



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 11:04 pm GMT

PDB ID : 7B70
EMDB ID : EMD-12063
Title : TRAPPCore plus C8 (355-596) and C11 (1-718) from MiniTRAPPIII
Authors : Galindo, A.; Munro, S.; Planelles-Herrero, V.J.
Deposited on : 2020-12-09
Resolution : 4.00 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

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.dev43
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) : 2.31.3

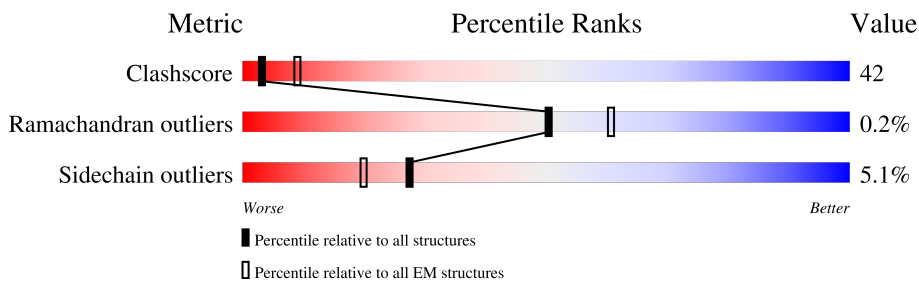
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



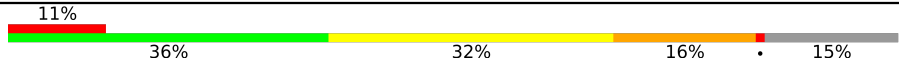

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	178	
1	G	178	
2	B	152	
3	C	145	
4	D	219	
5	E	139	
6	F	194	
7	H	138	

Continued on next page...

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Mol	Chain	Length	Quality of chain
8	I	246	
9	J	718	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 17084 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 Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	165	Total	C	N	O	S	0	0
			1337	847	229	253	8		
1	G	169	Total	C	N	O	S	0	0
			1363	861	233	261	8		

- Molecule 2 is a protein called GEO08327p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	151	Total	C	N	O	S	0	0
			1226	780	211	227	8		

- Molecule 3 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	145	Total	C	N	O	S	0	0
			1204	792	194	216	2		

- Molecule 4 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	219	Total	C	N	O	S	0	0
			1741	1125	279	330	7		

- Molecule 5 is a protein called Probable trafficking protein particle complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	139	Total	C	N	O	S	0	0
			1177	759	199	214	5		

- Molecule 6 is a protein called Trafficking protein particle complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	164	1333	852	225	250	6	0	0

- Molecule 7 is a protein called TRAPPC2L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	138	1089	697	179	207	6	0	0

- Molecule 8 is a protein called FI18195p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	208	1710	1096	301	301	12	0	0

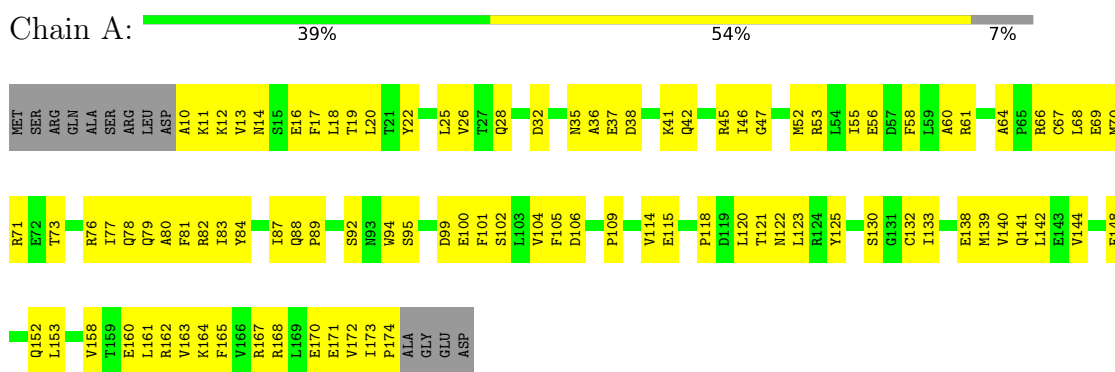
- Molecule 9 is a protein called Trafficking protein particle complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	614	4904	3125	864	882	33	0	0

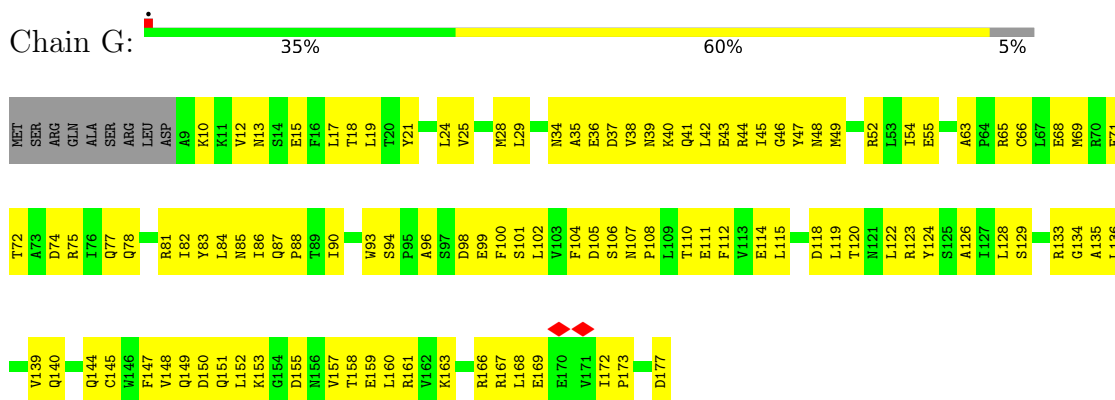
3 Residue-property plots [i](#)

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.

