wwPDB EM Validation Summary Report

Apr 11, 2024 – 04:28 pm BST

PDB ID	:	8QYL
EMDB ID	:	EMD-18757
Title	:	Human 20S proteasome assembly intermediate structure 2
Authors	:	Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.; Walsh Jr, R.M.; Goodall, E.A.
Deposited on	:	2023-10-26
Resolution	:	2.67 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:

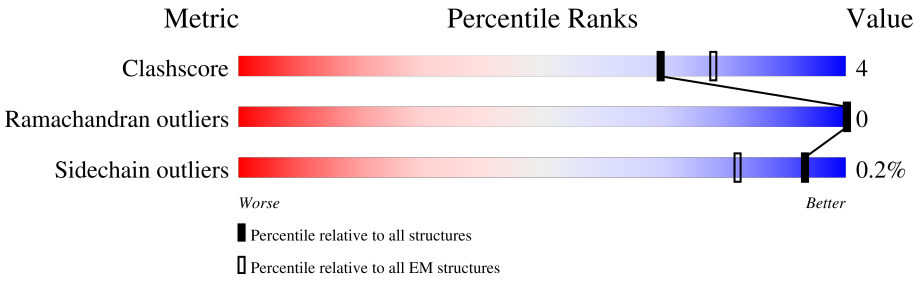
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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 <=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	234	92% 6%
2	B	261	90% 7%
3	C	248	90% 6%
4	D	242	77% 17% 5%
5	E	264	86% 6% 8%
6	F	255	82% 12% 6%
7	G	246	91% 8%
8	H	141	62% 6% 31%

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Mol	Chain	Length	Quality of chain
9	I	288	6% 81% 11% 7%
10	J	265	82% 12% 6%
11	K	332	61% 8% 31%
12	L	205	81% 7% 12%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 20997 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	231	1791	1147	305	333	6	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	244	1916	1213	328	365	10	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	240	1880	1180	334	361	5	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	230	1760	1109	291	348	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ACE	-	acetylation	UNP P28066

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	242	1898	1190	342	354	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	acetylation	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	240	Total	C	N	O	S	0	0
			1876	1189	320	356	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	243	Total	C	N	O	S	0	0
			1892	1200	316	363	13		

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	97	Total	C	N	O	S	0	0
			777	492	130	151	4		

- Molecule 9 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	267	Total	C	N	O	S	0	0
			2128	1363	355	392	18		

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	250	Total	C	N	O	S	0	0
			1956	1261	321	360	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP Q969U7

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	229	Total	C	N	O	S	0	0
			1701	1081	292	318	10		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	238O	GLU	-	expression tag	UNP Q99436
K	238P	ASP	-	expression tag	UNP Q99436
K	238Q	LEU	-	expression tag	UNP Q99436
K	238R	TYR	-	expression tag	UNP Q99436
K	238S	PHE	-	expression tag	UNP Q99436
K	238T	GLN	-	expression tag	UNP Q99436
K	238U	SER	-	expression tag	UNP Q99436
K	238V	VAL	-	expression tag	UNP Q99436
K	238W	ASP	-	expression tag	UNP Q99436
K	238X	SER	-	expression tag	UNP Q99436
K	238Y	ALA	-	expression tag	UNP Q99436
K	238Z	TRP	-	expression tag	UNP Q99436
K	239A	SER	-	expression tag	UNP Q99436
K	239B	HIS	-	expression tag	UNP Q99436
K	239C	PRO	-	expression tag	UNP Q99436
K	239D	GLN	-	expression tag	UNP Q99436
K	239E	PHE	-	expression tag	UNP Q99436
K	239F	GLU	-	expression tag	UNP Q99436
K	239G	LYS	-	expression tag	UNP Q99436
K	239H	GLY	-	expression tag	UNP Q99436
K	239I	GLY	-	expression tag	UNP Q99436
K	239J	GLY	-	expression tag	UNP Q99436
K	239K	SER	-	expression tag	UNP Q99436
K	239L	GLY	-	expression tag	UNP Q99436
K	239M	GLY	-	expression tag	UNP Q99436
K	239N	GLY	-	expression tag	UNP Q99436
K	239O	SER	-	expression tag	UNP Q99436
K	239P	GLY	-	expression tag	UNP Q99436
K	239Q	GLY	-	expression tag	UNP Q99436
K	239R	SER	-	expression tag	UNP Q99436
K	239S	ALA	-	expression tag	UNP Q99436
K	239T	TRP	-	expression tag	UNP Q99436
K	239U	SER	-	expression tag	UNP Q99436
K	239V	HIS	-	expression tag	UNP Q99436
K	239W	PRO	-	expression tag	UNP Q99436
K	239X	GLN	-	expression tag	UNP Q99436
K	239Y	PHE	-	expression tag	UNP Q99436
K	239Z	GLU	-	expression tag	UNP Q99436
K	240A	LYS	-	expression tag	UNP Q99436
K	247	UNK	-	expression tag	UNP Q99436
K	248	UNK	-	expression tag	UNP Q99436
K	249	UNK	-	expression tag	UNP Q99436

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Chain	Residue	Modelled	Actual	Comment	Reference
K	250	UNK	-	expression tag	UNP Q99436
K	251	UNK	-	expression tag	UNP Q99436
K	252	UNK	-	expression tag	UNP Q99436
K	253	UNK	-	expression tag	UNP Q99436
K	254	UNK	-	expression tag	UNP Q99436
K	255	UNK	-	expression tag	UNP Q99436
K	256	UNK	-	expression tag	UNP Q99436
K	257	UNK	-	expression tag	UNP Q99436
K	258	UNK	-	expression tag	UNP Q99436
K	259	UNK	-	expression tag	UNP Q99436
K	260	UNK	-	expression tag	UNP Q99436
K	261	UNK	-	expression tag	UNP Q99436
K	262	UNK	-	expression tag	UNP Q99436

- Molecule 12 is a protein called Proteasome subunit beta type-3.

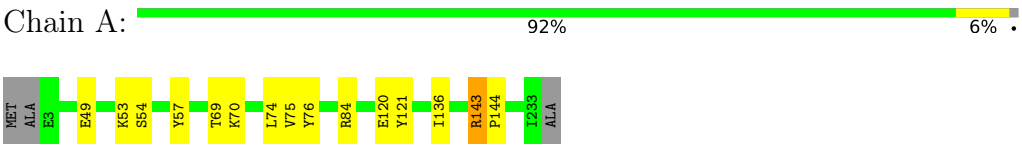
Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	181	Total	C	N	O	S	0	0
			1422	912	237	257	16		

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.

