wwPDB EM Validation Summary Report (i)

Feb 24, 2024 – 08:41 AM EST

PDB ID	:	7LS6
EMDB ID	:	EMD-23503
Title	:	Cryo-EM structure of Pre-15S proteasome core particle assembly intermediate purified from Pre3-1 proteasome mutant (G34D)
Authors	:	Schnell, H.M.; Walsh Jr, R.M.; Rawson, S.; Hanna, J.W.
Deposited on	:	2021-02-17
Resolution	:	3.17 Å(reported)
Based on initial model	:	4G4S

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 (i) 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 (i)) were used in the production of this report:

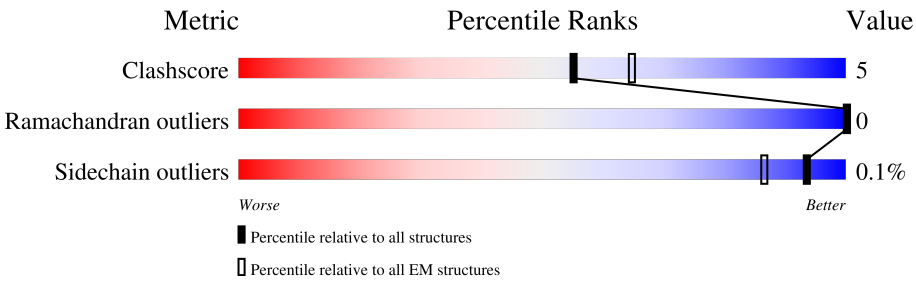
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.17 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	252	88% 9% •
2	B	250	87% 12% •
3	C	258	78% 13% 9%
4	D	254	81% 11% 7%
5	E	260	83% 12% •
6	F	234	92% 8%
7	G	288	73% 12% 15%
8	H	148	7% 66% 14% 20%

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Mol	Chain	Length	Quality of chain
9	I	261	69% 9% 21%
10	J	205	77% 8% 16%
11	K	198	11% 88% 9%
12	O	276	72% 15% 13%
13	P	267	6% 86% 10%
14	L	287	9% 48% 13% 38%
15	M	241	35% 56% 10% 34%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 50103 atoms, of which 25006 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	H	N	O	S		
1	A	245	3852	1226	1924	324	370	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	247	3791	1204	1900	312	372	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	234	3676	1165	1840	304	364	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	235	3700	1153	1859	322	362	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	249	3827	1204	1903	324	388	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	234	3614	1134	1811	313	351	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	245	3795	1208	1894	330	359	4	0	0

- Molecule 8 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	118	1875	584	927	170	188	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	205	3101	982	1547	269	298	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	173	2699	878	1346	213	255	7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	191	3066	973	1536	259	292	6	0	0

- Molecule 12 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	O	240	3768	1216	1898	290	351	13	0	0

- Molecule 13 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	P	257	4133	1351	2046	333	395	8	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	L	177	2723	879	1347	233	256	8	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-6.

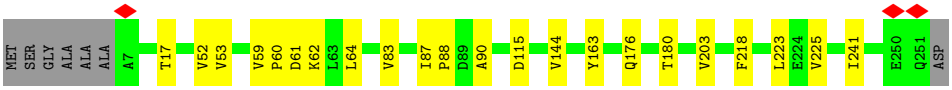
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	M	160	2483	807	1228	210	234	4	0	0

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.

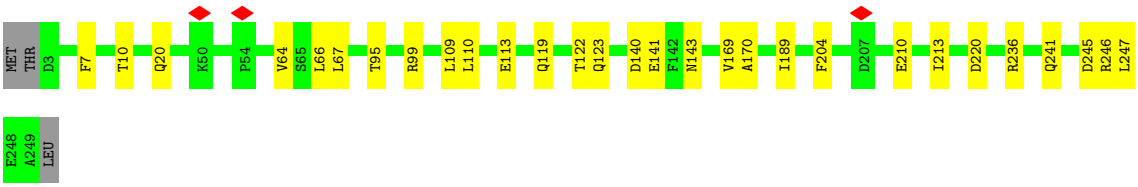
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



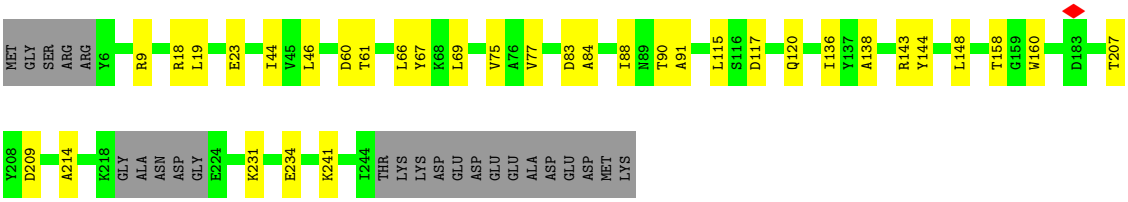
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



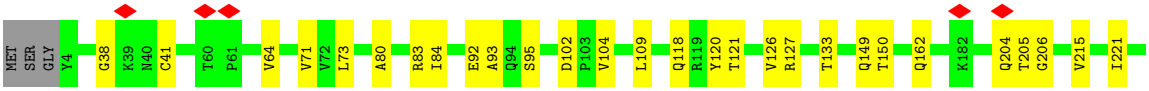
• Molecule 3: Proteasome subunit alpha type-3

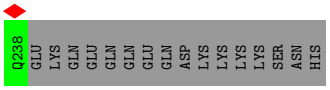
Chain C:



• Molecule 4: Proteasome subunit alpha type-4

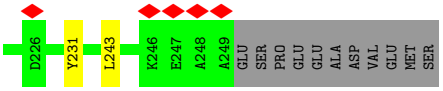
Chain D:





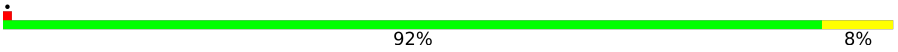
• Molecule 5: Proteasome subunit alpha type-5

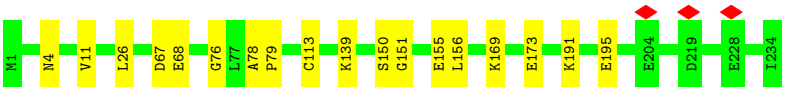
Chain E:



• Molecule 6: Proteasome subunit alpha type-6

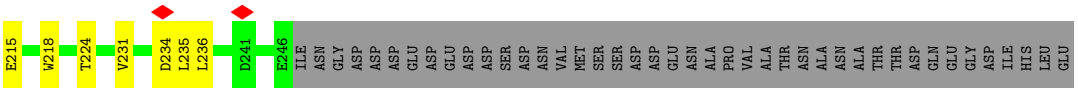
Chain F:





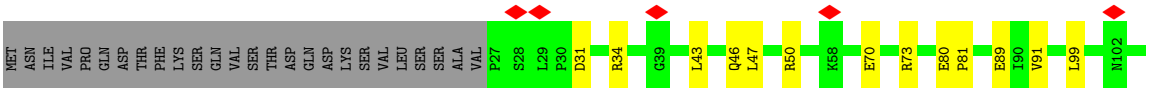
• Molecule 7: Proteasome subunit alpha type-7

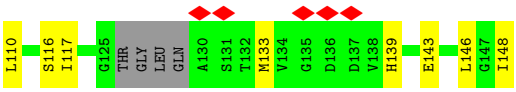
Chain G:



