



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2023 – 04:35 PM EDT

PDB ID : 8T0M
EMDB ID : EMD-40944
Title : Proteasome 20S core particle from Pre1-1 Pre4-1 Double mutant
Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.; Velez, B.; Hanna, J.
Deposited on : 2023-06-01
Resolution : 2.40 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:

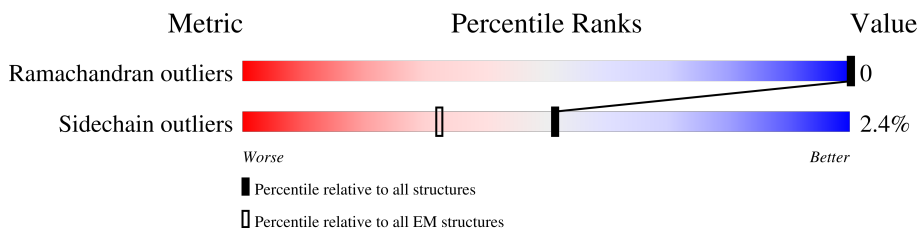
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




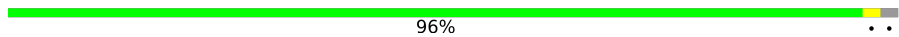
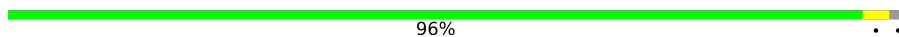







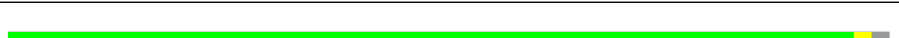


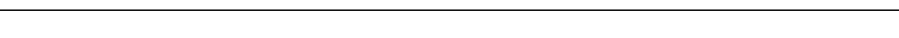
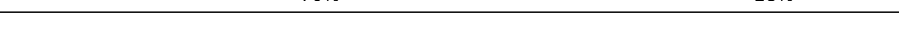
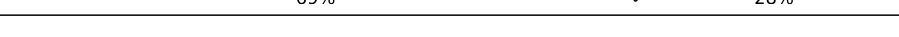



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	252	89% 9%
1	O	252	89% 9%
2	B	250	97% ..
2	P	250	97% ..
3	C	258	90% 8%
3	Q	258	90% 8%
4	D	254	85% 13%
4	R	254	85% 13%
5	E	260	87% 13%

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Mol	Chain	Length	Quality of chain
5	S	260	 86% 13%
6	F	234	 96%
6	T	234	 96%
7	G	288	 82% 16%
7	U	288	 82% 16%
8	H	215	 82% 15%
8	V	215	 82% 15%
9	I	261	 77% 23%
9	W	261	 77% 23%
10	J	205	 95%
10	X	205	 95%
11	K	198	 98%
11	Y	198	 97%
12	L	287	 70% 28%
12	Z	287	 69% 28%
13	M	241	 90% 9%
13	a	241	 90% 9%
14	N	251	 82% 16%
14	b	251	 82% 16%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 47538 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	229	Total	C	N	O	S	0	0
			1805	1152	301	344	8		
1	O	229	Total	C	N	O	S	0	0
			1805	1152	301	344	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		
2	P	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	237	Total	C	N	O	S	0	0
			1861	1177	313	368	3		
3	Q	237	Total	C	N	O	S	0	0
			1861	1177	313	368	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	221	Total	C	N	O	S	0	0
			1727	1084	298	341	4		
4	R	221	Total	C	N	O	S	0	0
			1727	1084	298	341	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1750	1097	294	352	7		
5	S	227	Total	C	N	O	S	0	0
			1750	1097	294	352	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	230	Total	C	N	O	S	0	0
			1765	1110	305	346	4		
6	T	230	Total	C	N	O	S	0	0
			1765	1110	305	346	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	U	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	183	Total	C	N	O	S	0	0
			1424	905	234	278	7		
8	V	183	Total	C	N	O	S	0	0
			1424	905	234	278	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	202	Total	C	N	O	S	0	0
			1550	985	266	293	6		
9	W	202	Total	C	N	O	S	0	0
			1550	985	266	293	6		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	200	Total	C	N	O	S	0	0
			1551	991	254	298	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	200	1551	991	254	298	8	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	194	1558	993	263	297	5	0	0
11	Y	194	1558	993	263	297	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	conflict	UNP P22141
Y	142	PHE	SER	conflict	UNP P22141

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	207	1617	1029	275	306	7	0	0
12	Z	207	1617	1029	275	306	7	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	220	1737	1101	300	332	4	0	0
13	a	220	1737	1101	300	332	4	0	0

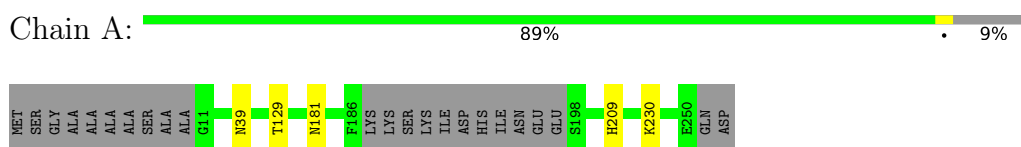
- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	211	1639	1037	281	315	6	0	0
14	b	211	1639	1037	281	315	6	0	0

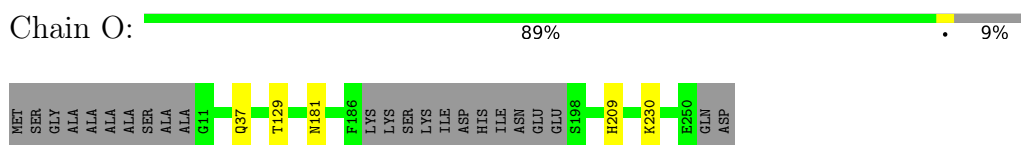
3 Residue-property plots [i](#)

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.

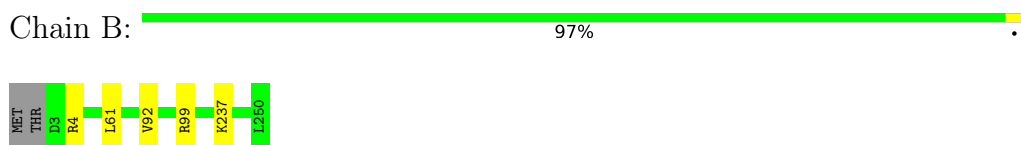
- Molecule 1: Proteasome subunit alpha type-1



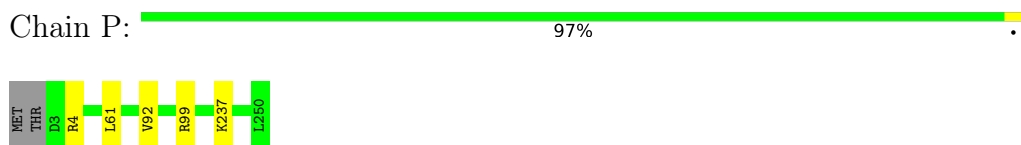
- Molecule 1: Proteasome subunit alpha type-1



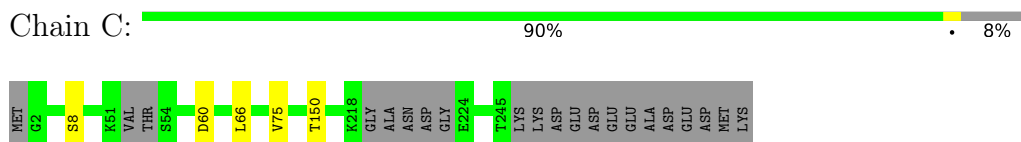
- Molecule 2: Proteasome subunit alpha type-2




