



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2023 – 03:38 pm GMT

PDB ID : 8BF9
EMDB ID : EMD-16017
Title : Molecular view of ER membrane remodeling by the Sec61/TRAP translocon.
Authors : Karki, S.; Javanainen, M.; Tranter, D.; Rehan, S.; Huiskonen, J.; Happonen, L.; Paavilainen, V.
Deposited on : 2022-10-24
Resolution : 2.69 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:

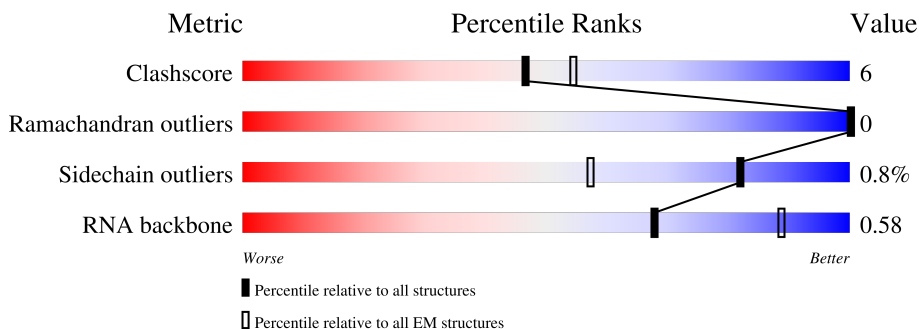
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.69 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.








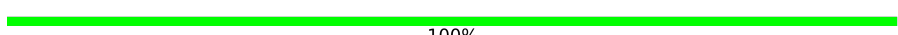






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	5	3662	29% 16% . 52%
2	8	156	38% 20% . 37%
3	A	353	41% . 55%
4	B	186	. 80% . 18%
5	D	173	77% 6% 16%
6	G	185	76% 9% . 15%
7	P	184	70% 12% 18%

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Mol	Chain	Length	Quality of chain
8	R	196	 39% 59%
9	U	128	 59% 6% 34%
10	X	156	 70% 6% 24%
11	Y	134	 83% 13% . .
12	C	475	 65% 15% 19%
13	b	29	 100%
14	d	125	 84% 16%
15	g	81	 69% 31%
16	h	123	 90% 10%
17	j	97	 74% 25%
18	k	70	 93% 7%
19	l	51	 92% 8%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 55482 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 RNA chain called RNA (1766).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	1766	37945	16901	6985	12293	1766	0	0

- Molecule 2 is a RNA chain called RNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	8	98	2098	935	380	685	98	0	0

- Molecule 3 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	158	1115	709	191	213	2	0	0

- Molecule 4 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	152	1026	644	184	196	2	0	0

- Molecule 5 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	145	943	573	171	197	2	0	0

- Molecule 6 is a protein called Translocon-associated protein subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	G	158	1055	655	195	205	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	151	1178	738	226	206	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	181	THR	MET	conflict	UNP W5Q9T9

- Molecule 8 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	R	81	599	366	128	102	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	HIS	conflict	UNP W5PLN0

- Molecule 9 is a protein called RL22 protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	U	84	630	404	112	113	1	0	0

- Molecule 10 is a protein called Ribosomal protein L23/L25 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	119	966	617	182	166	1	0	0

- Molecule 11 is a protein called RL26 protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Y	130	1051	656	214	178	3	0	0

- Molecule 12 is a protein called Sec61a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	386	Total	C	N	O	S	0	0
			2974	1960	478	517	19		

- Molecule 13 is a protein called Sec61b.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	b	29	Total	C	N	O	0	0
			146	87	29	30		

- Molecule 14 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	105	Total	C	N	O	S	0	0
			865	541	169	153	2		

- Molecule 15 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	56	Total	C	N	O	S	0	0
			443	294	77	70	2		

- Molecule 16 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	111	Total	C	N	O	S	0	0
			928	590	186	151	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	119	PHE	TYR	conflict	UNP A0A6P3TAC5

- Molecule 17 is a protein called Ribosomal protein L37.

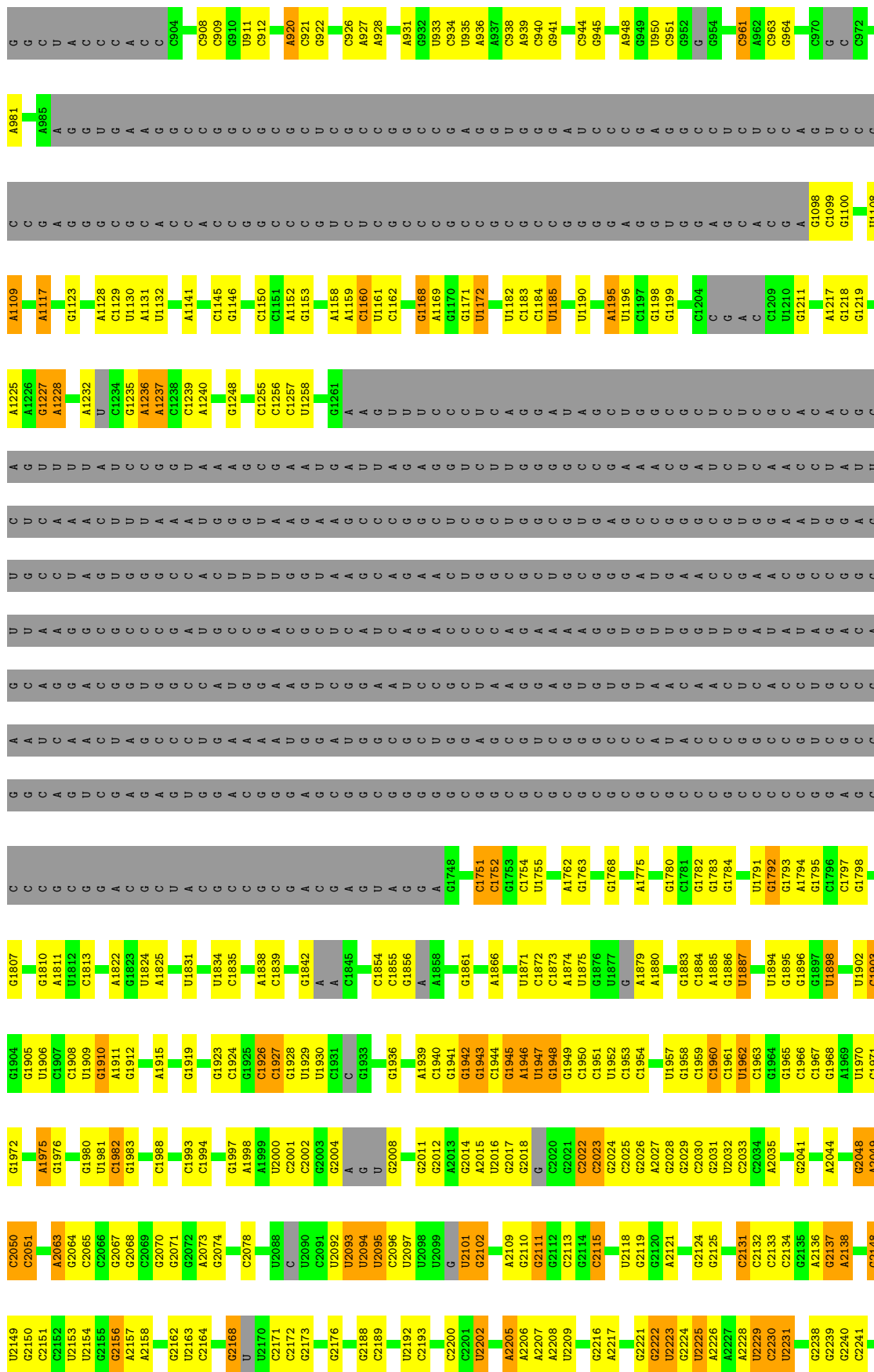
Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	73	Total	C	N	O	S	0	0
			575	357	126	88	4		

- Molecule 18 is a protein called Large ribosomal subunit protein eL38.