• Molecule 8: Proteasome maturation factor UMP1

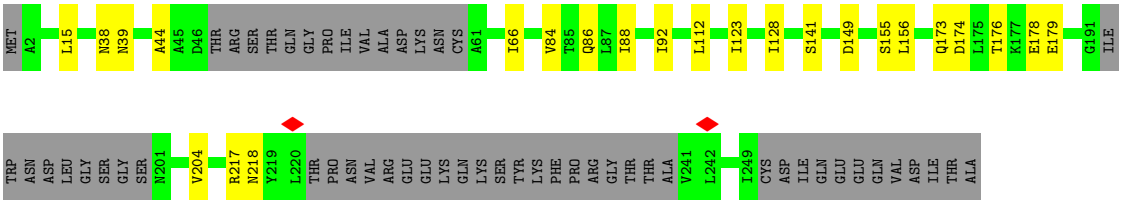
Chain H:



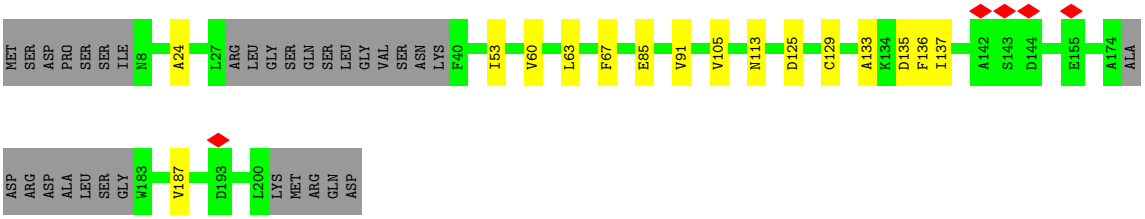


• Molecule 9: Proteasome subunit beta type-2

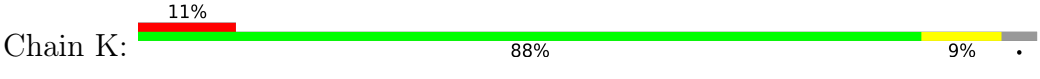
Chain I:

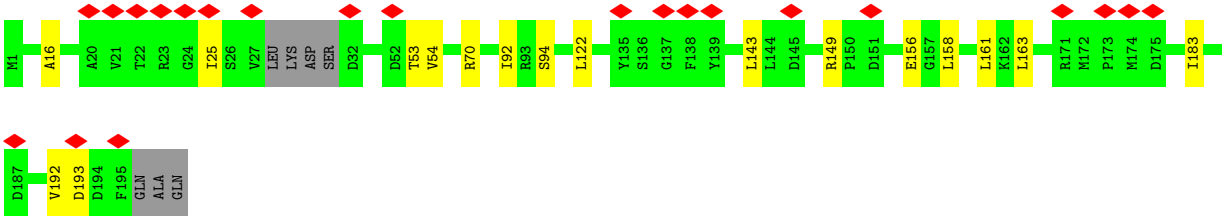


• Molecule 10: Proteasome subunit beta type-3

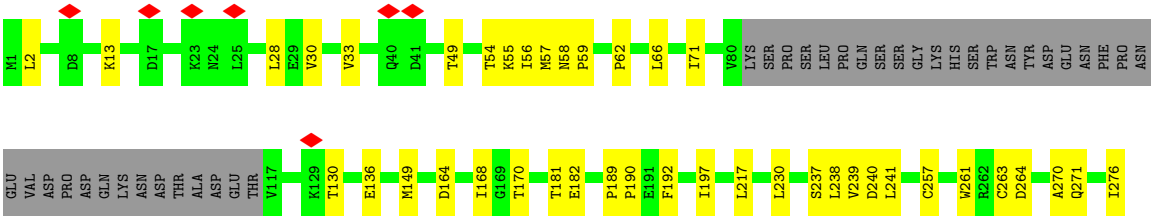


• Molecule 11: Proteasome subunit beta type-4

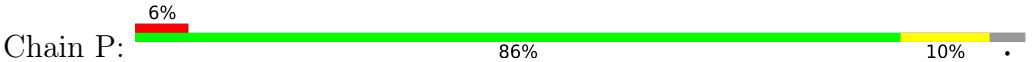


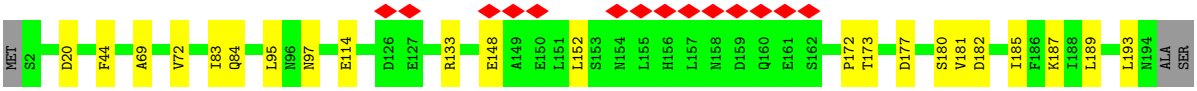


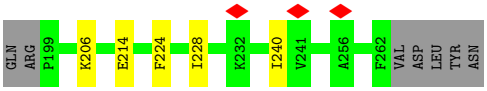
• Molecule 12: Proteasome chaperone 1



• Molecule 13: Proteasome assembly chaperone 2

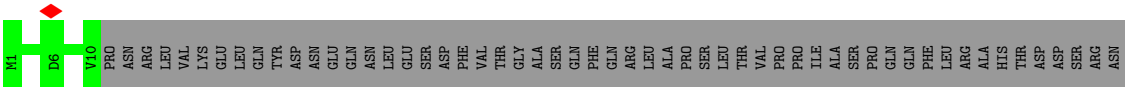


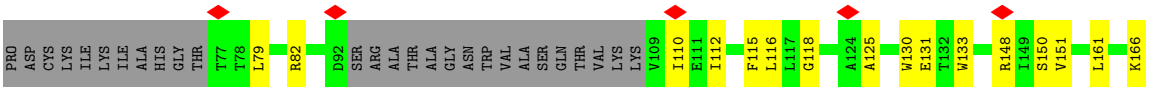


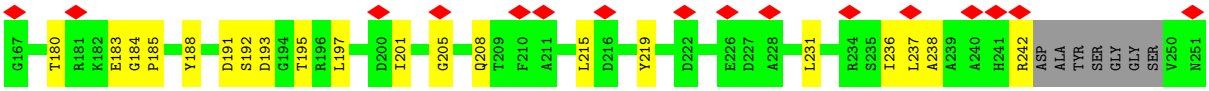


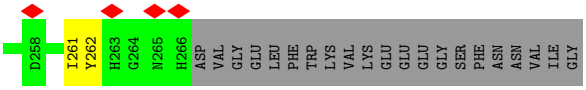
• Molecule 14: Proteasome subunit beta type-5

Chain L:



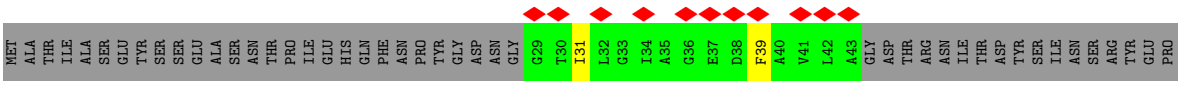


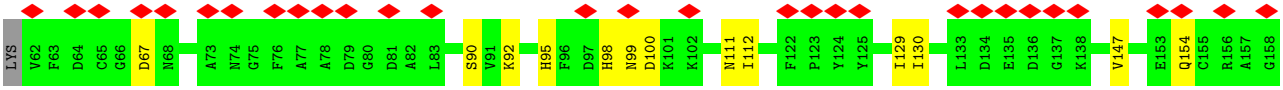


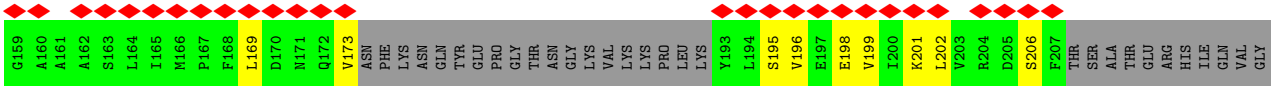


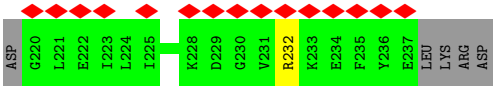
• Molecule 15: Proteasome subunit beta type-6