- Molecule 2: Proteasome subunit alpha type-2

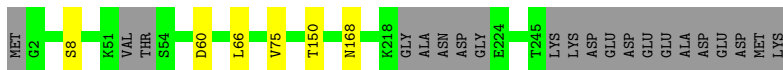


- Molecule 3: Proteasome subunit alpha type-3




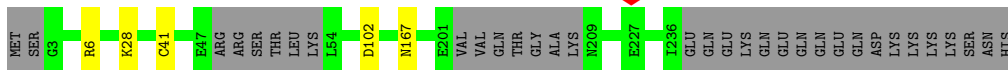
- Molecule 3: Proteasome subunit alpha type-3

Chain Q:  90% 8%




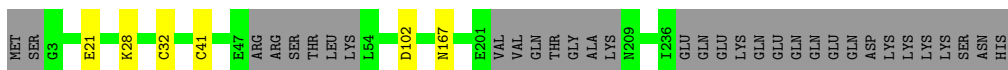
- Molecule 4: Proteasome subunit alpha type-4

Chain D:  85% 13%




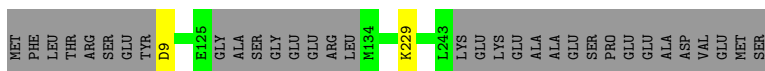
- Molecule 4: Proteasome subunit alpha type-4

Chain R:  85% 13%




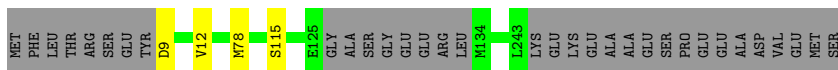
- Molecule 5: Proteasome subunit alpha type-5

Chain E:  87% 13%



- Molecule 5: Proteasome subunit alpha type-5

Chain S:  86% 13%



- Molecule 6: Proteasome subunit alpha type-6

Chain F:  96% 2%



- Molecule 6: Proteasome subunit alpha type-6

Chain T:  96% 2%



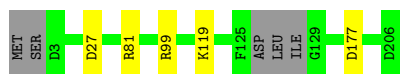
- Molecule 7: Proteasome subunit alpha type-7

Chain J:  95%



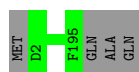
- Molecule 10: Proteasome subunit beta type-3

Chain X:  95%



- Molecule 11: Proteasome subunit beta type-4

Chain K:  98%



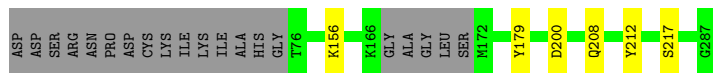
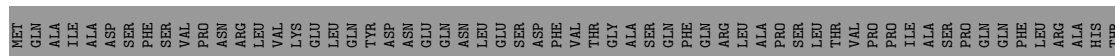
- Molecule 11: Proteasome subunit beta type-4

Chain Y:  97%



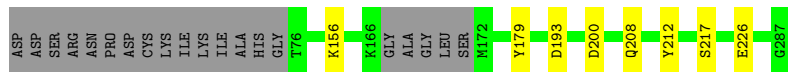
- Molecule 12: Proteasome subunit beta type-5

Chain L:  70% 28%



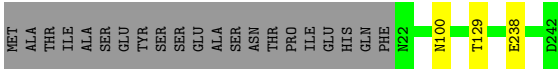
- Molecule 12: Proteasome subunit beta type-5

Chain Z:  69% 28%

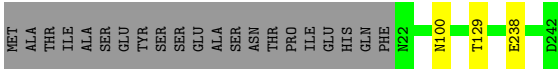
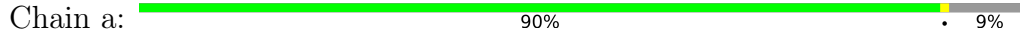


- Molecule 13: Proteasome subunit beta type-6

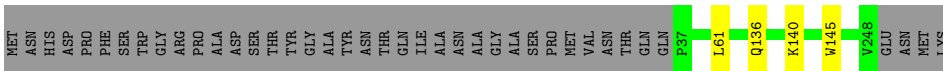
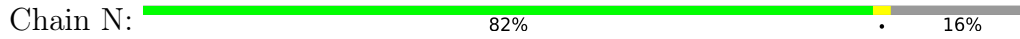
Chain M:  90% 9%



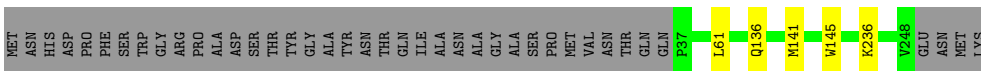
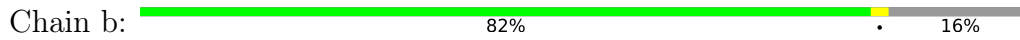
- Molecule 13: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	766100	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 ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.963	Depositor
Minimum map value	-4.126	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.426	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.29	0/1841	0.50	0/2495
1	O	0.28	0/1841	0.50	0/2495
2	B	0.28	0/1937	0.48	0/2622
2	P	0.27	0/1937	0.47	0/2622
3	C	0.27	0/1889	0.50	0/2553
3	Q	0.27	0/1889	0.49	0/2553
4	D	0.27	0/1754	0.51	0/2376
4	R	0.26	0/1754	0.50	0/2376
5	E	0.25	0/1774	0.50	0/2392
5	S	0.25	0/1774	0.47	0/2392
6	F	0.26	0/1792	0.49	0/2422
6	T	0.26	0/1792	0.48	0/2422
7	G	0.27	0/1925	0.46	0/2599
7	U	0.27	0/1925	0.46	0/2599
8	H	0.26	0/1451	0.48	0/1961
8	V	0.26	0/1451	0.47	0/1961
9	I	0.26	0/1575	0.48	0/2131
9	W	0.26	0/1575	0.48	0/2131
10	J	0.28	0/1580	0.49	0/2130
10	X	0.28	0/1580	0.48	0/2130
11	K	0.27	0/1587	0.51	0/2140
11	Y	0.26	0/1587	0.52	0/2140
12	L	0.26	0/1653	0.49	0/2235
12	Z	0.26	0/1653	0.48	0/2235
13	M	0.27	0/1774	0.49	0/2392
13	a	0.27	0/1774	0.49	0/2392
14	N	0.27	0/1666	0.52	0/2262
14	b	0.27	0/1666	0.51	0/2262
All	All	0.27	0/48396	0.49	0/65420

