



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2024 – 05:28 PM EST

PDB ID : 6MEM
EMDB ID : EMD-9107
Title : A unique supramolecular organization of photosystem I in the moss
Physcomitrella patens
Authors : Iwai, M.; Grob, P.
Deposited on : 2018-09-06
Resolution : 11.60 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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

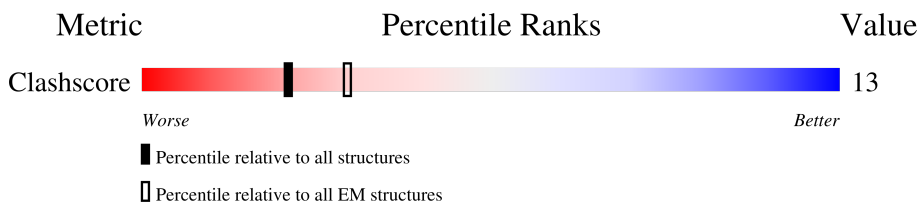
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

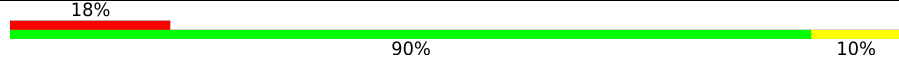
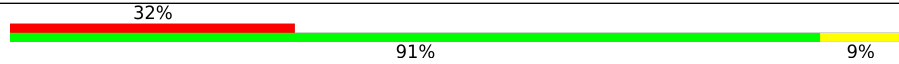
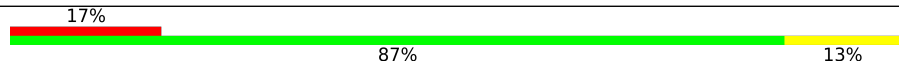
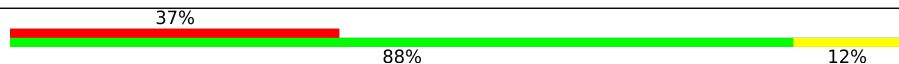
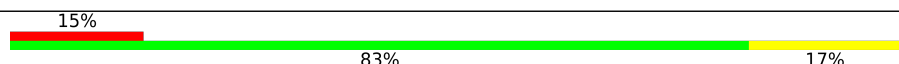
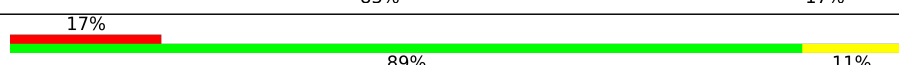
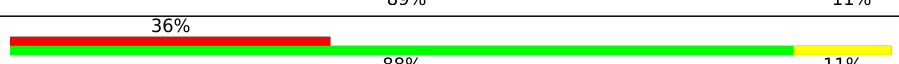
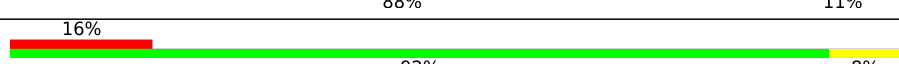
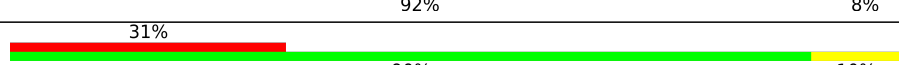
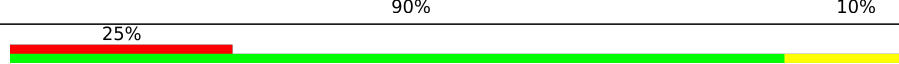
The reported resolution of this entry is 11.60 Å.

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

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	193	
2	B	195	
3	C	208	
4	D	206	
5	E	221	
6	F	218	
7	G	219	
8	H	198	
9	I	196	
10	J	743	

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Mol	Chain	Length	Quality of chain
11	K	223	
12	L	733	
13	M	224	
14	N	80	
15	O	225	
16	P	143	
17	Q	66	
18	R	154	
19	S	97	
20	T	88	
21	U	30	
22	V	42	
23	W	77	
24	X	157	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 29561 atoms, of which 4906 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 Chlorophyll A/B binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A	193	1157	579	192	193	193	0	0

- Molecule 2 is a protein called Chlorophyll A/B binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	B	195	1169	585	194	195	195	0	0

- Molecule 3 is a protein called Chlorophyll A/B binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	C	208	1247	624	207	208	208	0	0

- Molecule 4 is a protein called Chlorophyll A/B binding protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	D	206	1235	618	205	206	206	0	0

- Molecule 5 is a protein called Chlorophyll A/B binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	E	221	1325	663	220	221	221	0	0

- Molecule 6 is a protein called Chlorophyll A/B binding protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	F	218	1307	654	217	218	218	0	0

- Molecule 7 is a protein called Chlorophyll A/B binding protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
7	G	218	1307	654	217	218	218	0	0

- Molecule 8 is a protein called Chlorophyll A/B binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
8	H	198	1187	594	197	198	198	0	0

- Molecule 9 is a protein called Chlorophyll A/B binding protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
9	I	196	1175	588	195	196	196	0	0

- Molecule 10 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
10	J	743	4457	2229	742	743	743	0	0

- Molecule 11 is a protein called Chlorophyll A/B binding protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
11	K	223	1337	669	222	223	223	0	0

- Molecule 12 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
12	L	733	4397	2199	732	733	733	0	0

- Molecule 13 is a protein called Chlorophyll A/B binding protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
13	M	223	1337	669	222	223	223	0	0

- Molecule 14 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	80	Total	C	H	N	O	0	0
			479	240	79	80	80		

- Molecule 15 is a protein called Chlorophyll A/B binding protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	223	Total	C	H	N	O	0	0
			1337	669	222	223	223		

- Molecule 16 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	143	Total	C	H	N	O	0	0
			857	429	142	143	143		

- Molecule 17 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	66	Total	C	H	N	O	0	0
			395	198	65	66	66		

- Molecule 18 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	154	Total	C	H	N	O	0	0
			923	462	153	154	154		

- Molecule 19 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	97	Total	C	H	N	O	0	0
			581	291	96	97	97		

- Molecule 20 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	H	N	O	0	0
			527	264	87	88	88		

- Molecule 21 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
21	U	30	179	90	29	30	30	0	0

- Molecule 22 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
22	V	41	245	123	40	41	41	0	0

- Molecule 23 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
23	W	77	460	231	75	77	77	0	0

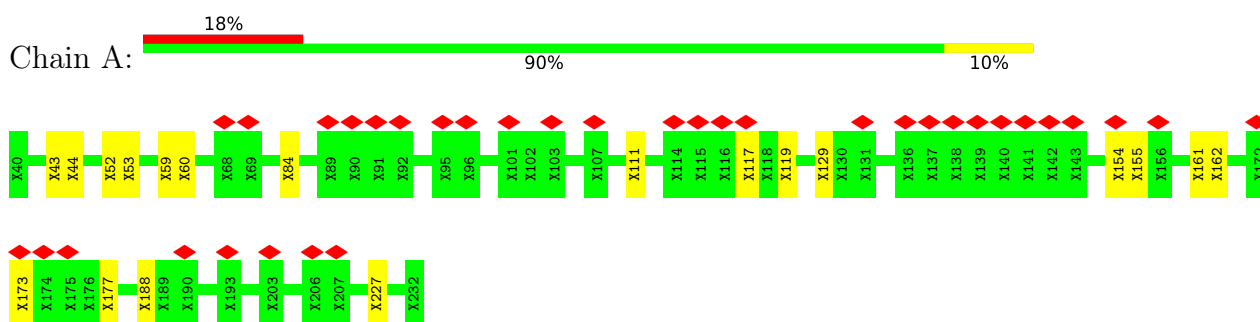
- Molecule 24 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
24	X	157	941	471	156	157	157	0	0

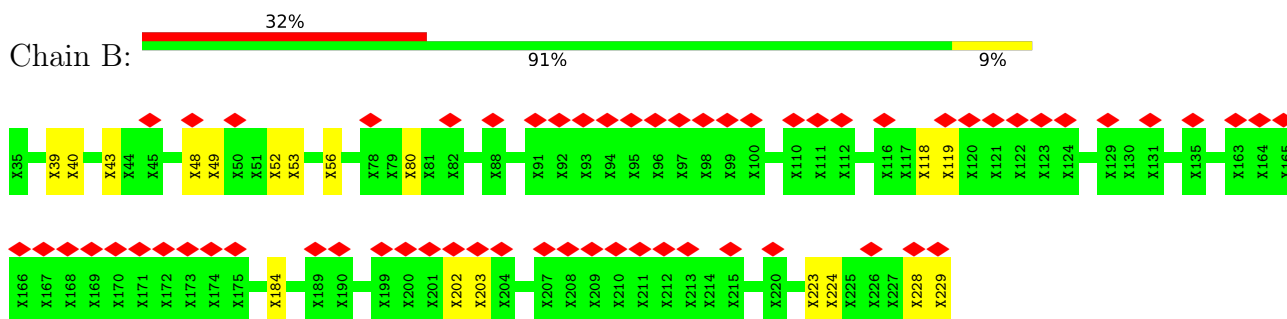
3 Residue-property plots [i](#)

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.