Chain M:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95288	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 ($e^-/Å^2$)	55.94	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.894	Depositor
Minimum map value	-1.672	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.5	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	0.26	0/1966	0.48	0/2663
2	B	0.26	0/1928	0.47	0/2611
3	C	0.26	0/1865	0.48	0/2525
4	D	0.25	0/1870	0.50	0/2534
5	E	0.25	0/1951	0.50	0/2628
6	F	0.26	0/1831	0.50	0/2473
7	G	0.27	0/1941	0.46	0/2621
8	H	0.25	0/964	0.50	0/1301
9	I	0.25	0/1580	0.49	0/2139
10	J	0.27	0/1380	0.46	0/1864
11	K	0.25	0/1557	0.48	0/2098
12	O	0.26	0/1914	0.45	0/2597
13	P	0.25	0/2138	0.45	0/2904
14	L	0.26	0/1404	0.49	0/1896
15	M	0.27	0/1279	0.49	0/1721
All	All	0.26	0/25568	0.48	0/34575

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)

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	1928	1924	1921	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1891	1900	1899	19	0
3	C	1836	1840	1838	24	0
4	D	1841	1859	1856	25	0
5	E	1924	1903	1902	22	0
6	F	1803	1811	1809	13	0
7	G	1901	1894	1892	26	0
8	H	948	927	926	22	0
9	I	1554	1547	1542	17	0
10	J	1353	1346	1343	9	0
11	K	1530	1536	1535	11	0
12	O	1870	1898	1897	32	0
13	P	2087	2046	2045	19	0
14	L	1376	1347	1341	26	0
15	M	1255	1228	1223	18	0
All	All	25097	25006	24969	267	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 5.

The worst 5 of 267 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)
14:L:191:ASP:OD1	14:L:192:SER:N	2.09	0.86
13:P:20:ASP:OD1	13:P:84:GLN:NE2	2.09	0.85
9:I:176:THR:OG1	9:I:179:GLU:OE1	1.98	0.81
5:E:44:GLU:OE2	5:E:192:THR:OG1	1.98	0.81
9:I:128:ILE:HD11	9:I:156:LEU:HD23	1.64	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	
1	A	243/252 (96%)	239 (98%)	4 (2%)	0	100	100
2	B	245/250 (98%)	244 (100%)	1 (0%)	0	100	100
3	C	230/258 (89%)	223 (97%)	7 (3%)	0	100	100
4	D	233/254 (92%)	228 (98%)	5 (2%)	0	100	100
5	E	247/260 (95%)	245 (99%)	2 (1%)	0	100	100
6	F	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
7	G	243/288 (84%)	239 (98%)	4 (2%)	0	100	100
8	H	114/148 (77%)	114 (100%)	0	0	100	100
9	I	197/261 (76%)	193 (98%)	4 (2%)	0	100	100
10	J	167/205 (82%)	164 (98%)	3 (2%)	0	100	100
11	K	187/198 (94%)	183 (98%)	4 (2%)	0	100	100
12	O	236/276 (86%)	229 (97%)	7 (3%)	0	100	100
13	P	253/267 (95%)	238 (94%)	15 (6%)	0	100	100
14	L	169/287 (59%)	167 (99%)	2 (1%)	0	100	100
15	M	152/241 (63%)	148 (97%)	4 (3%)	0	100	100
All	All	3148/3679 (86%)	3082 (98%)	66 (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	207/210 (99%)	207 (100%)	0	100	100
2	B	206/209 (99%)	206 (100%)	0	100	100
3	C	197/216 (91%)	196 (100%)	1 (0%)	88	95
4	D	208/226 (92%)	208 (100%)	0	100	100
5	E	205/215 (95%)	205 (100%)	0	100	100
6	F	193/193 (100%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	202/239 (84%)	201 (100%)	1 (0%)	88	95
8	H	108/136 (79%)	107 (99%)	1 (1%)	78	91
9	I	165/214 (77%)	165 (100%)	0	100	100
10	J	146/173 (84%)	146 (100%)	0	100	100
11	K	169/175 (97%)	169 (100%)	0	100	100
12	O	217/251 (86%)	217 (100%)	0	100	100
13	P	235/244 (96%)	235 (100%)	0	100	100
14	L	142/235 (60%)	142 (100%)	0	100	100
15	M	130/201 (65%)	129 (99%)	1 (1%)	81	92
All	All	2730/3137 (87%)	2726 (100%)	4 (0%)	93	98

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

Mol	Chain	Res	Type
3	C	241	LYS
7	G	72	ARG
8	H	73	ARG
15	M	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
2	B	139	HIS
7	G	64	ASN

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.

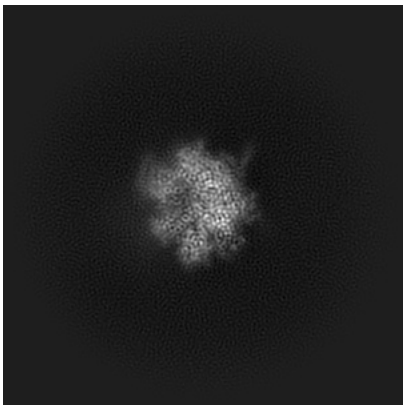
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23503. These allow visual inspection of the internal detail of the map and identification of artifacts.

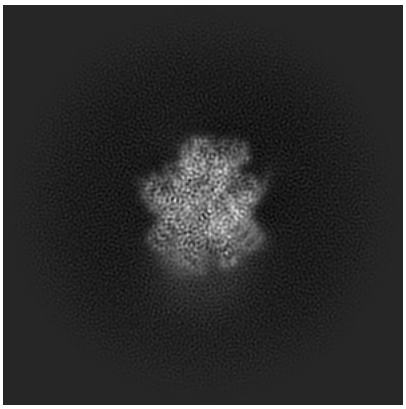
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

