wwPDB EM Validation Summary Report (i)

Aug 15, 2022 – 04:45 pm BST

PDB ID	:	7QPD
EMDB ID	:	EMD-14119
Title	:	Structure of the human MHC I peptide-loading complex editing module
Authors	:	Domnick, A.; Susac, L.; Trowitzsch, S.; Thomas, C.; Tampe, R.
Deposited on	:	2022-01-03
Resolution	:	3.73 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 (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:

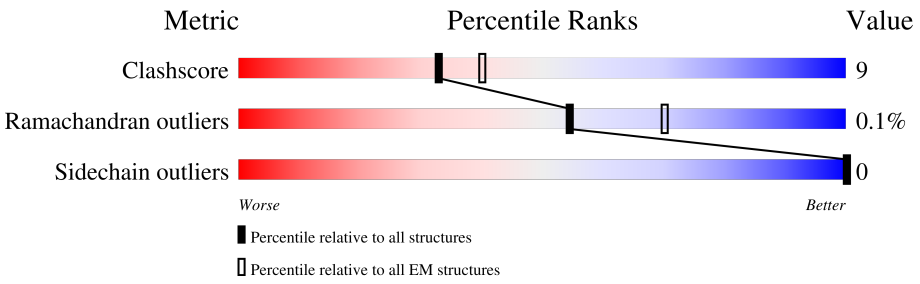
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.73 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	B	99	69% 31%
2	T	428	. 64% 17% 19%
3	E	481	. 79% 17% 5%
4	M	341	67% 14% 20%
5	C	400	26% 73% 18% 9%
6	A	3	33% 67%
7	D	7	29% 71%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11521 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	99	803	512	138	150	3	0	0

- Molecule 2 is a protein called Tapasin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	348	2569	1656	449	453	11	0	0

- Molecule 3 is a protein called Protein disulfide-isomerase A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	459	3365	2152	585	615	13	0	0

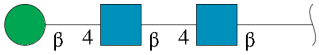
- Molecule 4 is a protein called HLA class I histocompatibility antigen, A-3 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	274	2110	1330	379	392	9	0	0

- Molecule 5 is a protein called Calreticulin.

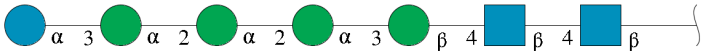
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	364	2552	1625	434	487	6	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	A	3	39	22	2	15	0	0

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



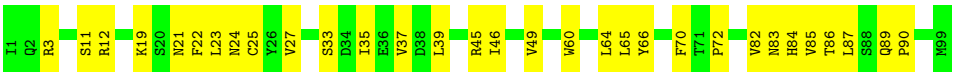
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	D	7	83	46	2	35	0	0

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.

