CYS:SG	2.51	0.84
1:A:458:SER:OG	1:A:516:GLU:OE1	1.96	0.84
3:C:51:ILE:HG21	3:C:158:ILE:HD11	1.60	0.82
5:E:45:TYR:OH	5:E:210:GLU:OE1	1.96	0.82
3:C:43:ARG:NH2	9:N:225:ASN:OD1	2.19	0.76
2:B:84:ARG:NH1	2:B:85:ALA:O	2.18	0.76
2:B:216:ARG:NH2	2:B:229:ASP:O	2.20	0.74
4:D:105:GLU:OE2	4:D:169:TYR:OH	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:9:SER:OG	6:G:11:ASP:OD1	2.05	0.73
1:A:339:ARG:NH1	9:M:521:ASP:OD2	2.23	0.72
1:A:341:ILE:HD11	1:A:378:VAL:HG21	1.72	0.71
6:H:38:ASP:OD1	6:H:42:THR:OG1	2.09	0.70
5:F:185:SER:OG	5:F:186:GLU:OE1	2.10	0.69
4:D:114:LEU:HD12	4:D:114:LEU:O	1.93	0.69
6:H:190:GLN:HE22	7:I:13:THR:HG21	1.58	0.69
1:A:226:SER:OG	1:A:231:ASP:OD2	2.06	0.68
1:A:257:LYS:NZ	1:A:390:GLU:OE2	2.26	0.68
5:F:203:LEU:HD23	5:F:207:ILE:HD11	1.76	0.68
9:M:463:ASP:O	9:M:466:GLY:N	2.27	0.67
9:M:497:TYR:O	9:M:534:ARG:NH1	2.27	0.67
5:E:221:ALA:HB2	5:E:233:LEU:HD22	1.75	0.67
1:A:190:ASP:OD2	1:A:212:ARG:NH1	2.28	0.65
3:C:36:ARG:HG3	3:C:187:ILE:HD12	1.77	0.65
1:A:36:ASN:HD22	1:A:36:ASN:N	1.94	0.64
5:E:206:ILE:HG23	5:E:207:ILE:HG23	1.78	0.63
1:A:654:GLN:O	1:A:655:THR:OG1	2.13	0.63
2:B:122:ILE:HD12	2:B:125:GLU:HB2	1.81	0.63
1:A:417:GLY:O	1:A:584:ARG:NH2	2.32	0.63
3:C:1:MET:HE1	3:C:6:LEU:HD13	1.82	0.62
3:C:51:ILE:HG21	3:C:158:ILE:CD1	2.29	0.62
5:E:185:SER:OG	5:F:135:GLU:OE2	2.16	0.61
6:H:148:ILE:HD13	6:H:176:LEU:HD13	1.81	0.61
6:G:199:PHE:O	6:G:202:ASN:ND2	2.34	0.60
6:H:190:GLN:NE2	7:I:13:THR:CG2	2.45	0.59
6:H:62:TYR:O	6:H:94:MET:HE3	2.02	0.59
2:B:218:THR:O	2:B:218:THR:HG22	2.03	0.58
1:A:666:LEU:HD22	1:A:675:LYS:HB2	1.86	0.58
1:A:164:GLU:OE2	1:A:168:ASN:ND2	2.37	0.58
1:A:58:LEU:O	1:A:80:ARG:NH2	2.37	0.57
1:A:669:SER:O	1:A:670:SER:OG	2.20	0.57
9:M:445:ASN:OD1	9:M:446:GLU:N	2.37	0.57
3:C:36:ARG:NH2	3:C:159:PHE:O	2.37	0.57
3:C:68:ALA:HB3	3:C:75:GLU:OE1	2.04	0.57
1:A:163:ARG:NH1	1:A:625:GLU:OE2	2.38	0.56
1:A:52:ASP:OD1	1:A:57:ARG:NH2	2.39	0.56
4:D:56:SER:O	4:D:63:ILE:HG21	2.05	0.56
1:A:609:SER:O	1:A:613:THR:HG23	2.05	0.56
4:D:29:GLU:OE2	4:D:222:LYS:NZ	2.39	0.56
4:D:127:LEU:HD22	4:D:149:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:105:ASN:OD1	5:F:170:ARG:NH1	2.39	0.55
7:I:96:ILE:HG23	7:I:98:GLU:HG3	1.89	0.54
2:B:78:LYS:NZ	2:B:79:ASN:OD1	2.40	0.54
7:I:25:LYS:NZ	7:I:29:ASP:OD2	2.40	0.54
1:A:36:ASN:N	1:A:36:ASN:ND2	2.54	0.54
6:H:181:LEU:HD12	7:I:12:ILE:HD13	1.88	0.54
5:E:7:SER:HB2	5:E:180:THR:HG21	1.89	0.54
8:K:1:MET:HE2	8:L:1:MET:HE3	1.89	0.54
2:B:138:ASP:OD1	2:B:139:GLU:N	2.40	0.54
6:G:124:THR:HG23	6:G:124:THR:O	2.07	0.54
6:H:31:LEU:HD12	6:H:94:MET:CB	2.38	0.53
1:A:735:GLN:NE2	1:A:739:GLU:OE2	2.41	0.52
1:A:144:TYR:CE2	1:A:148:LEU:HD11	2.45	0.52
1:A:661:SER:O	1:A:664:THR:OG1	2.21	0.52
6:H:151:GLN:NE2	6:H:202:ASN:OD1	2.42	0.52
5:F:203:LEU:HD23	5:F:207:ILE:CD1	2.41	0.51
6:H:31:LEU:HD12	6:H:94:MET:HB2	1.93	0.51
1:A:542:GLY:HA3	1:A:570:ILE:HG21	1.93	0.51
4:D:144:SER:OG	4:D:146:ASP:OD1	2.29	0.50
5:E:90:ARG:NH2	5:E:134:LYS:O	2.44	0.50
5:F:91:ALA:HB1	5:F:155:GLU:HB3	1.94	0.50
6:H:27:PHE:O	6:H:95:LYS:NZ	2.35	0.50
1:A:337:SER:N	1:A:380:GLU:O	2.45	0.49
3:C:174:ASN:OD1	3:C:175:GLY:N	2.46	0.49
1:A:95:ARG:HD2	1:A:189:MET:HE3	1.94	0.49
2:B:83:LEU:HD22	2:B:109:PRO:HB2	1.95	0.49
4:D:45:ILE:CG2	4:D:63:ILE:HG23	2.42	0.49
1:A:440:LEU:HD23	1:A:533:ILE:HD12	1.93	0.48
6:G:30:VAL:O	6:G:95:LYS:NZ	2.41	0.48