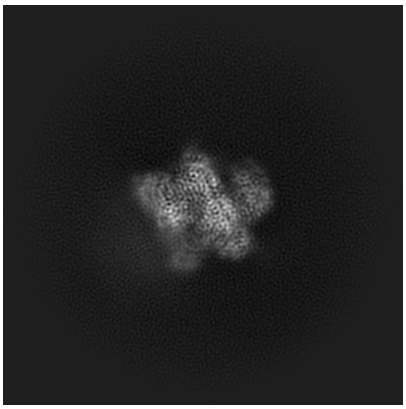
6.1.1 Primary map



X

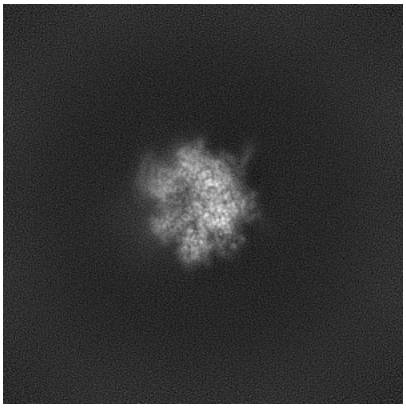


Y

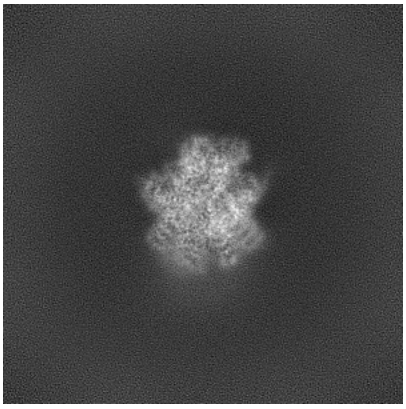


Z

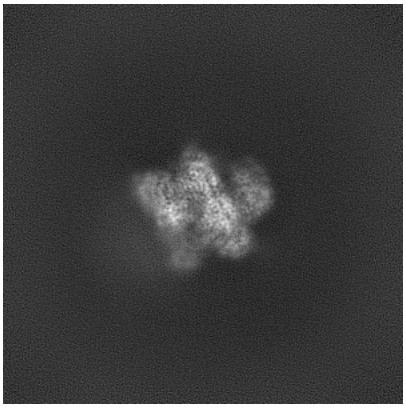
6.1.2 Raw map



X



Y

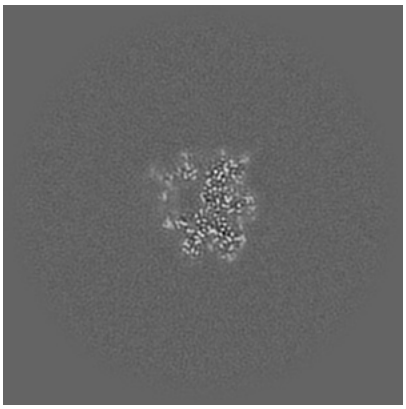


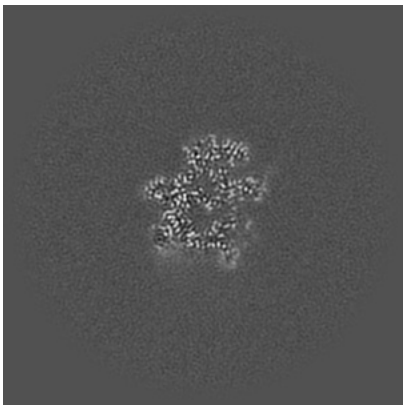
Z

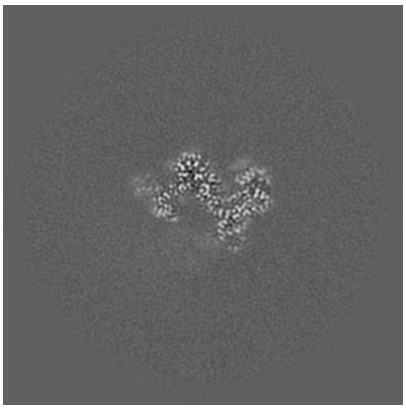
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

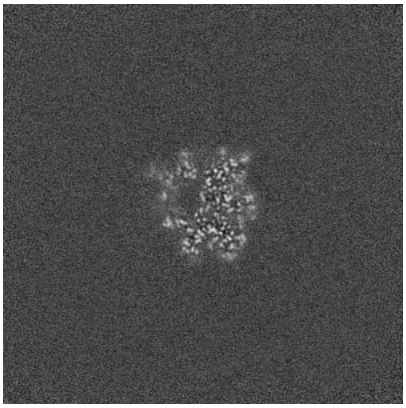
6.2.1 Primary map

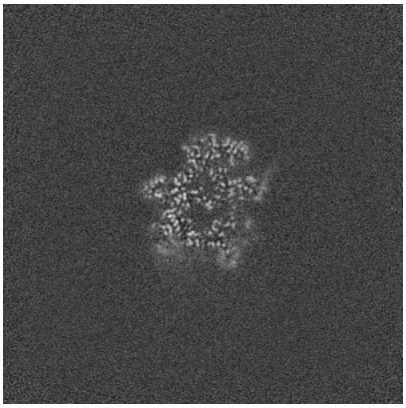

X Index: 180

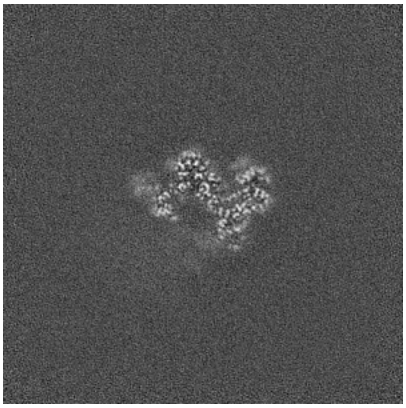

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

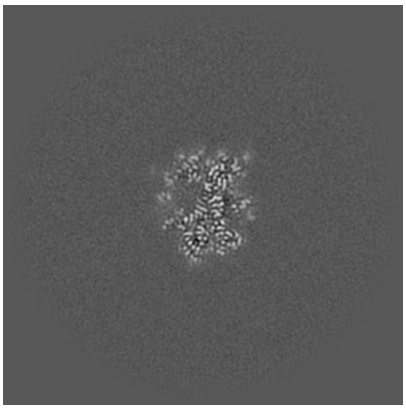

Y Index: 180


Z Index: 180

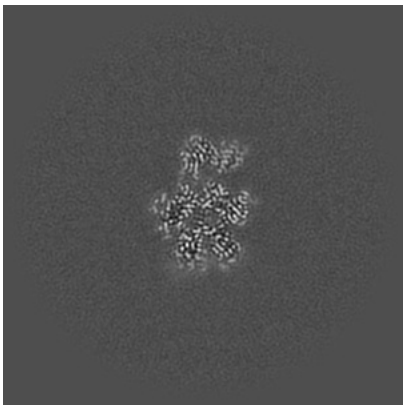
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