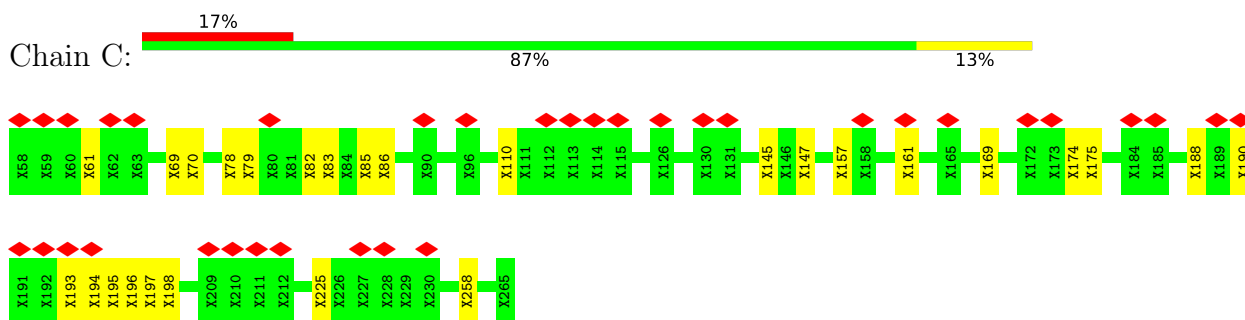
- Molecule 1: Chlorophyll A/B binding protein 1



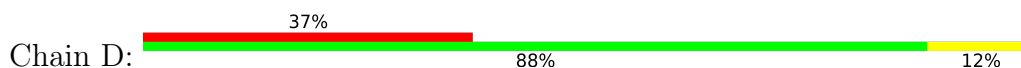
- Molecule 2: Chlorophyll A/B binding protein 5

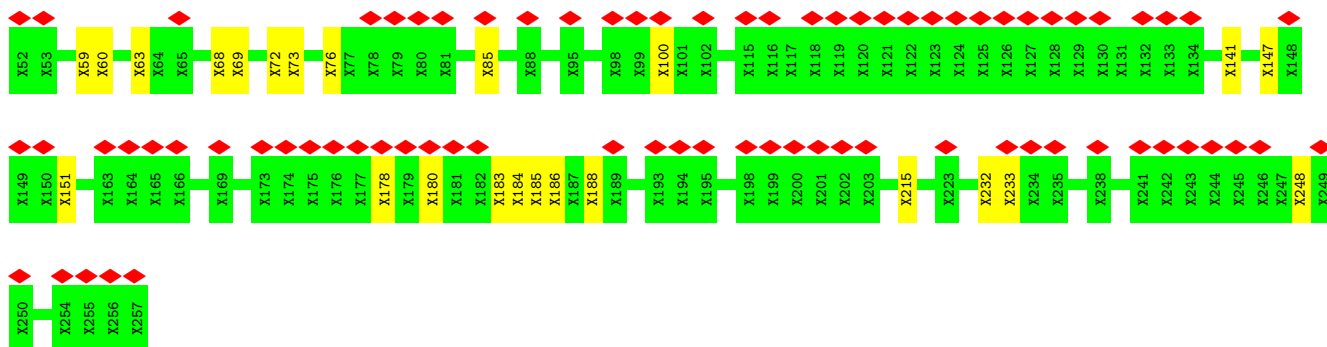


- Molecule 3: Chlorophyll A/B binding protein 3

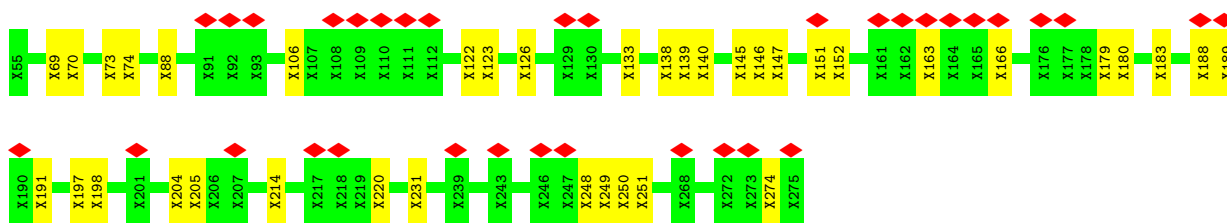
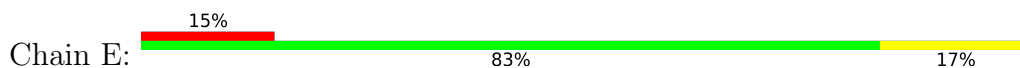


- Molecule 4: Chlorophyll A/B binding protein 7

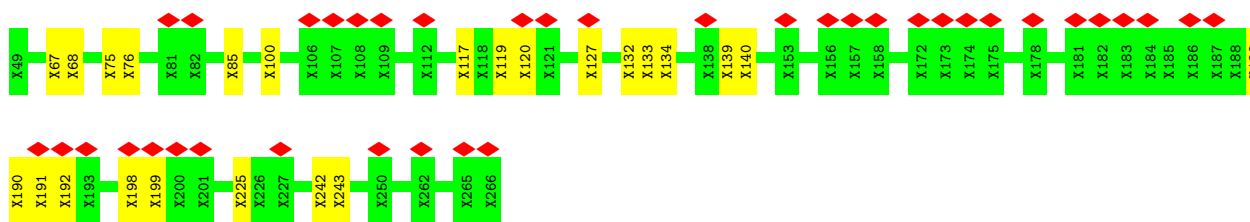
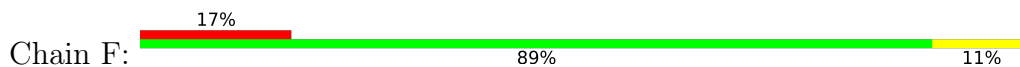




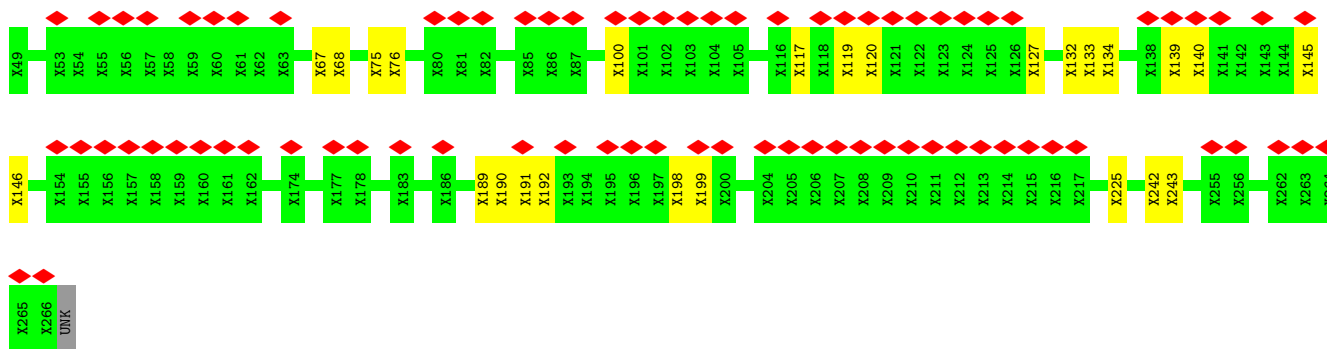
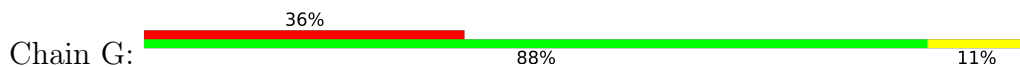
- Molecule 5: Chlorophyll A/B binding protein 4