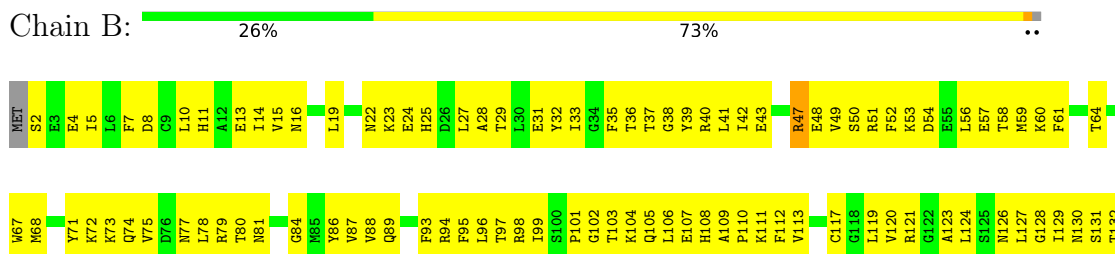
- Molecule 1: Trafficking protein particle complex subunit

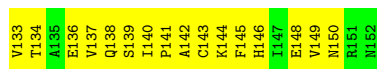


- Molecule 1: Trafficking protein particle complex subunit

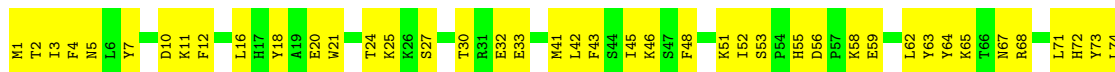


- Molecule 2: GEO08327p1

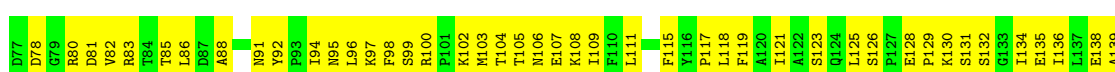
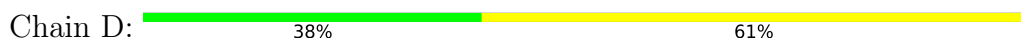




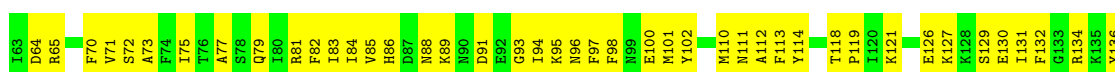
• Molecule 3: Trafficking protein particle complex subunit



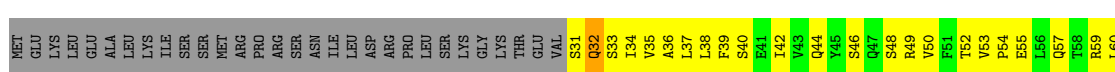
• Molecule 4: Trafficking protein particle complex subunit



• Molecule 5: Probable trafficking protein particle complex subunit 2

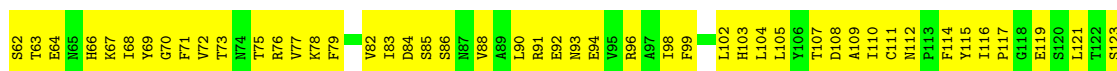
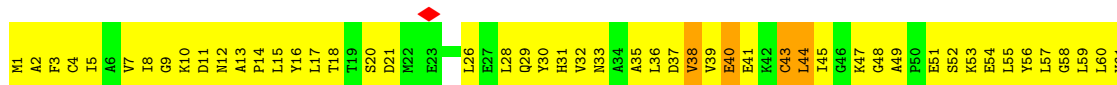
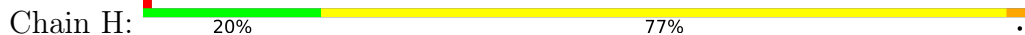


• Molecule 6: Trafficking protein particle complex subunit 5

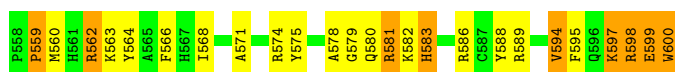
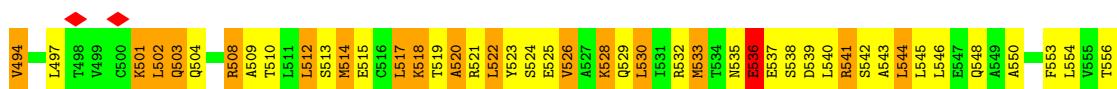
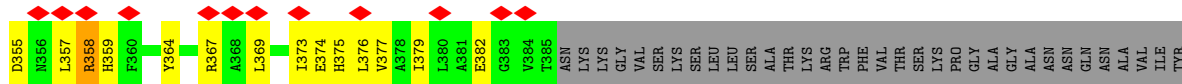




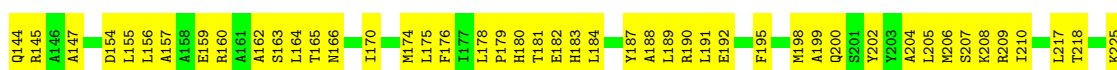
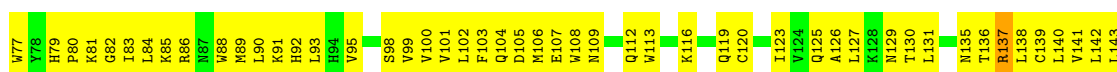
• Molecule 7: TRAPPC2L