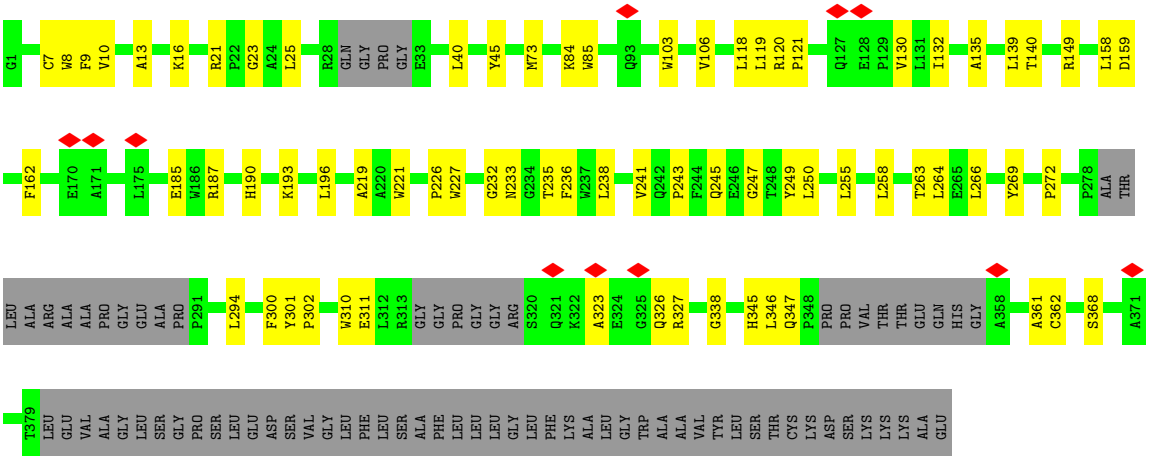
- Molecule 1: Beta-2-microglobulin

Chain B:



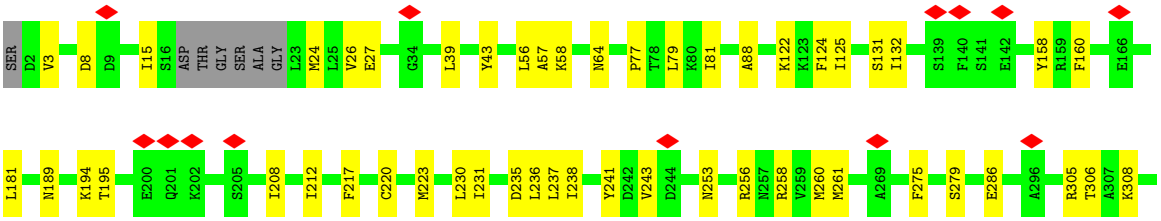
- Molecule 2: Tapasin

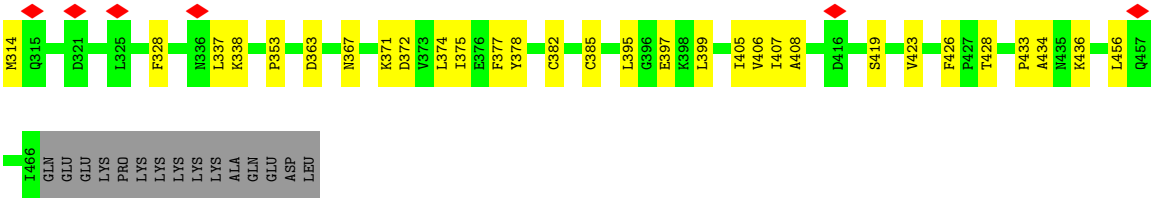
Chain T:



- Molecule 3: Protein disulfide-isomerase A3

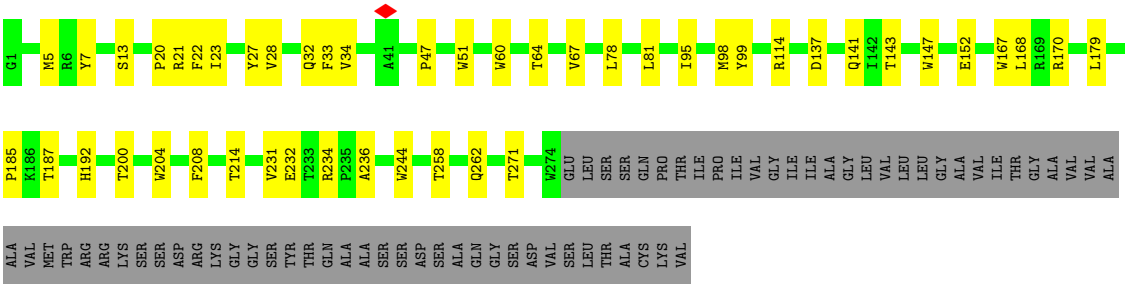
Chain E:





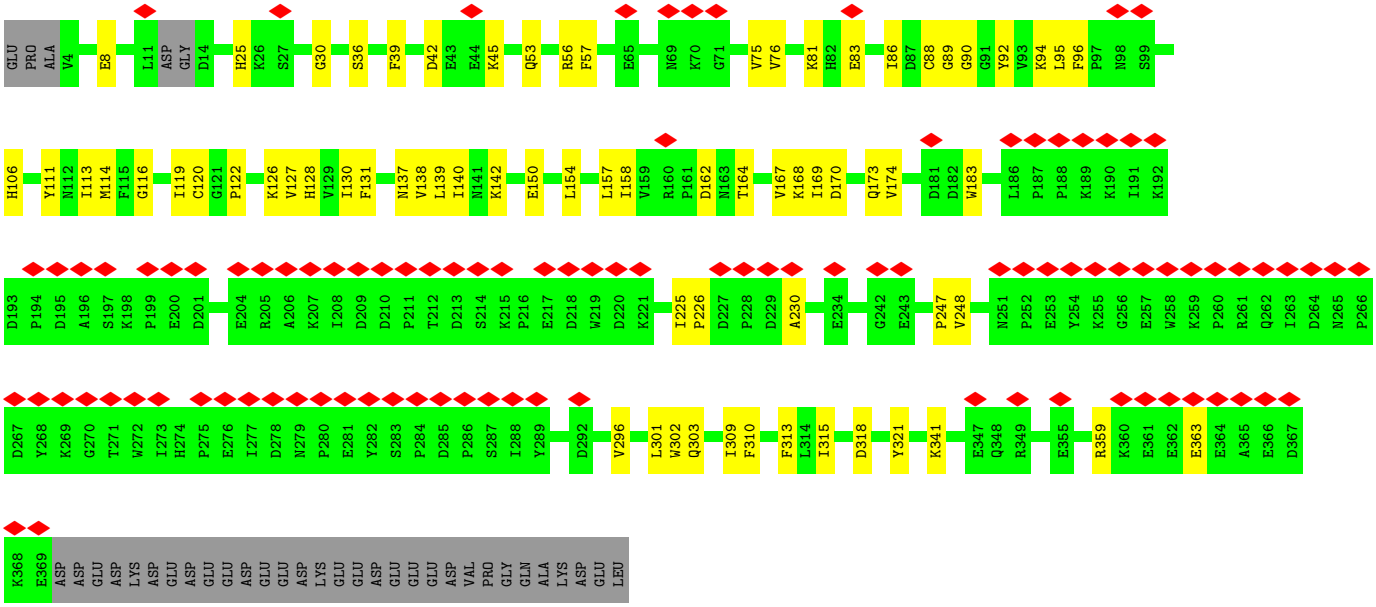
• Molecule 4: HLA class I histocompatibility antigen, A-3 alpha chain

Chain M:



• Molecule 5: Calreticulin

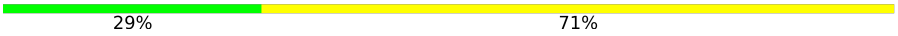
Chain C:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

• Molecule 7: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.857	Depositor
Minimum map value	-0.635	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG, GLC

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	B	0.32	0/826	0.54	0/1121
2	T	0.30	0/2656	0.52	0/3650
3	E	0.30	0/3446	0.46	0/4688
4	M	0.31	0/2169	0.53	0/2961
5	C	0.33	0/2619	0.48	0/3585
All	All	0.31	0/11716	0.50	0/16005

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	B	803	0	749	21	0
2	T	2569	0	2462	50	0
3	E	3365	0	3043	49	0
4	M	2110	0	1912	31	0
5	C	2552	0	2081	50	0
6	A	39	0	34	2	0
7	D	83	0	70	2	0
All	All	11521	0	10351	202	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 9.