7:I:25:LYS:HE3	7:I:72:MET:HE2	1.95	0.48
1:A:191:ALA:HB1	1:A:420:TYR:CE2	2.49	0.48
5:F:206:ILE:HG23	5:F:207:ILE:HG23	1.96	0.48
3:C:70:SER:OG	3:C:71:GLY:N	2.46	0.47
1:A:594:LYS:NZ	1:A:623:PHE:O	2.45	0.47
2:B:64:LEU:O	2:B:116:ARG:NH2	2.45	0.47
5:E:106:GLU:OE2	5:E:167:TYR:OH	2.30	0.47
5:E:8:ASN:OD1	5:F:138:LYS:NZ	2.43	0.47
1:A:253:VAL:HG21	1:A:393:VAL:HG13	1.96	0.47
7:I:11:ALA:HB1	7:I:33:ILE:CD1	2.46	0.46
6:G:109:SER:O	6:G:113:THR:OG1	2.29	0.46
2:B:39:ILE:HD12	2:B:47:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HG23	1:A:171:LEU:HD12	1.97	0.46
1:A:341:ILE:CD1	1:A:378:VAL:HG21	2.44	0.46
5:E:40:GLU:O	5:E:44:ASN:ND2	2.48	0.46
1:A:191:ALA:HB2	1:A:197:GLU:HB2	1.98	0.46
6:H:112:SER:OG	6:H:200:ILE:O	2.30	0.45
7:I:101:ILE:C	7:I:102:LEU:HD22	2.42	0.45
4:D:83:LYS:NZ	4:D:157:LEU:HD11	2.31	0.45
1:A:658:LEU:HD23	1:A:663:ILE:HD11	1.99	0.45
3:C:107:ILE:HG22	3:C:130:CYS:SG	2.57	0.45
6:H:6:LEU:HG	6:H:142:VAL:HG22	1.99	0.45
1:A:30:ASN:HB2	1:A:386:MET:HE1	2.00	0.44
1:A:412:HIS:ND1	1:A:413:PHE:O	2.51	0.44
8:K:11:ILE:O	8:K:15:LEU:HD23	2.17	0.44
5:E:44:ASN:ND2	5:E:238:GLU:OE1	2.51	0.44
4:D:65:ARG:O	4:D:203:ASN:ND2	2.51	0.44
1:A:437:TYR:HB2	1:A:537:MET:HG3	1.99	0.44
5:F:108:VAL:CG2	5:F:164:ILE:HG23	2.47	0.44
5:E:85:ILE:O	5:E:85:ILE:HG23	2.18	0.44
6:H:178:ALA:HA	7:I:12:ILE:HD12	1.98	0.43
6:G:122:LYS:O	6:G:122:LYS:HG3	2.18	0.43
5:F:44:ASN:ND2	5:F:238:GLU:O	2.51	0.43
6:G:152:THR:OG1	7:I:42:MET:HE1	2.18	0.43
9:M:453:ASN:OD1	9:M:455:TYR:N	2.51	0.43
4:D:15:ASN:O	4:D:22:ASN:ND2	2.48	0.42
5:E:117:ILE:HG23	5:E:143:ARG:HB2	2.00	0.42
5:F:146:THR:OG1	5:F:147:THR:N	2.52	0.42
3:C:69:ILE:N	3:C:75:GLU:OE1	2.39	0.42
2:B:9:LYS:NZ	2:B:137:ASP:OD1	2.47	0.42
5:F:106:GLU:OE2	5:F:167:TYR:OH	2.36	0.42
7:I:1:MET:HE1	7:I:43:LEU:HB2	2.02	0.42
3:C:57:GLN:OE1	3:C:165:ALA:HB3	2.19	0.42
1:A:400:ILE:HD13	1:A:592:THR:HG23	2.02	0.41
6:H:31:LEU:HD12	6:H:94:MET:HB3	2.02	0.41
7:I:33:ILE:HD11	7:I:72:MET:SD	2.60	0.41
9:M:489:ILE:HG21	9:M:494:ARG:HD3	2.03	0.41
1:A:134:ILE:HD13	1:A:151:LEU:HD21	2.03	0.41
1:A:203:ILE:HD12	1:A:400:ILE:HD11	2.03	0.41
1:A:493:GLU:OE2	2:B:184:TYR:OH	2.35	0.41
9:M:444:ILE:HD13	9:M:471:VAL:HG21	2.03	0.41
1:A:415:ILE:HD12	1:A:415:ILE:H	1.86	0.41
1:A:657:THR:O	1:A:657:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:5:GLU:OE2	6:G:98:ARG:NH1	2.51	0.41
5:E:108:VAL:CG2	5:E:164:ILE:HG23	2.50	0.41
5:E:38:GLN:HE21	5:E:203:LEU:HD13	1.86	0.40
2:B:63:GLU:OE2	2:B:116:ARG:NH2	2.54	0.40
1:A:342:LEU:HD13	1:A:361:GLU:HA	2.02	0.40
4:D:118:ASP:OD1	4:D:119:GLY:N	2.54	0.40
5:F:111:ASN:OD1	5:F:112:ALA:N	2.54	0.40
6:G:170:ILE:HD11	7:I:35:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	647/806 (80%)	636 (98%)	11 (2%)	0	100	100
2	B	222/236 (94%)	217 (98%)	5 (2%)	0	100	100
3	C	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
4	D	224/230 (97%)	213 (95%)	11 (5%)	0	100	100
5	E	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
5	F	228/238 (96%)	216 (95%)	12 (5%)	0	100	100
6	G	173/215 (80%)	168 (97%)	4 (2%)	1 (1%)	21	55
6	H	184/215 (86%)	180 (98%)	4 (2%)	0	100	100
7	I	105/114 (92%)	101 (96%)	4 (4%)	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
9	M	122/842 (14%)	116 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
All	All	2451/6697 (37%)	2369 (97%)	81 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	162	ASP