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/252 (89%)	223 (99%)	2 (1%)	0	100	100
1	O	225/252 (89%)	224 (100%)	1 (0%)	0	100	100
2	B	246/250 (98%)	243 (99%)	3 (1%)	0	100	100
2	P	246/250 (98%)	245 (100%)	1 (0%)	0	100	100
3	C	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
3	Q	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
4	D	215/254 (85%)	209 (97%)	6 (3%)	0	100	100
4	R	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
5	E	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
5	S	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
6	F	228/234 (97%)	223 (98%)	5 (2%)	0	100	100
6	T	228/234 (97%)	225 (99%)	3 (1%)	0	100	100
7	G	240/288 (83%)	238 (99%)	2 (1%)	0	100	100
7	U	240/288 (83%)	238 (99%)	2 (1%)	0	100	100
8	H	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
8	V	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
9	I	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
9	W	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
10	J	196/205 (96%)	190 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	196/205 (96%)	192 (98%)	4 (2%)	0	100	100
11	K	192/198 (97%)	190 (99%)	2 (1%)	0	100	100
11	Y	192/198 (97%)	188 (98%)	4 (2%)	0	100	100
12	L	203/287 (71%)	201 (99%)	2 (1%)	0	100	100
12	Z	203/287 (71%)	200 (98%)	3 (2%)	0	100	100
13	M	218/241 (90%)	213 (98%)	5 (2%)	0	100	100
13	a	218/241 (90%)	214 (98%)	4 (2%)	0	100	100
14	N	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
14	b	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
All	All	5994/6908 (87%)	5908 (99%)	86 (1%)	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	194/210 (92%)	189 (97%)	5 (3%)	46	66
1	O	194/210 (92%)	189 (97%)	5 (3%)	46	66
2	B	207/209 (99%)	202 (98%)	5 (2%)	49	68
2	P	207/209 (99%)	202 (98%)	5 (2%)	49	68
3	C	199/216 (92%)	194 (98%)	5 (2%)	47	67
3	Q	199/216 (92%)	193 (97%)	6 (3%)	41	61
4	D	195/226 (86%)	190 (97%)	5 (3%)	46	66
4	R	195/226 (86%)	189 (97%)	6 (3%)	40	60
5	E	188/215 (87%)	186 (99%)	2 (1%)	73	87
5	S	188/215 (87%)	184 (98%)	4 (2%)	53	72
6	F	189/193 (98%)	184 (97%)	5 (3%)	46	66
6	T	189/193 (98%)	183 (97%)	6 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	200/239 (84%)	193 (96%)	7 (4%)	36	55
7	U	200/239 (84%)	195 (98%)	5 (2%)	47	67
8	H	153/178 (86%)	147 (96%)	6 (4%)	32	50
8	V	153/178 (86%)	147 (96%)	6 (4%)	32	50
9	I	169/214 (79%)	169 (100%)	0	100	100
9	W	169/214 (79%)	169 (100%)	0	100	100
10	J	168/173 (97%)	163 (97%)	5 (3%)	41	61
10	X	168/173 (97%)	163 (97%)	5 (3%)	41	61
11	K	172/175 (98%)	172 (100%)	0	100	100
11	Y	172/175 (98%)	171 (99%)	1 (1%)	86	94
12	L	167/235 (71%)	161 (96%)	6 (4%)	35	54
12	Z	167/235 (71%)	159 (95%)	8 (5%)	25	41
13	M	183/201 (91%)	180 (98%)	3 (2%)	62	79
13	a	183/201 (91%)	180 (98%)	3 (2%)	62	79
14	N	180/212 (85%)	176 (98%)	4 (2%)	52	71
14	b	180/212 (85%)	175 (97%)	5 (3%)	43	63
All	All	5128/5792 (88%)	5005 (98%)	123 (2%)	51	68

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	145	TRP
12	Z	200	ASP
3	Q	75	VAL
12	Z	193	ASP
14	b	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	K	166	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.

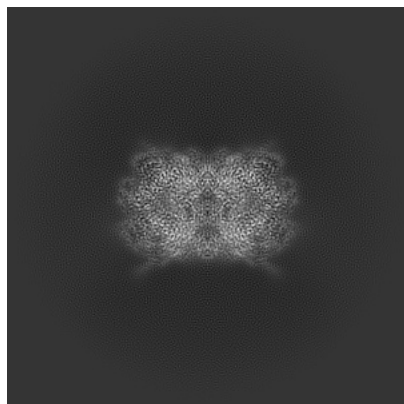
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40944. These allow visual inspection of the internal detail of the map and identification of artifacts.

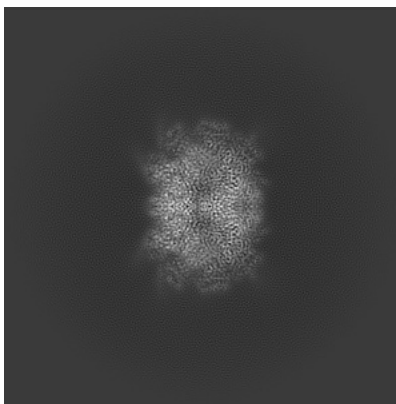
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

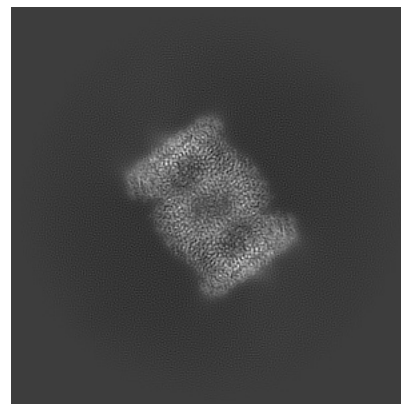
6.1.1 Primary map



X

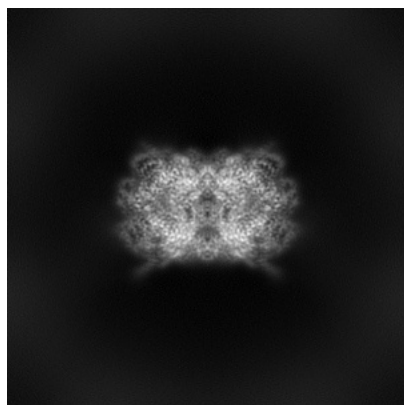


Y

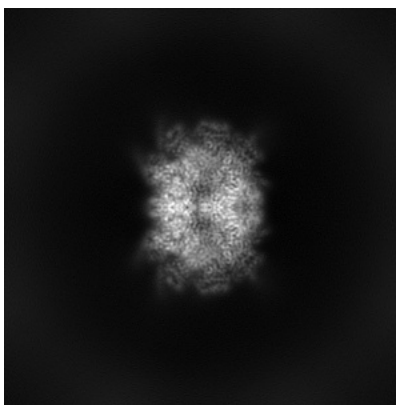


Z

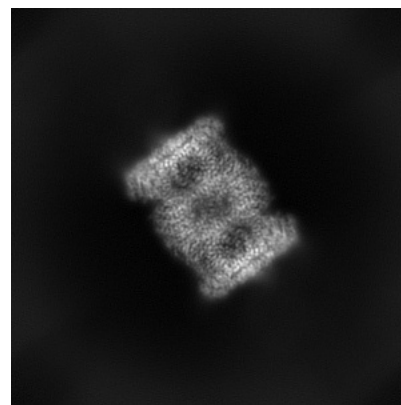
6.1.2 Raw map



X



Y

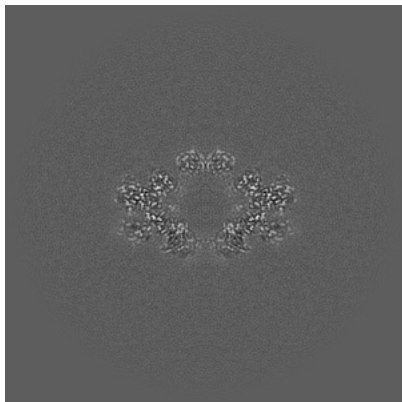


Z

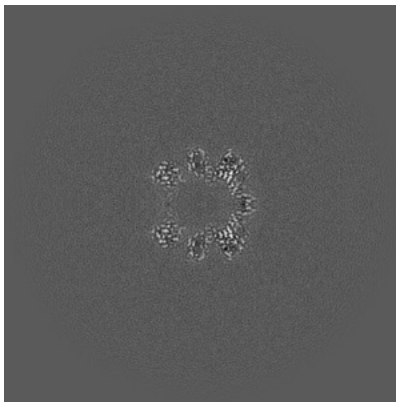
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