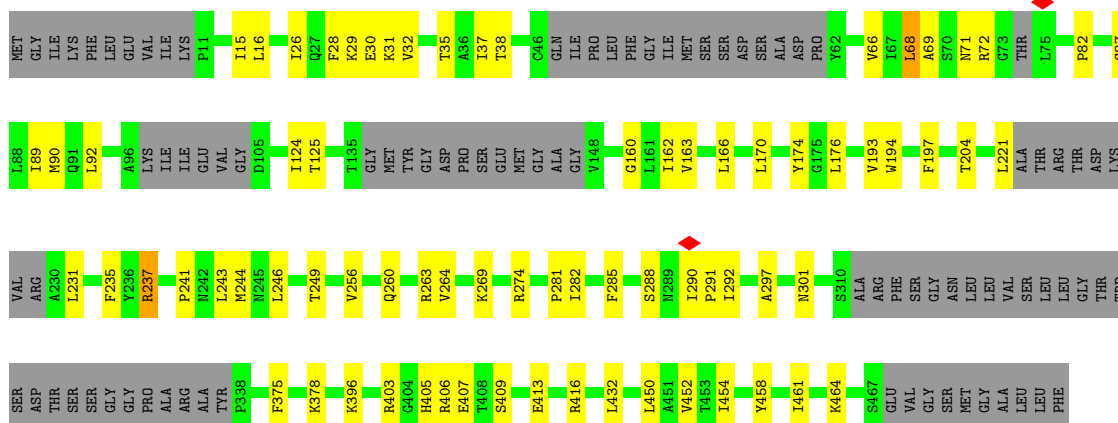
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	k	65	528	339	96	92	1	0	0

- Molecule 19 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	1	47	417	266	92	58	1	0	0



Chain C:  65% 15% 19%




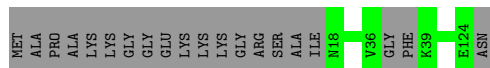
- Molecule 13: Sec61b

Chain b:  100%

There are no outlier residues recorded for this chain.

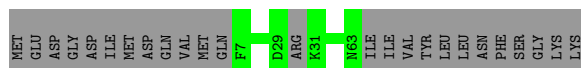
- Molecule 14: Large ribosomal subunit protein eL31

Chain d:  84% 16%



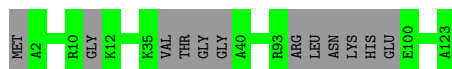
- Molecule 15: Protein transport protein Sec61 subunit gamma

Chain g:  69% 31%



- Molecule 16: Large ribosomal subunit protein uL29

Chain h:  90% 10%



- Molecule 17: Ribosomal protein L37

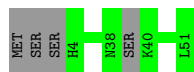
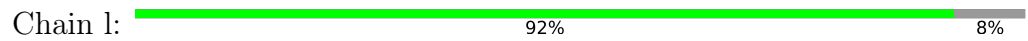
Chain j:  74% 25%



- Molecule 18: Large ribosomal subunit protein eL38



- Molecule 19: 60S ribosomal protein L39



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61177	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.312	Depositor
Minimum map value	-1.535	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.00275	Depositor
Map size (Å)	664.0, 664.0, 664.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	5	0.47	0/42441	0.82	8/66129 (0.0%)
2	8	0.47	0/2342	0.84	1/3641 (0.0%)
3	A	0.25	0/1140	0.45	0/1551
4	B	0.25	0/1051	0.48	0/1435
5	D	0.25	0/956	0.46	0/1309
6	G	0.23	0/1070	0.44	0/1459
7	P	0.34	0/1204	0.54	0/1621
8	R	0.35	0/602	0.61	0/801
9	U	0.33	0/634	0.53	0/846
10	X	0.29	0/983	0.51	0/1321
11	Y	0.28	0/1064	0.64	2/1414 (0.1%)
12	C	0.25	0/3034	0.46	1/4108 (0.0%)
14	d	0.27	0/878	0.56	0/1181
15	g	0.25	0/452	0.42	0/604
16	h	0.28	0/932	0.52	0/1225
17	j	0.32	0/585	0.61	0/770
18	k	0.29	0/533	0.52	0/707
19	l	0.27	0/426	0.55	0/561
All	All	0.43	0/60327	0.76	12/90683 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	51	LYS	CB-CA-C	-12.40	85.61	110.40
1	5	3179	C	O4'-C1'-N1	6.35	113.28	108.20
1	5	2275	A	OP2-P-O3'	6.15	118.74	105.20
1	5	2281	U	O4'-C1'-N1	6.15	113.12	108.20
11	Y	51	LYS	N-CA-C	-5.94	94.96	111.00

There are no chirality outliers.

There are no planarity outliers.

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	5	37945	0	19142	426	0
2	8	2098	0	1063	20	0
3	A	1115	0	918	8	0
4	B	1026	0	842	3	0
5	D	943	0	728	5	0
6	G	1055	0	869	10	0
7	P	1178	0	1154	15	0
8	R	599	0	613	3	0
9	U	630	0	582	5	0
10	X	966	0	1028	8	0
11	Y	1051	0	1105	11	0
12	C	2974	0	3054	43	0
13	b	146	0	32	0	0
14	d	865	0	892	0	0
15	g	443	0	460	0	0
16	h	928	0	1050	0	0
17	j	575	0	588	0	0
18	k	528	0	574	0	0
19	l	417	0	447	0	0
All	All	55482	0	35141	535	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 6.

The worst 5 of 535 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)
4:B:63:SER:O	4:B:112:THR:HB	1.74	0.87
5:D:101:THR:HA	5:D:136:VAL:O	1.77	0.84
1:5:2063:A:N6	1:5:2206:A:OP2	2.11	0.83
1:5:1927:C:H1'	1:5:2463:G:H22	1.45	0.81
1:5:2483:A:H62	1:5:2614:G:H21	1.29	0.80

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	
3	A	152/353 (43%)	143 (94%)	9 (6%)	0	100	100
4	B	148/186 (80%)	133 (90%)	15 (10%)	0	100	100
5	D	139/173 (80%)	132 (95%)	7 (5%)	0	100	100
6	G	156/185 (84%)	152 (97%)	4 (3%)	0	100	100
7	P	149/184 (81%)	144 (97%)	5 (3%)	0	100	100
8	R	75/196 (38%)	71 (95%)	4 (5%)	0	100	100
9	U	68/128 (53%)	63 (93%)	5 (7%)	0	100	100
10	X	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
11	Y	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
12	C	371/475 (78%)	356 (96%)	15 (4%)	0	100	100
14	d	101/125 (81%)	98 (97%)	3 (3%)	0	100	100
15	g	52/81 (64%)	52 (100%)	0	0	100	100
16	h	103/123 (84%)	100 (97%)	3 (3%)	0	100	100
17	j	68/97 (70%)	65 (96%)	3 (4%)	0	100	100
18	k	61/70 (87%)	61 (100%)	0	0	100	100
19	l	43/51 (84%)	40 (93%)	3 (7%)	0	100	100
All	All	1929/2717 (71%)	1848 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	92/312 (30%)	91 (99%)	1 (1%)	73	90
4	B	79/154 (51%)	79 (100%)	0	100	100
5	D	71/145 (49%)	70 (99%)	1 (1%)	67	86
6	G	81/164 (49%)	79 (98%)	2 (2%)	47	76
7	P	119/163 (73%)	119 (100%)	0	100	100
8	R	58/175 (33%)	58 (100%)	0	100	100
9	U	58/114 (51%)	58 (100%)	0	100	100
10	X	103/133 (77%)	103 (100%)	0	100	100
11	Y	112/124 (90%)	112 (100%)	0	100	100
12	C	319/396 (81%)	312 (98%)	7 (2%)	52	79
14	d	94/110 (86%)	94 (100%)	0	100	100
15	g	46/72 (64%)	46 (100%)	0	100	100
16	h	99/110 (90%)	99 (100%)	0	100	100
17	j	55/80 (69%)	54 (98%)	1 (2%)	59	83
18	k	58/65 (89%)	58 (100%)	0	100	100
19	l	42/48 (88%)	42 (100%)	0	100	100
All	All	1486/2365 (63%)	1474 (99%)	12 (1%)	82	93