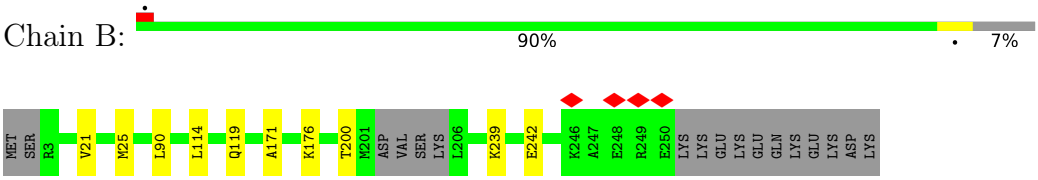
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



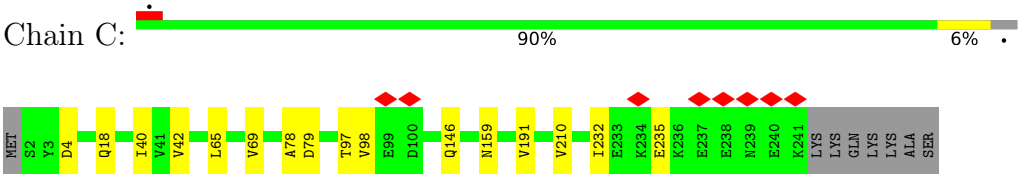
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



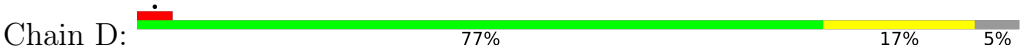
• Molecule 3: Proteasome subunit alpha type-7

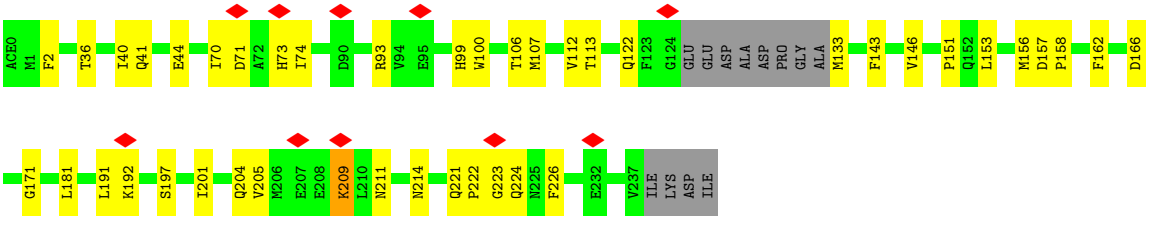
Chain C:



• Molecule 4: Proteasome subunit alpha type-5

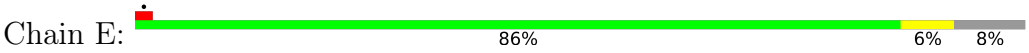
Chain D:





• Molecule 5: Proteasome subunit alpha type-1

Chain E:

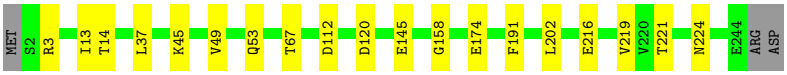


• Molecule 6: Proteasome subunit alpha type-3

Chain F:

• Molecule 7: Proteasome subunit alpha type-6

Chain G:

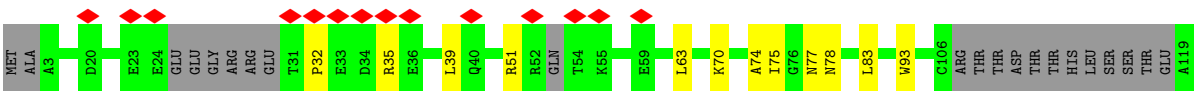


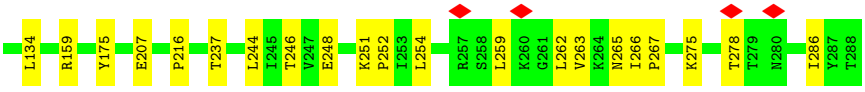
• Molecule 8: Proteasome maturation protein

Chain H:

• Molecule 9: Proteasome assembly chaperone 1

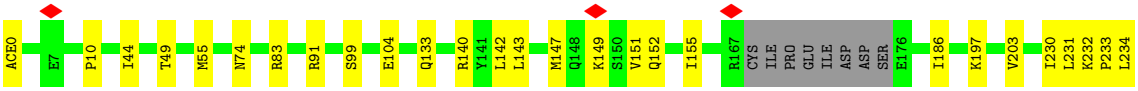
Chain I:

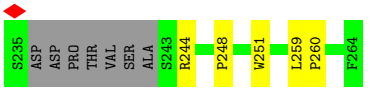




• Molecule 10: Proteasome assembly chaperone 2

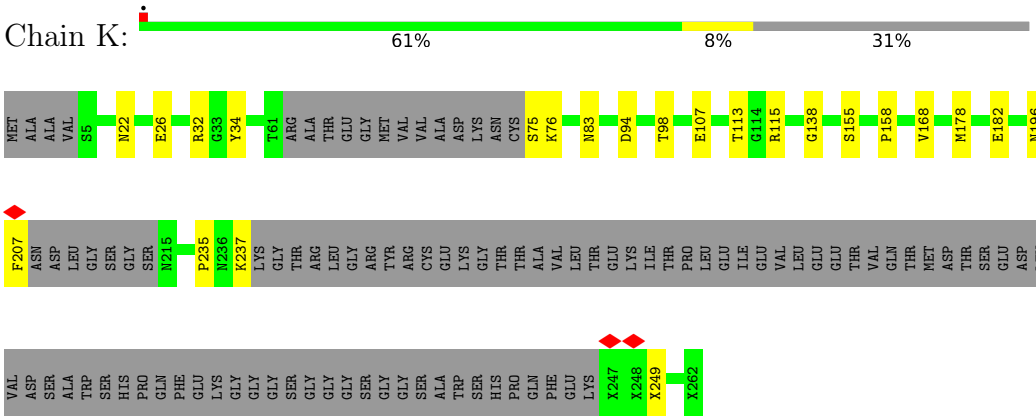
Chain J:





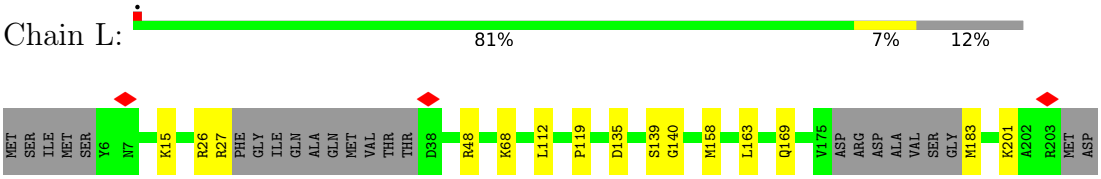
• Molecule 11: Proteasome subunit beta type-7

Chain K:



• Molecule 12: Proteasome subunit beta type-3

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	322874	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 ($e^-/Å^2$)	66.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.894	Depositor
Minimum map value	-1.773	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	255.36, 255.36, 255.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/1830	0.50	0/2480
2	B	0.27	0/1945	0.50	0/2620
3	C	0.25	0/1906	0.49	0/2573
4	D	0.26	0/1785	0.50	0/2410
5	E	0.26	0/1932	0.52	0/2611
6	F	0.28	0/1911	0.49	0/2574
7	G	0.28	0/1926	0.49	0/2603
8	H	0.26	0/790	0.47	0/1063
9	I	0.26	0/2171	0.49	0/2940
10	J	0.26	0/1996	0.47	0/2701
11	K	0.26	0/1652	0.48	0/2235
12	L	0.26	0/1448	0.51	0/1951
All	All	0.27	0/21292	0.49	0/28761

There are no bond length outliers.

There are no bond angle outliers.

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	1791	0	1783	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1916	0	1927	7	0
3	C	1880	0	1893	9	0
4	D	1760	0	1746	29	0
5	E	1898	0	1885	11	0
6	F	1876	0	1858	20	0
7	G	1892	0	1898	15	0
8	H	777	0	774	4	0
9	I	2128	0	2147	19	0
10	J	1956	0	1999	19	0
11	K	1701	0	1652	14	0
12	L	1422	0	1445	10	0
All	All	20997	0	21007	156	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.