• Molecule 8: FI18195p1



• Molecule 9: Trafficking protein particle complex subunit 11



PRO	LYS	ASN	PHE	GLU	LYS	ASN	MET	ARG	LEU	GLU	GLY	S676	L680	F681	S683	T684	E685	A686	Q687	Q688	M692	T693	Q694	L695	V698	R699	L700	E701	A702	H703	M704	G705	T706	D707	Q708	V709	T714	N718														
Q599	L600	F601	V602	L605	T606	D607	I608	P609	L610	R611	I612	R613	S614	F615	H616	L619	A620	D621	P625	Q626	ASN	SER	TYR	LYS	LEU	GLU	ALA	LEU	LYS	TYR	PHE	CYS	PHE	G705	T706	D707	Q708	V709	T714	N718												
D523	Q524	R527	I528	L529	I530	W535	Q536	V541	P542	F543	M544	P545	K546	P551	Q554	A555	L556	W557	T558	S559	A560	L561	A562	N563	V564	K565	S566	PRO	ILE	GLN	ILE	ASP	LEU	LEU	LYS	VAL	ASN	ASP	VAL	V579	E580	M581	T584	L590	S591	N592	D593	D594	L595	L596	Q597	L598
K443	C444	R445	R446	F447	R448	K449	I453	D454	M455	A456	E457	E458	Y459	L460	K461	S462	L471	Y472	M475	L476	Y479	K483	W484	T485	T486	I487	F488	T489	L492	R497	C498	A499	L500	L501	V505	A506	D507	Y508	I509	S512	V513	E514	A515	L516	S517	L518	R519	H520	Q521	S522		
M367	E368	A369	Y370	M373	S377	GLU	ALA	THR	THR	THR	PRO	ILE	GLN	ASN	PRO	LEU	SER	LEU	TYR	THR	GLU	PHE	PHE	GLY	ILE	ARG	ALA	VAL	LYS	THR	GLY	ASP	LEU	V406	Q409	N412	L415	C416	D417	Q418	E419	R420	S421	Y422	I428	M436	A437	Q438	F439	R440	I441	Y442
L226	Q229	F230	K231	L232	G233	F234	V235	M238	R239	Q240	S243	T244	Q245	Q246	K247	H248	Y249	A252	N255	L256	D257	E258	I259	R260	I261	C266	I269	K270	A273	G274	F275	L276	N277	Y278	K279	I280	L283	M284	F285	K286	L287	K288	T289	P290	R291	D292	A293	I294	N295	Q296		
F297	I298	I299	H300	K303	H304	K305	R307	F310	K311	D312	L313	A314	F315	E316	H317	H318	A319	W320	L321	Q324	H325	L331	F332	C333	F334	A335	I336	G339	L343	Q344	T345	H347	P348	G349	I350	Y351	Y352	H353	K354	A355	A356	E357	F358	V359	M360	K361	R362	R363	D364	A365	A366	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	486758	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 ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	502.56, 502.56, 502.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2564, 1.2564, 1.2564	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1360	0.63	0/1841
1	G	0.39	0/1386	0.56	0/1876
2	B	0.43	0/1250	0.61	0/1686
3	C	0.40	0/1237	0.58	0/1675
4	D	0.42	0/1776	0.64	1/2406 (0.0%)
5	E	0.42	0/1207	0.57	1/1623 (0.1%)
6	F	0.40	0/1359	0.60	0/1833
7	H	0.46	0/1108	0.73	1/1498 (0.1%)
8	I	0.60	0/1749	0.66	0/2360
9	J	0.34	0/5004	0.55	0/6769
All	All	0.42	0/17436	0.60	3/23567 (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
4	D	0	1
6	F	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	197	LEU	CB-CG-CD1	8.39	125.27	111.00
5	E	36	LEU	CA-CB-CG	5.46	127.86	115.30
7	H	38	VAL	CB-CA-C	5.08	121.06	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	214	ILE	Peptide
6	F	134	ILE	Peptide

5.2 Too-close contacts [i](#)

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	1337	0	1334	103	0
1	G	1363	0	1352	110	0
2	B	1226	0	1217	161	0
3	C	1204	0	1213	104	0
4	D	1741	0	1768	164	0
5	E	1177	0	1151	101	0
6	F	1333	0	1338	142	0
7	H	1089	0	1099	175	0
8	I	1710	0	1682	193	0
9	J	4904	0	4942	340	0
All	All	17084	0	17096	1438	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 42.

The worst 5 of 1438 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)
8:I:510:THR:HG21	8:I:533:MET:CE	1.41	1.49
8:I:575:TYR:CA	8:I:579:GLY:HA3	1.38	1.47
8:I:575:TYR:HA	8:I:579:GLY:CA	1.42	1.45
8:I:514:MET:CG	8:I:526:VAL:HG11	1.53	1.38
8:I:537:GLU:OE1	8:I:545:LEU:HD11	1.24	1.35

There are no symmetry-related clashes.

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	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
1	G	167/178 (94%)	150 (90%)	17 (10%)	0	100	100
2	B	149/152 (98%)	124 (83%)	25 (17%)	0	100	100
3	C	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	D	217/219 (99%)	177 (82%)	40 (18%)	0	100	100
5	E	137/139 (99%)	122 (89%)	15 (11%)	0	100	100
6	F	162/194 (84%)	145 (90%)	17 (10%)	0	100	100
7	H	136/138 (99%)	114 (84%)	21 (15%)	1 (1%)	22	61
8	I	204/246 (83%)	183 (90%)	17 (8%)	4 (2%)	7	40
9	J	604/718 (84%)	544 (90%)	60 (10%)	0	100	100
All	All	2082/2307 (90%)	1829 (88%)	248 (12%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	435	TYR
8	I	520	ALA
8	I	559	PRO
7	H	43	CYS
8	I	536	GLU

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	149/159 (94%)	149 (100%)	0	100	100
1	G	151/159 (95%)	151 (100%)	0	100	100
2	B	136/137 (99%)	135 (99%)	1 (1%)	84	90
3	C	133/133 (100%)	133 (100%)	0	100	100
4	D	199/199 (100%)	198 (100%)	1 (0%)	88	93
5	E	129/129 (100%)	128 (99%)	1 (1%)	81	89
6	F	149/177 (84%)	148 (99%)	1 (1%)	84	90
7	H	120/120 (100%)	118 (98%)	2 (2%)	60	78
8	I	173/204 (85%)	89 (51%)	84 (49%)	0	0
9	J	526/621 (85%)	520 (99%)	6 (1%)	73	85
All	All	1865/2038 (92%)	1769 (95%)	96 (5%)	27	52