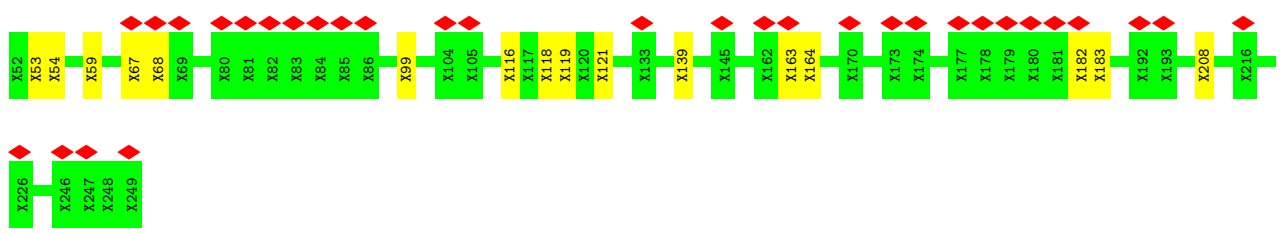
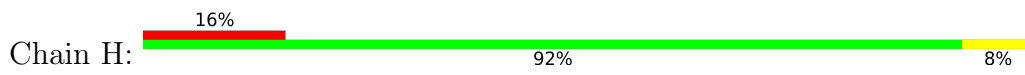
- Molecule 6: Chlorophyll A/B binding protein 9



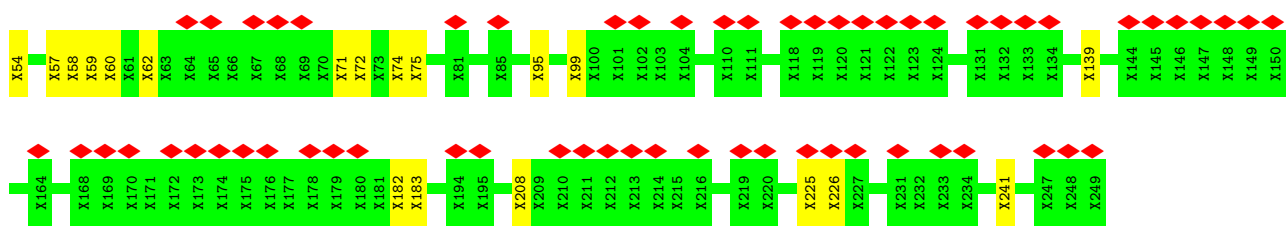
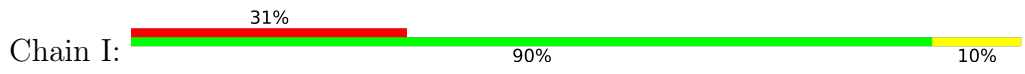
- Molecule 7: Chlorophyll A/B binding protein 8



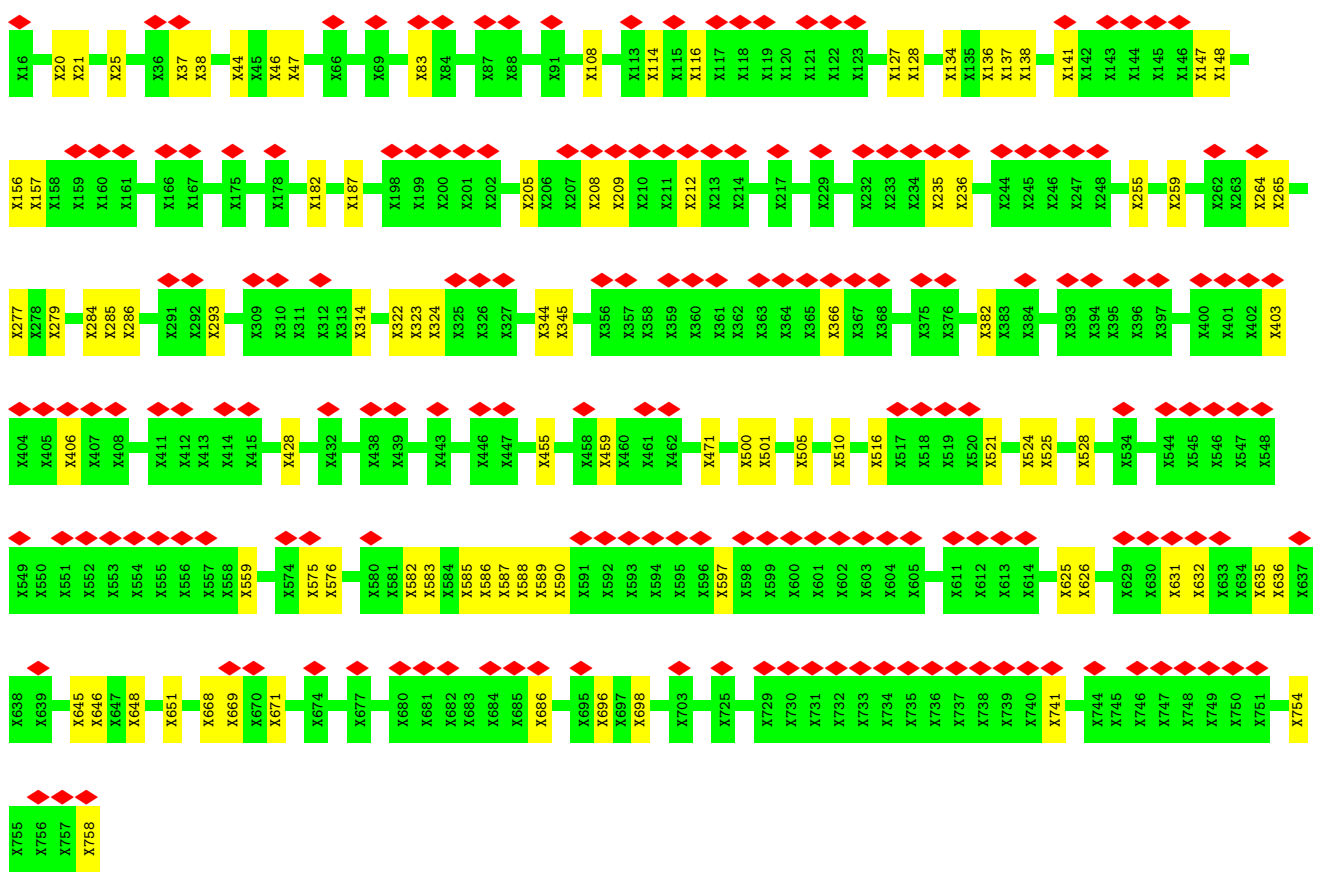
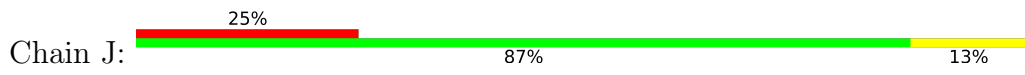
- Molecule 8: Chlorophyll A/B binding protein 2