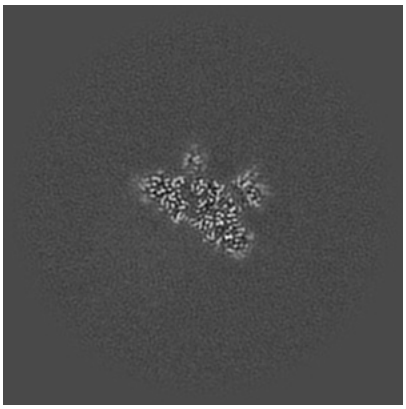
6.3.1 Primary map



X Index: 183

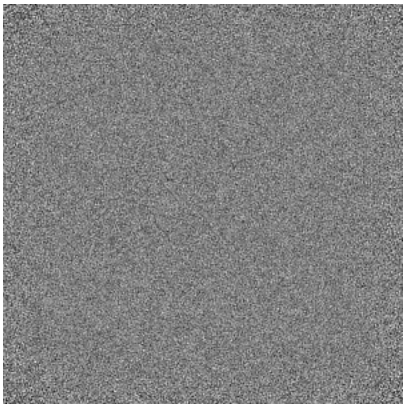


Y Index: 193

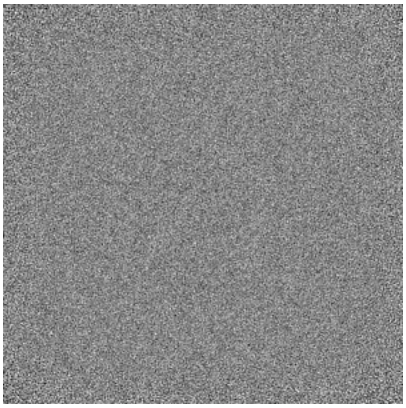


Z Index: 166

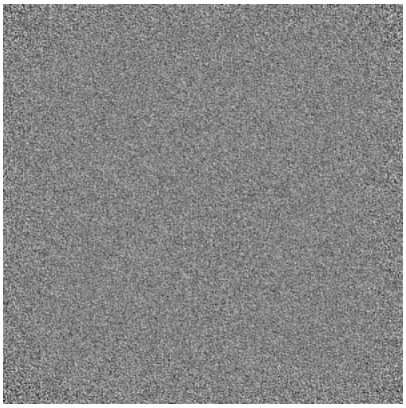
6.3.2 Raw map



X Index: 0



Y Index: 0

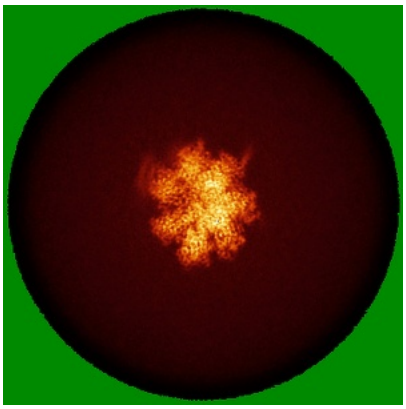


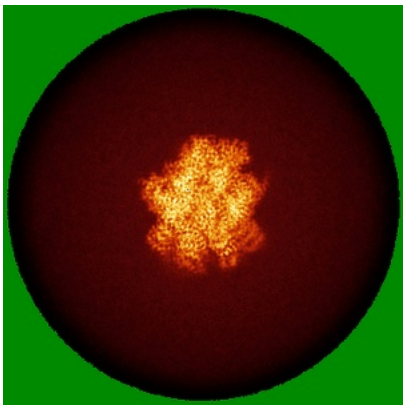
Z Index: 0

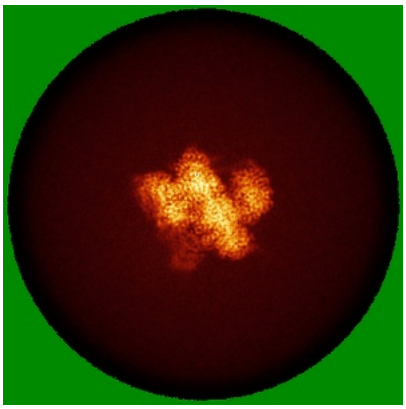
The images above show the largest variance slices of the map in three orthogonal directions.

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

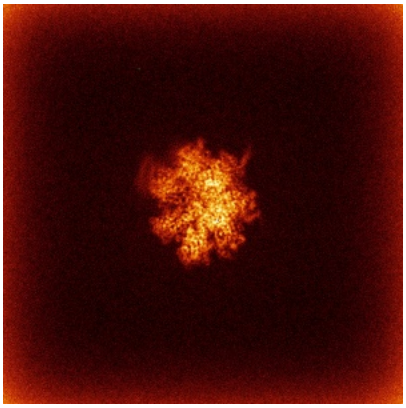
6.4.1 Primary map

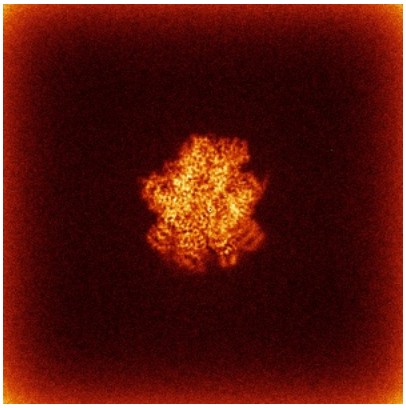

X

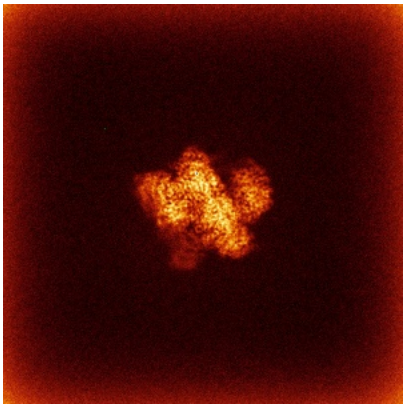

Y


Z

6.4.2 Raw map


X

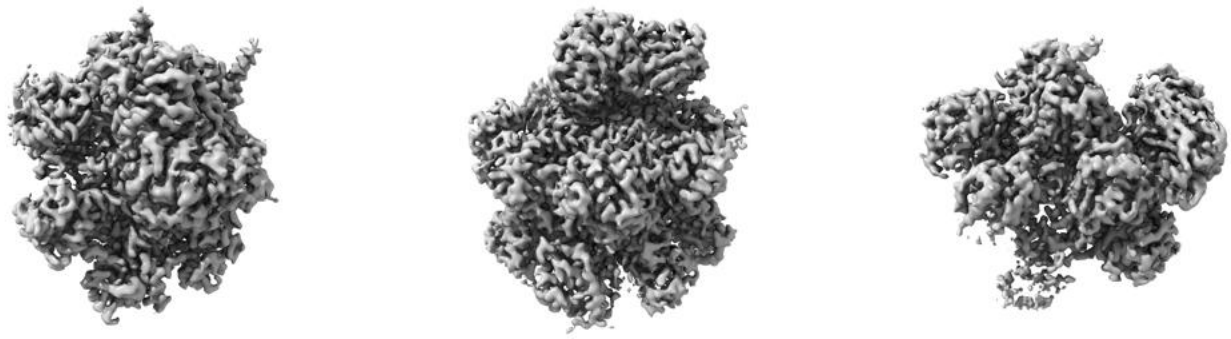

Y


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



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.

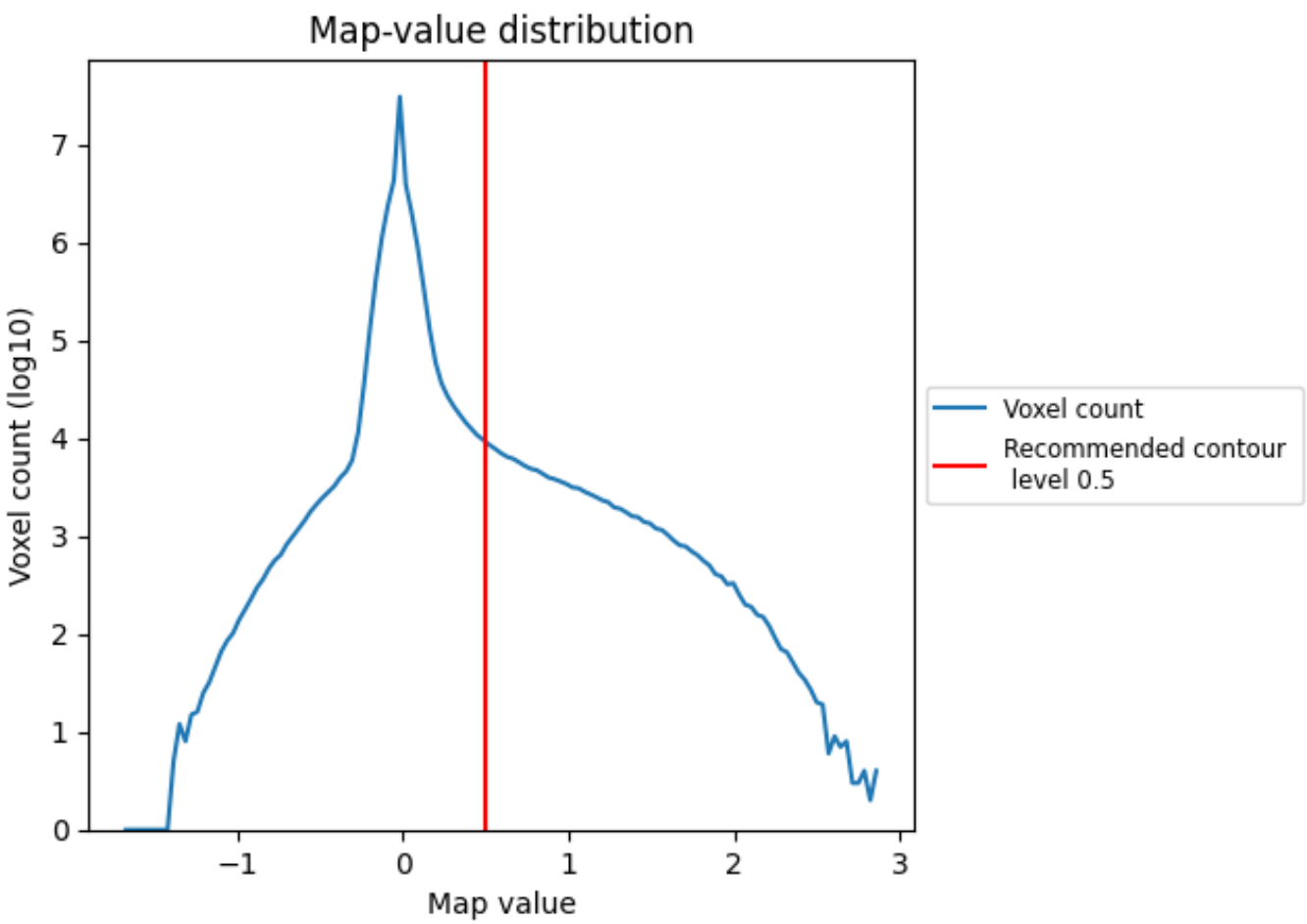
6.6 Mask visualisation (i)