5.3.2 Protein sidechains ⓘ

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%)	586 (100%)	2 (0%)	86	87
2	B	206/215 (96%)	206 (100%)	0	100	100
3	C	208/208 (100%)	208 (100%)	0	100	100
4	D	207/210 (99%)	207 (100%)	0	100	100
5	E	211/211 (100%)	211 (100%)	0	100	100
5	F	208/211 (99%)	206 (99%)	2 (1%)	68	78
6	G	168/203 (83%)	167 (99%)	1 (1%)	78	83
6	H	177/203 (87%)	177 (100%)	0	100	100
7	I	100/106 (94%)	100 (100%)	0	100	100
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%)	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
All	All	2259/5777 (39%)	2254 (100%)	5 (0%)	85	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	200	GLN
5	F	13	LEU
5	F	17	ILE
6	G	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	121	ASN
1	A	131	GLN
1	A	145	ASN
1	A	200	GLN
3	C	94	ASN
4	D	165	ASN
5	E	38	GLN
5	E	44	ASN
5	F	15	ASN
5	F	16	ASN
6	G	92	GLN
6	G	190	GLN
6	H	190	GLN
9	M	456	GLN
9	M	469	ASN
9	N	231	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

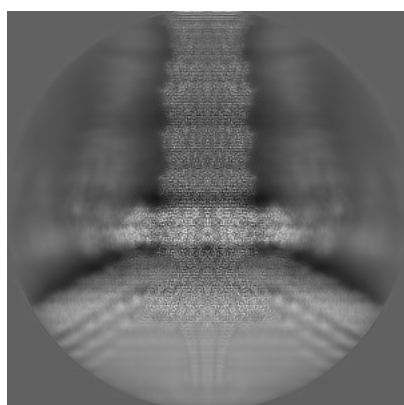
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14092. These allow visual inspection of the internal detail of the map and identification of artifacts.

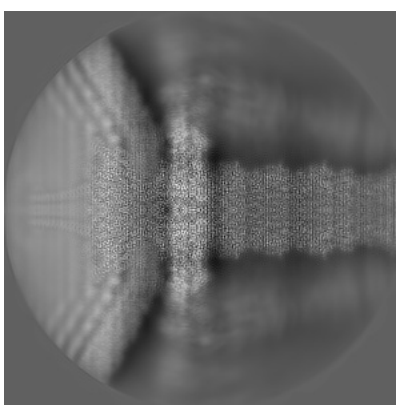
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

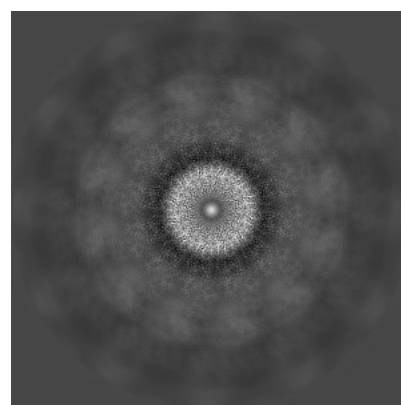
6.1.1 Primary map



X



Y

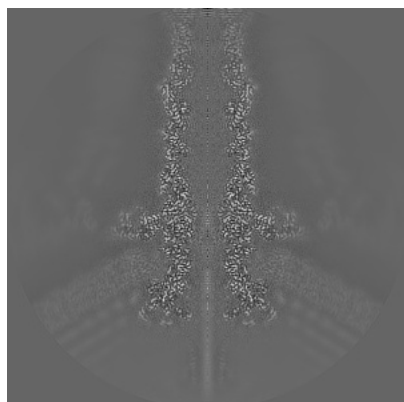


Z

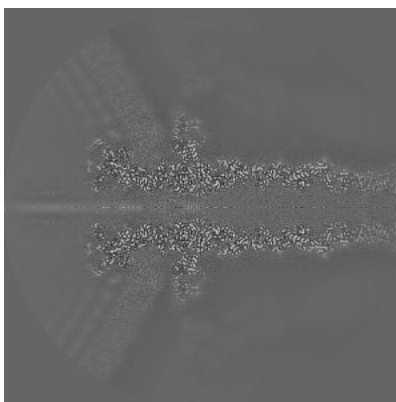
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