The worst 5 of 156 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)
1:A:143:ARG:NH1	1:A:144:PRO:O	2.23	0.71
11:K:22:ASN:O	11:K:26:GLU:HG3	1.91	0.71
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.74	0.69
1:A:84:ARG:NH1	7:G:120:ASP:OD1	2.25	0.69
10:J:0:ACE:H1	10:J:49:THR:HG22	1.77	0.67

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	229/234 (98%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	240/261 (92%)	237 (99%)	3 (1%)	0	100	100
3	C	238/248 (96%)	236 (99%)	2 (1%)	0	100	100
4	D	226/242 (93%)	218 (96%)	8 (4%)	0	100	100
5	E	240/264 (91%)	234 (98%)	6 (2%)	0	100	100
6	F	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
8	H	95/141 (67%)	92 (97%)	3 (3%)	0	100	100
9	I	259/288 (90%)	253 (98%)	6 (2%)	0	100	100
10	J	244/265 (92%)	236 (97%)	8 (3%)	0	100	100
11	K	207/332 (62%)	206 (100%)	1 (0%)	0	100	100
12	L	175/205 (85%)	166 (95%)	9 (5%)	0	100	100
All	All	2632/2981 (88%)	2570 (98%)	62 (2%)	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	186/191 (97%)	185 (100%)	1 (0%)	88	95
2	B	202/221 (91%)	202 (100%)	0	100	100
3	C	200/211 (95%)	200 (100%)	0	100	100
4	D	193/203 (95%)	191 (99%)	2 (1%)	76	90
5	E	205/224 (92%)	205 (100%)	0	100	100
6	F	197/212 (93%)	197 (100%)	0	100	100
7	G	207/210 (99%)	207 (100%)	0	100	100
8	H	90/128 (70%)	89 (99%)	1 (1%)	73	89
9	I	242/262 (92%)	242 (100%)	0	100	100
10	J	223/237 (94%)	223 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	174/257 (68%)	174 (100%)	0	100 100
12	L	154/174 (88%)	154 (100%)	0	100 100
All	All	2273/2530 (90%)	2269 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ARG
4	D	192	LYS
4	D	209	LYS
8	H	68	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
9	I	103	ASN
8	H	90	GLN
4	D	221	GLN
4	D	214	ASN
7	G	53	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.

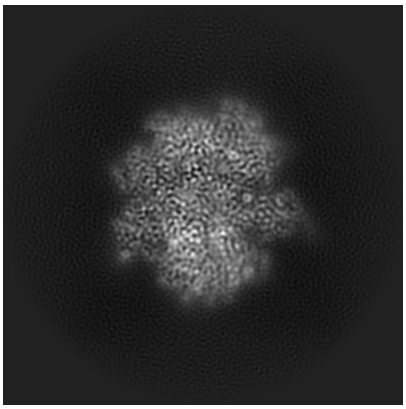
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18757. These allow visual inspection of the internal detail of the map and identification of artifacts.

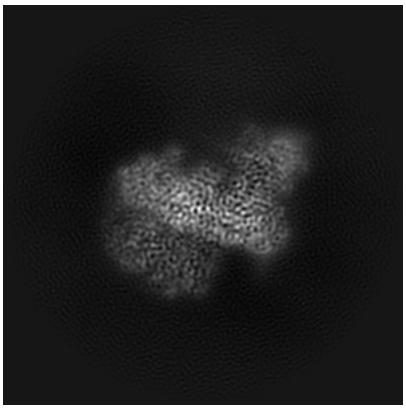
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

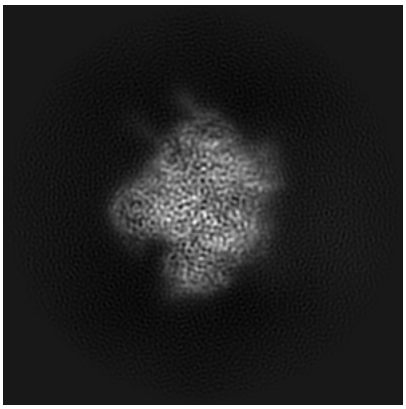
6.1.1 Primary map



X

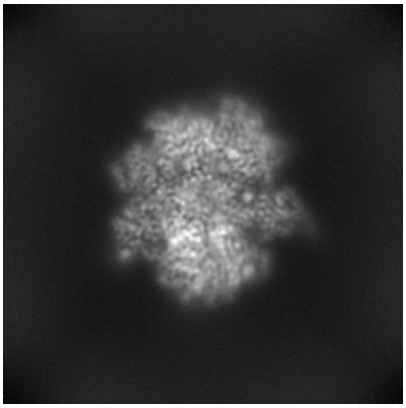


Y

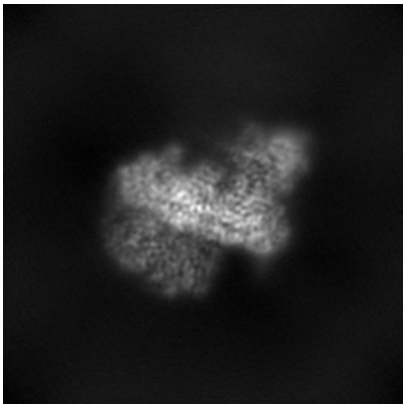


Z

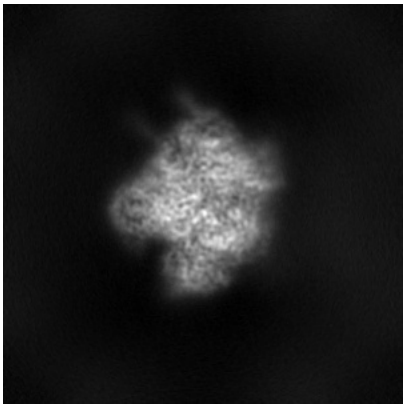
6.1.2 Raw map



X



Y

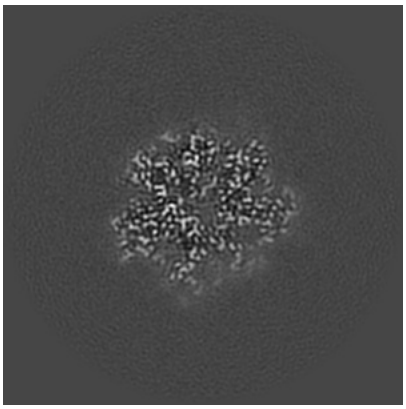


Z

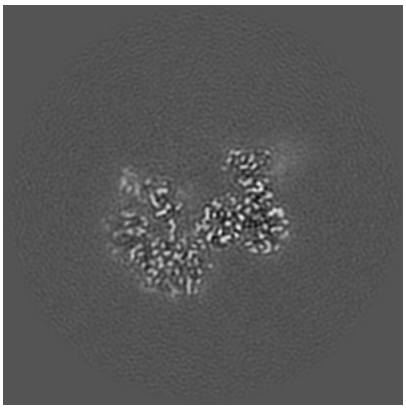
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