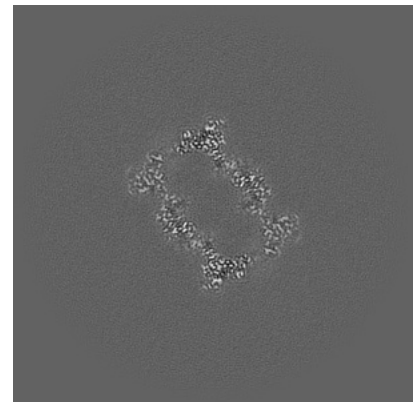
6.2.1 Primary map



X Index: 180

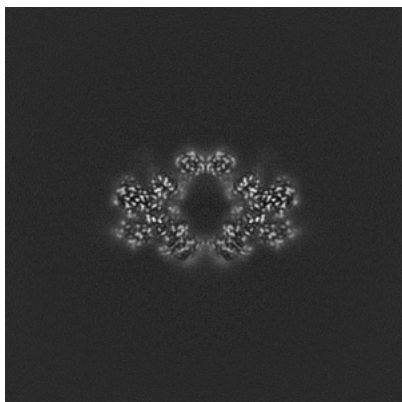


Y Index: 180

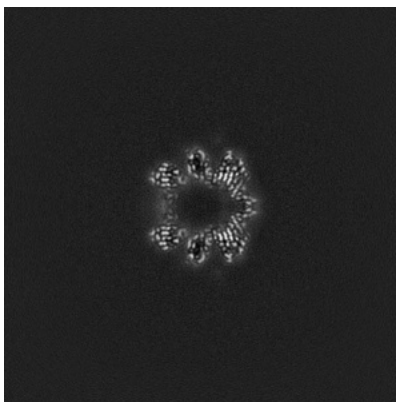


Z Index: 180

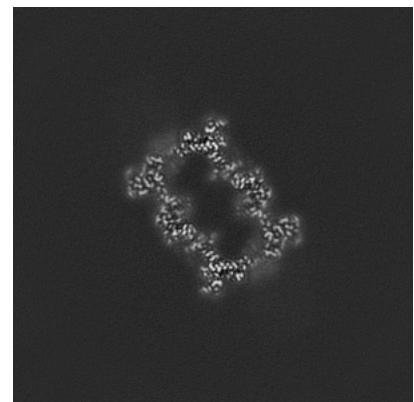
6.2.2 Raw map



X Index: 180



Y Index: 180

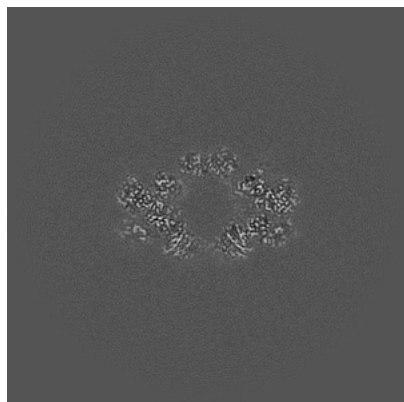


Z Index: 180

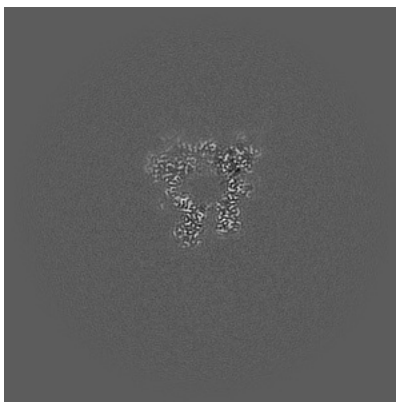
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

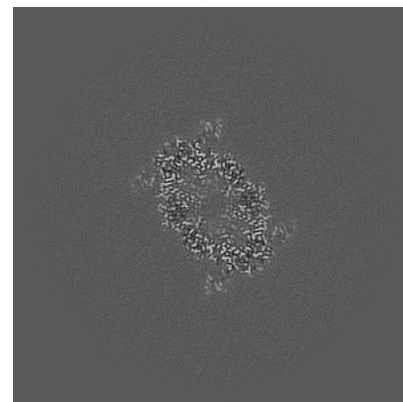
6.3.1 Primary map



X Index: 178

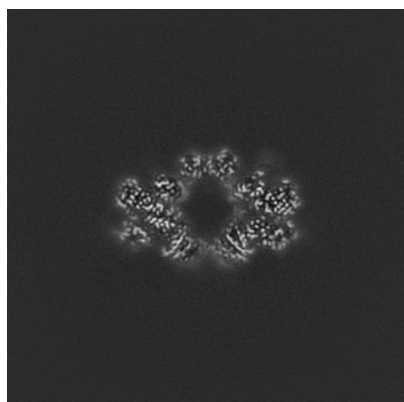


Y Index: 140

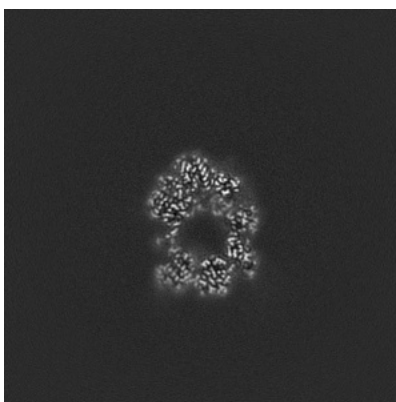


Z Index: 203

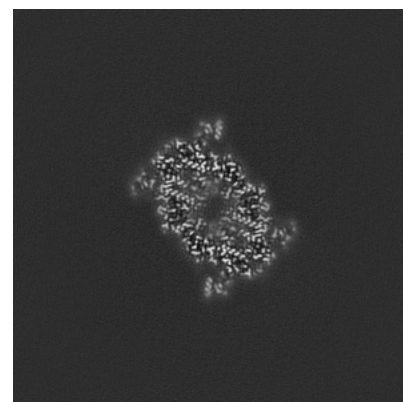
6.3.2 Raw map



X Index: 178



Y Index: 204

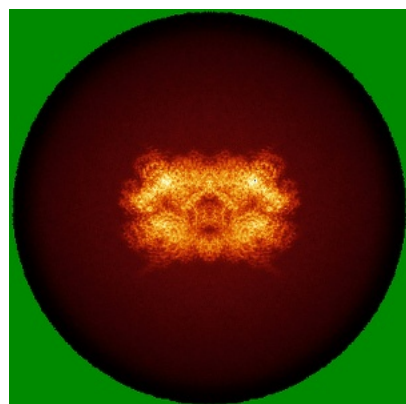


Z Index: 203

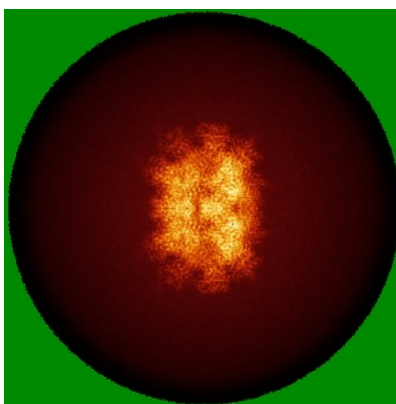
The images above show the largest variance slices of the map in three orthogonal directions.