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	C	263	ARG
12	C	281	PRO
17	j	64	MET
12	C	290	ILE
6	G	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
11	Y	24	HIS
14	d	18	ASN
16	h	108	GLN
15	g	63	ASN
10	X	57	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	1724/3662 (47%)	262 (15%)	15 (0%)
2	8	93/156 (59%)	18 (19%)	0
All	All	1817/3818 (47%)	280 (15%)	15 (0%)

5 of 280 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	42	A
1	5	58	G
1	5	59	A
1	5	98	A
1	5	108	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	2101	U
1	5	2746	U
1	5	2137	G
1	5	3198	U
1	5	2405	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

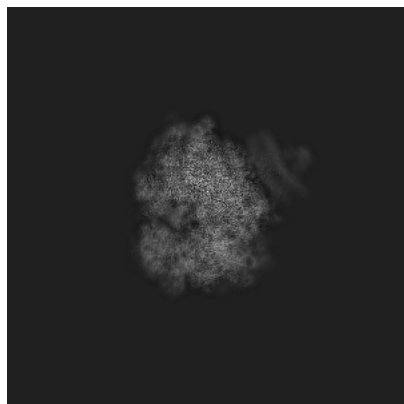
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16017. These allow visual inspection of the internal detail of the map and identification of artifacts.

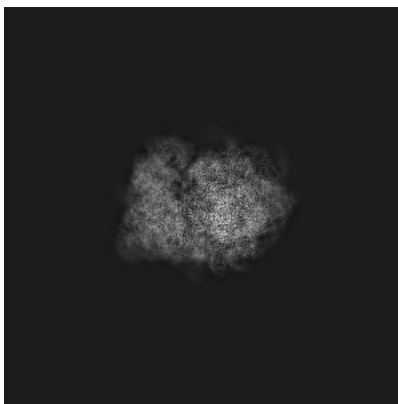
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

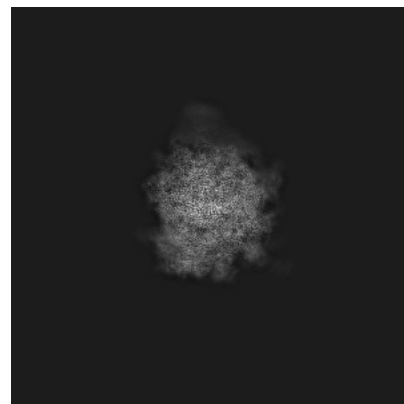
6.1.1 Primary map



X

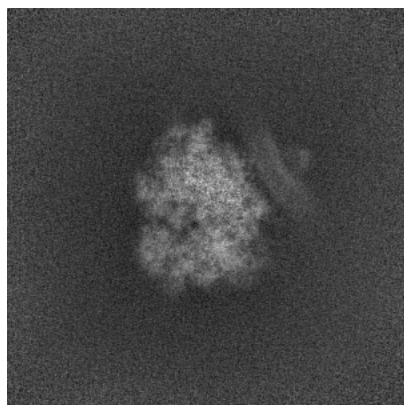


Y

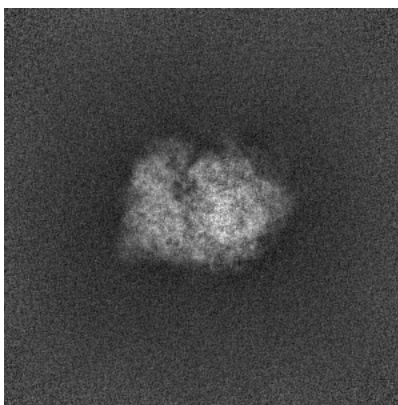


Z

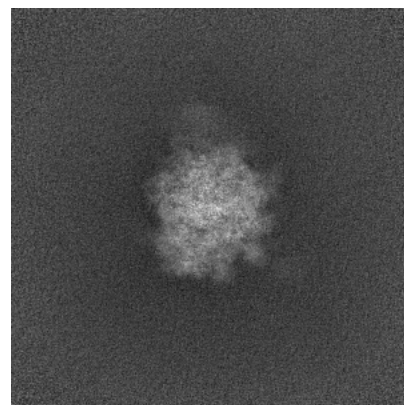
6.1.2 Raw map



X



Y

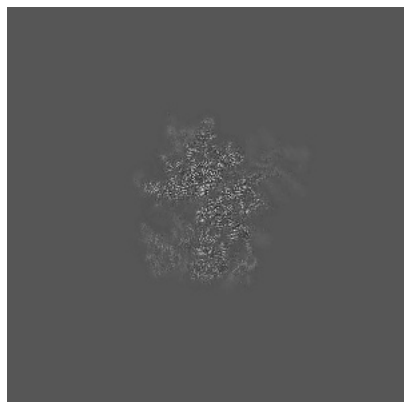


Z

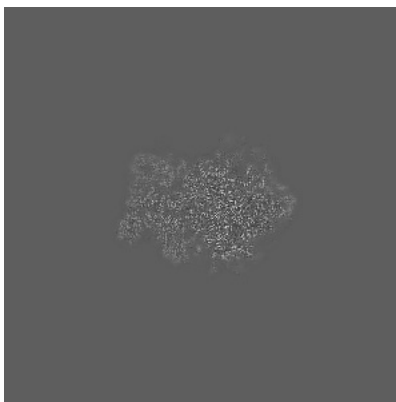
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