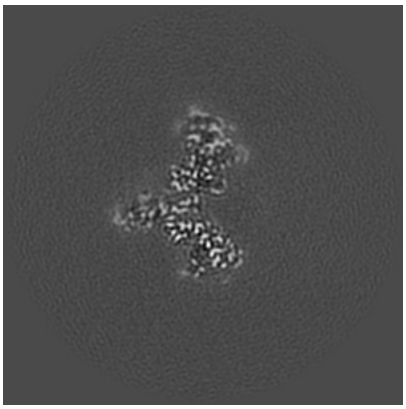
6.2.1 Primary map



X Index: 150

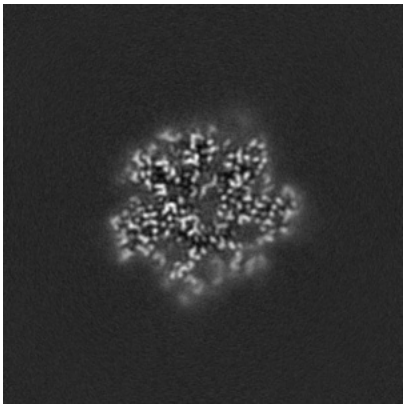


Y Index: 150

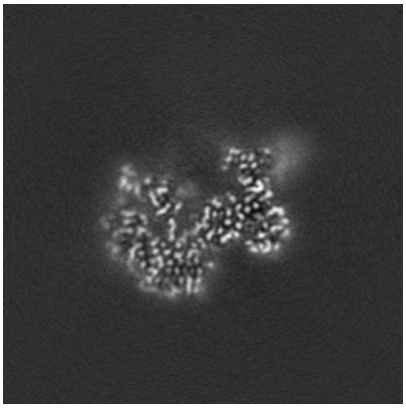


Z Index: 150

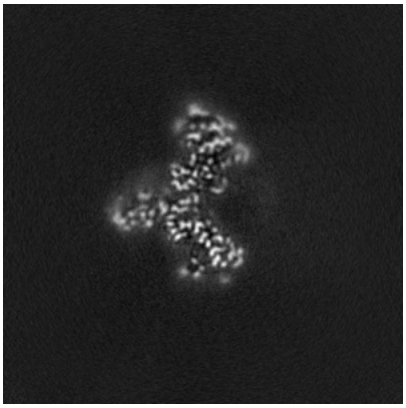
6.2.2 Raw map



X Index: 150



Y Index: 150

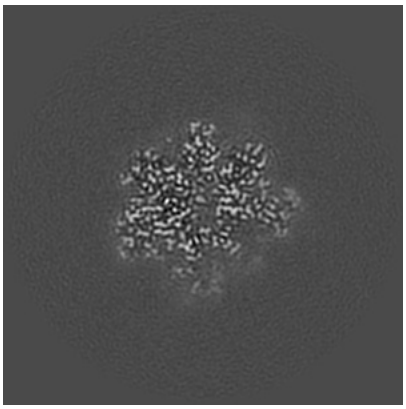


Z Index: 150

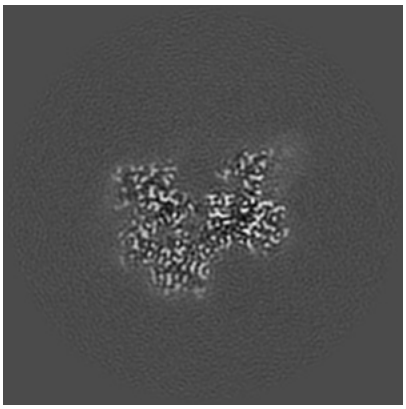
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

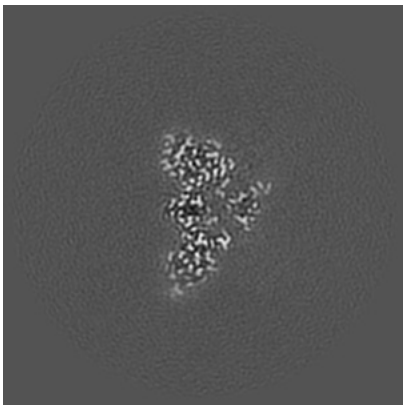
6.3.1 Primary map



X Index: 147

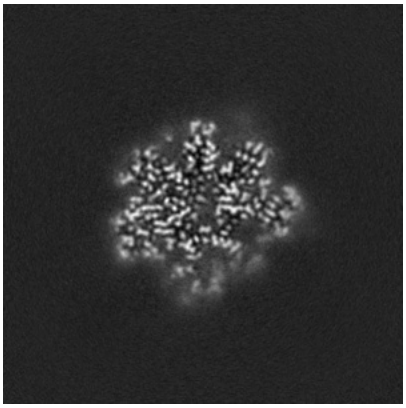


Y Index: 142

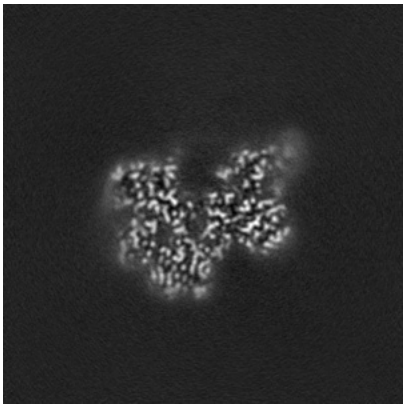


Z Index: 176

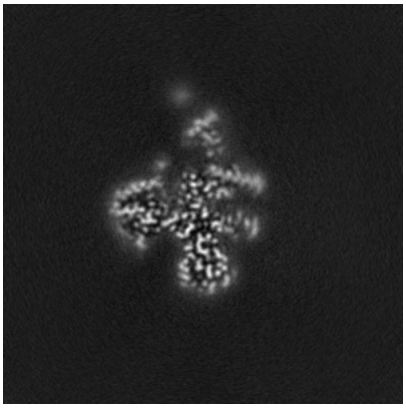
6.3.2 Raw map



X Index: 147



Y Index: 141

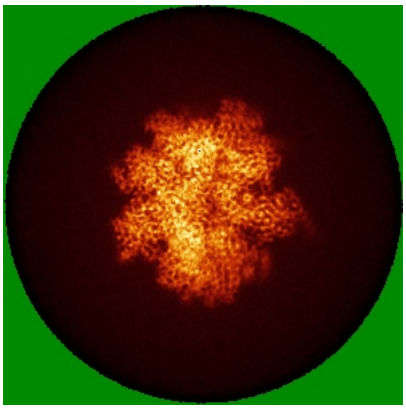


Z Index: 129

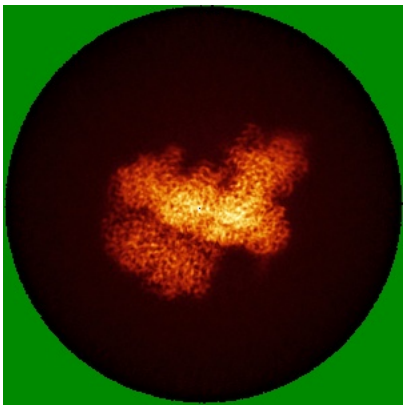
The images above show the largest variance slices of the map in three orthogonal directions.