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

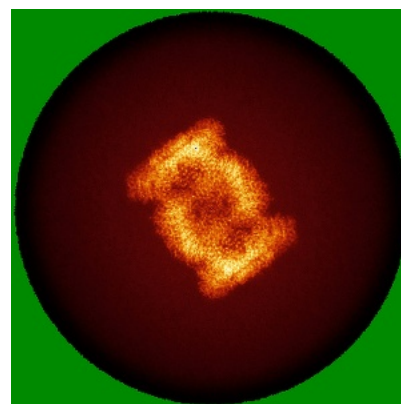
6.4.1 Primary map



X

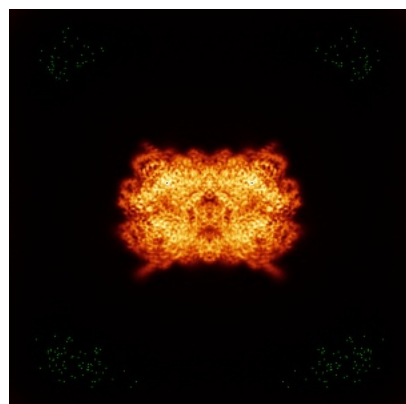


Y

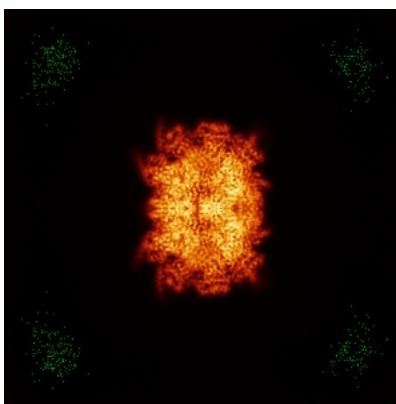


Z

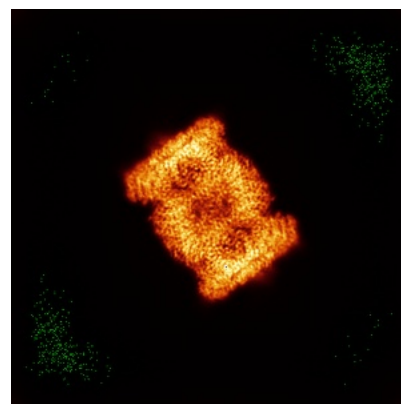
6.4.2 Raw map



X



Y

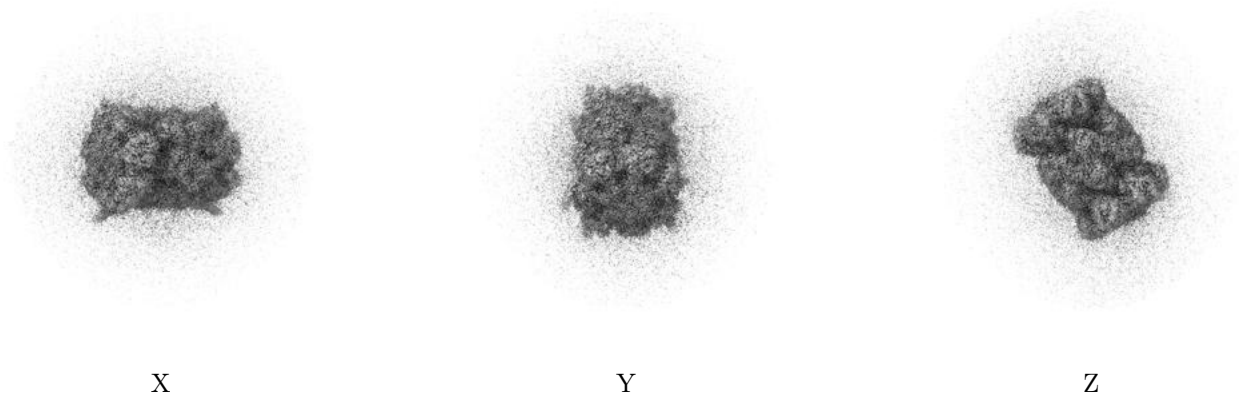


Z

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.

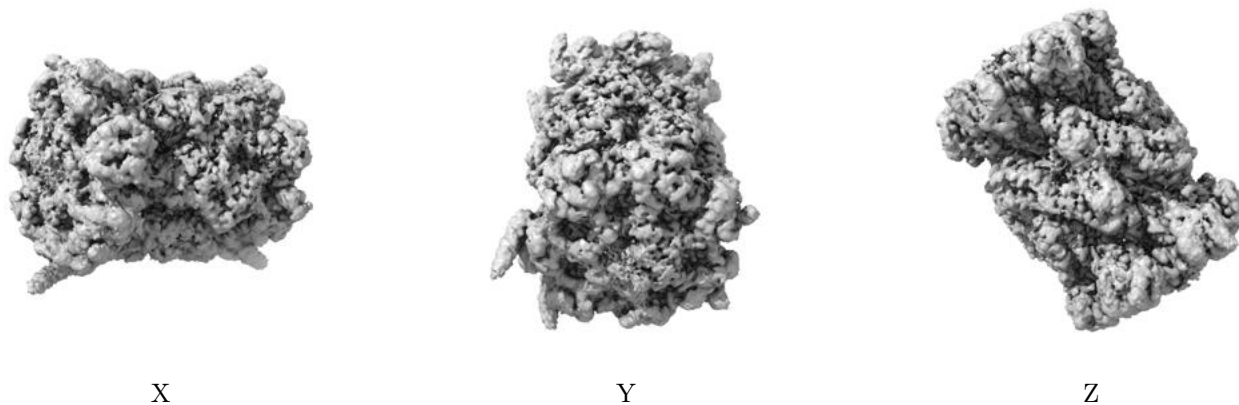
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.426. 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.

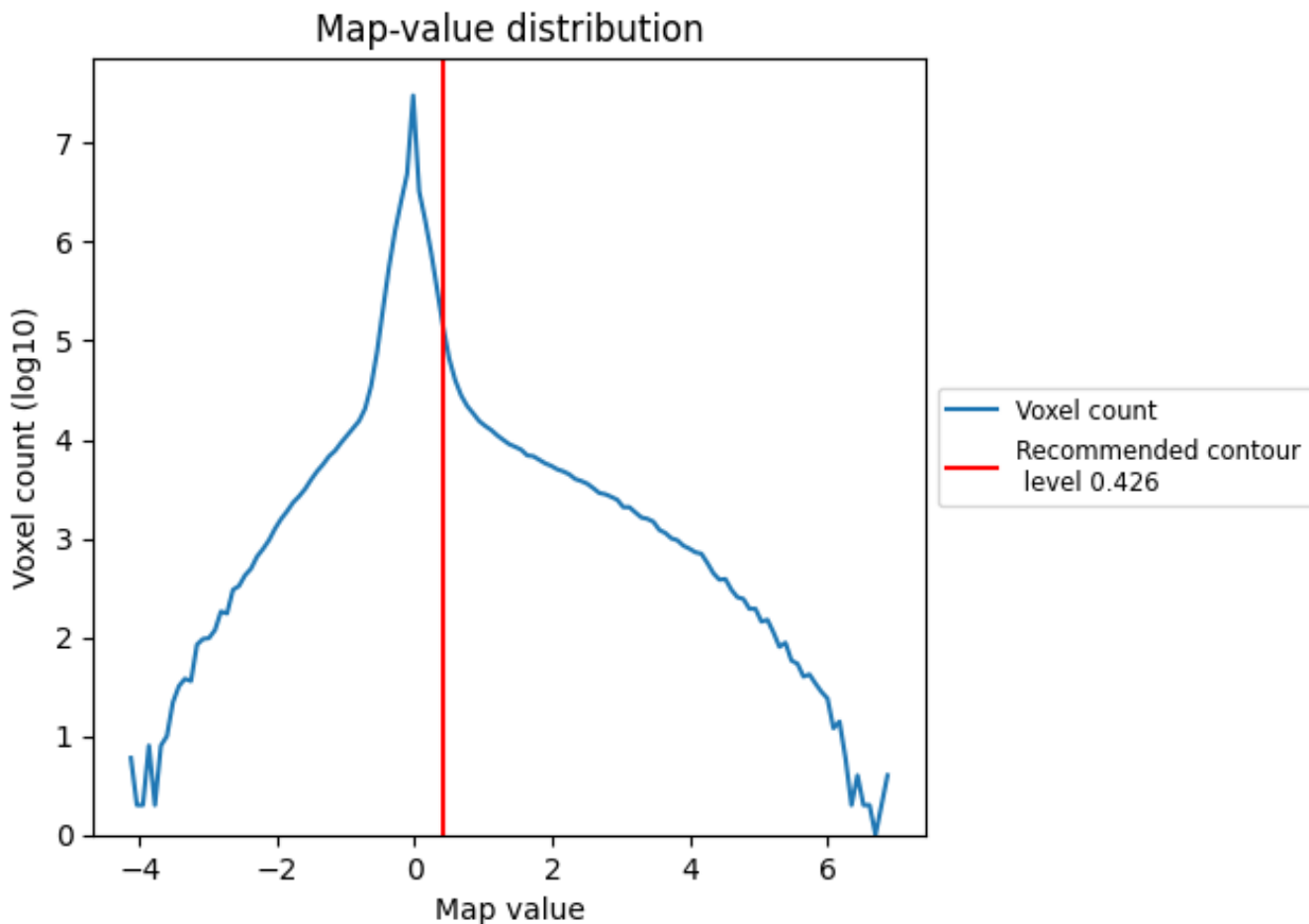
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