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	525	GLU
8	I	556	THR
8	I	528	LYS
8	I	540	LEU
8	I	562	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	33	HIS
9	J	129	ASN
9	J	119	GLN
9	J	318	HIS
5	E	38	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

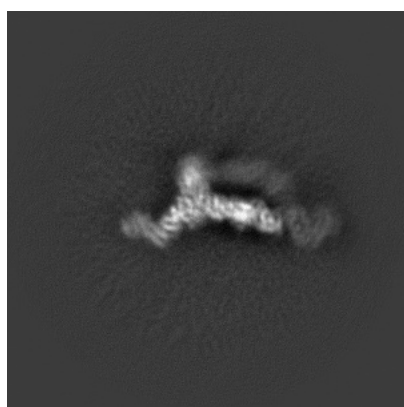
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12063. These allow visual inspection of the internal detail of the map and identification of artifacts.

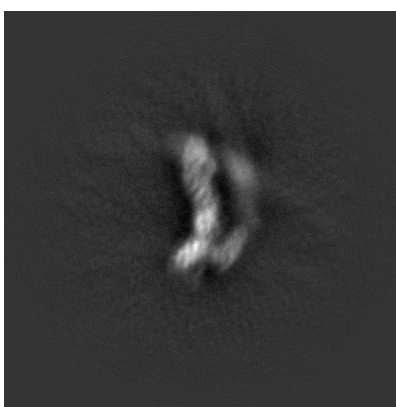
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

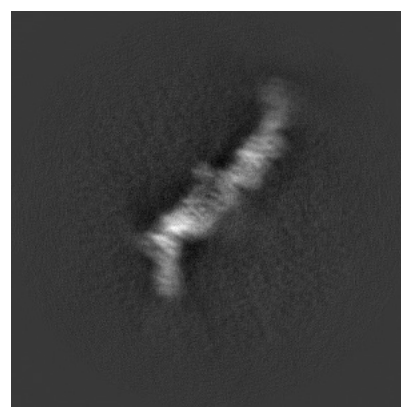
6.1.1 Primary map



X



Y

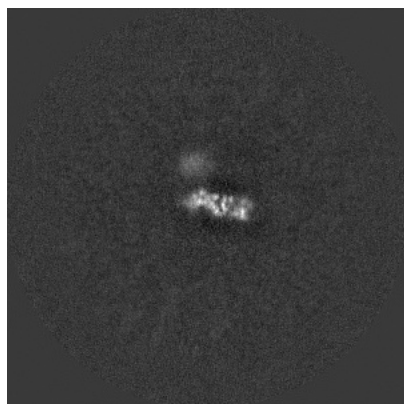


Z

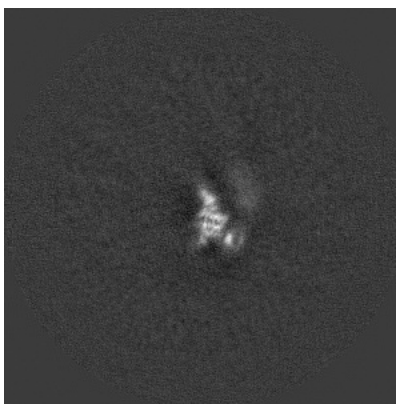
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

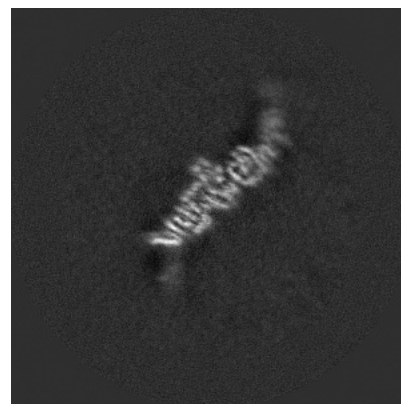
6.2.1 Primary map



X Index: 200



Y Index: 200

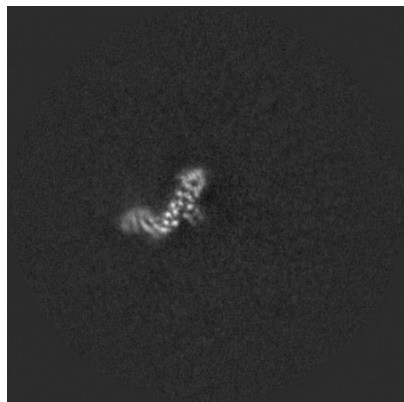


Z Index: 200

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

6.3 Largest variance slices [i](#)

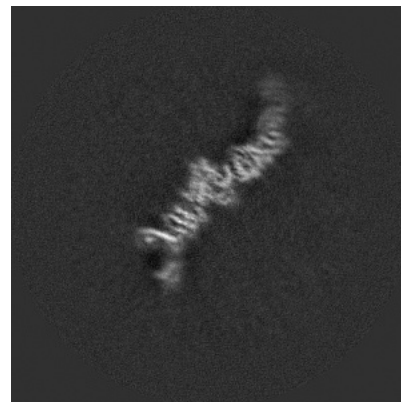
6.3.1 Primary map



X Index: 158



Y Index: 182



Z Index: 195

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_12063_msk_1.map [i](#)