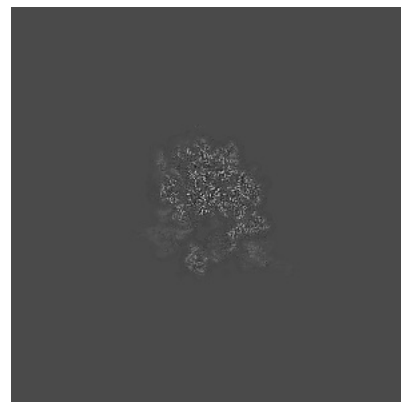
6.2.1 Primary map



X Index: 400

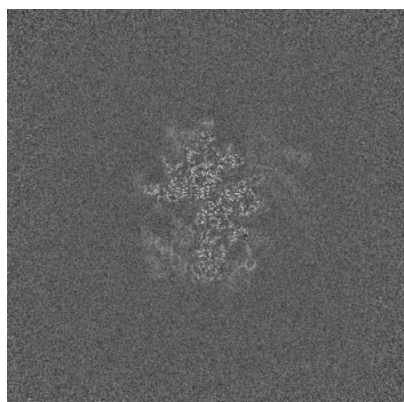


Y Index: 400

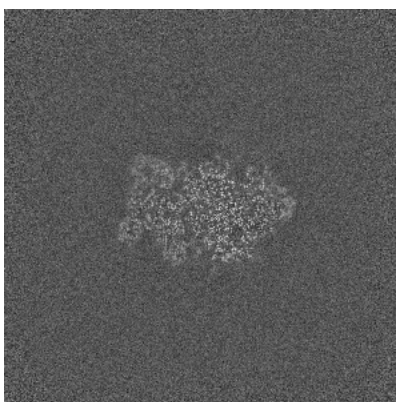


Z Index: 400

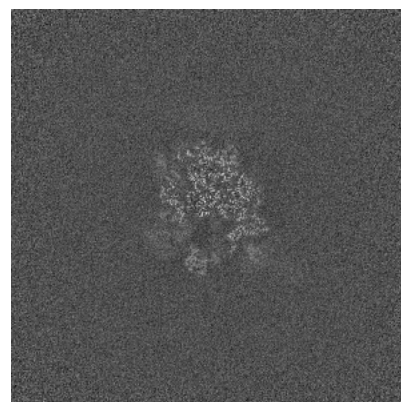
6.2.2 Raw map



X Index: 400



Y Index: 400

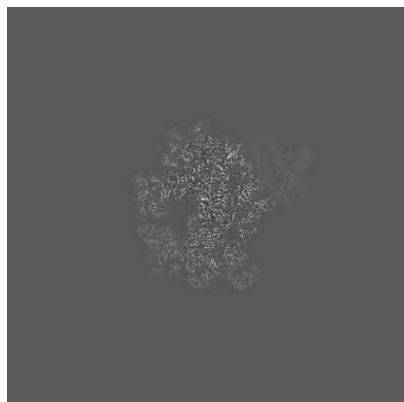


Z Index: 400

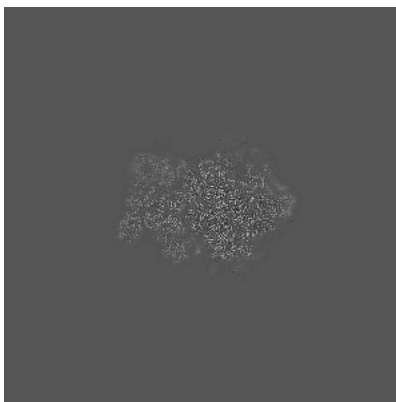
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

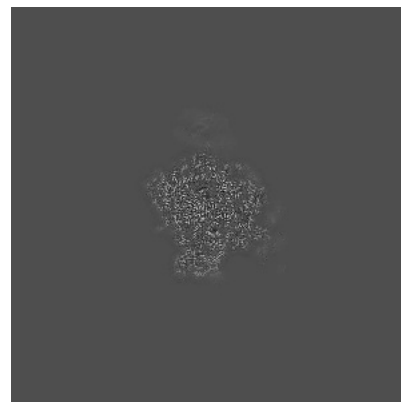
6.3.1 Primary map



X Index: 377

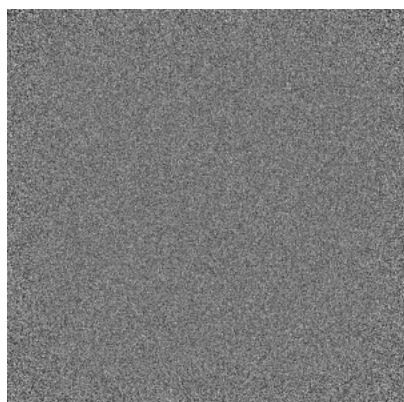


Y Index: 401

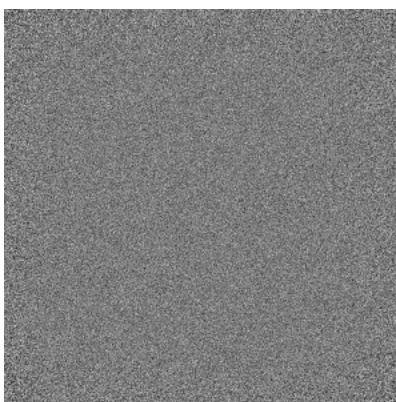


Z Index: 445

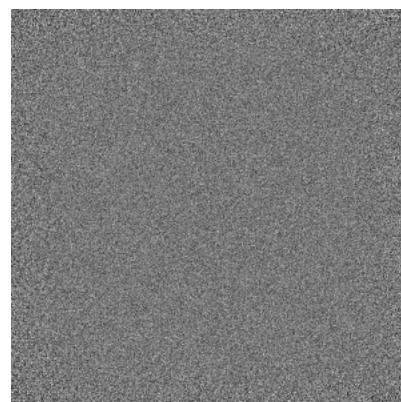
6.3.2 Raw map



X Index: 0



Y Index: 0

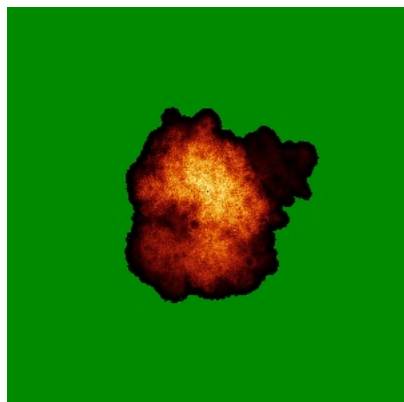


Z Index: 0

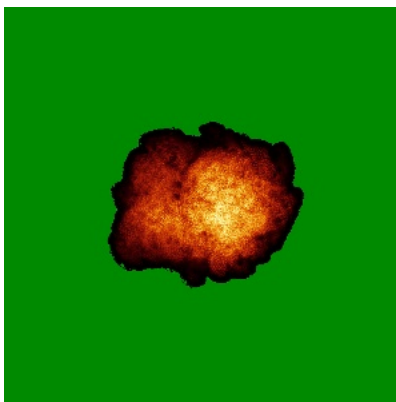
The images above show the largest variance slices of the map in three orthogonal directions.