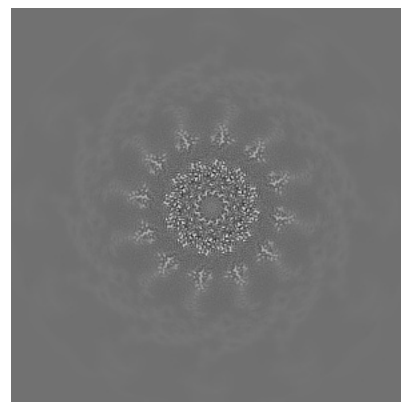
6.2.1 Primary map



X Index: 192



Y Index: 192

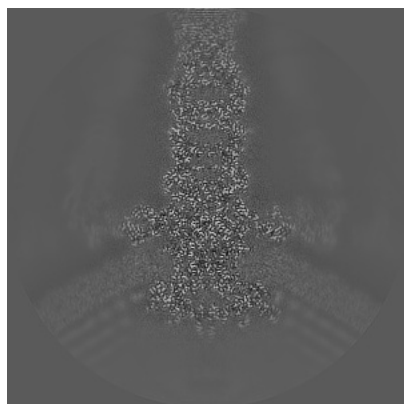


Z Index: 192

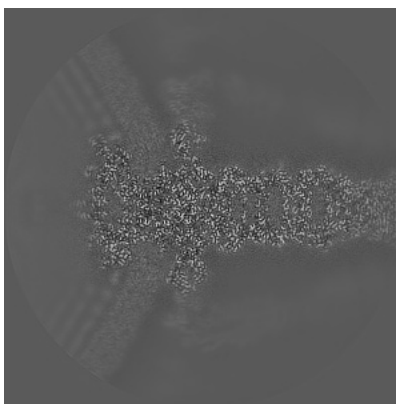
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

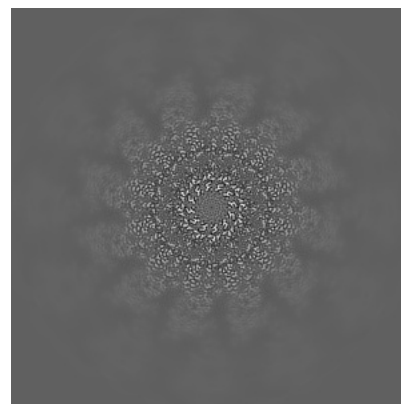
6.3.1 Primary map



X Index: 213



Y Index: 171

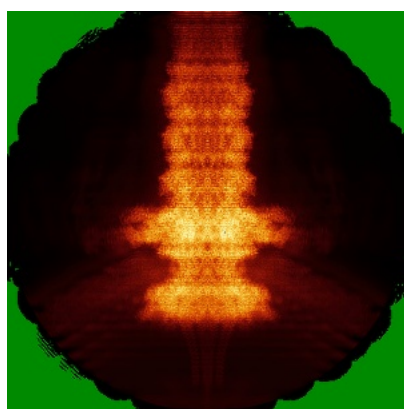


Z Index: 171

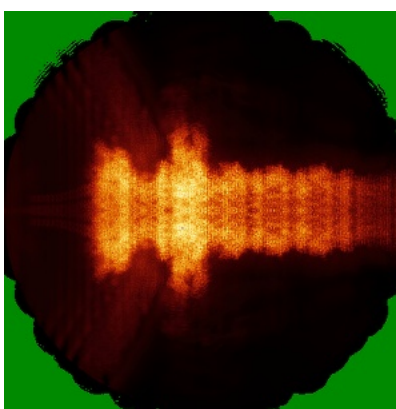
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