X



Y

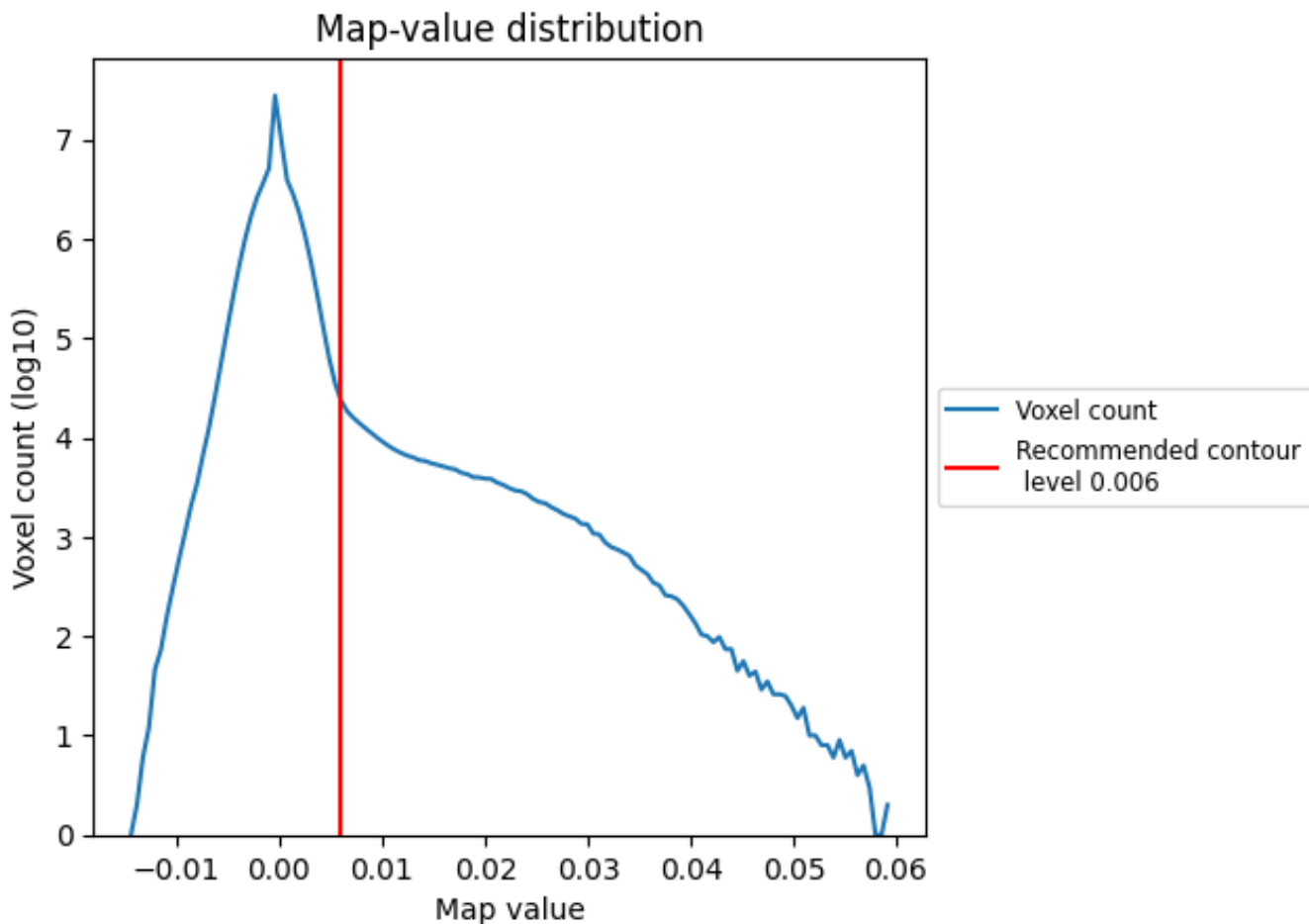


Z

7 Map analysis [i](#)

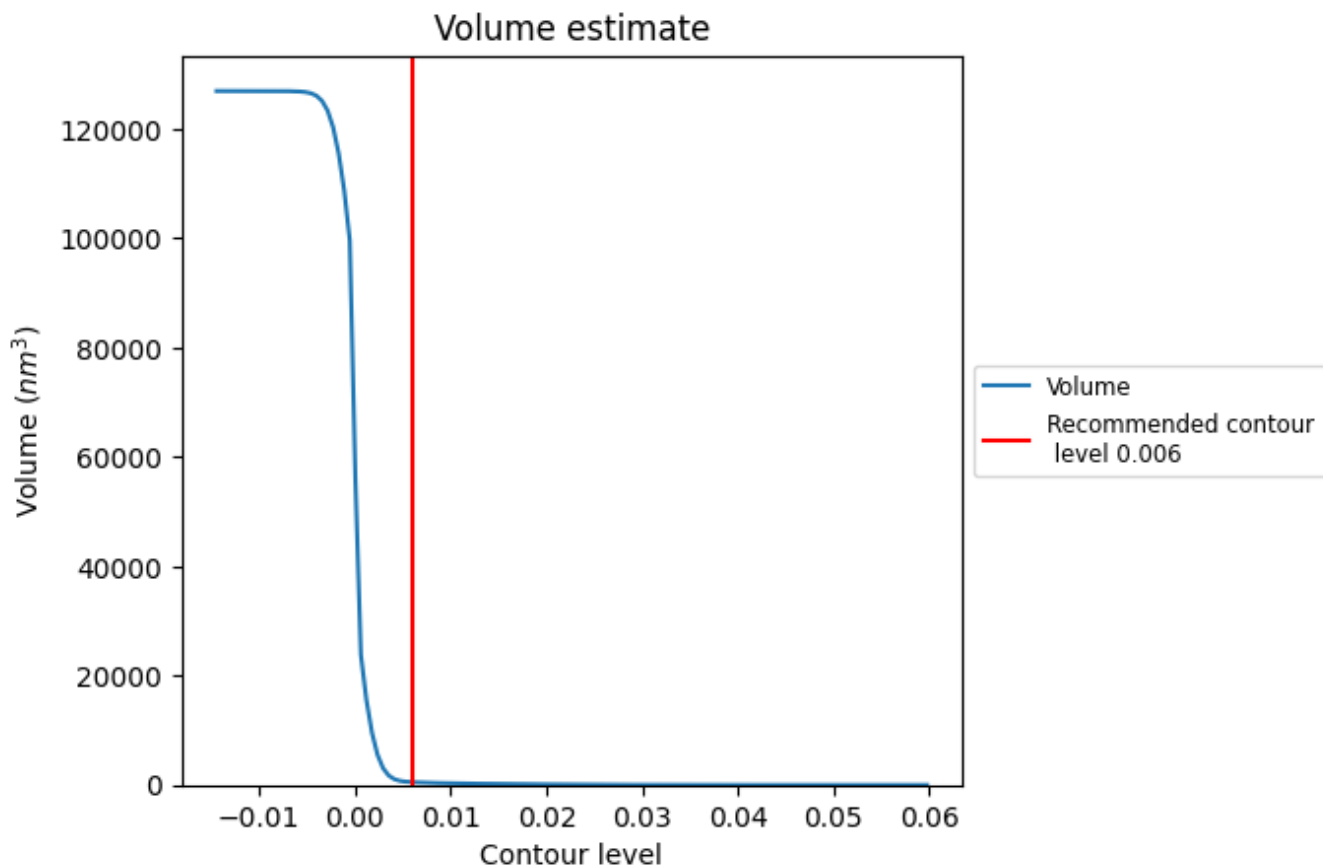
This section contains the results of statistical analysis of the map.