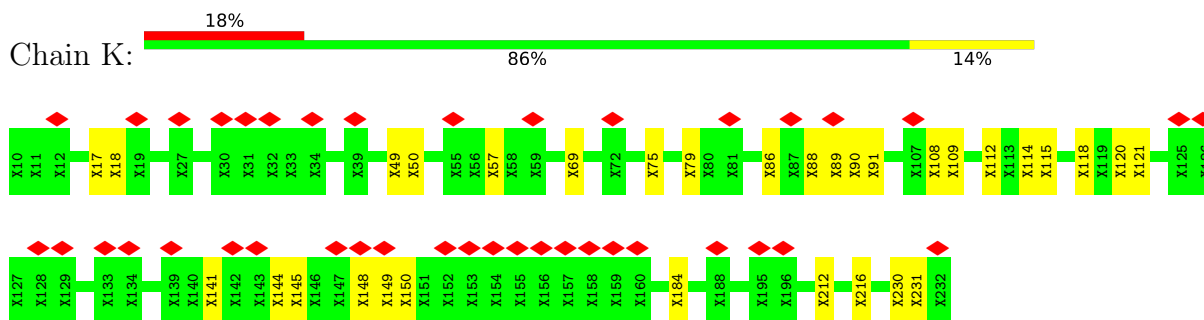
• Molecule 9: Chlorophyll A/B binding protein 6



• Molecule 10: PsaA



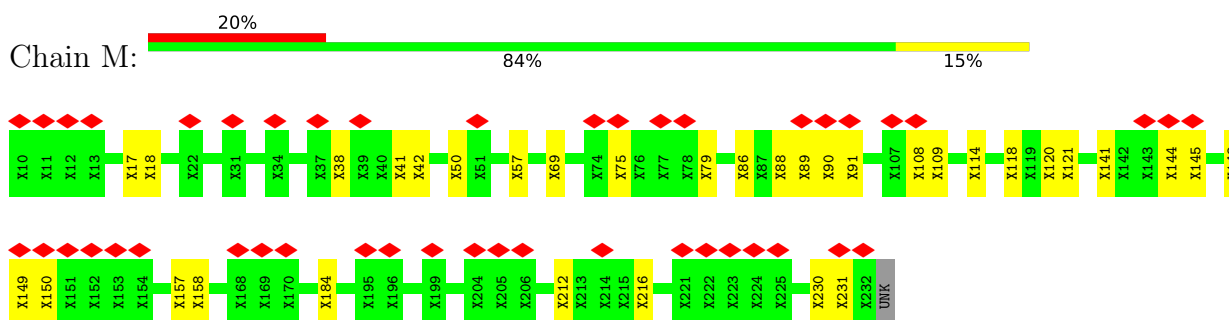
• Molecule 11: Chlorophyll A/B binding protein 10