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

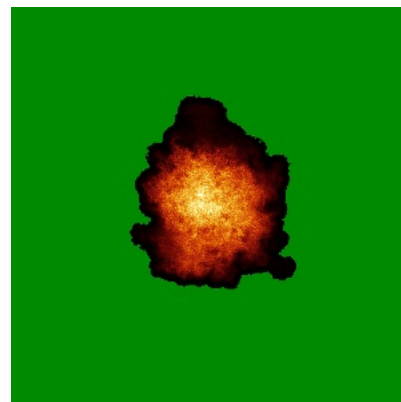
6.4.1 Primary map



X

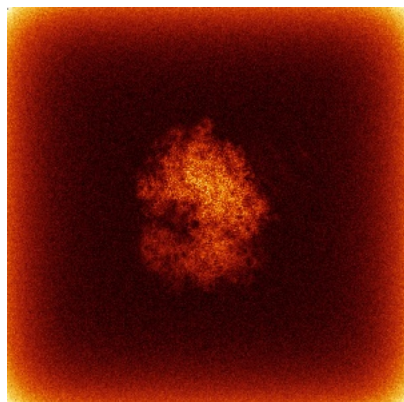


Y

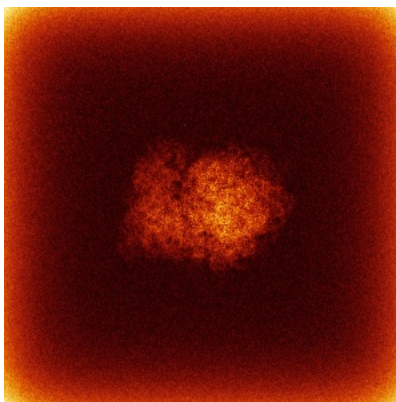


Z

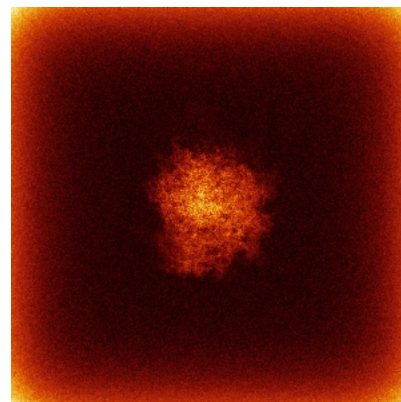
6.4.2 Raw map



X



Y

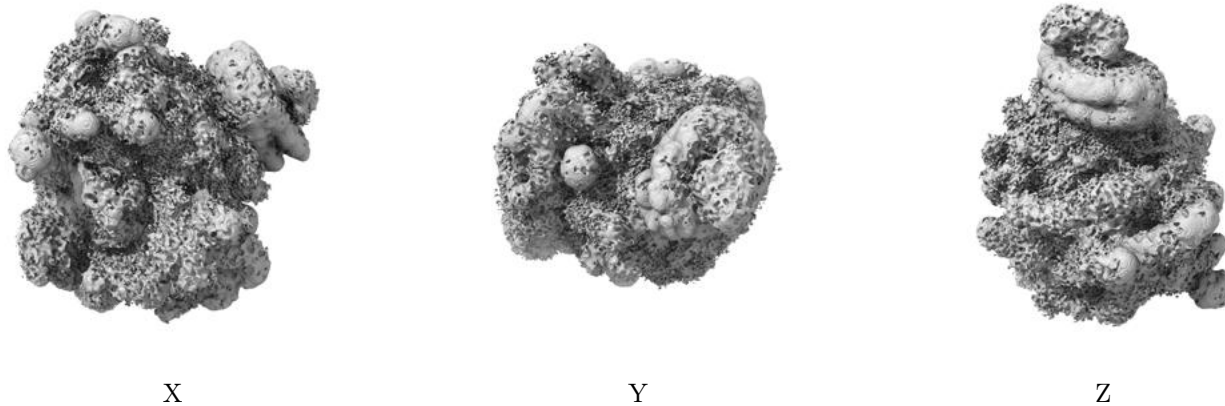


Z

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

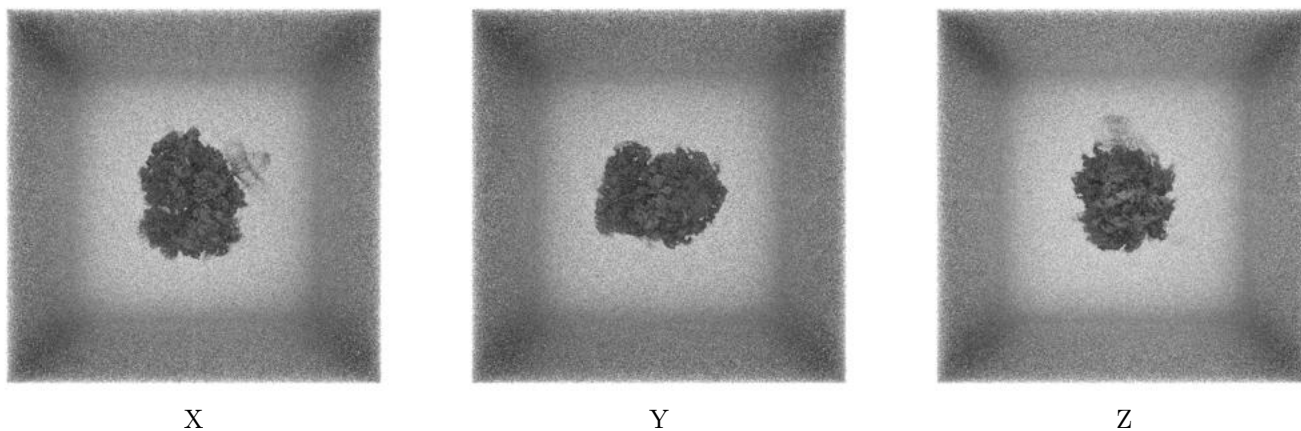
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

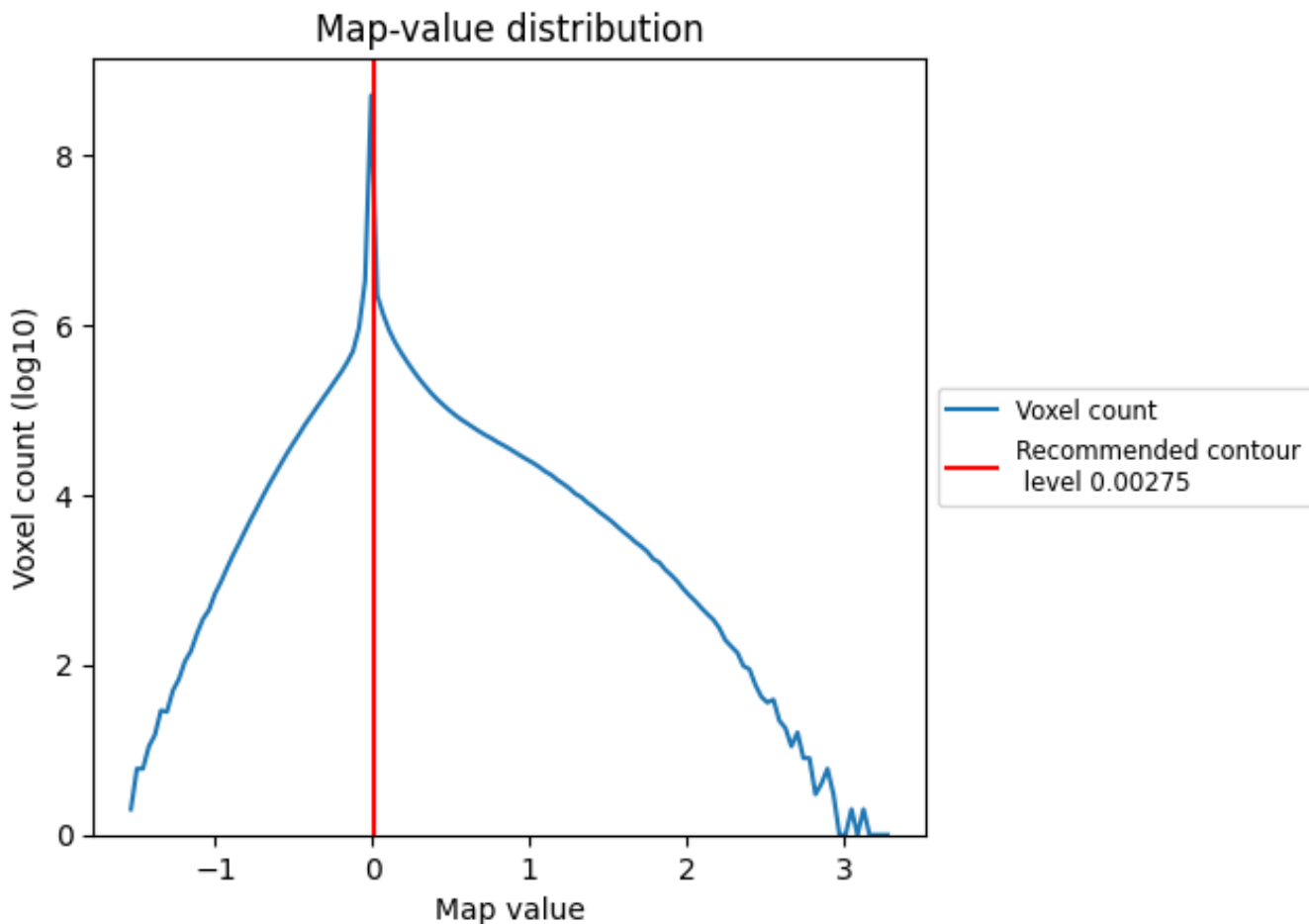
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