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.

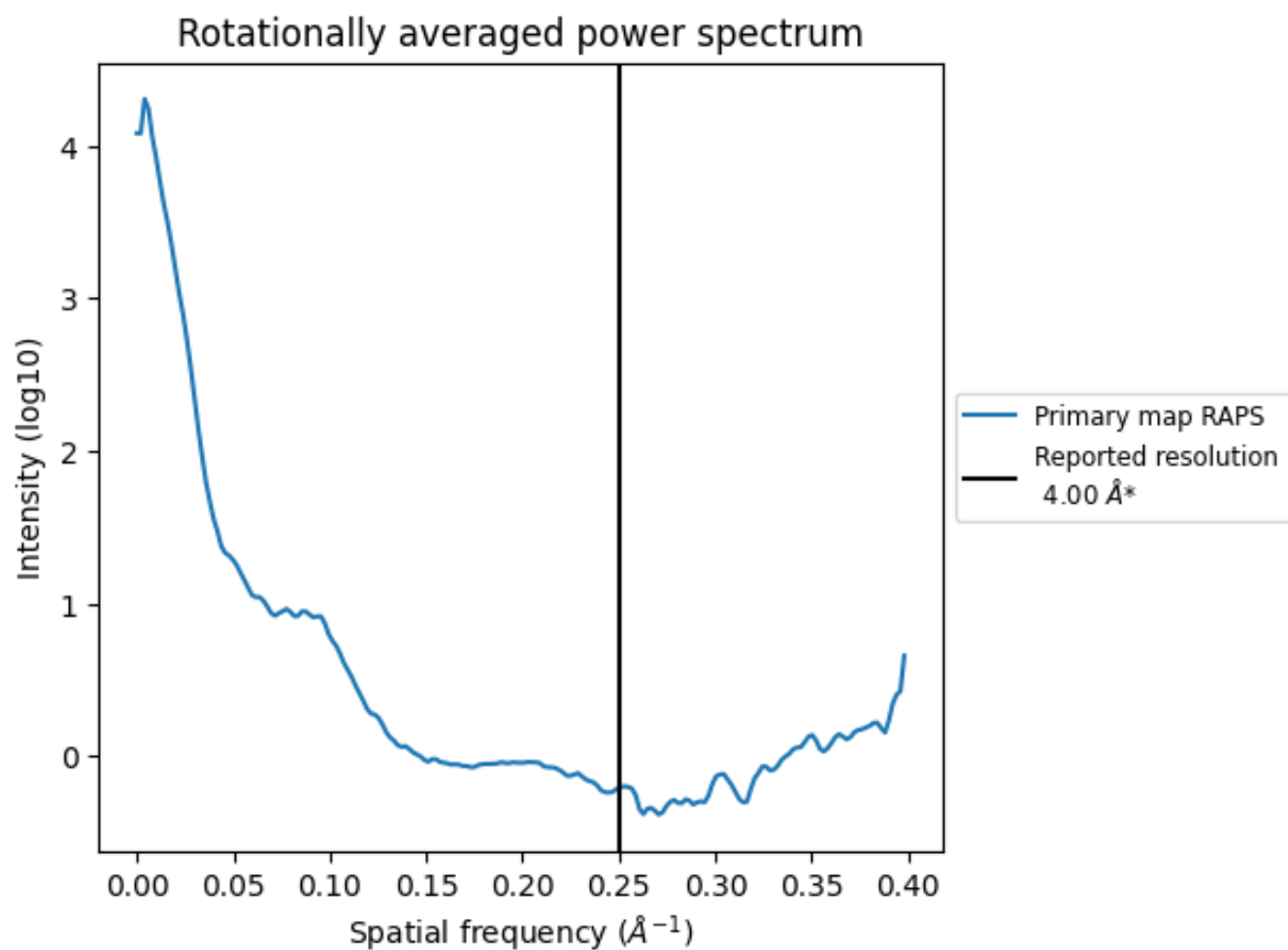
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 515 nm³; this corresponds to an approximate mass of 465 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 [\(i\)](#)