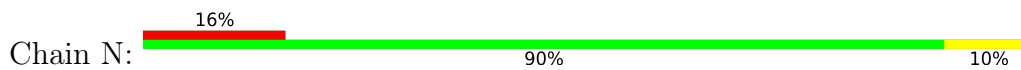
• Molecule 12: PsaB

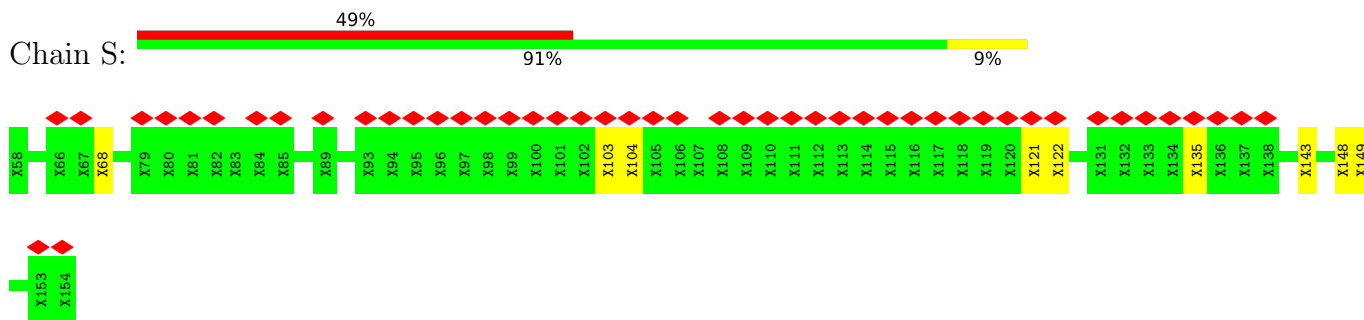


• Molecule 13: Chlorophyll A/B binding protein 11

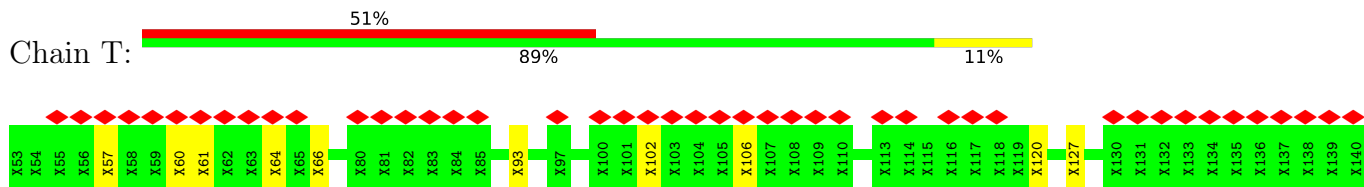


• Molecule 14: PsaC

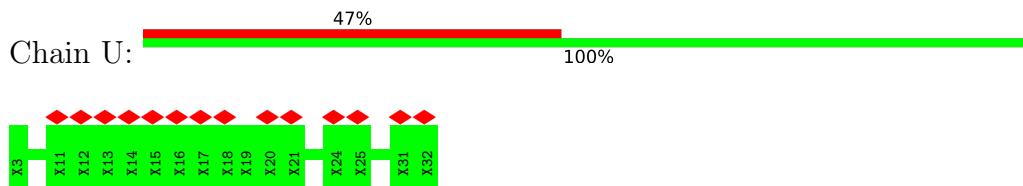




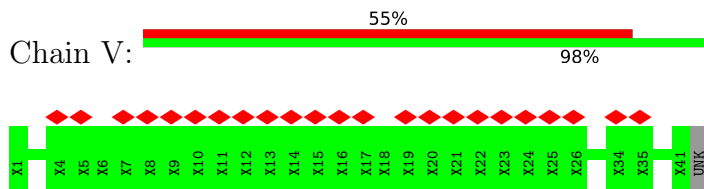
• Molecule 20: PsaH



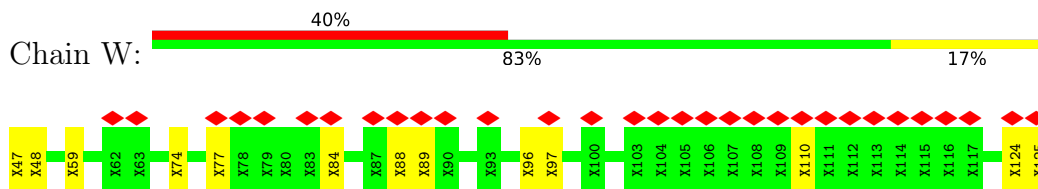
• Molecule 21: PsaI



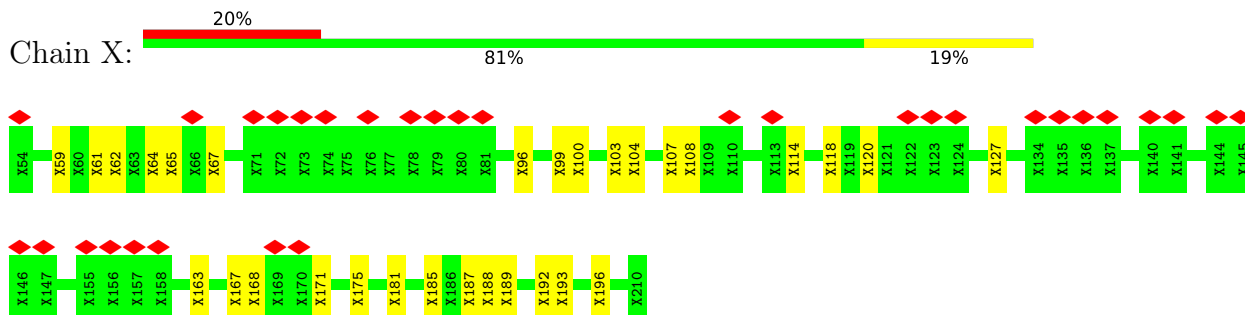
• Molecule 22: PsaJ



• Molecule 23: PsaK



• Molecule 24: PsaL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14412	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	-1900	Depositor
Maximum defocus (nm)	-4200	Depositor
Magnification	107140	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.691	Depositor
Minimum map value	-0.241	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.8, 2.8, 2.8	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	965	192	197	14	0
2	B	975	194	199	12	0
3	C	1040	207	213	20	0
4	D	1030	205	214	18	0
5	E	1105	220	226	28	0
6	F	1090	217	227	14	0
7	G	1090	217	227	15	0
8	H	990	197	202	10	0
9	I	980	195	203	13	0
10	J	3715	742	762	76	0
11	K	1115	222	229	21	0
12	L	3665	732	746	70	0
13	M	1115	222	230	20	0
14	N	400	79	84	13	0
15	O	1115	222	230	21	0
16	P	715	142	153	13	0
17	Q	330	65	70	2	0
18	R	770	153	157	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	485	96	99	6	0
20	T	440	87	90	9	0
21	U	150	29	32	0	0
22	V	205	40	43	0	0
23	W	385	75	87	8	0
24	X	785	156	160	32	0
All	All	24655	4906	5080	396	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 13.

The worst 5 of 396 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)
5:E:106:UNK:CB	5:E:231:UNK:CB	1.77	1.60
23:W:59:UNK:HA	23:W:110:UNK:CB	1.30	1.56
5:E:88:UNK:CB	10:J:21:UNK:HA	1.52	1.39
10:J:645:UNK:O	10:J:651:UNK:CB	1.70	1.37
19:S:68:UNK:HA	19:S:135:UNK:CB	1.56	1.35

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	80:UNK	C	83:UNK	N	6.55

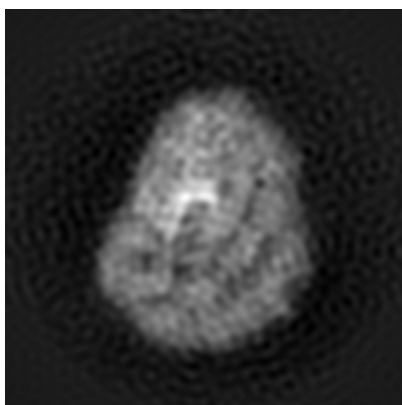
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9107. These allow visual inspection of the internal detail of the map and identification of artifacts.

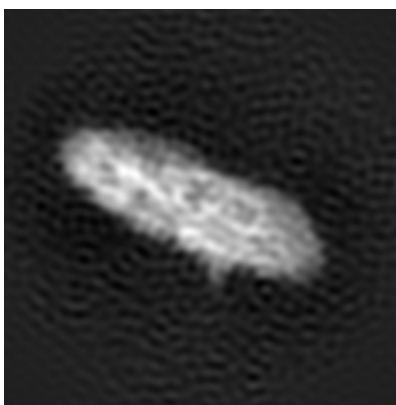
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

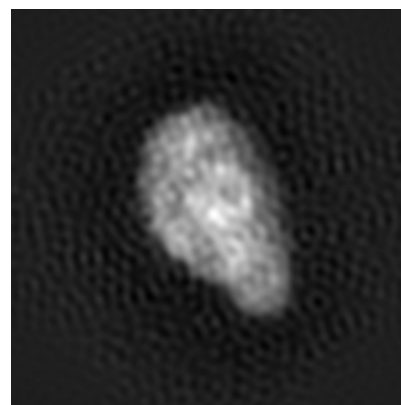
6.1.1 Primary map



X



Y

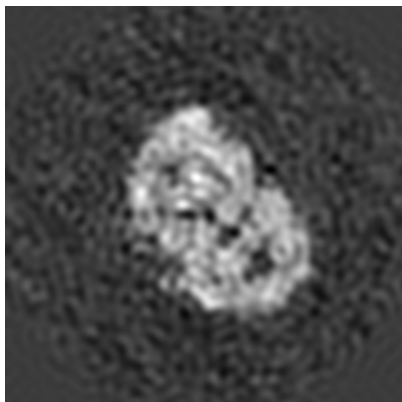


Z

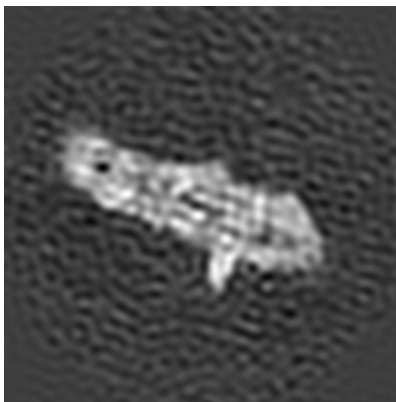
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

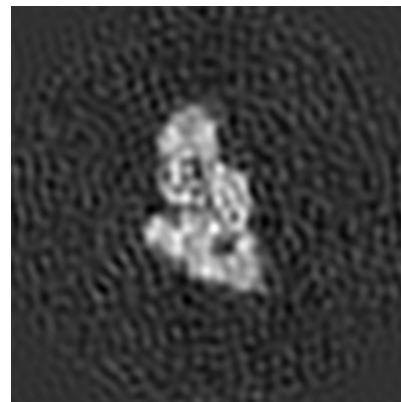
6.2.1 Primary map



X Index: 64



Y Index: 64

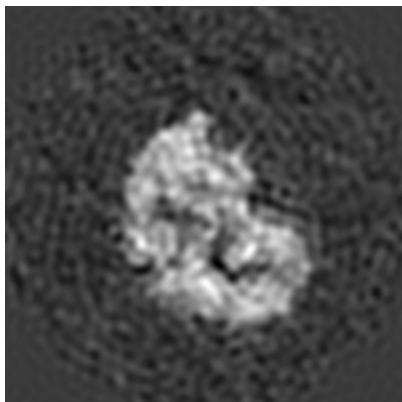


Z Index: 64

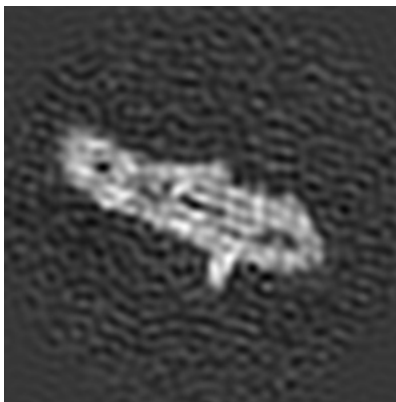
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

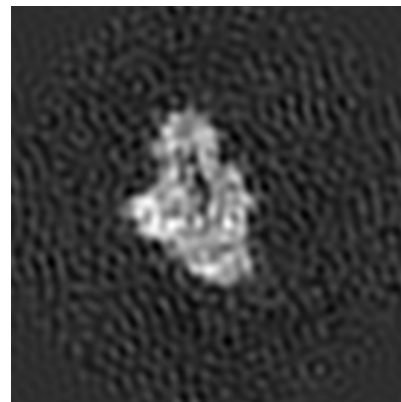
6.3.1 Primary map



X Index: 67



Y Index: 65

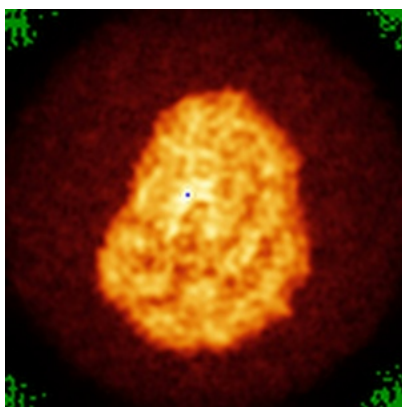


Z Index: 67

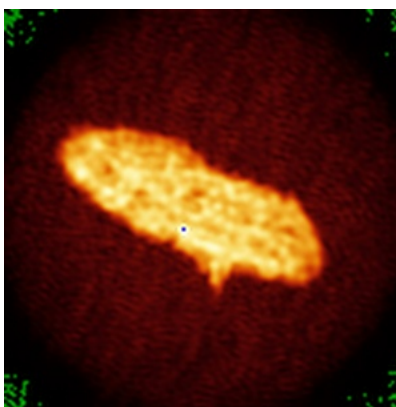
The images above show the largest variance slices of the map in three orthogonal directions.