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

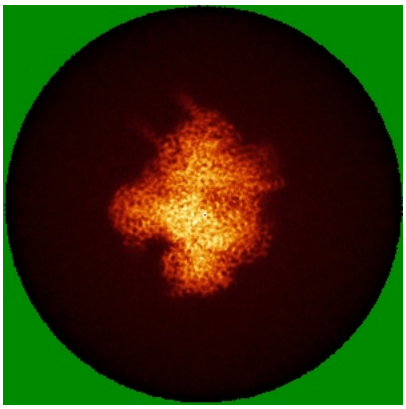
6.4.1 Primary map



X

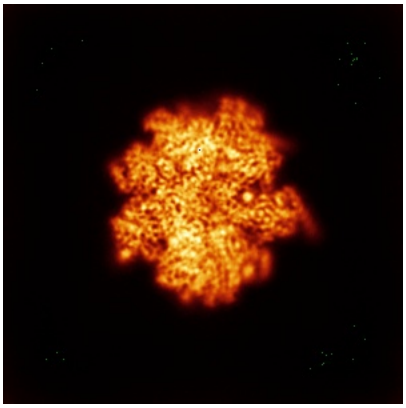


Y

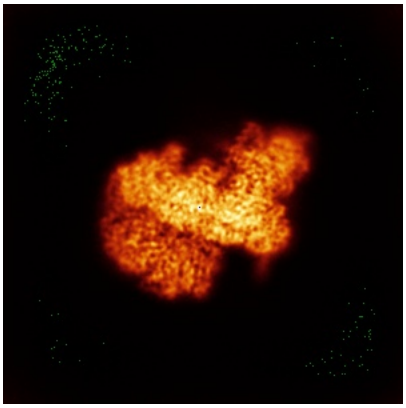


Z

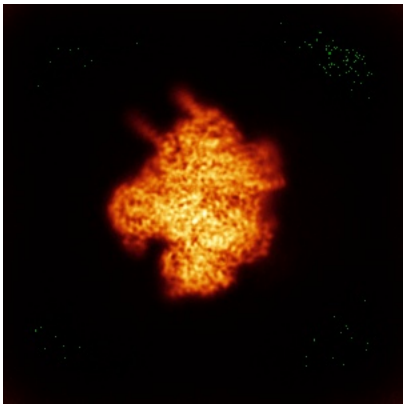
6.4.2 Raw map



X



Y

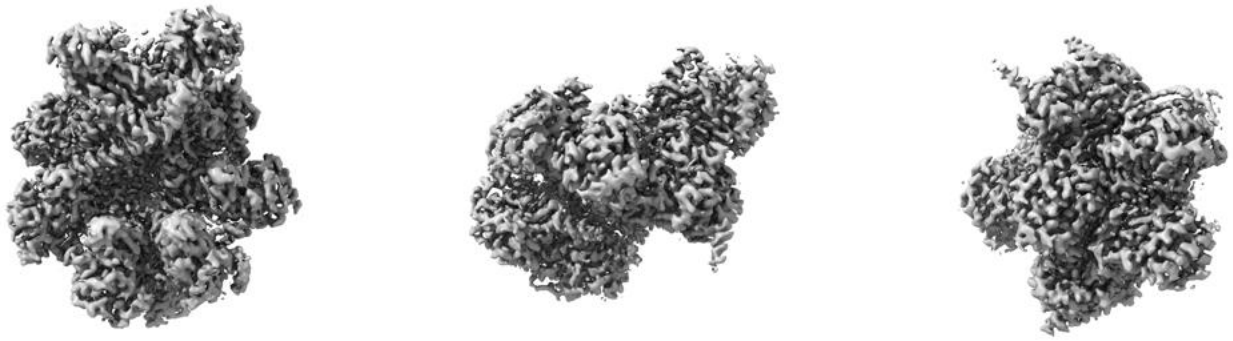


Z

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)

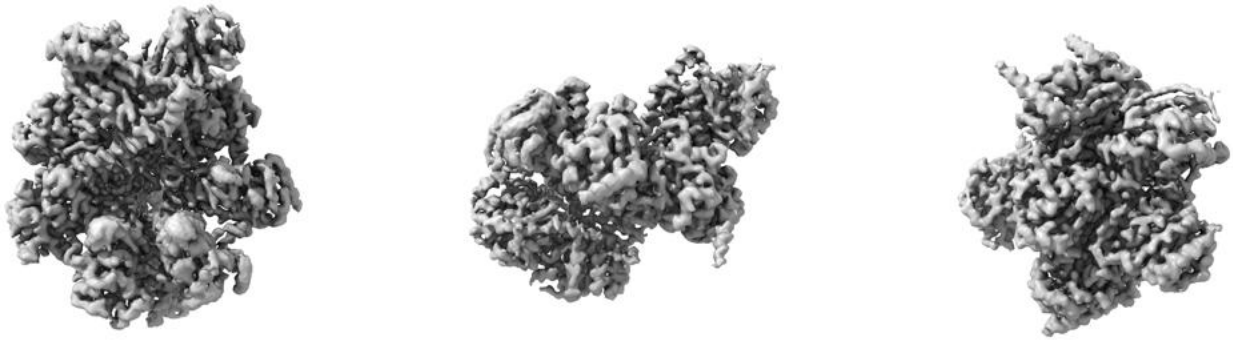
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



X Y Z

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.

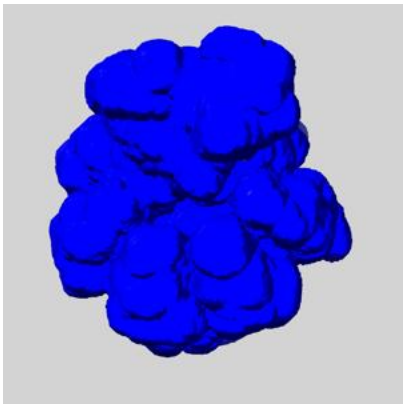
6.6 Mask visualisation (i)

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

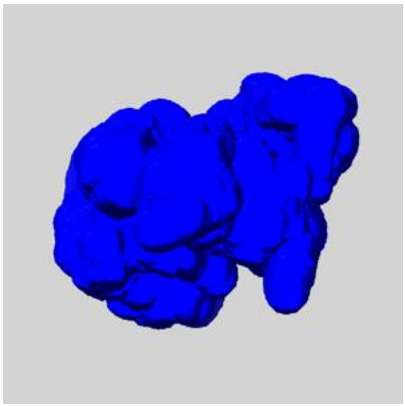
A mask typically either:

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

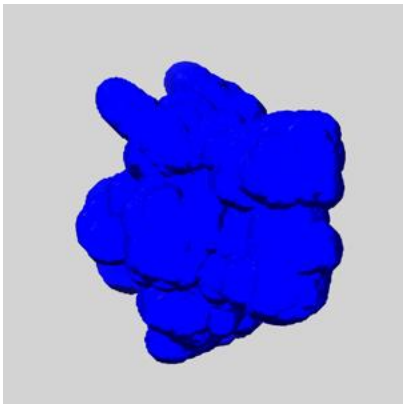
6.6.1 emd_18757_msk_1.map (i)