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

7 Map analysis (i)

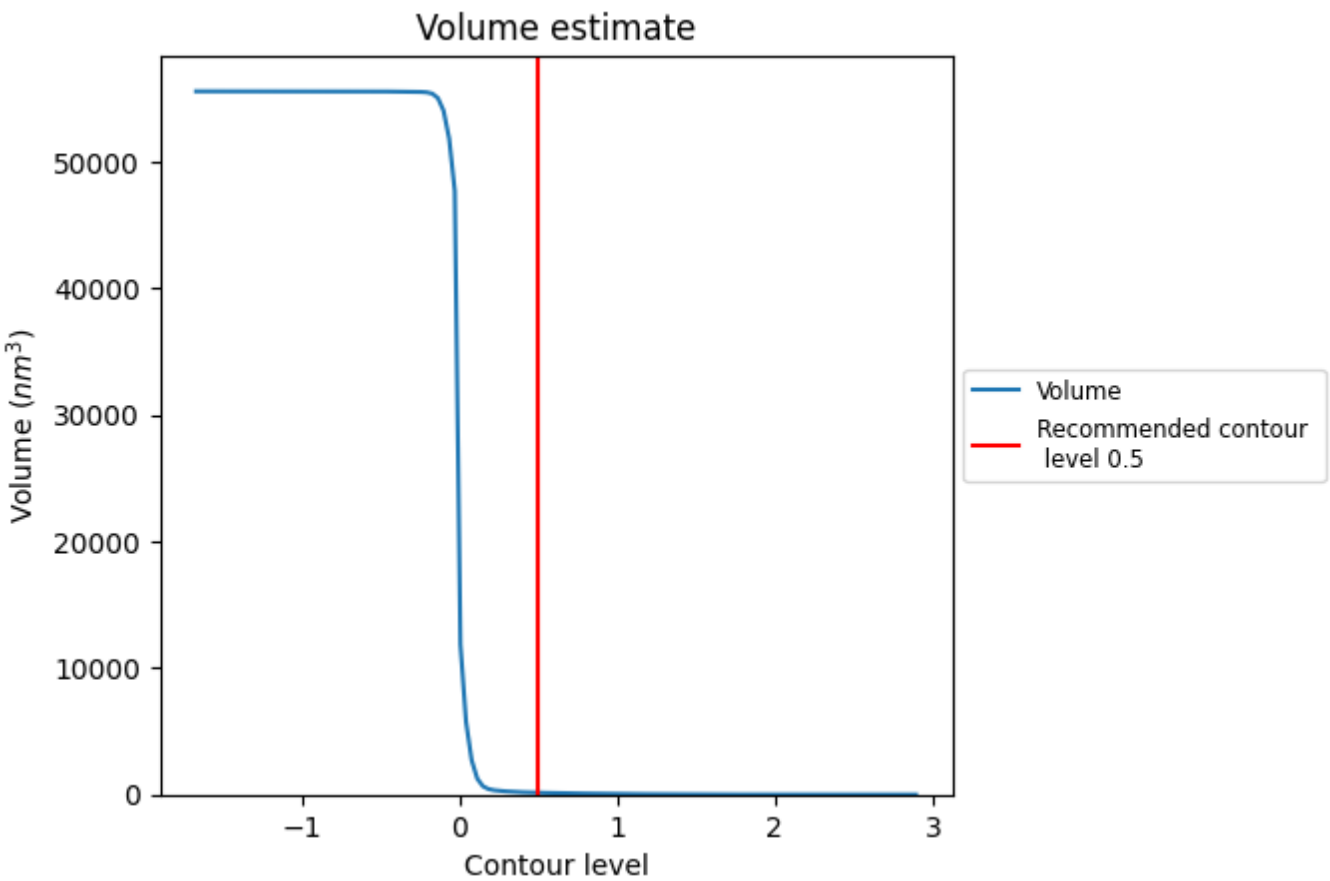
This section contains the results of statistical analysis of the map.

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.

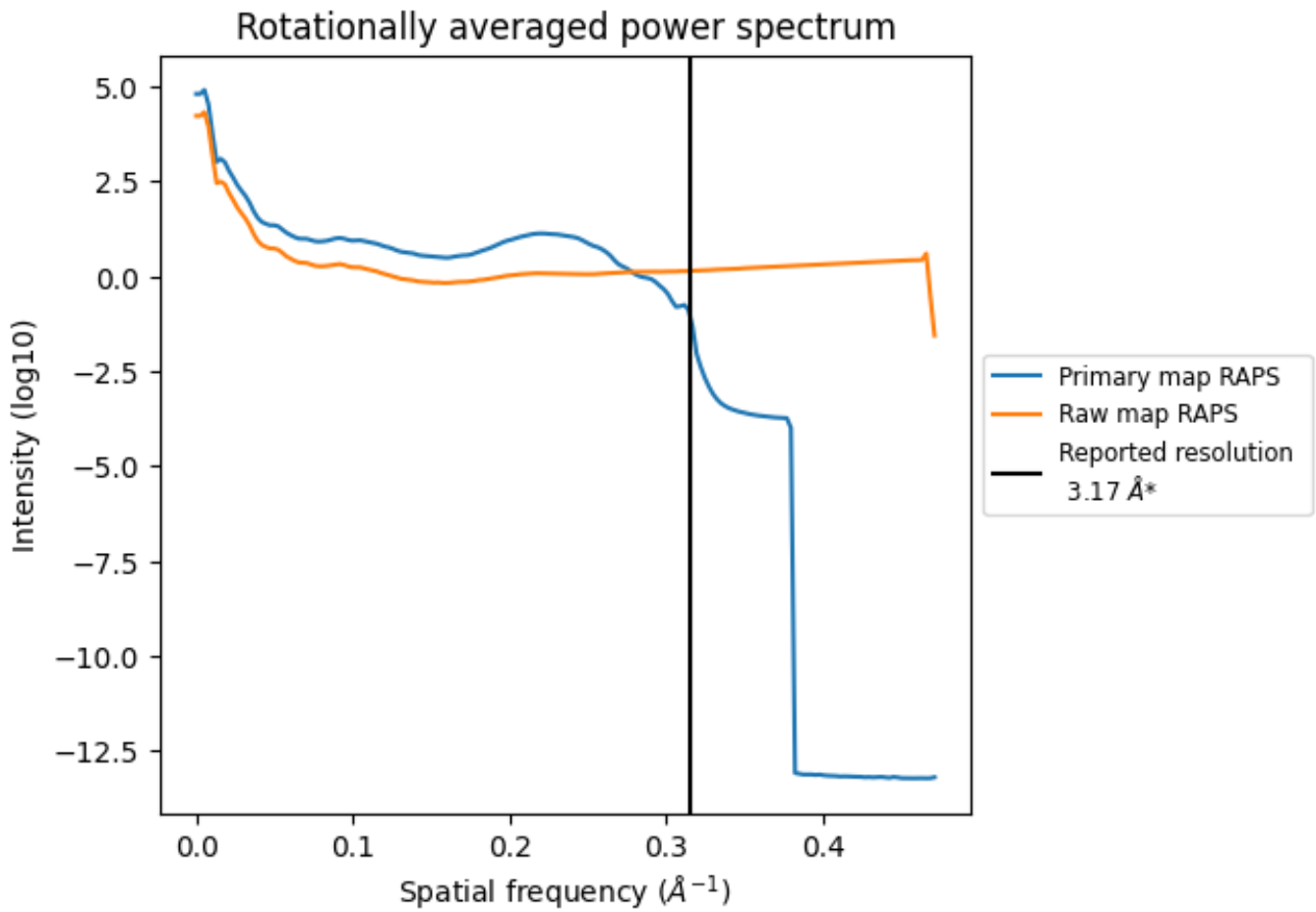
7.2 Volume estimate (i)