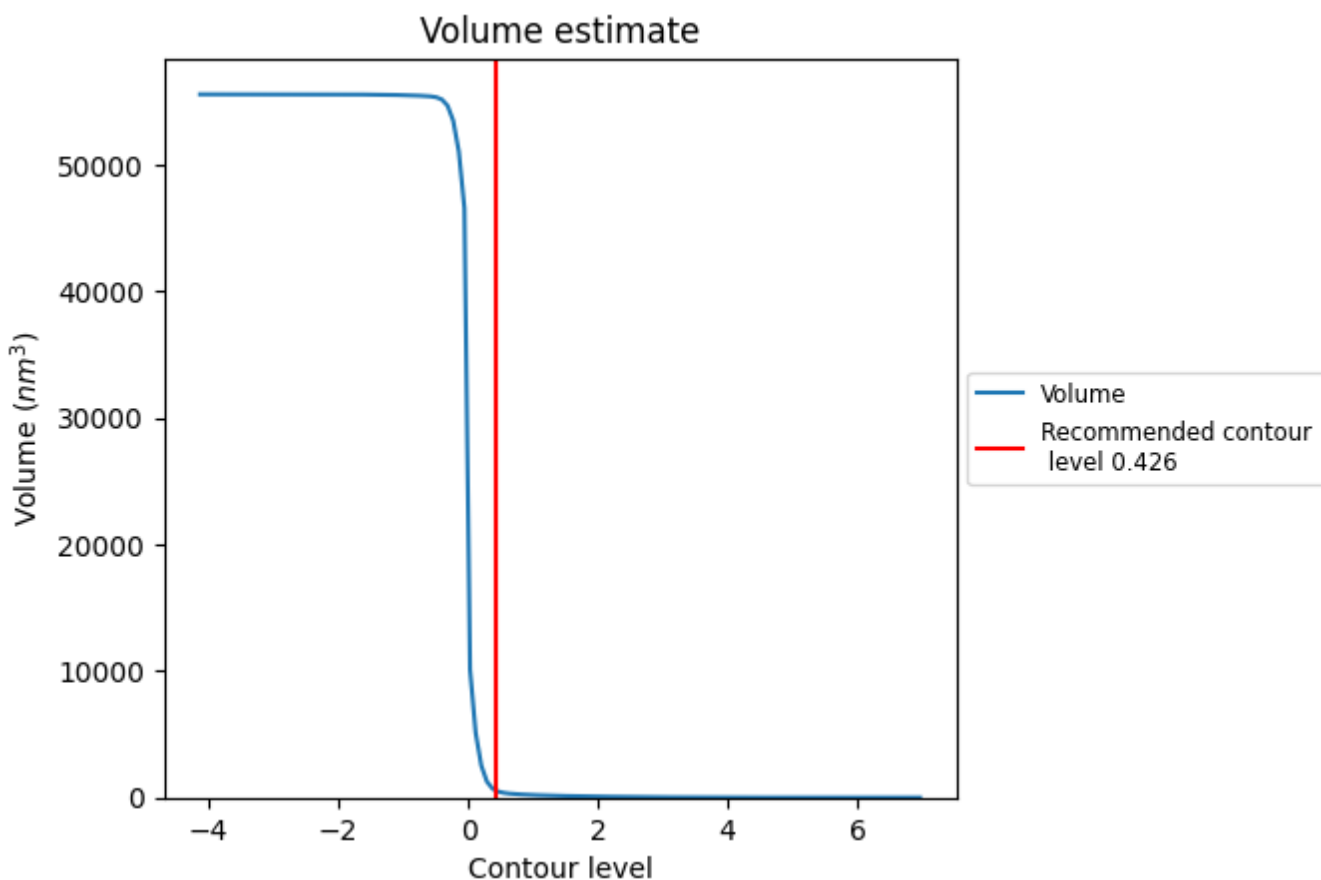
This section contains the results of statistical analysis of the map.

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.

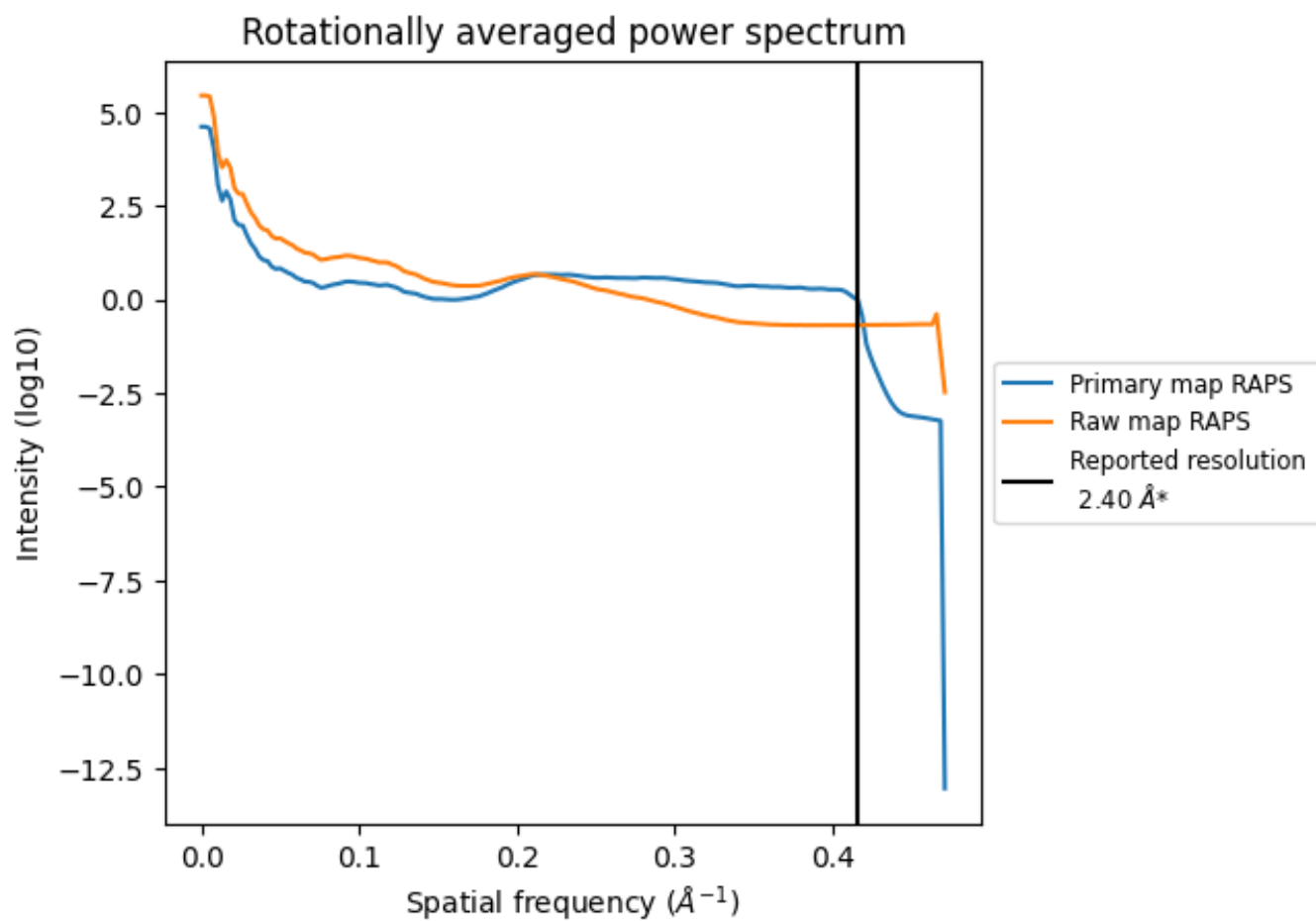
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 579 nm^3 ; this corresponds to an approximate mass of 523 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](#)