X



Y

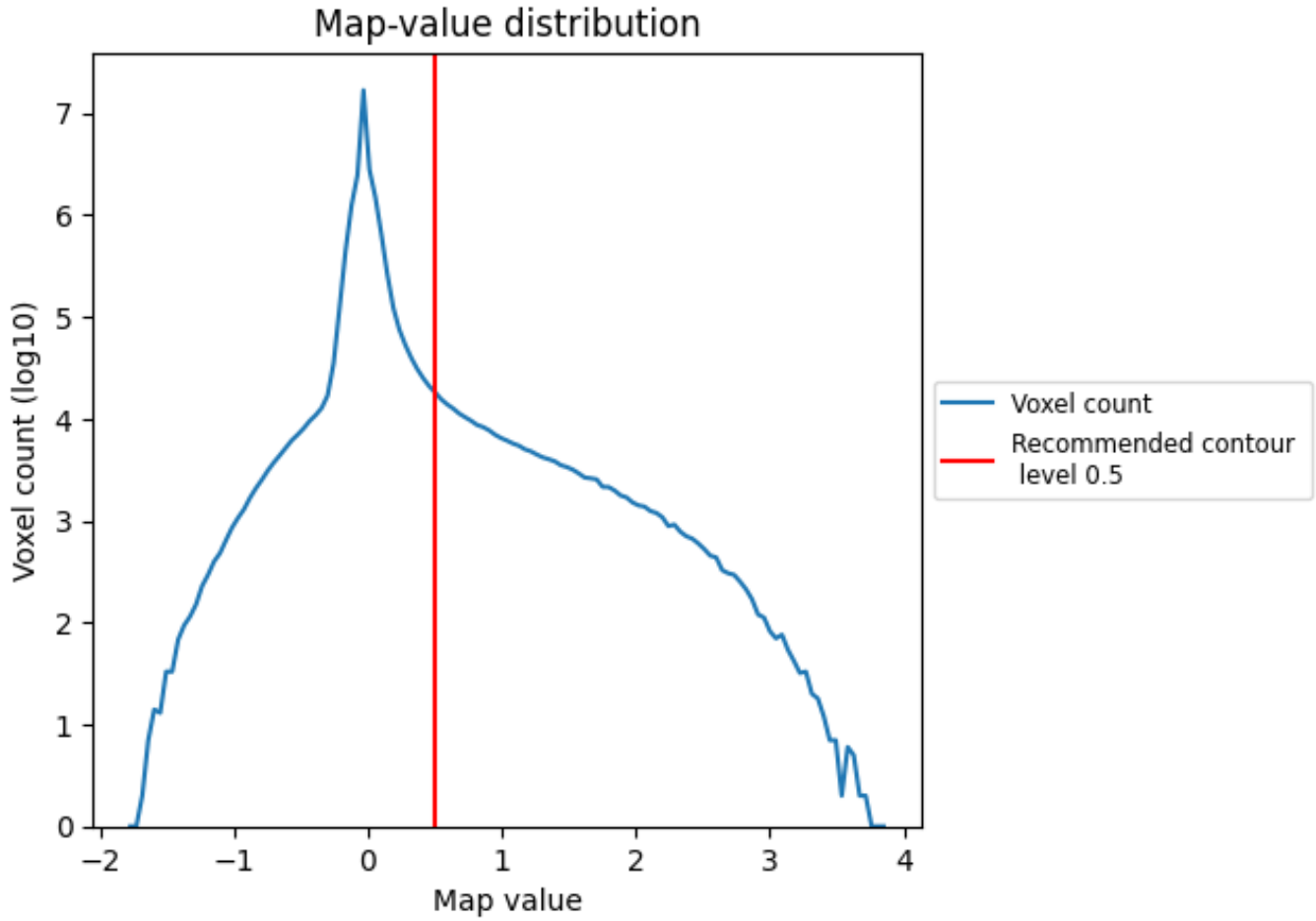


Z

7 Map analysis

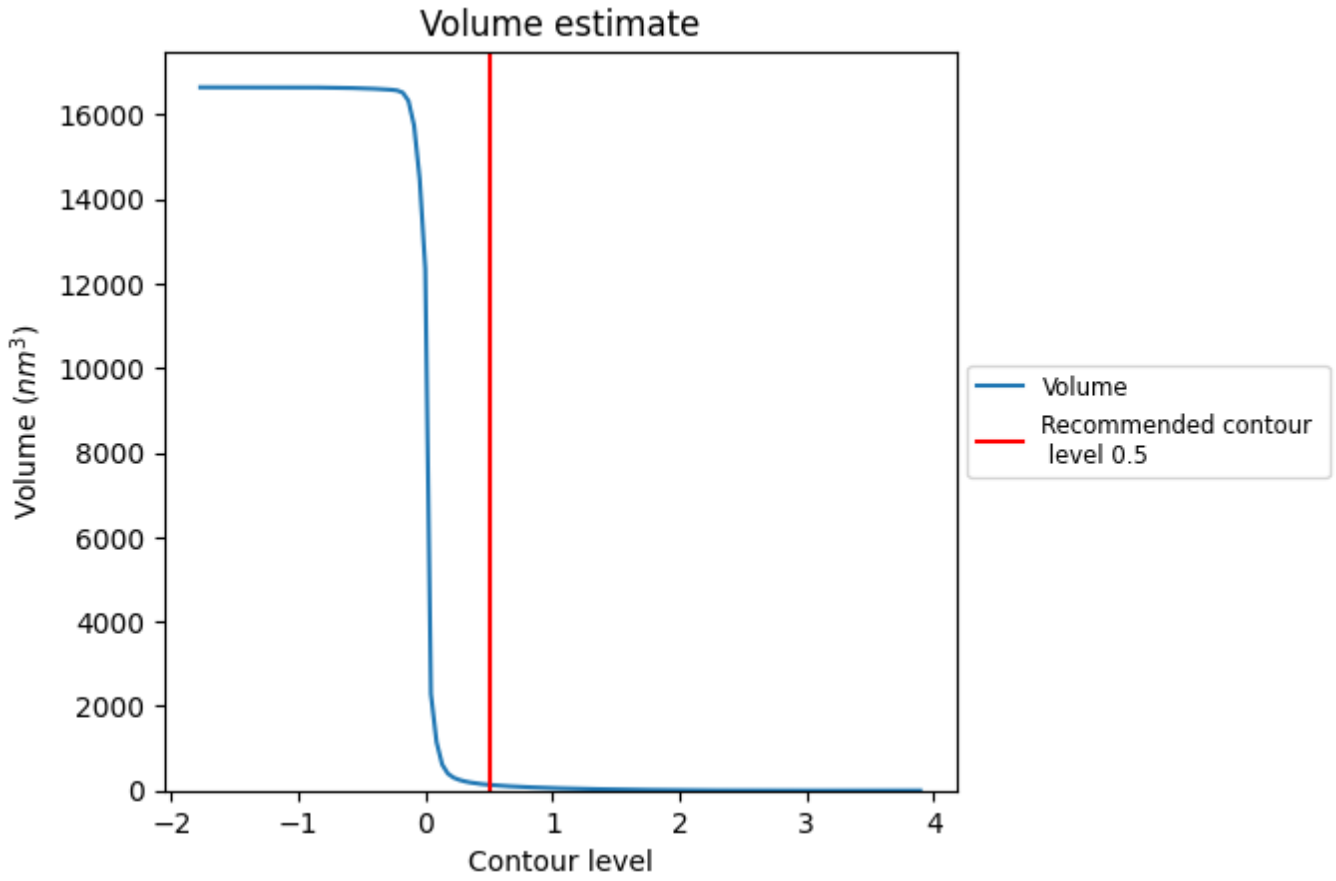
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