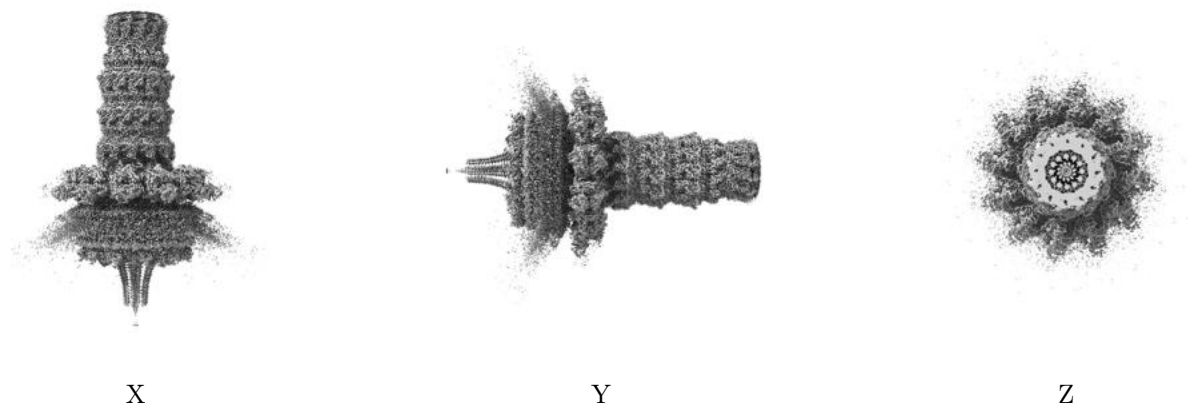


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

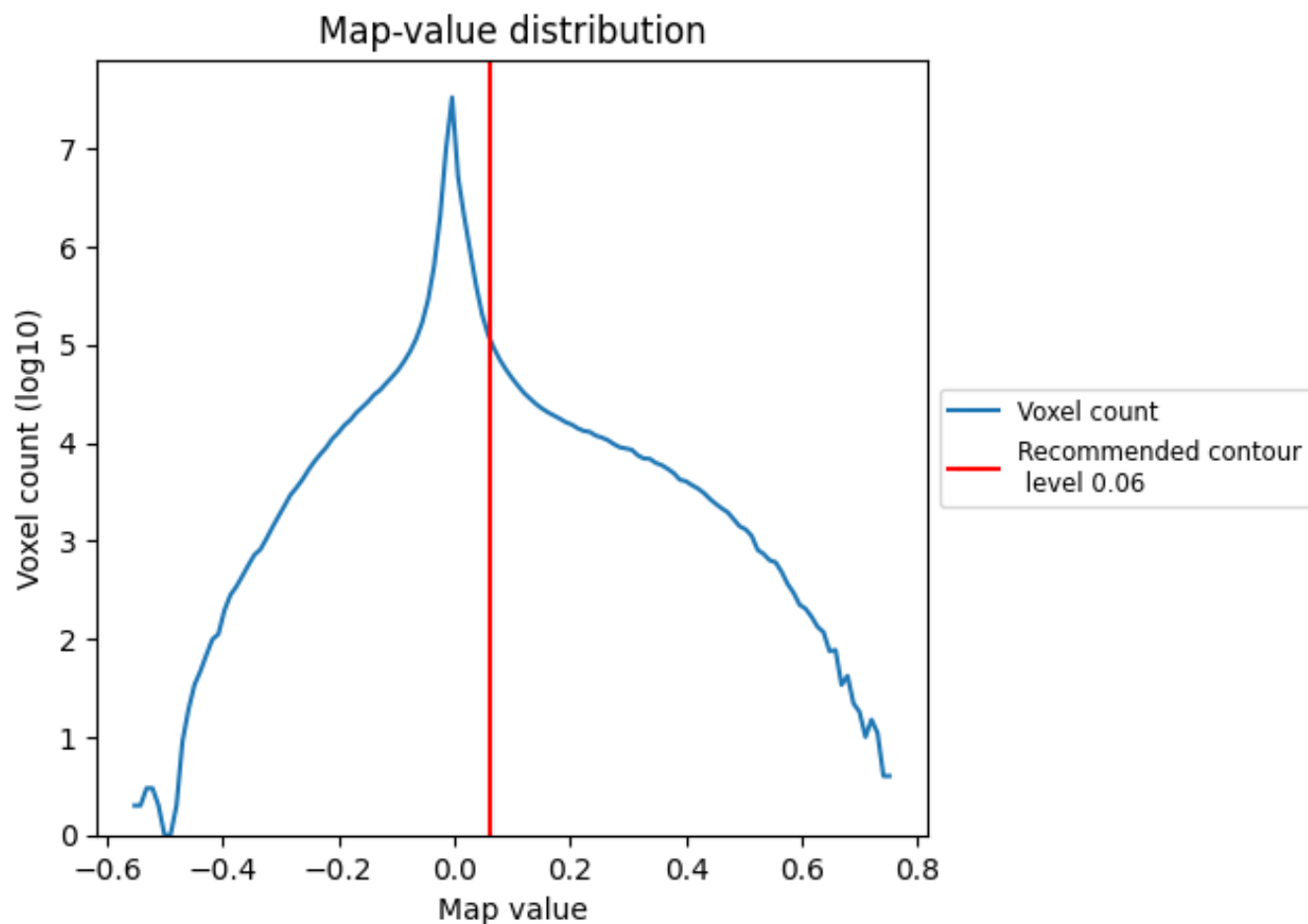
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