The volume at the recommended contour level is 146 nm^3; this corresponds to an approximate mass of 132 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)

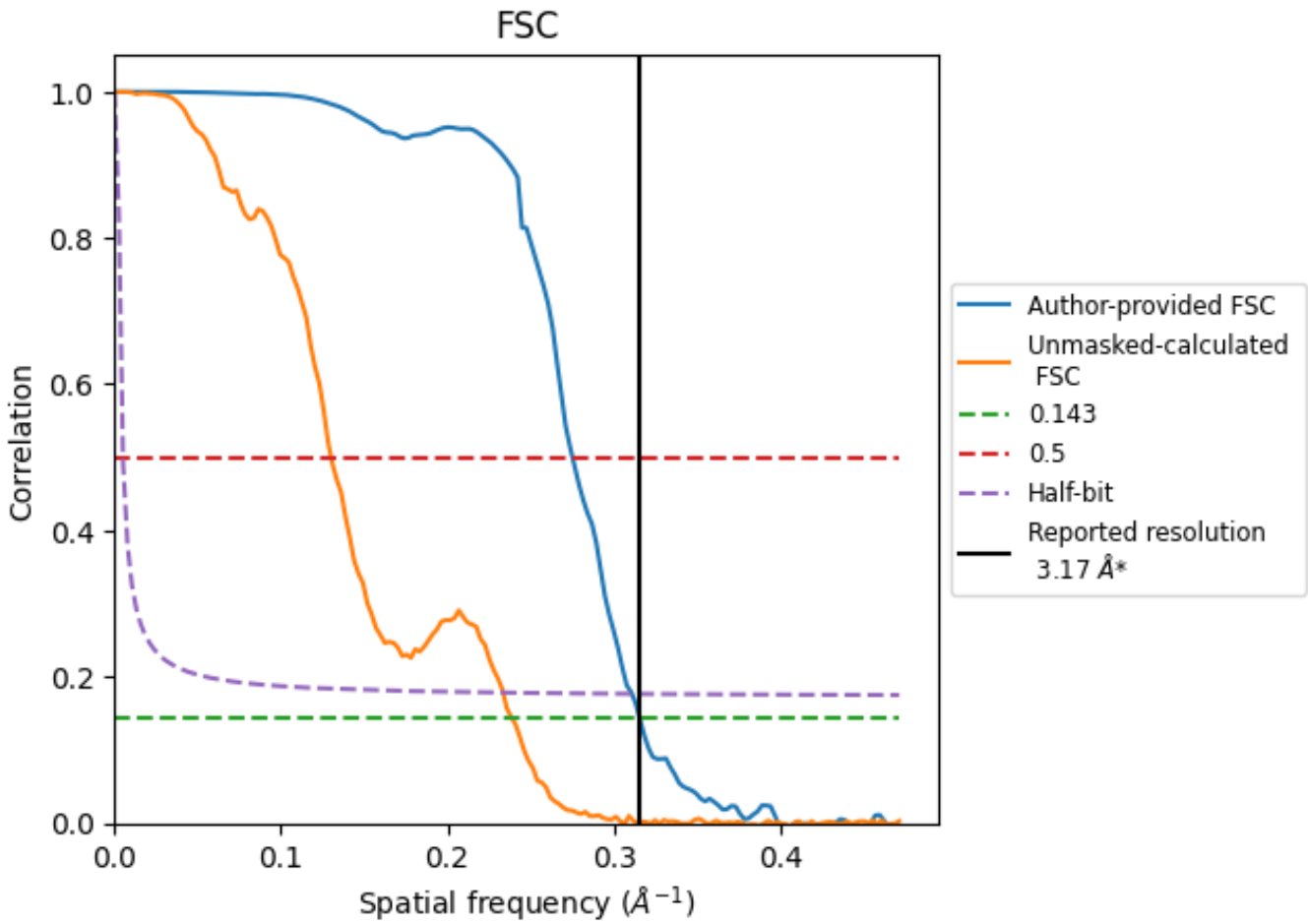


*Reported resolution corresponds to spatial frequency of 0.315 Å^{-1}

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 0.315 Å^{-1}

8.2 Resolution estimates (i)

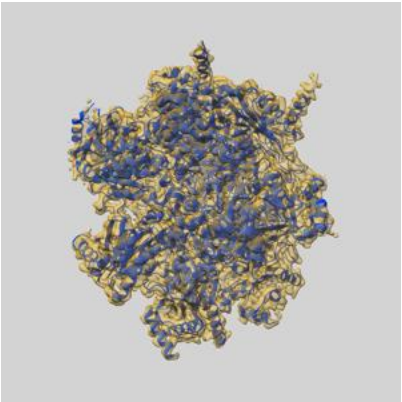
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.63	3.22
Unmasked-calculated*	4.19	7.68	4.28

*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 4.19 differs from the reported value 3.17 by more than 10 %

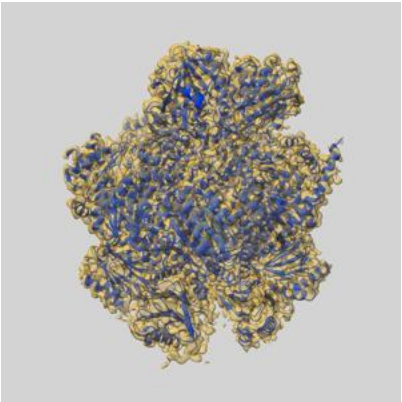
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23503 and PDB model 7LS6. Per-residue inclusion information can be found in section 3 on page 7.