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

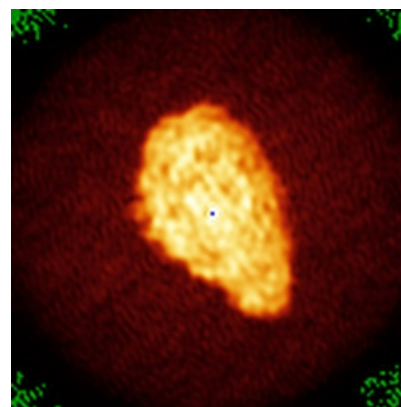
6.4.1 Primary map



X



Y

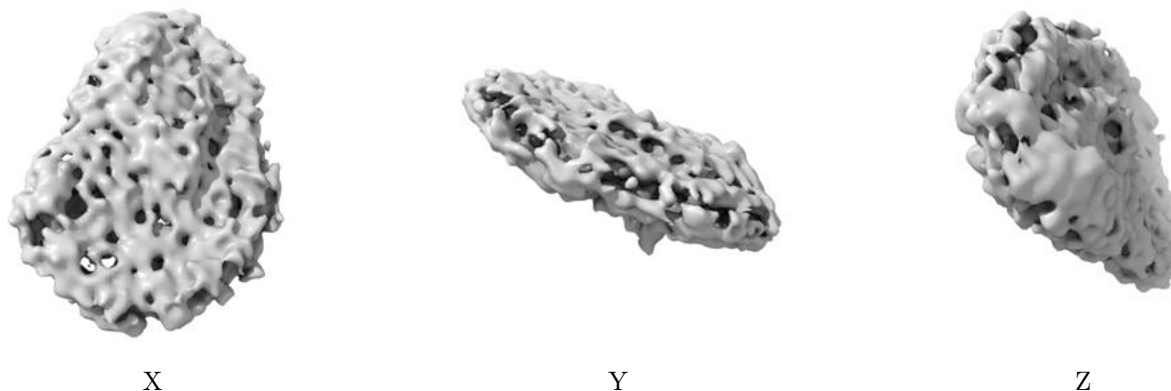


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

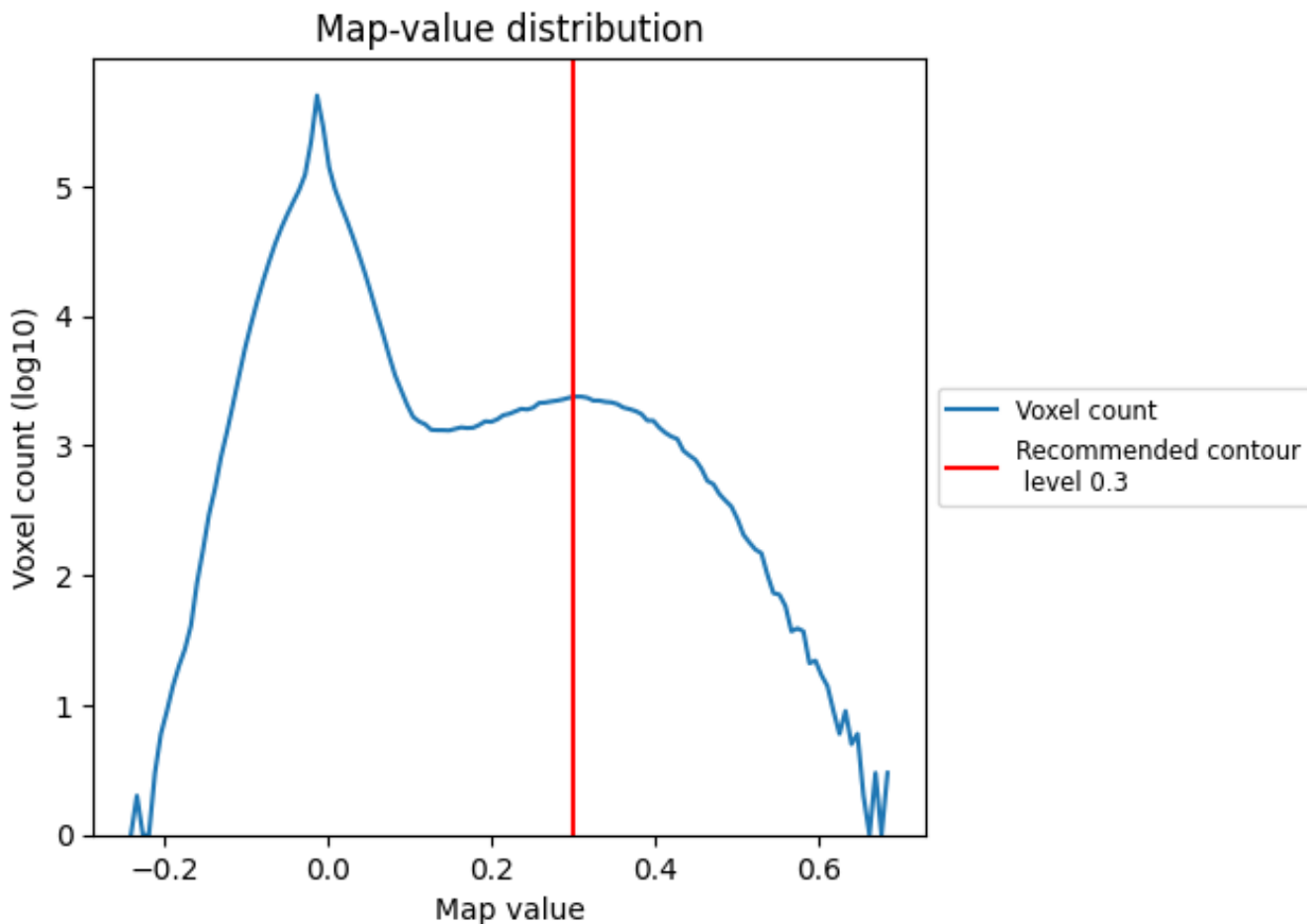
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