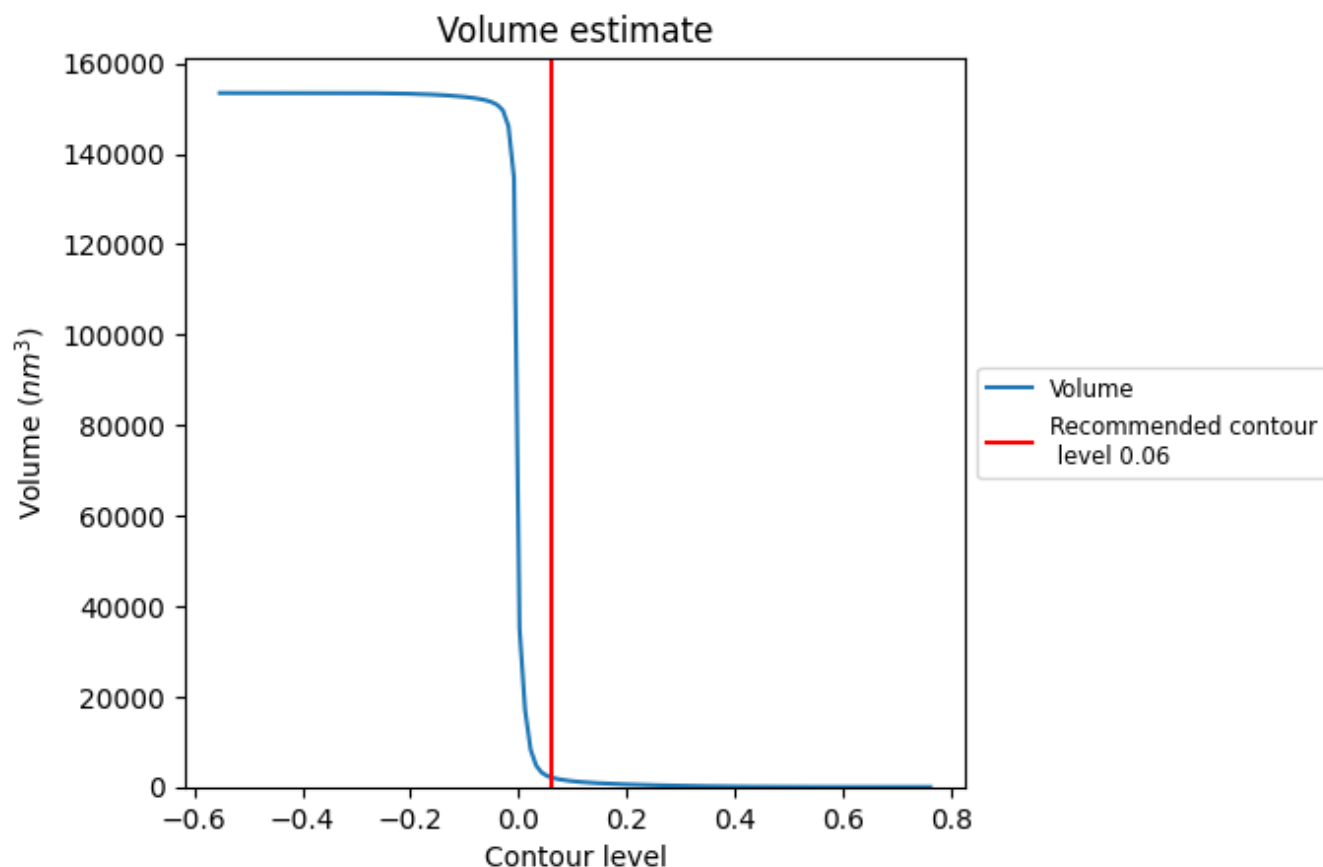
This section contains the results of statistical analysis of the map.

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.

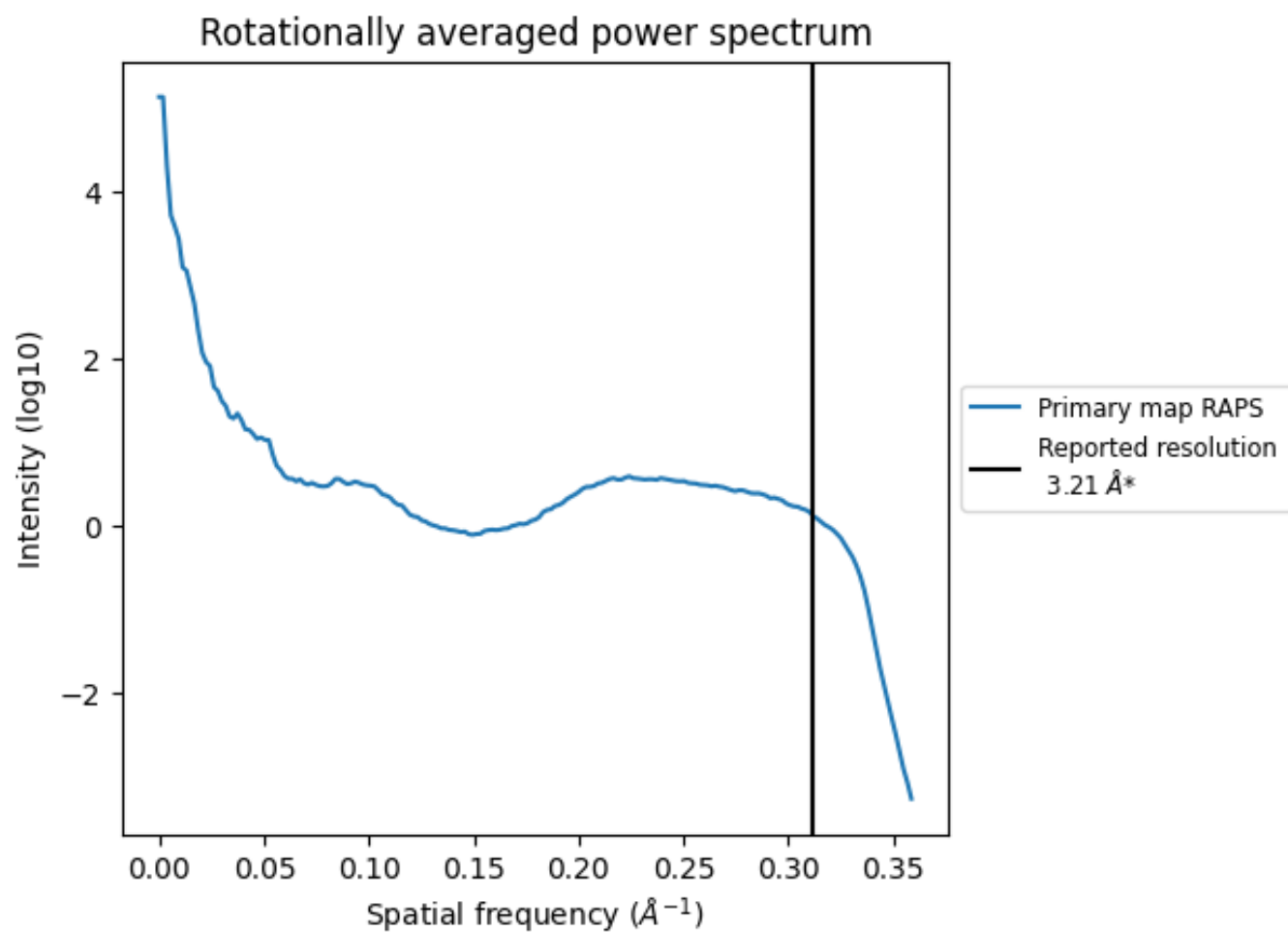
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2153 nm³; this corresponds to an approximate mass of 1945 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 ⓘ