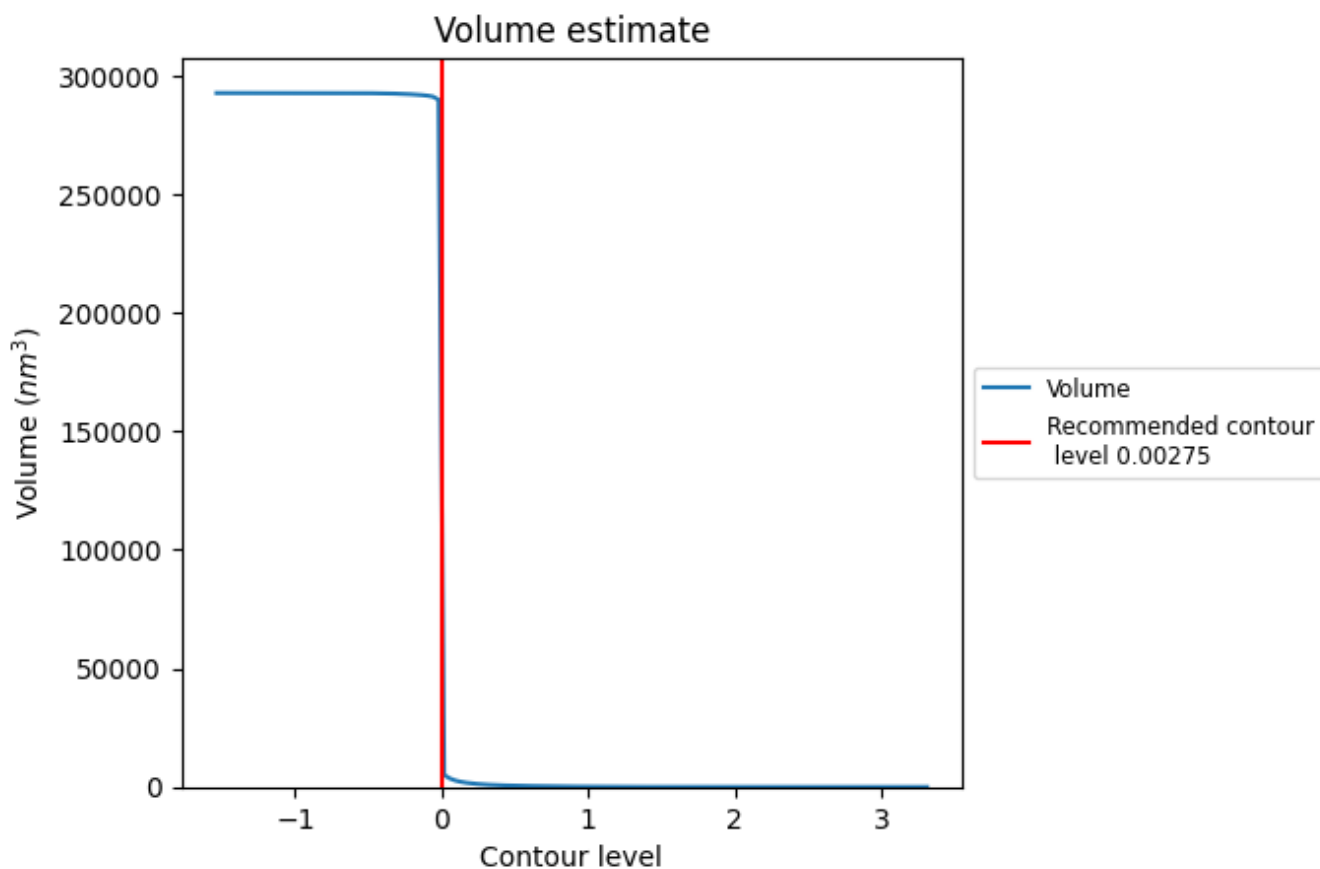
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

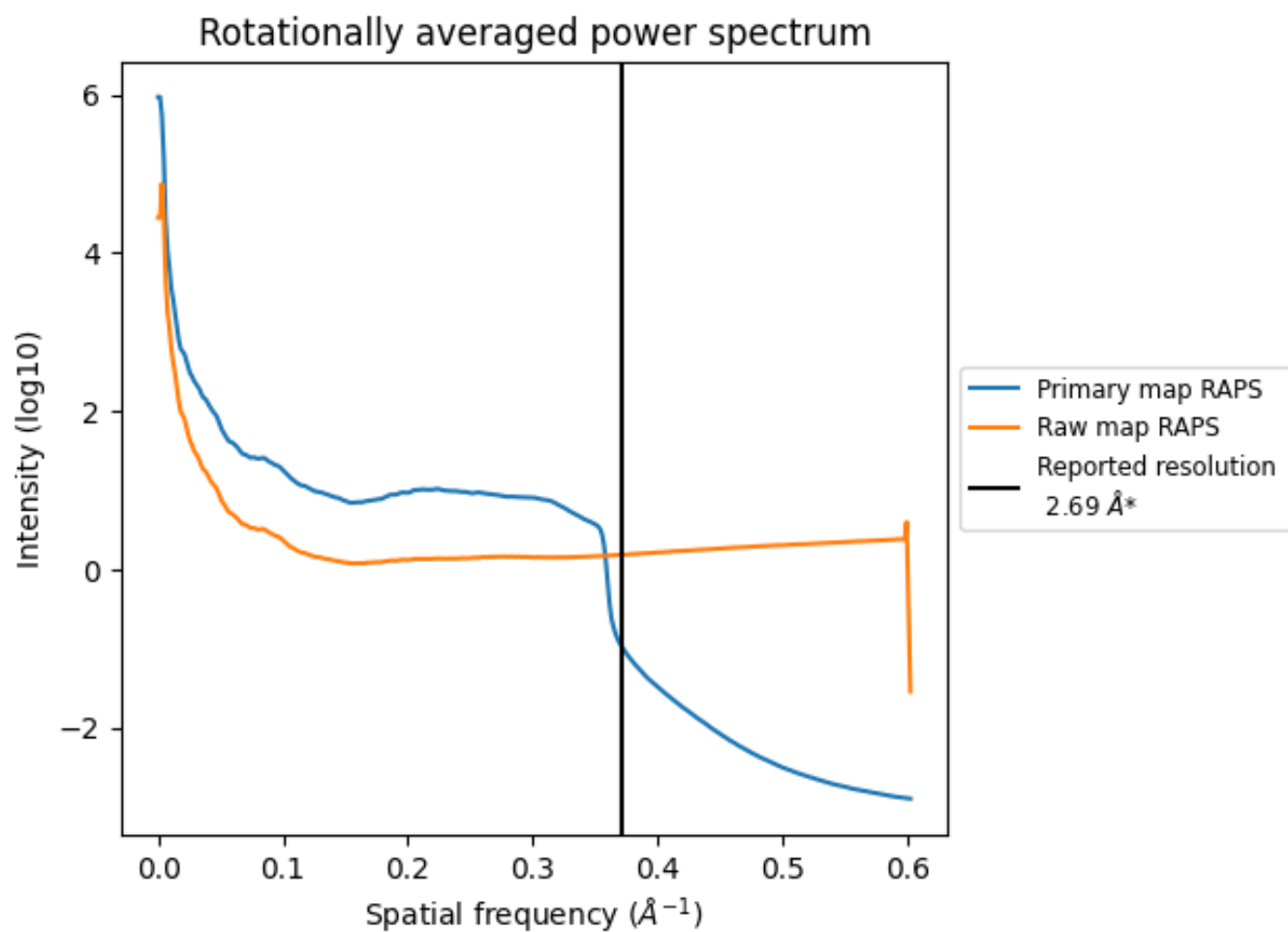
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 119533 nm³; this corresponds to an approximate mass of 107977 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