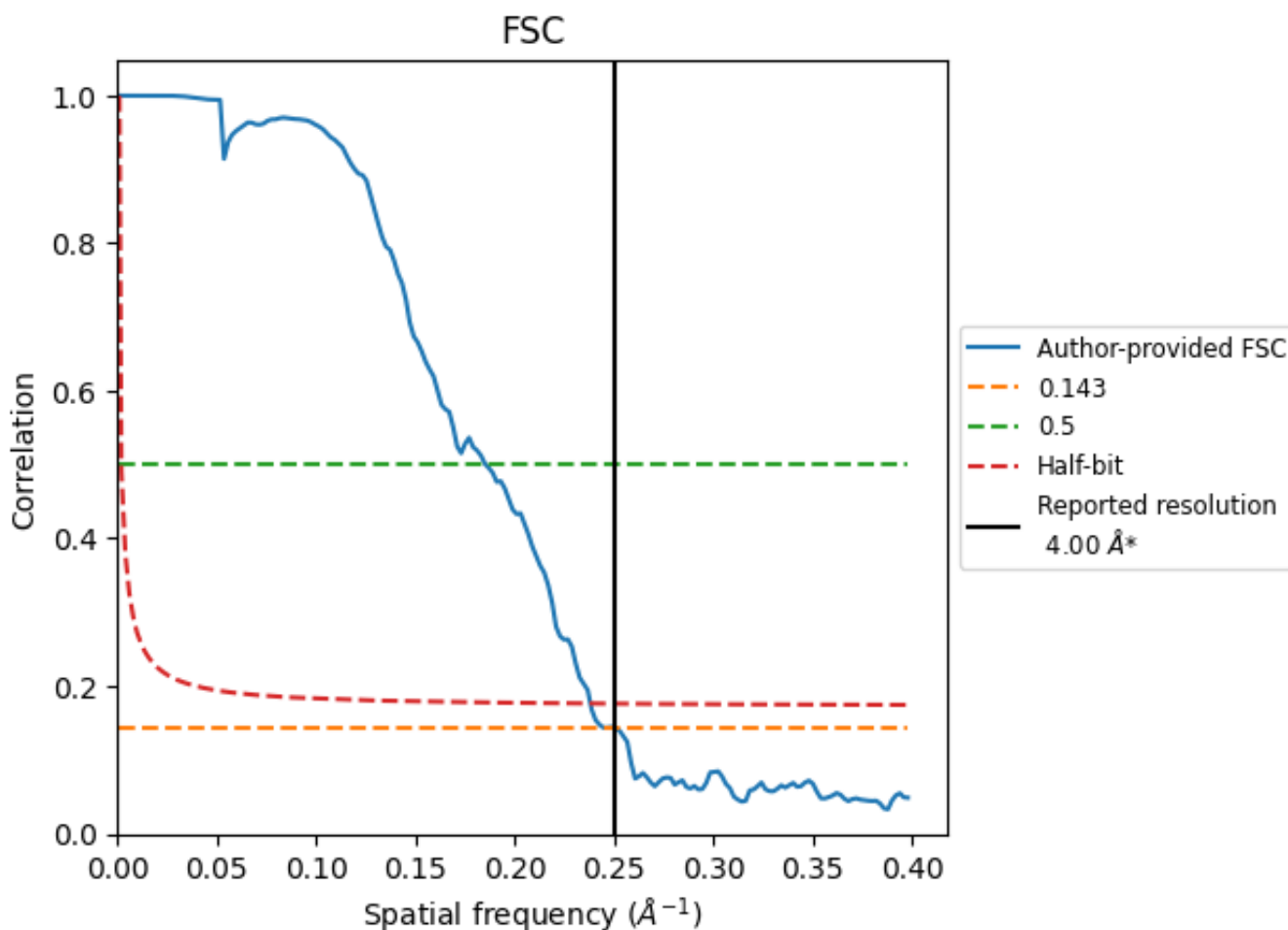


*Reported resolution corresponds to spatial frequency of 0.250\AA^{-1}

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

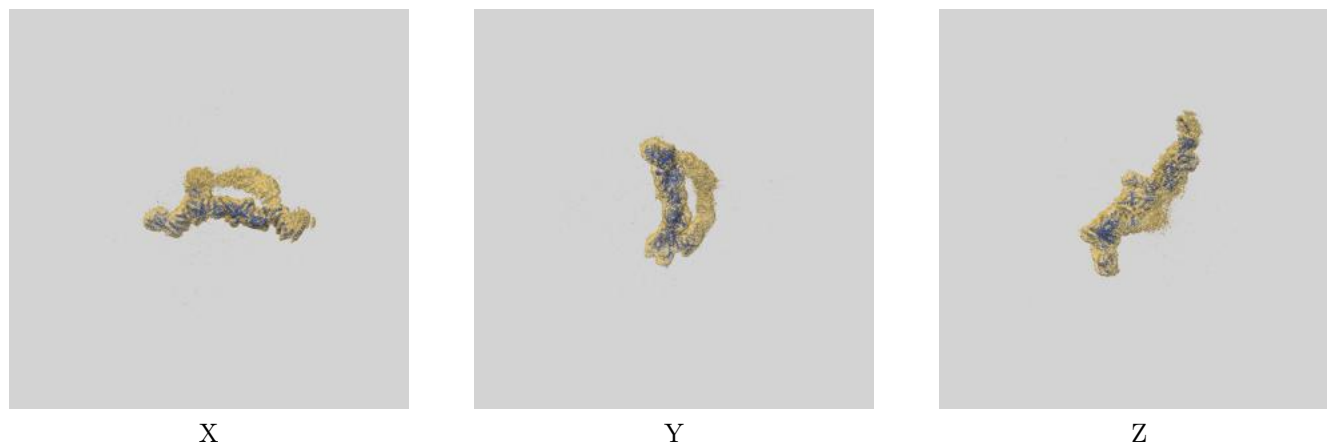
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	5.39	4.20
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