The worst 5 of 202 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:C:88:CYS:HA	5:C:120:CYS:HA	1.57	0.85
5:C:8:GLU:HB3	5:C:313:PHE:HB2	1.63	0.79
4:M:33:PHE:HD2	4:M:34:VAL:HG13	1.52	0.75
4:M:28:VAL:HG23	4:M:33:PHE:HE1	1.52	0.73
5:C:92:TYR:HA	5:C:116:GLY:HA3	1.69	0.73

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	B	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
2	T	338/428 (79%)	321 (95%)	17 (5%)	0	100	100
3	E	455/481 (95%)	435 (96%)	19 (4%)	1 (0%)	47	78
4	M	272/341 (80%)	261 (96%)	11 (4%)	0	100	100
5	C	360/400 (90%)	340 (94%)	20 (6%)	0	100	100
All	All	1522/1749 (87%)	1446 (95%)	75 (5%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	419	SER

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	B	87/94 (93%)	87 (100%)	0	100	100
2	T	257/338 (76%)	257 (100%)	0	100	100
3	E	307/414 (74%)	307 (100%)	0	100	100
4	M	200/282 (71%)	200 (100%)	0	100	100
5	C	209/361 (58%)	209 (100%)	0	100	100
All	All	1060/1489 (71%)	1060 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	T	242	GLN
2	T	261	GLN
2	T	326	GLN
3	E	384	HIS
4	M	191	HIS

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)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	1	2,6	14,14,15	0.51	0	17,19,21	1.28	2 (11%)
6	NAG	A	2	6	14,14,15	0.27	0	17,19,21	1.28	2 (11%)
6	BMA	A	3	6	11,11,12	0.55	0	15,15,17	0.80	0
7	NAG	D	1	4,7	14,14,15	0.36	0	17,19,21	0.35	0
7	NAG	D	2	7	14,14,15	0.17	0	17,19,21	0.47	0
7	BMA	D	3	7	11,11,12	0.73	0	15,15,17	0.98	0
7	MAN	D	4	7	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
7	MAN	D	5	7	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
7	MAN	D	6	7	11,11,12	0.61	0	15,15,17	1.07	2 (13%)
7	GLC	D	7	7	11,11,12	0.63	0	15,15,17	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	A	2	6	-	3/6/23/26	0/1/1/1
6	BMA	A	3	6	-	2/2/19/22	0/1/1/1
7	NAG	D	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3	7	-	1/2/19/22	0/1/1/1
7	MAN	D	4	7	-	0/2/19/22	0/1/1/1
7	MAN	D	5	7	-	0/2/19/22	0/1/1/1
7	MAN	D	6	7	-	0/2/19/22	0/1/1/1
7	GLC	D	7	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2	NAG	C2-N2-C7	4.29	129.01	122.90
6	A	1	NAG	C2-N2-C7	4.27	128.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	5	MAN	C1-O5-C5	2.41	115.46	112.19
7	D	4	MAN	O2-C2-C3	-2.39	105.34	110.14
7	D	5	MAN	O2-C2-C3	-2.32	105.49	110.14