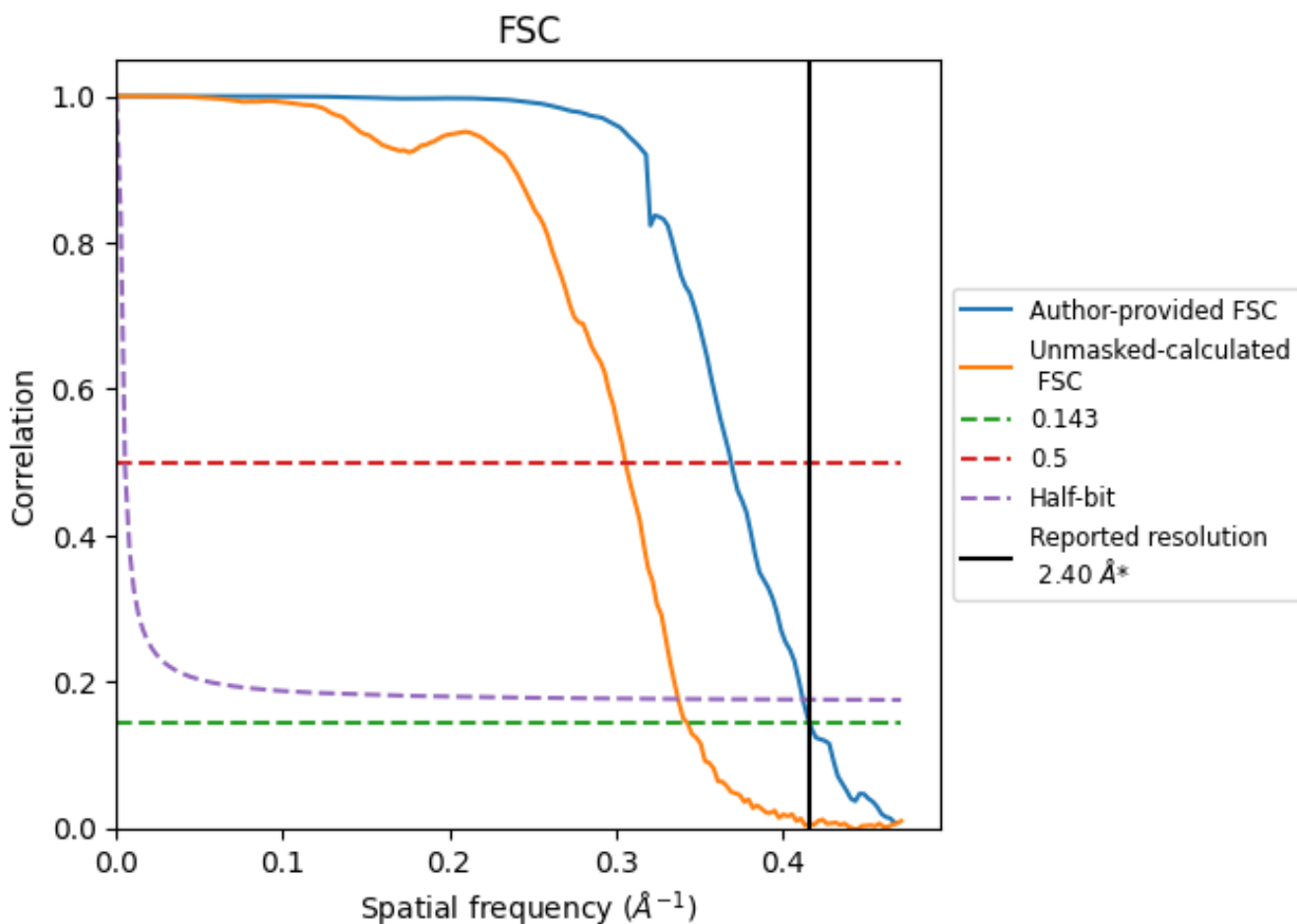


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 Å⁻¹

8.2 Resolution estimates

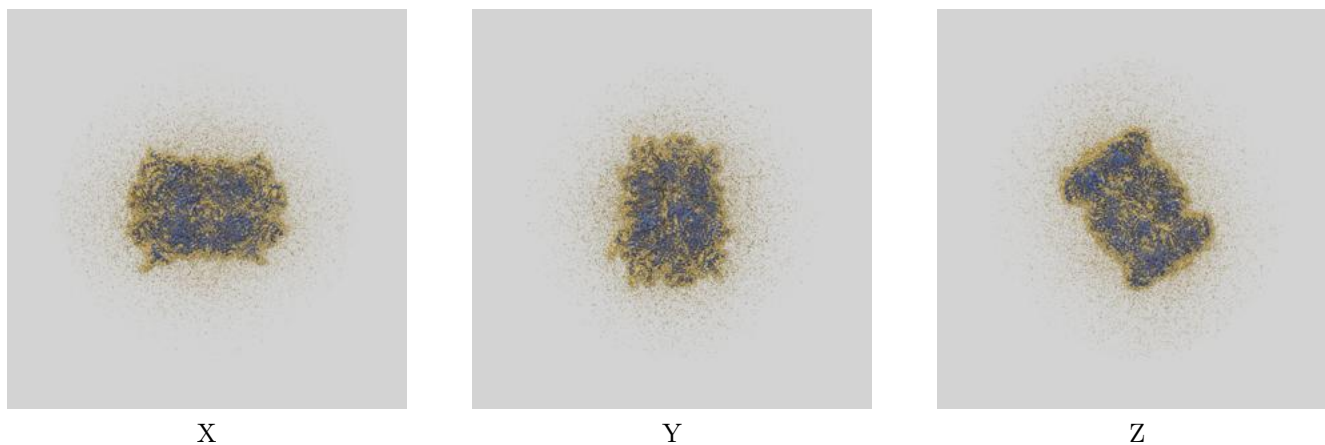
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.71	2.42
Unmasked-calculated*	2.91	3.27	2.96

*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 2.91 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