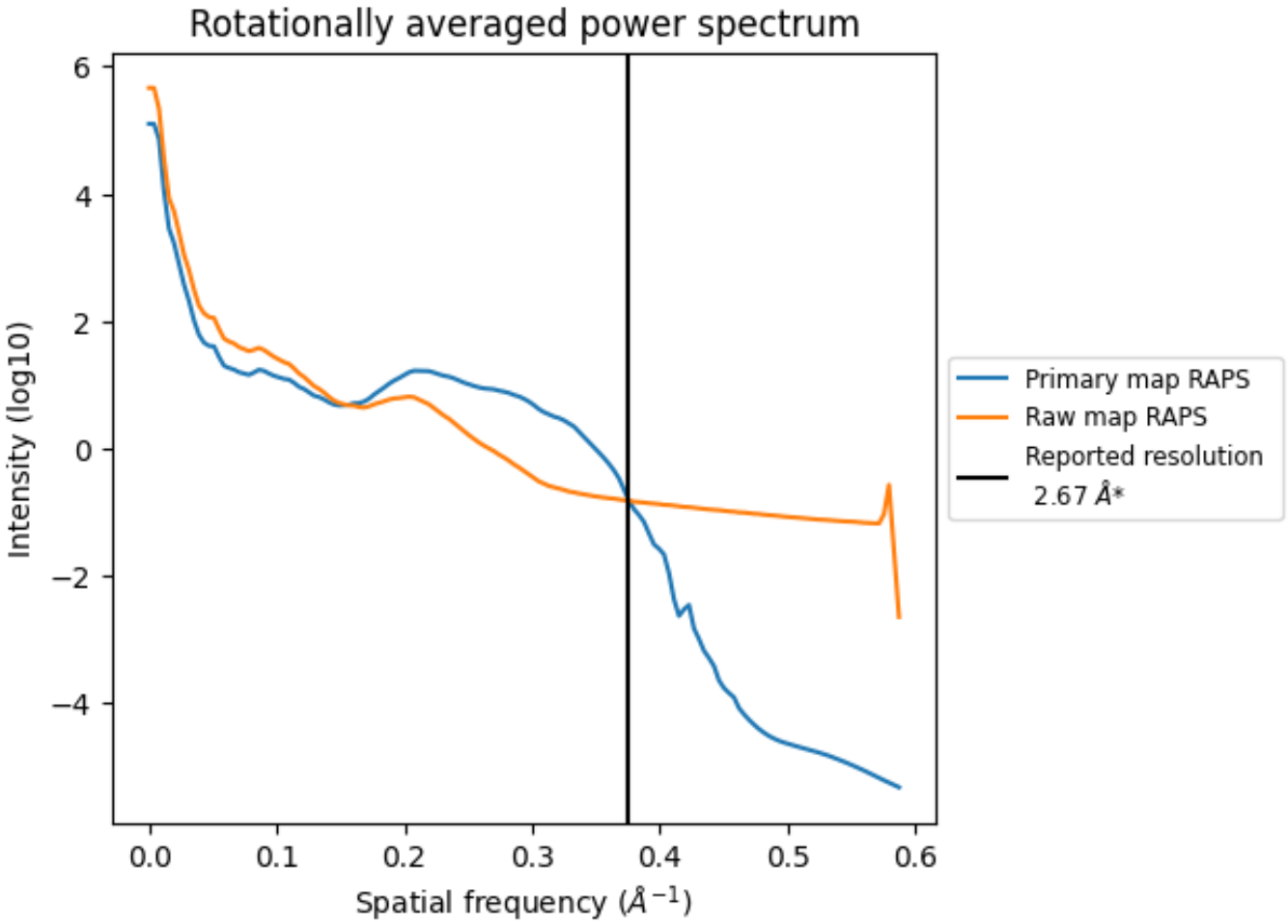
7.2 Volume estimate (i)



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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)

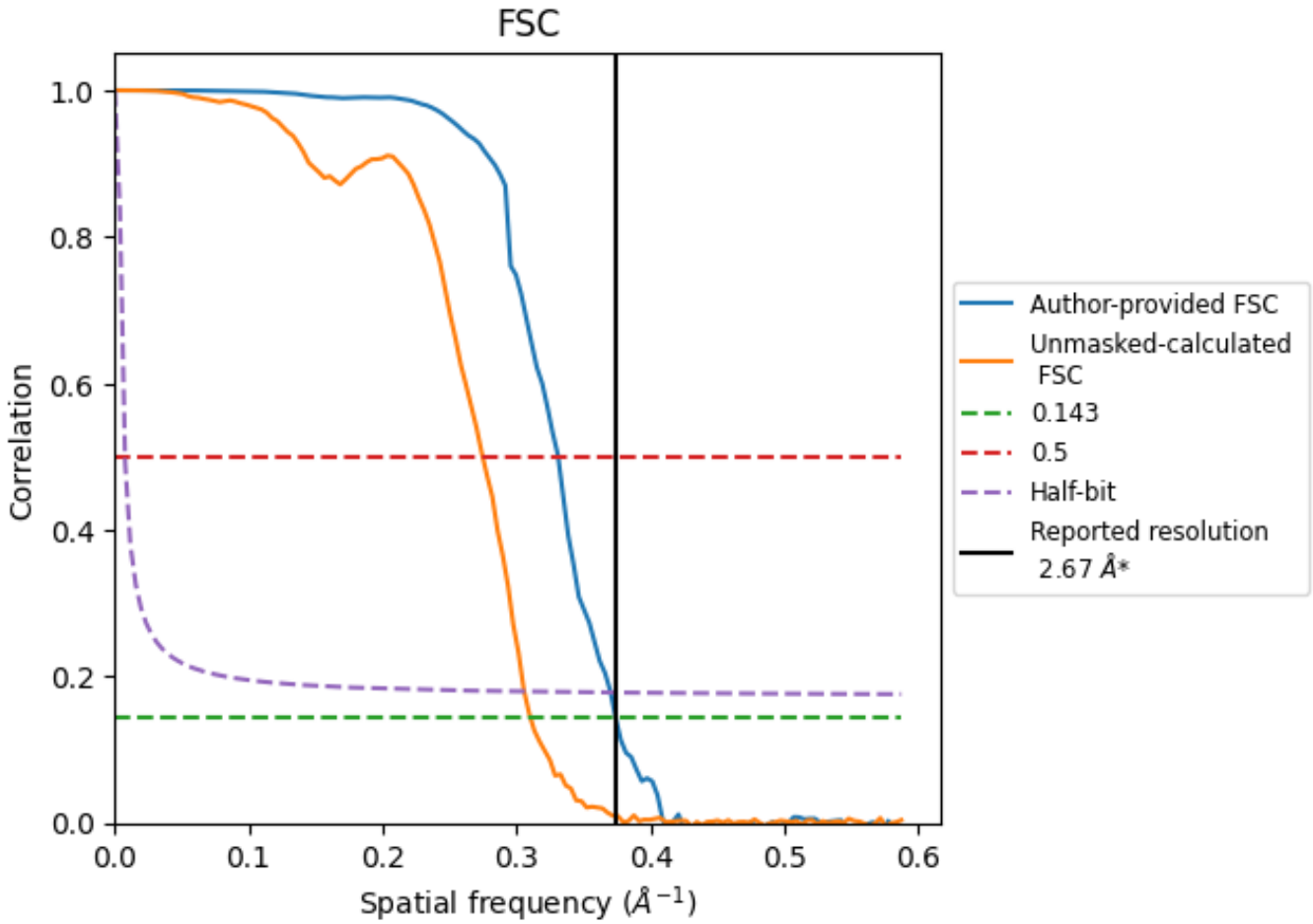


*Reported resolution corresponds to spatial frequency of 0.375 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.375 Å^{-1}

8.2 Resolution estimates (i)

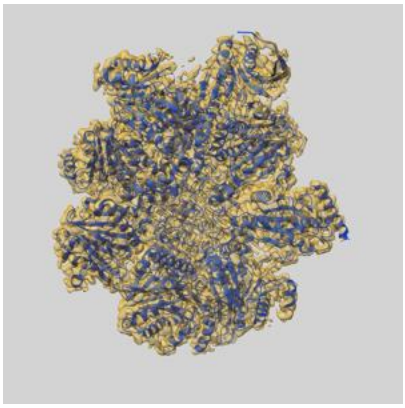
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.02	2.70
Unmasked-calculated*	3.22	3.64	3.27

*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 3.22 differs from the reported value 2.67 by more than 10 %

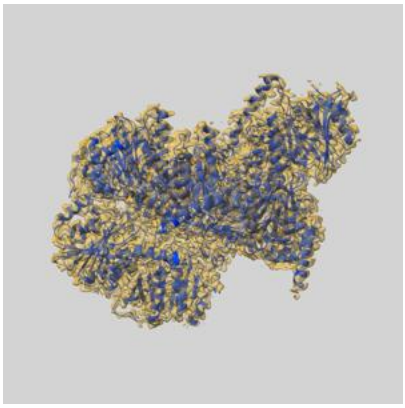
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18757 and PDB model 8QYL. Per-residue inclusion information can be found in section 3 on page 8.