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

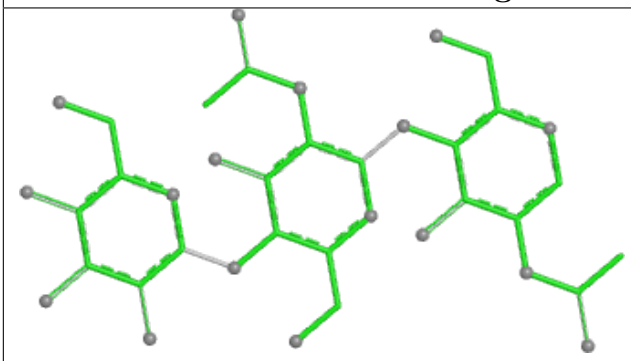
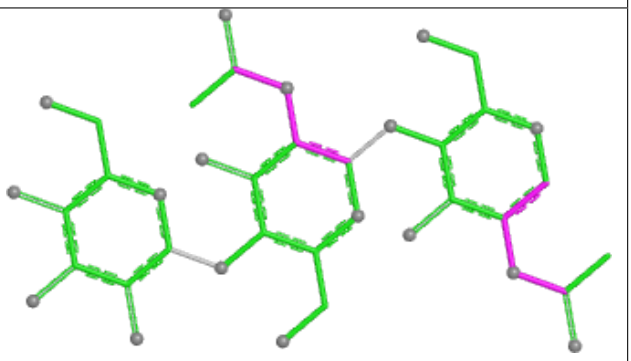
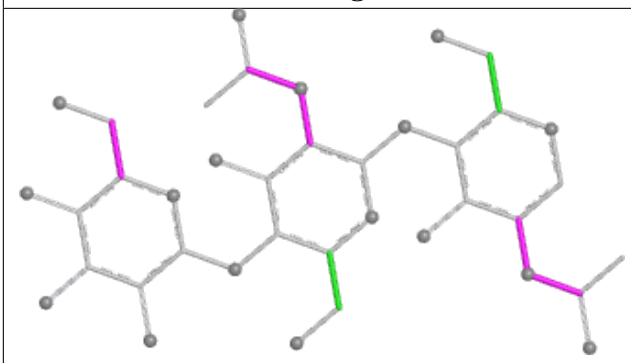
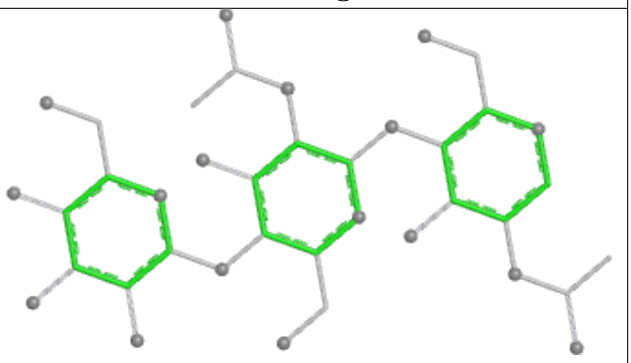
Mol	Chain	Res	Type	Atoms
7	D	1	NAG	C4-C5-C6-O6
6	A	1	NAG	C8-C7-N2-C2
6	A	1	NAG	O7-C7-N2-C2
6	A	2	NAG	C8-C7-N2-C2
6	A	2	NAG	O7-C7-N2-C2