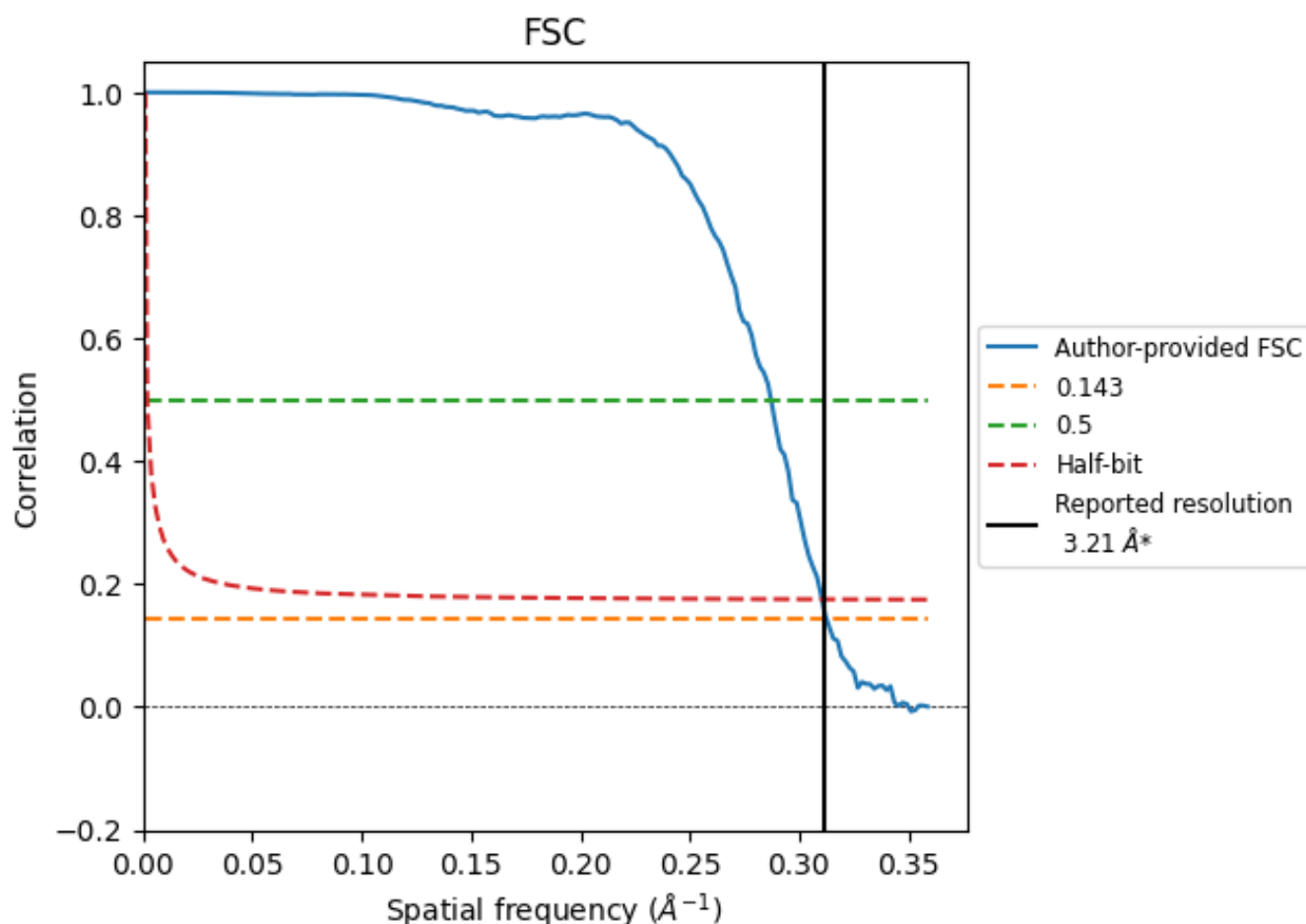


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.20	3.48	3.22
Unmasked-calculated*	-	-	-