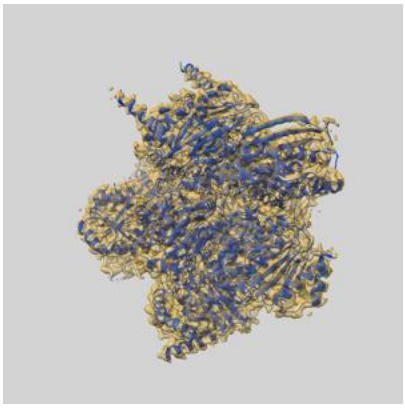
9.1 Map-model overlay



X



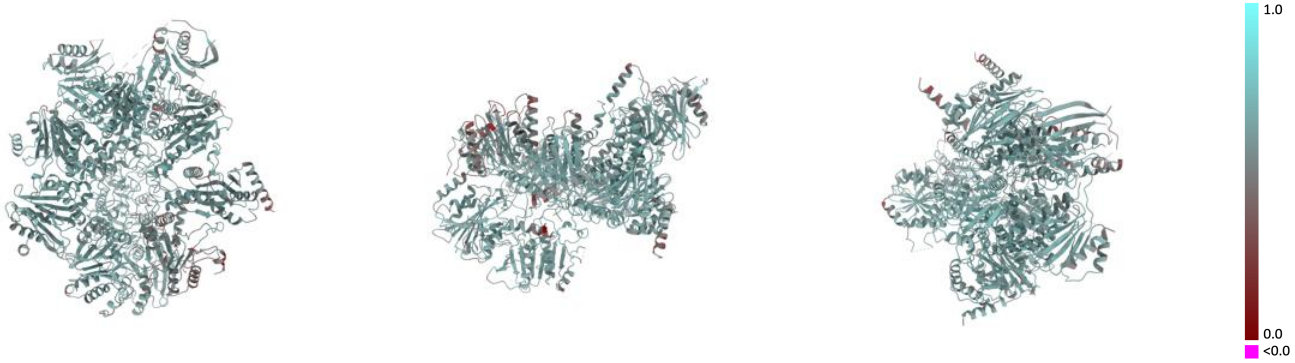
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

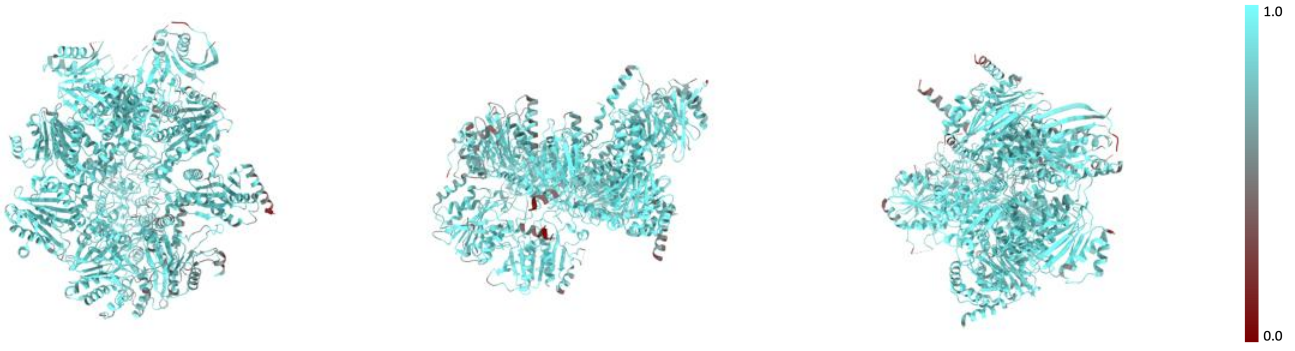
9.2 Q-score mapped to coordinate model



X Y Z

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.

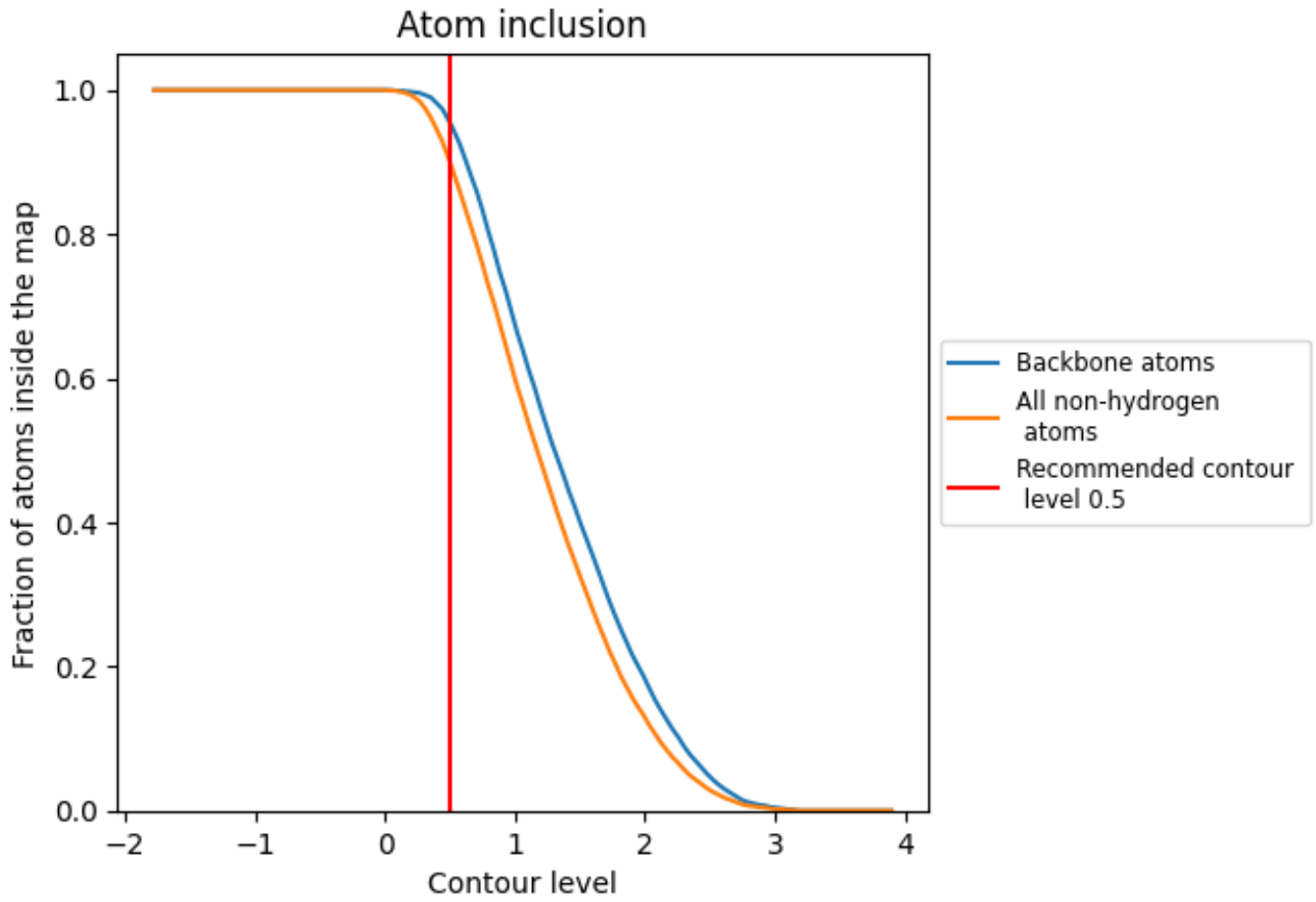
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.6010
A	0.9640	0.6320
B	0.9170	0.6180
C	0.8810	0.5880
D	0.7970	0.5190
E	0.9140	0.6020
F	0.9330	0.6190
G	0.9450	0.6270
H	0.9300	0.6250
I	0.8330	0.5870
J	0.9200	0.6110
K	0.9010	0.6050
L	0.8800	0.5890