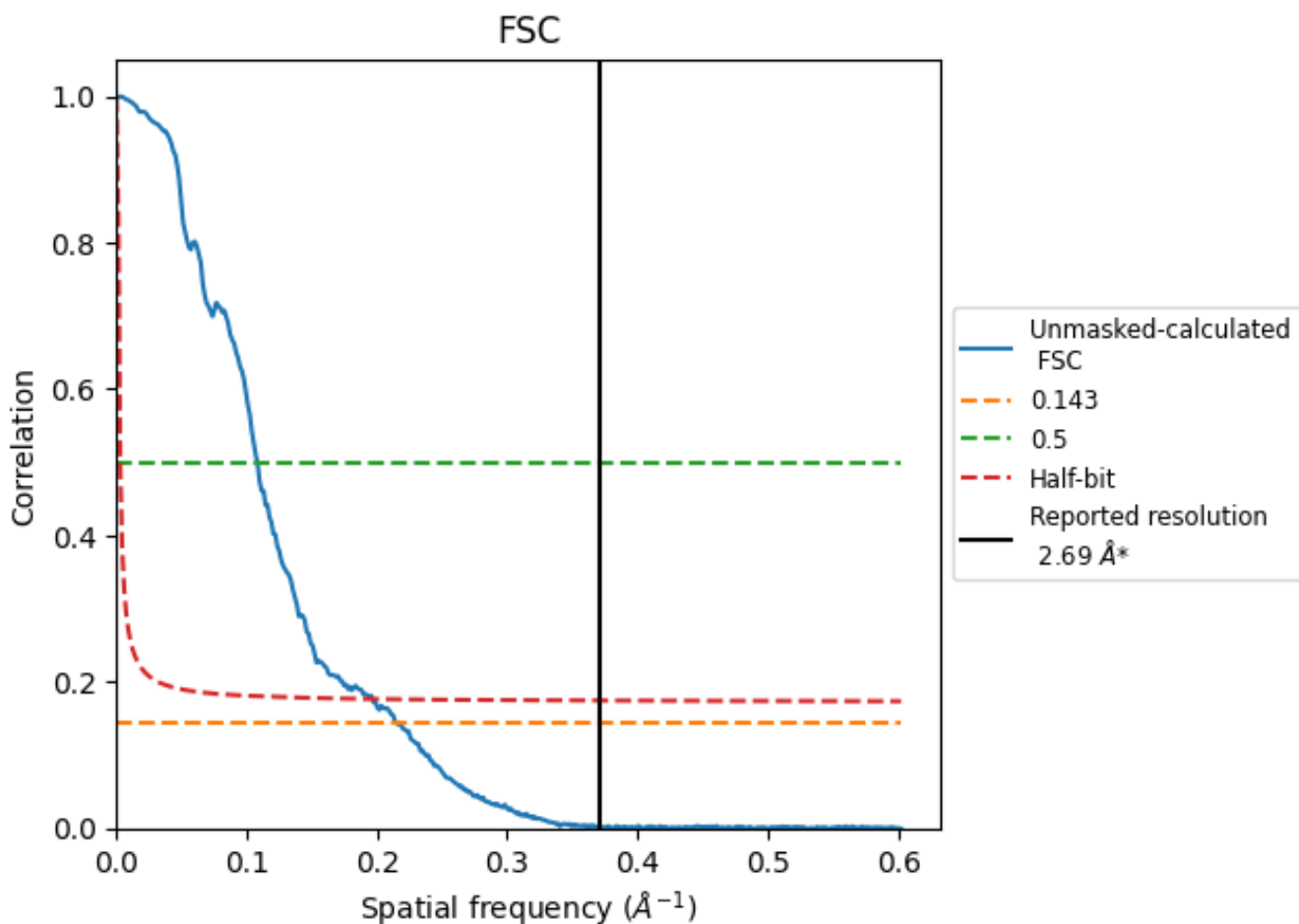


*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

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 0.372 Å⁻¹

8.2 Resolution estimates [i](#)

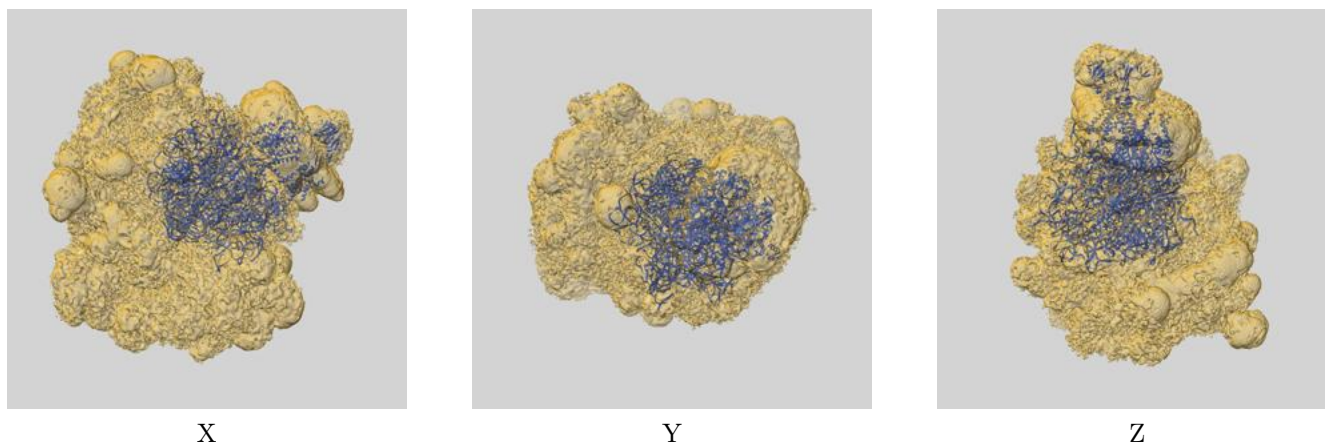
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.65	9.25	5.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.65 differs from the reported value 2.69 by more than 10 %