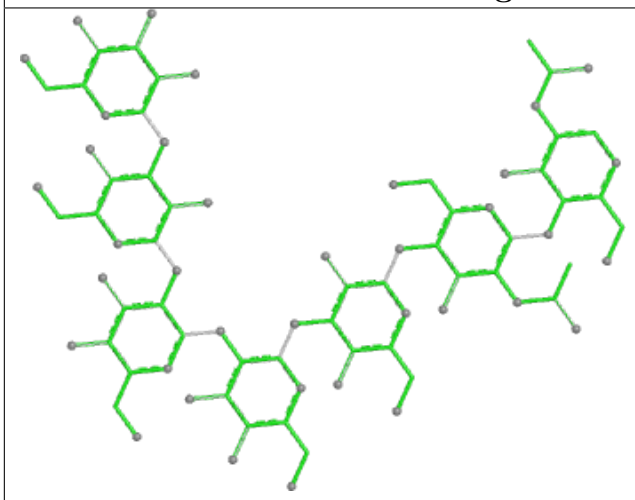
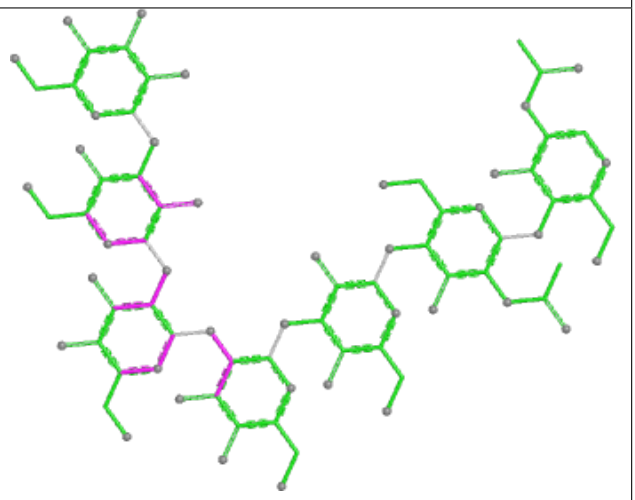
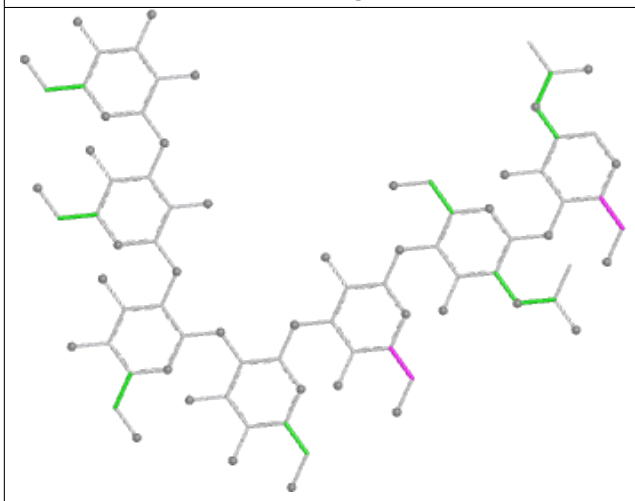
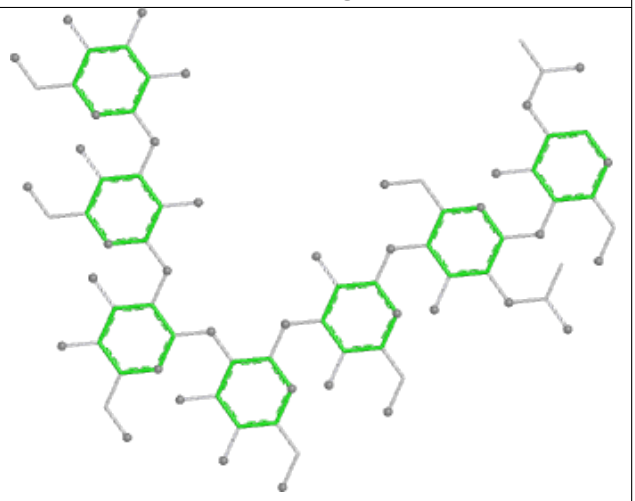
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2	NAG	1	0
6	A	1	NAG	1	0
7	D	1	NAG	1	0
7	D	3	BMA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain A	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

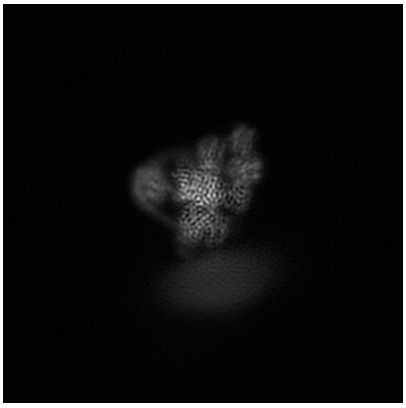
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14119. These allow visual inspection of the internal detail of the map and identification of artifacts.

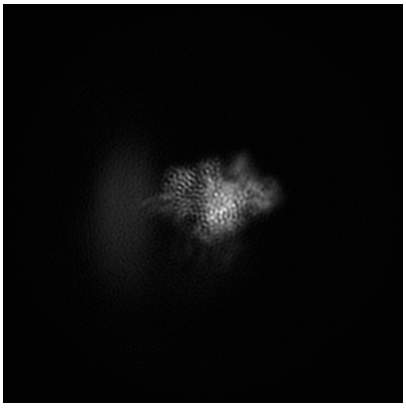
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