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

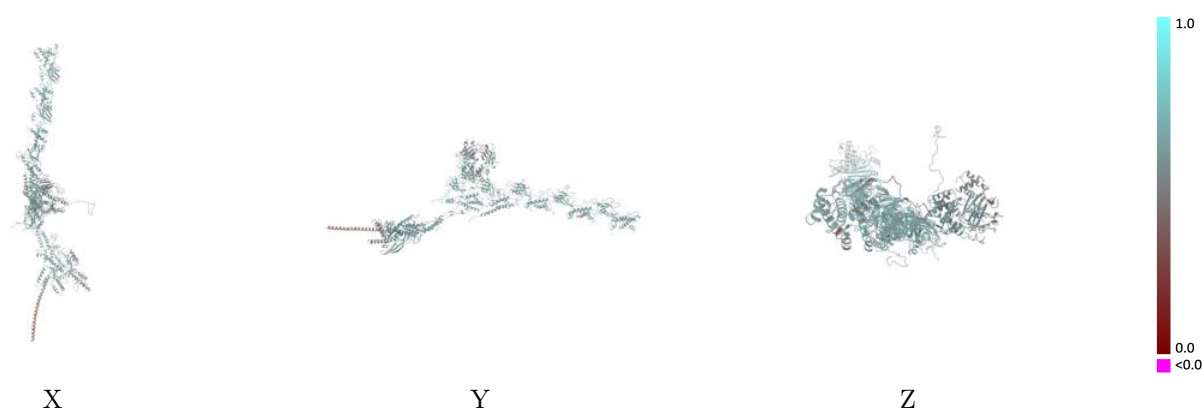
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14092 and PDB model 7QOJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

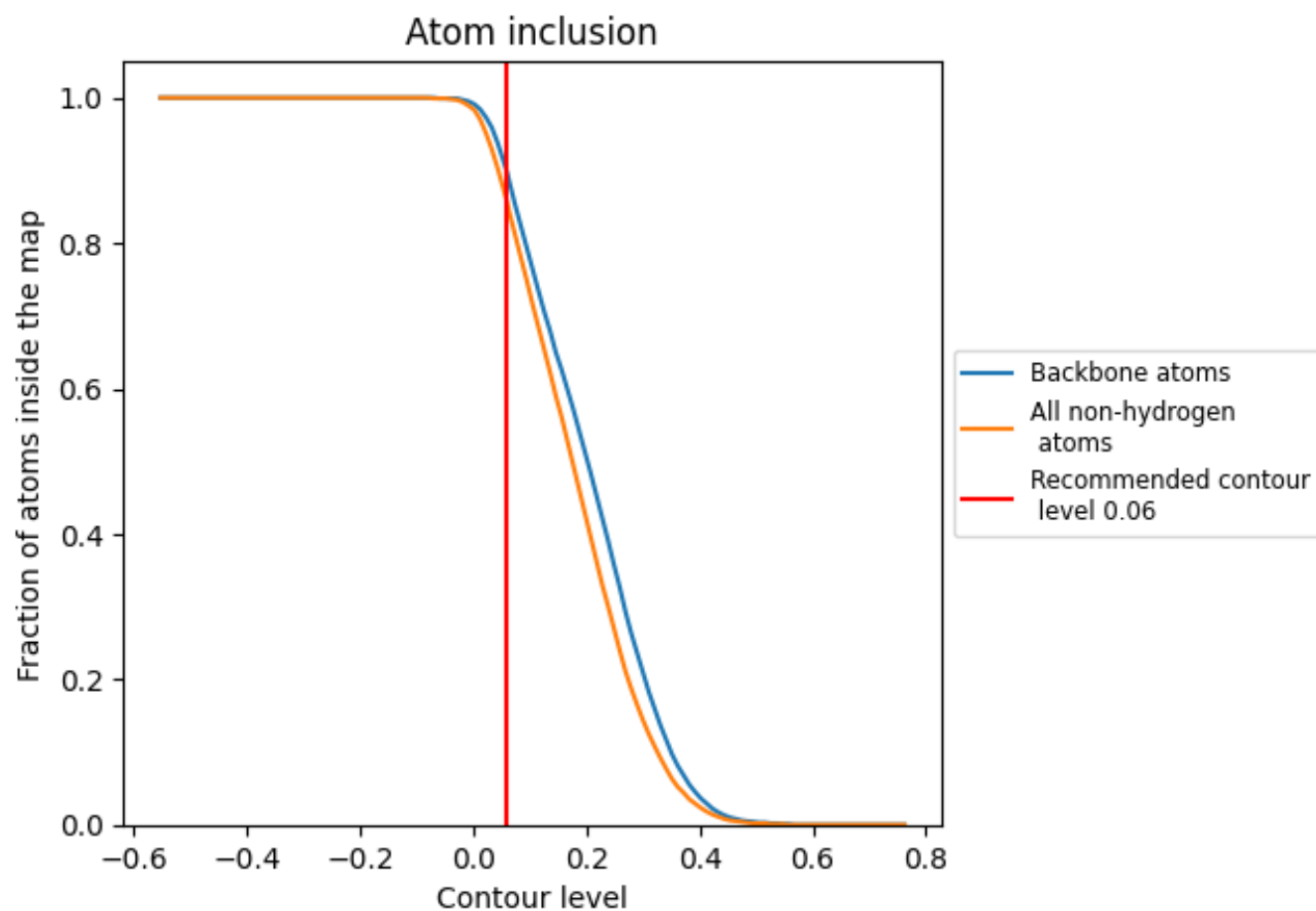


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.5620
A	0.8180	0.5510
B	0.9250	0.5980
C	0.9310	0.5950
D	0.9420	0.5930
E	0.9250	0.5880
F	0.9020	0.5760
G	0.8380	0.5430
H	0.8320	0.5270
I	0.8560	0.5440
J	0.7170	0.4820
K	0.7950	0.5120
L	0.7250	0.5230
M	0.6130	0.4970
N	0.7710	0.5300