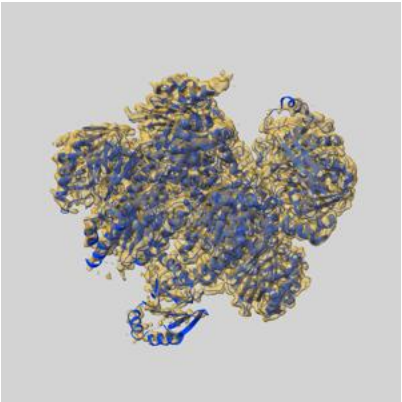
9.1 Map-model overlay (i)



X



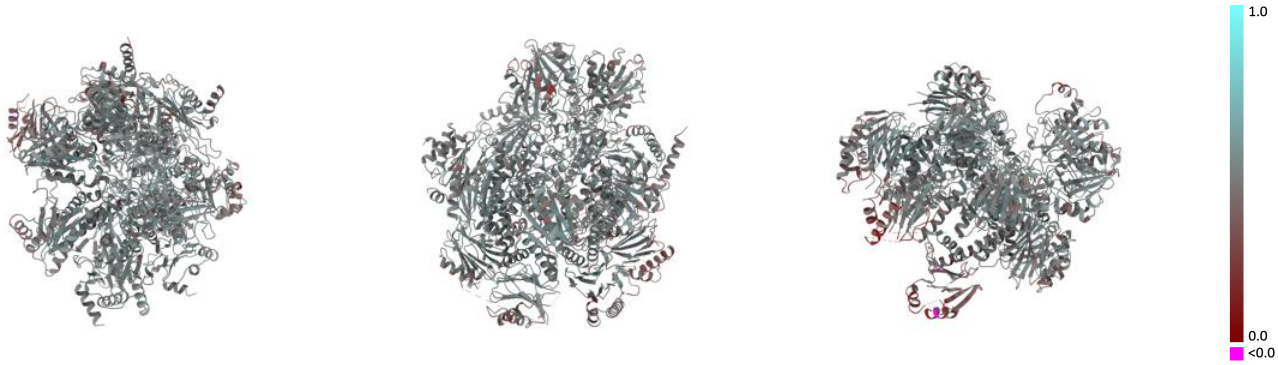
Y



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.

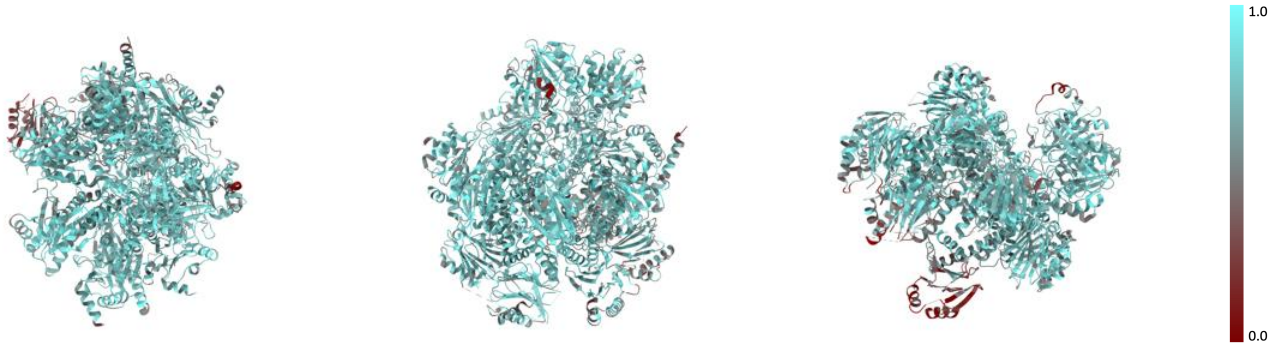
9.2 Q-score mapped to coordinate model (i)



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.

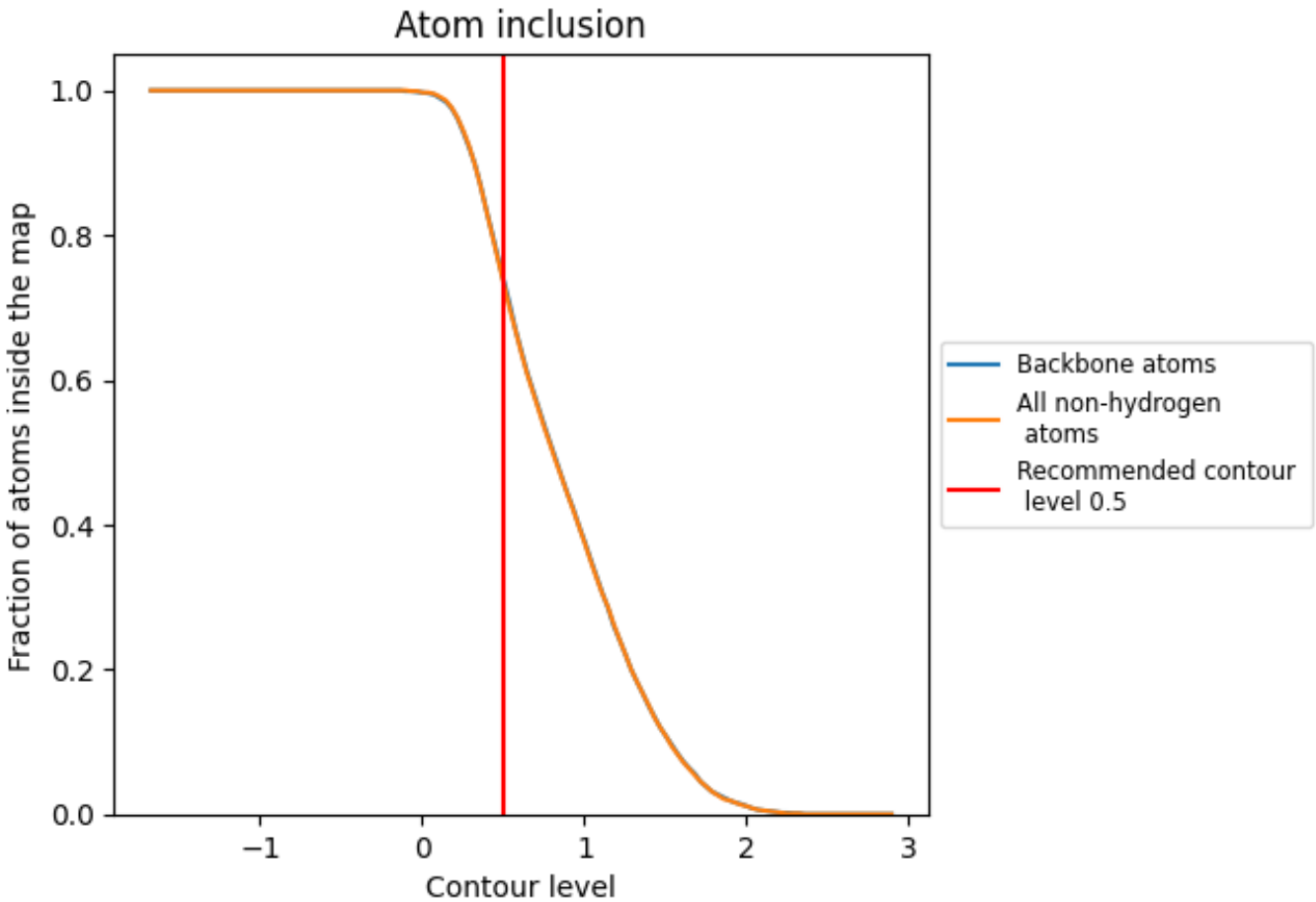
9.3 Atom inclusion mapped to coordinate model (i)



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, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7350	0.4900
A	0.7940	0.5100
B	0.7930	0.5150
C	0.7890	0.5130
D	0.7740	0.5060
E	0.7430	0.5010
F	0.7680	0.5050
G	0.7810	0.5040
H	0.7200	0.4960
I	0.7810	0.4960
J	0.7800	0.4990
K	0.7120	0.4740
L	0.6280	0.4240
M	0.4100	0.3860
O	0.7370	0.4890
P	0.7430	0.4900