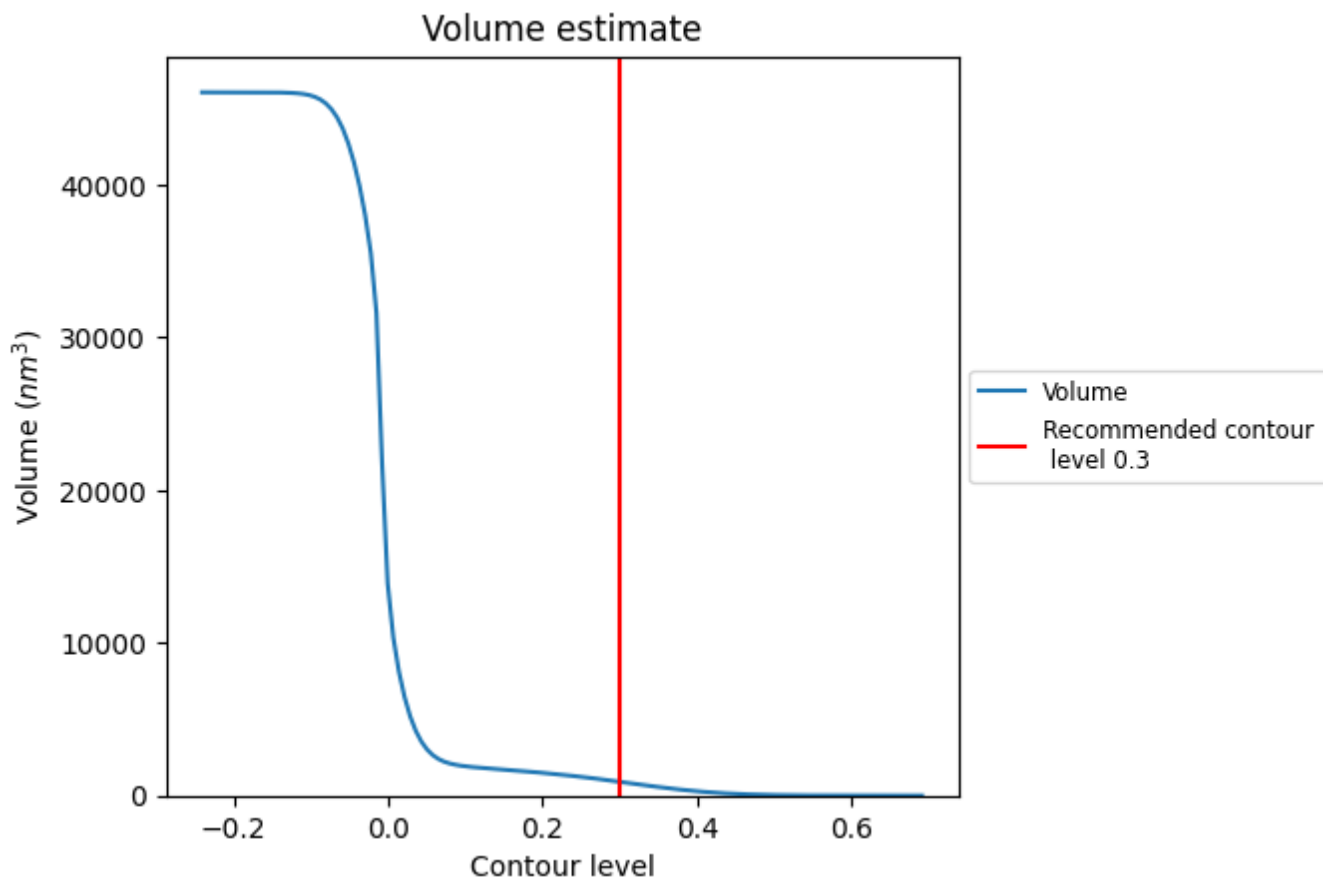
This section contains the results of statistical analysis of the map.

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.

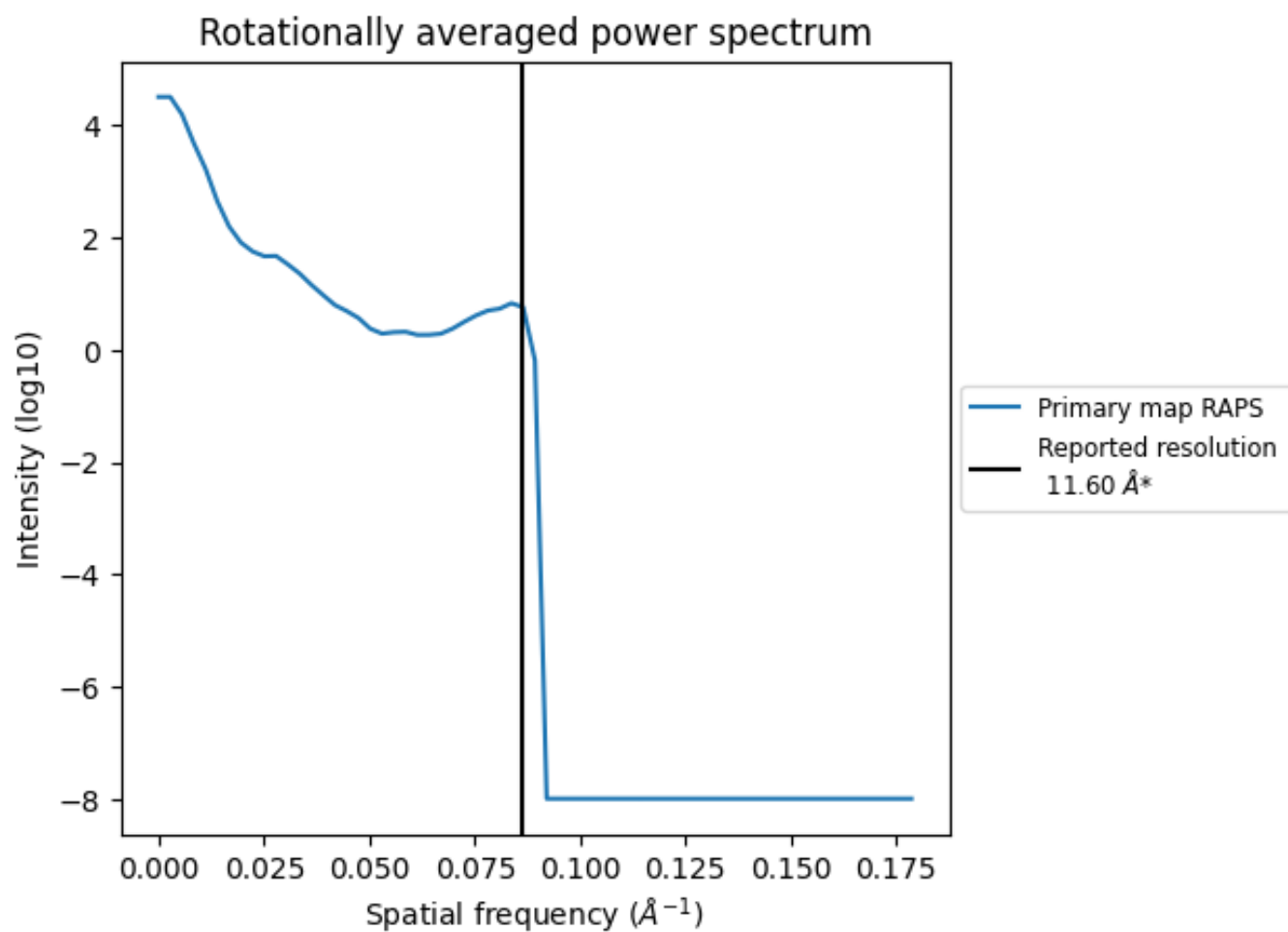
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 901 nm³; this corresponds to an approximate mass of 814 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 0.086 Å⁻¹

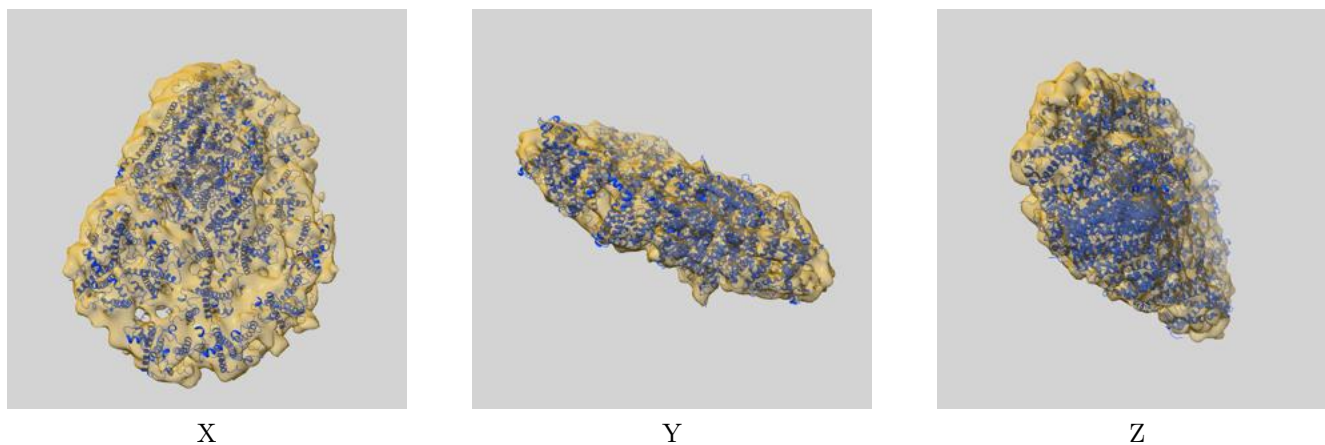
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