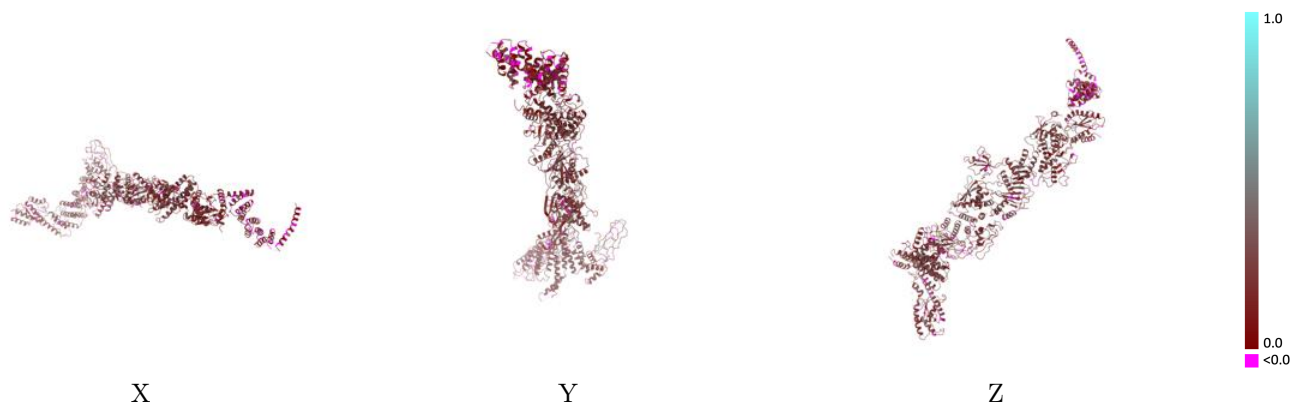
This section contains information regarding the fit between EMDB map EMD-12063 and PDB model 7B70. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



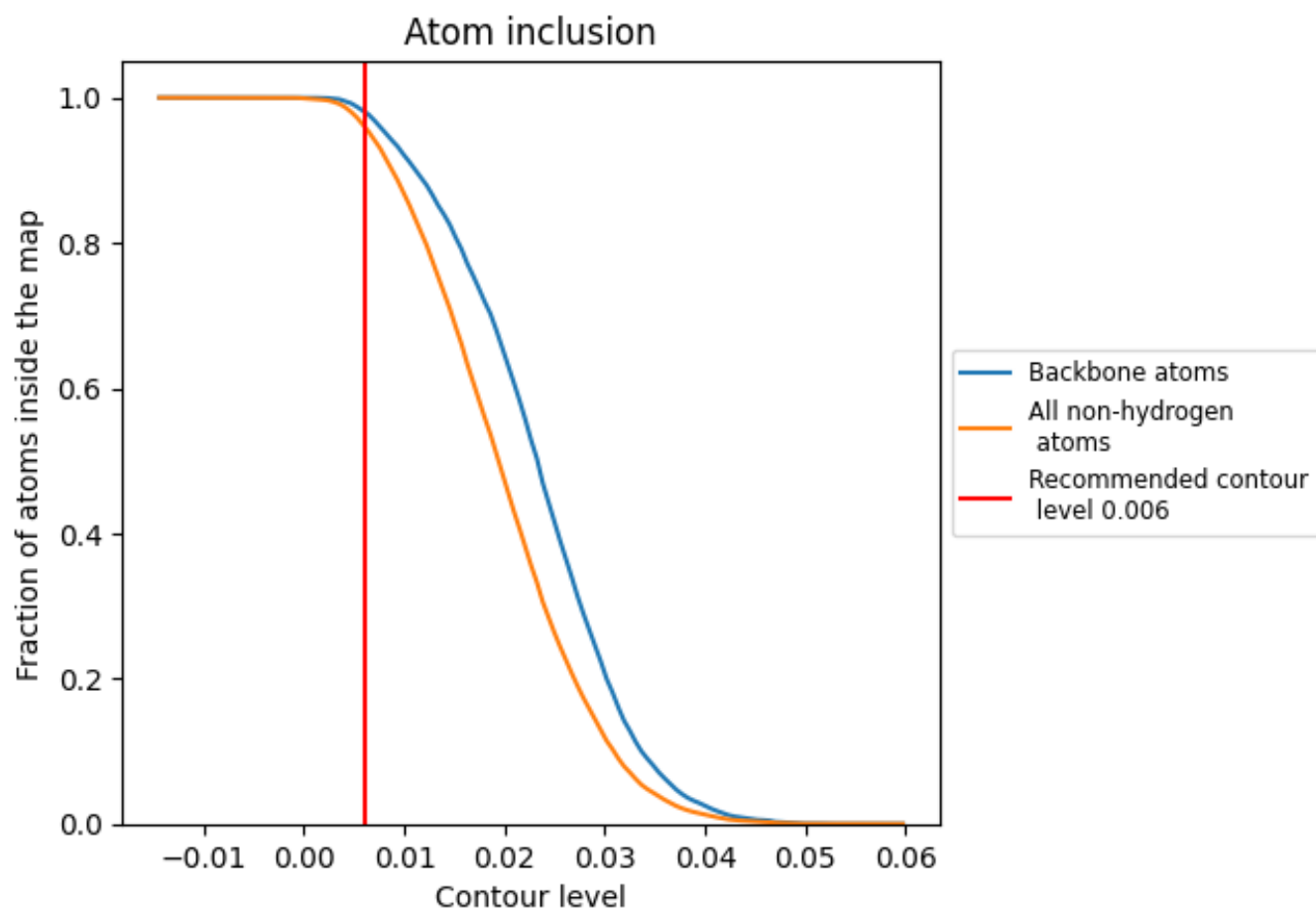
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9603	 0.1920
A	 0.9939	 0.2610
B	 0.9908	 0.1860
C	 0.9721	 0.2220
D	 0.9825	 0.2260
E	 0.9542	 0.1620
F	 0.9771	 0.2210
G	 0.9722	 0.1840
H	 0.9701	 0.2110
I	 0.7758	 0.0990
J	 0.9877	 0.1850