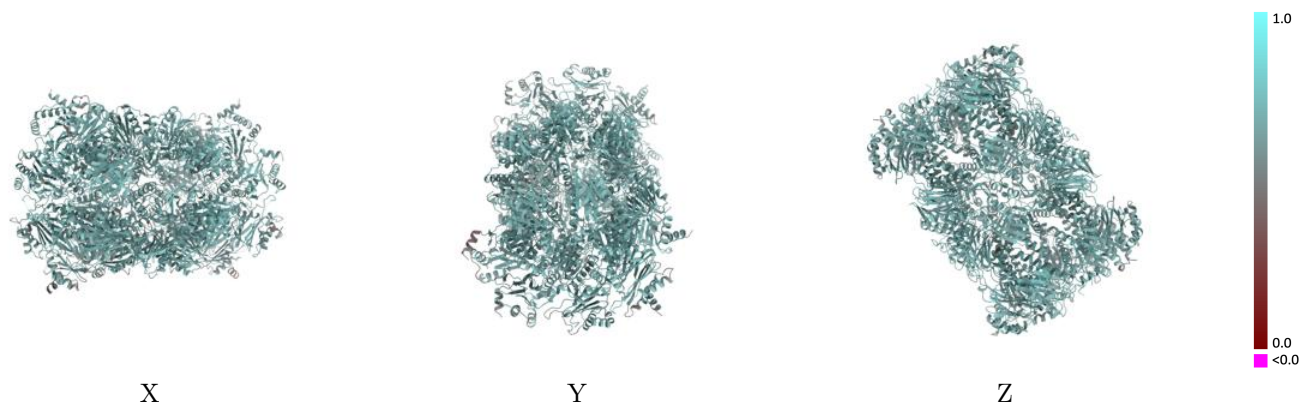
This section contains information regarding the fit between EMDB map EMD-40944 and PDB model 8T0M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



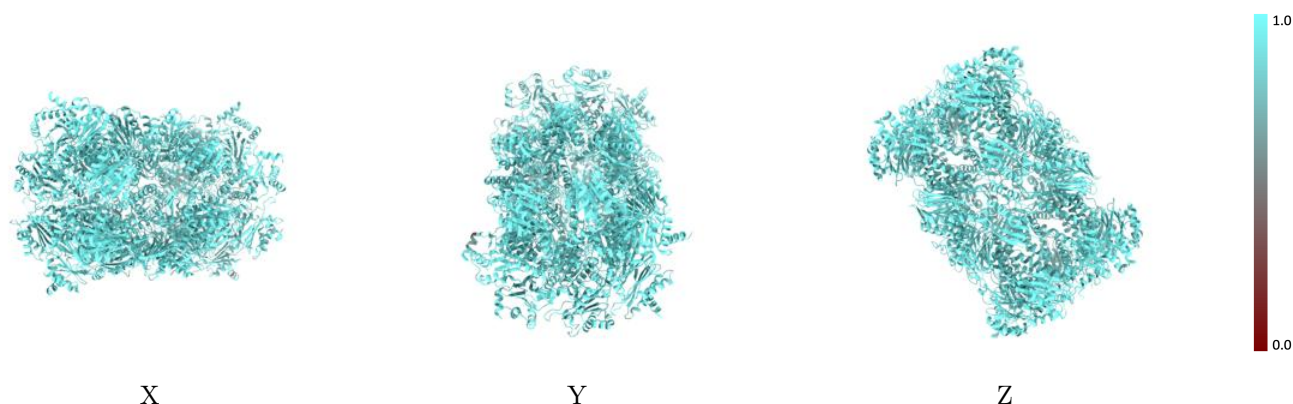
The images above show the 3D surface view of the map at the recommended contour level 0.426 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



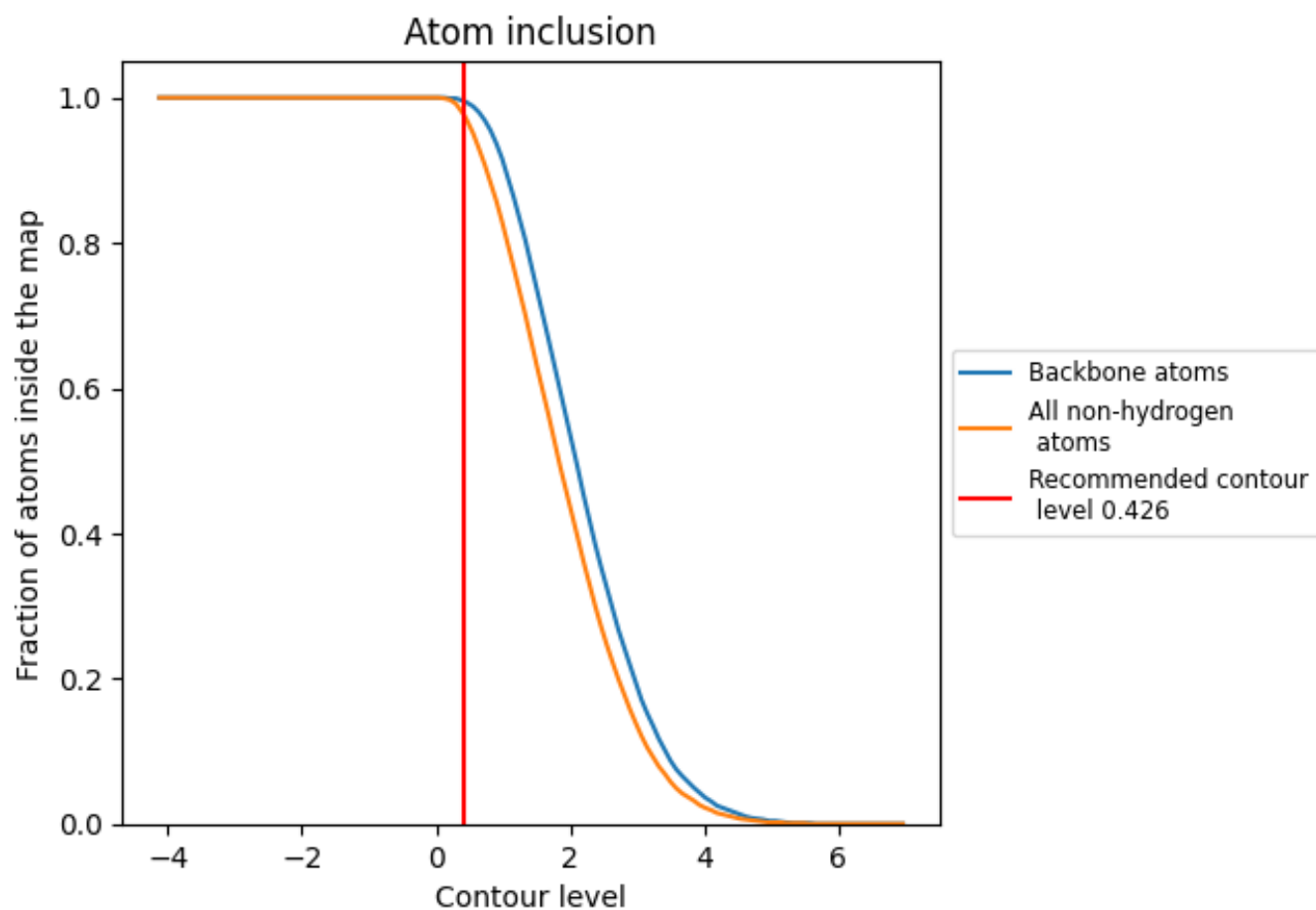
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.426).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.426) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6600
A	 0.9890	 0.6690
B	 0.9780	 0.6680
C	 0.9700	 0.6520
D	 0.9590	 0.6190
E	 0.9590	 0.6270
F	 0.9720	 0.6520
G	 0.9700	 0.6610
H	 0.9800	 0.6610
I	 0.9820	 0.6730
J	 0.9840	 0.6840
K	 0.9690	 0.6520
L	 0.9810	 0.6690
M	 0.9770	 0.6680
N	 0.9830	 0.6780
O	 0.9880	 0.6710
P	 0.9800	 0.6710
Q	 0.9730	 0.6550
R	 0.9600	 0.6200
S	 0.9600	 0.6300
T	 0.9710	 0.6520
U	 0.9710	 0.6600
V	 0.9790	 0.6600
W	 0.9810	 0.6730
X	 0.9840	 0.6840
Y	 0.9690	 0.6540
Z	 0.9800	 0.6710
a	 0.9740	 0.6700
b	 0.9830	 0.6790