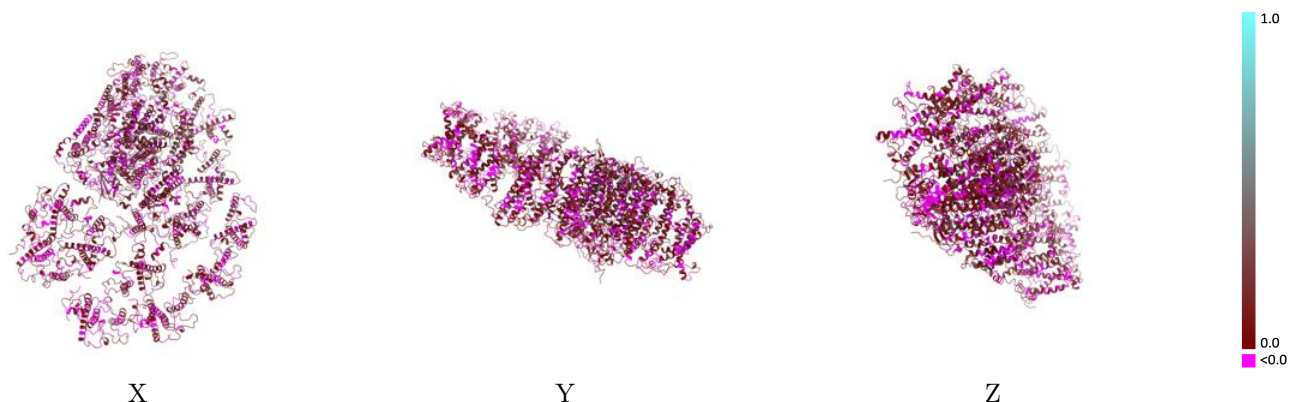
This section contains information regarding the fit between EMDB map EMD-9107 and PDB model 6MEM. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



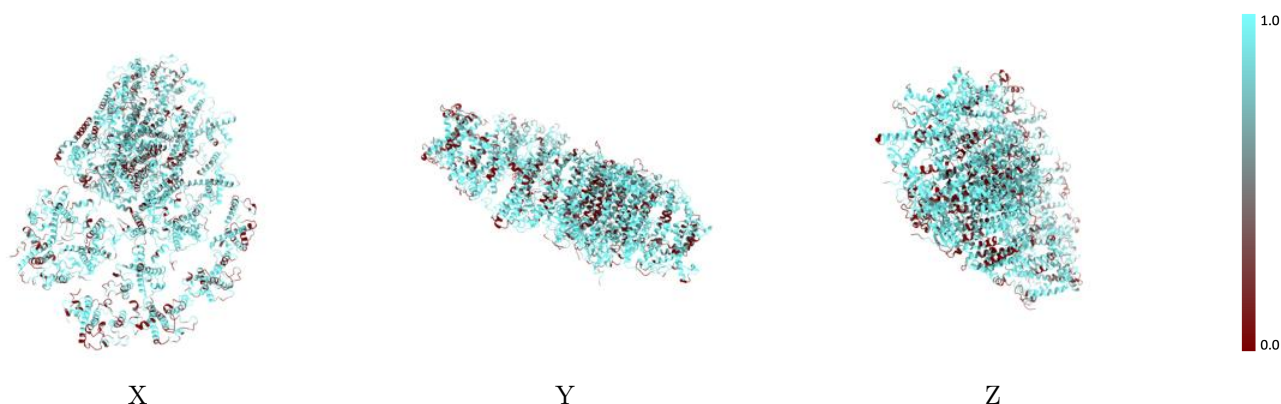
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



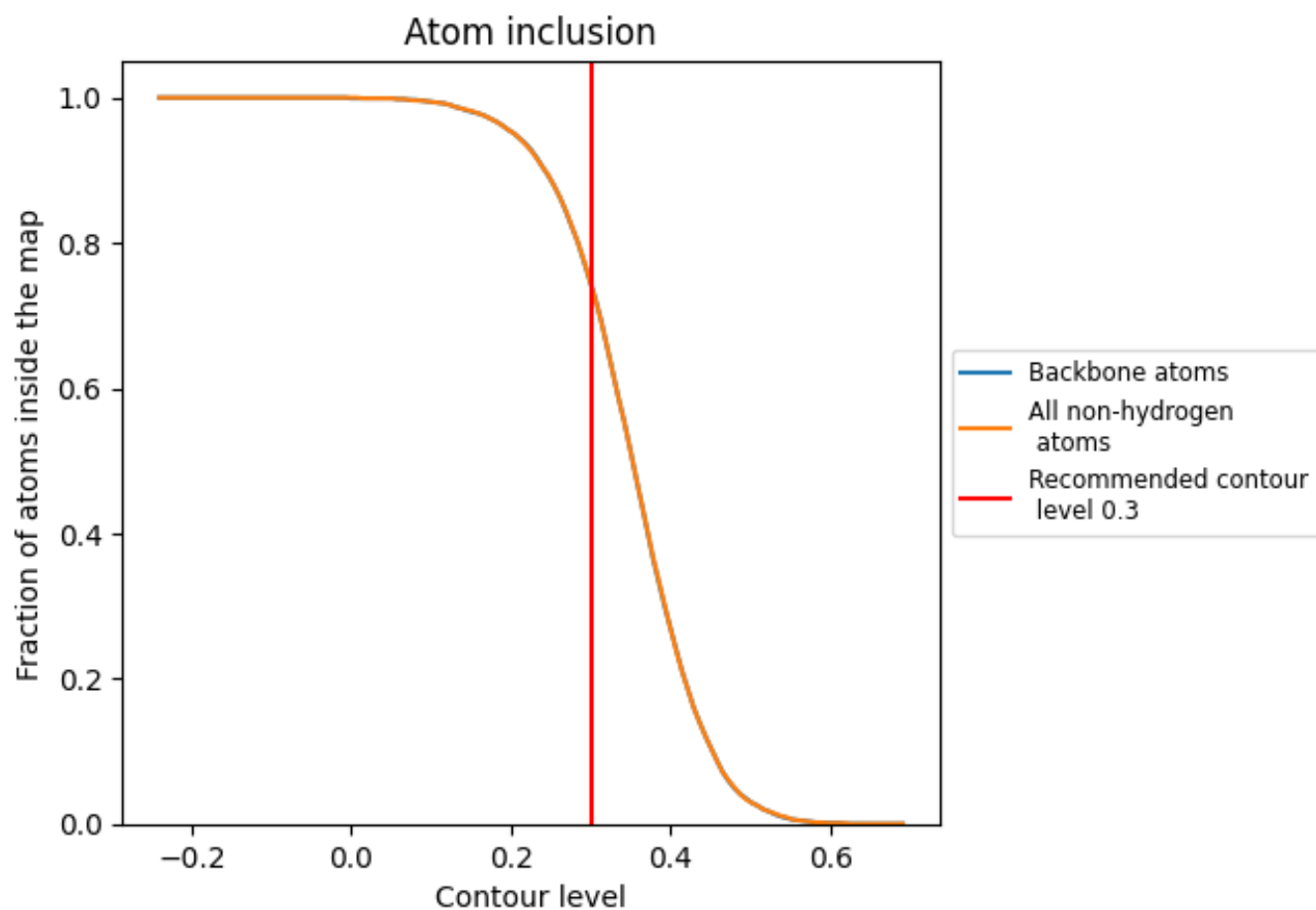
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).



















































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

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.0700
A	 0.8030	 0.0730
B	 0.6790	 0.0770
C	 0.8280	 0.0940
D	 0.6330	 0.0540
E	 0.8530	 0.0860
F	 0.7940	 0.0890
G	 0.6390	 0.0480
H	 0.8180	 0.0620
I	 0.6830	 0.0430
J	 0.7320	 0.0730
K	 0.7960	 0.0980
L	 0.8280	 0.0700
M	 0.7870	 0.0770
N	 0.8230	 0.0220
O	 0.6420	 0.0510
P	 0.7250	 0.0670
Q	 0.8520	 0.1140
R	 0.7290	 0.1250
S	 0.4950	 0.0080
T	 0.4640	 0.0120
U	 0.5600	 0.0810
V	 0.4630	 0.0510
W	 0.6030	 0.0510
X	 0.7900	 0.0730