9 Map-model fit [i](#)

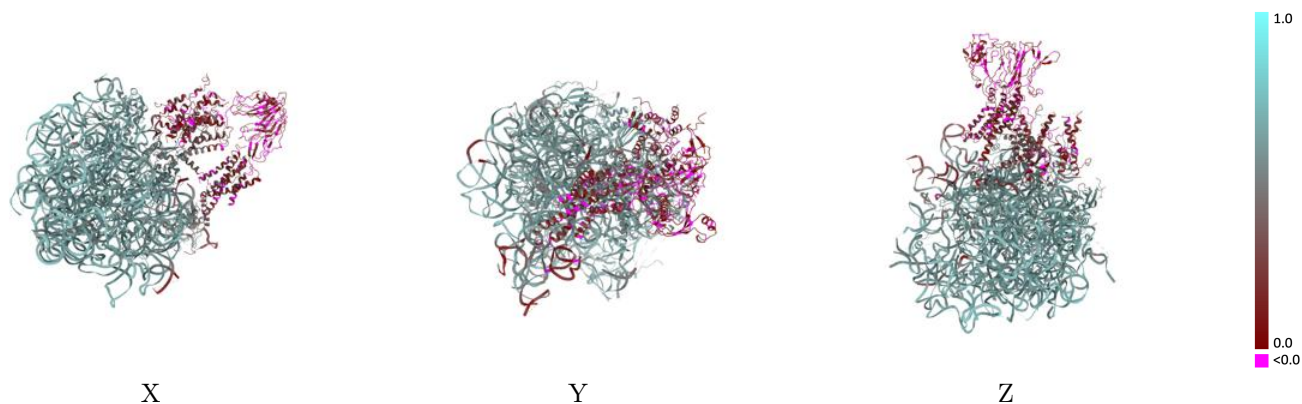
This section contains information regarding the fit between EMDB map EMD-16017 and PDB model 8BF9. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



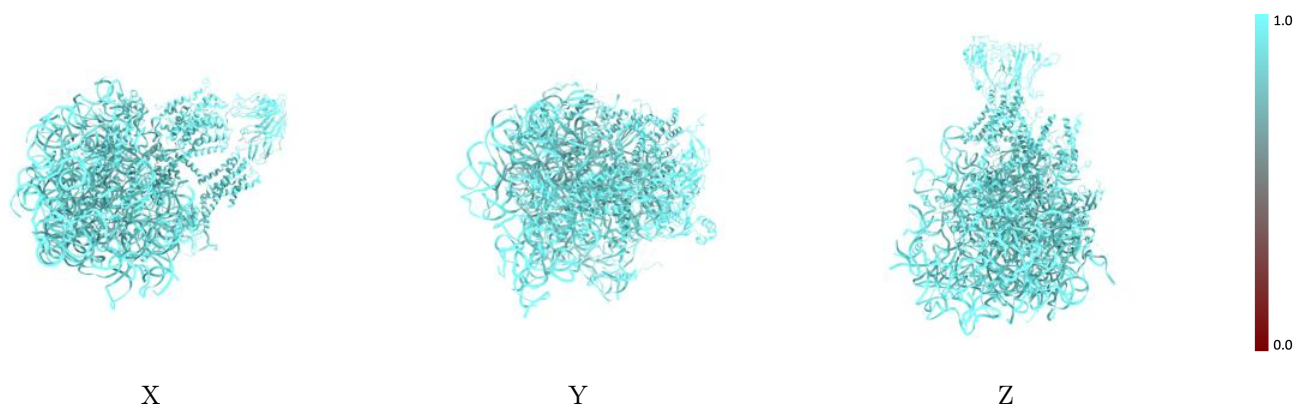
The images above show the 3D surface view of the map at the recommended contour level 0.00275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



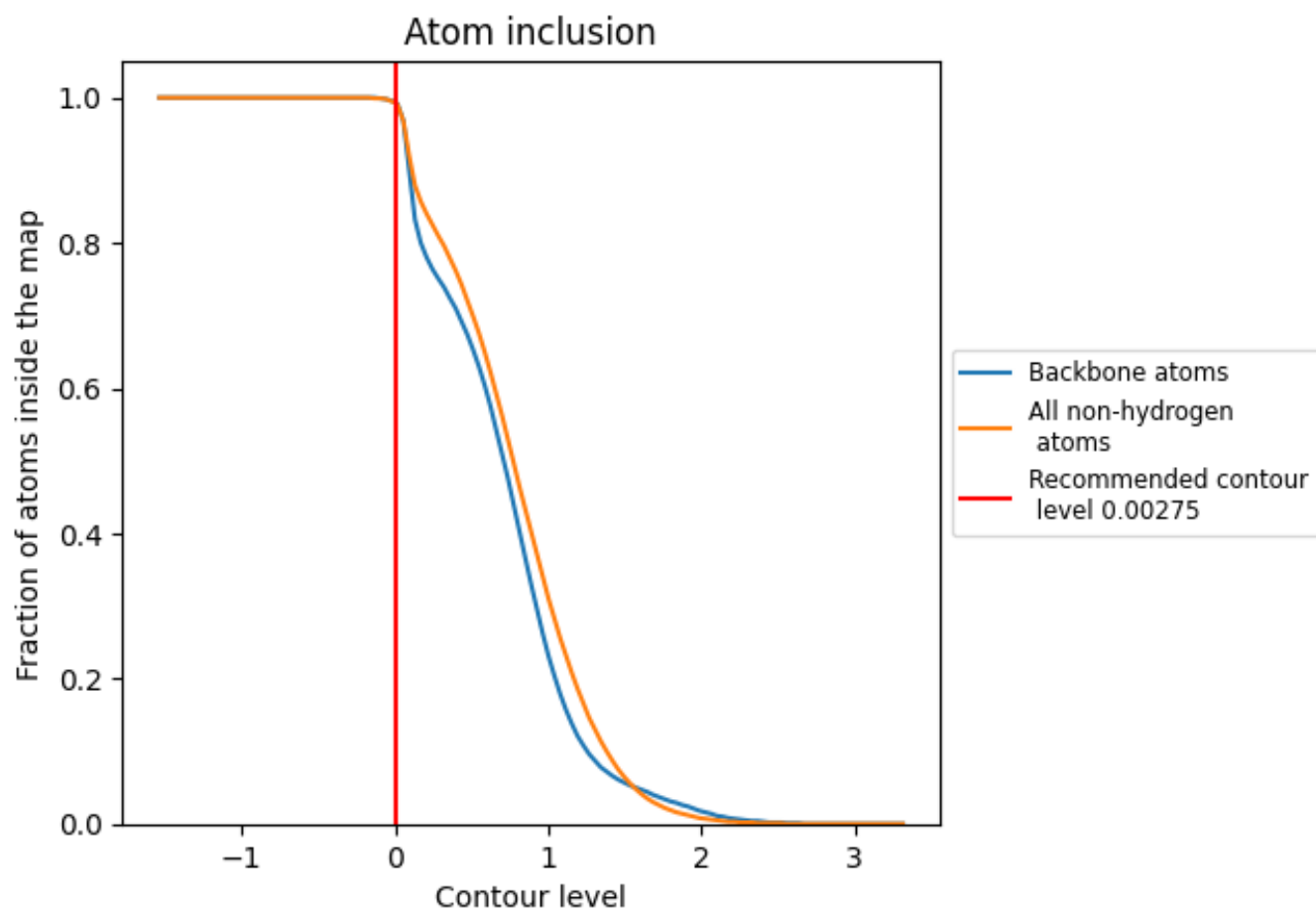
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00275).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9930	 0.5520
5	 0.9970	 0.6150
8	 0.9930	 0.5860
A	 0.9870	 0.0820
B	 0.9590	 0.0770
C	 0.9660	 0.2610
D	 0.9850	 0.0700
G	 0.9880	 0.1480
P	 0.9970	 0.6430
R	 0.9980	 0.6240
U	 0.9980	 0.5120
X	 0.9970	 0.6190
Y	 0.9940	 0.6180
b	 0.9930	 0.2180
d	 0.9950	 0.5970
g	 0.9590	 0.2830
h	 0.9940	 0.6030
j	 0.9980	 0.6520
k	 1.0000	 0.5650
l	 0.9950	 0.6320