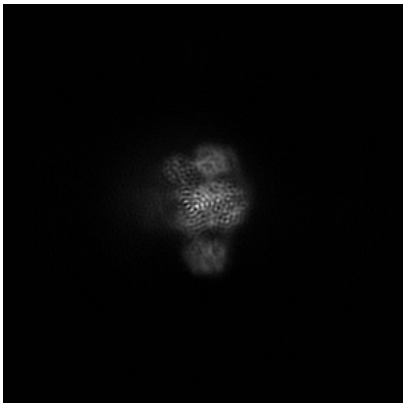
6.1.1 Primary map



X



Y



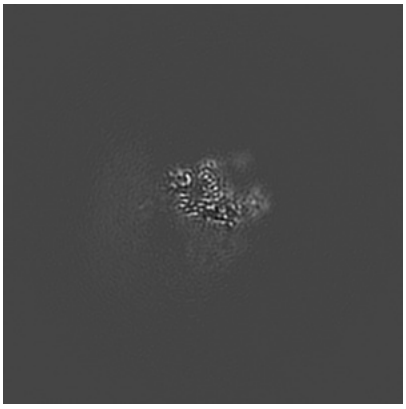
Z

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

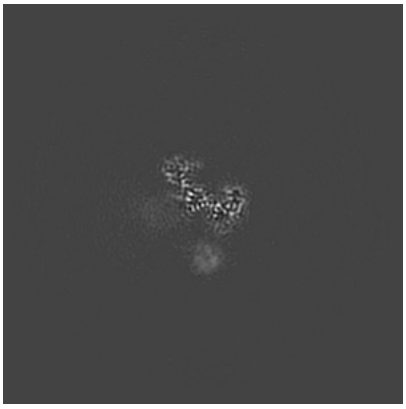
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



Y Index: 180

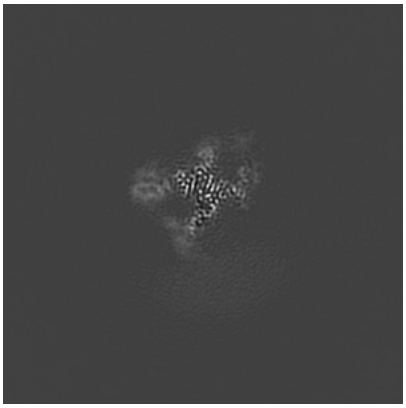


Z Index: 180

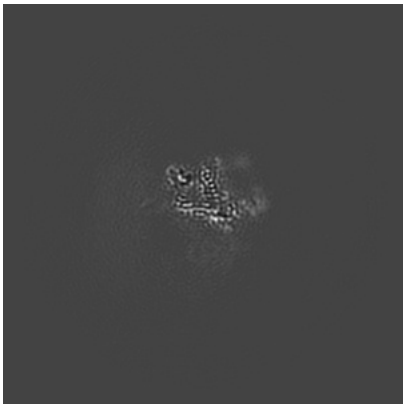
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 172



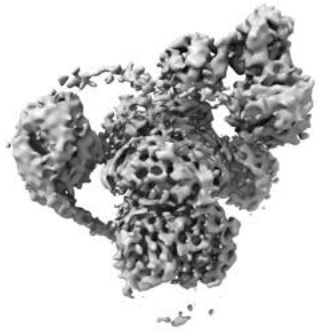
Y Index: 177

Z Index: 187

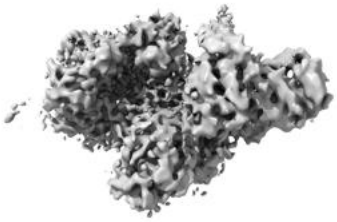
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

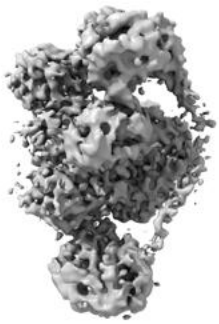
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

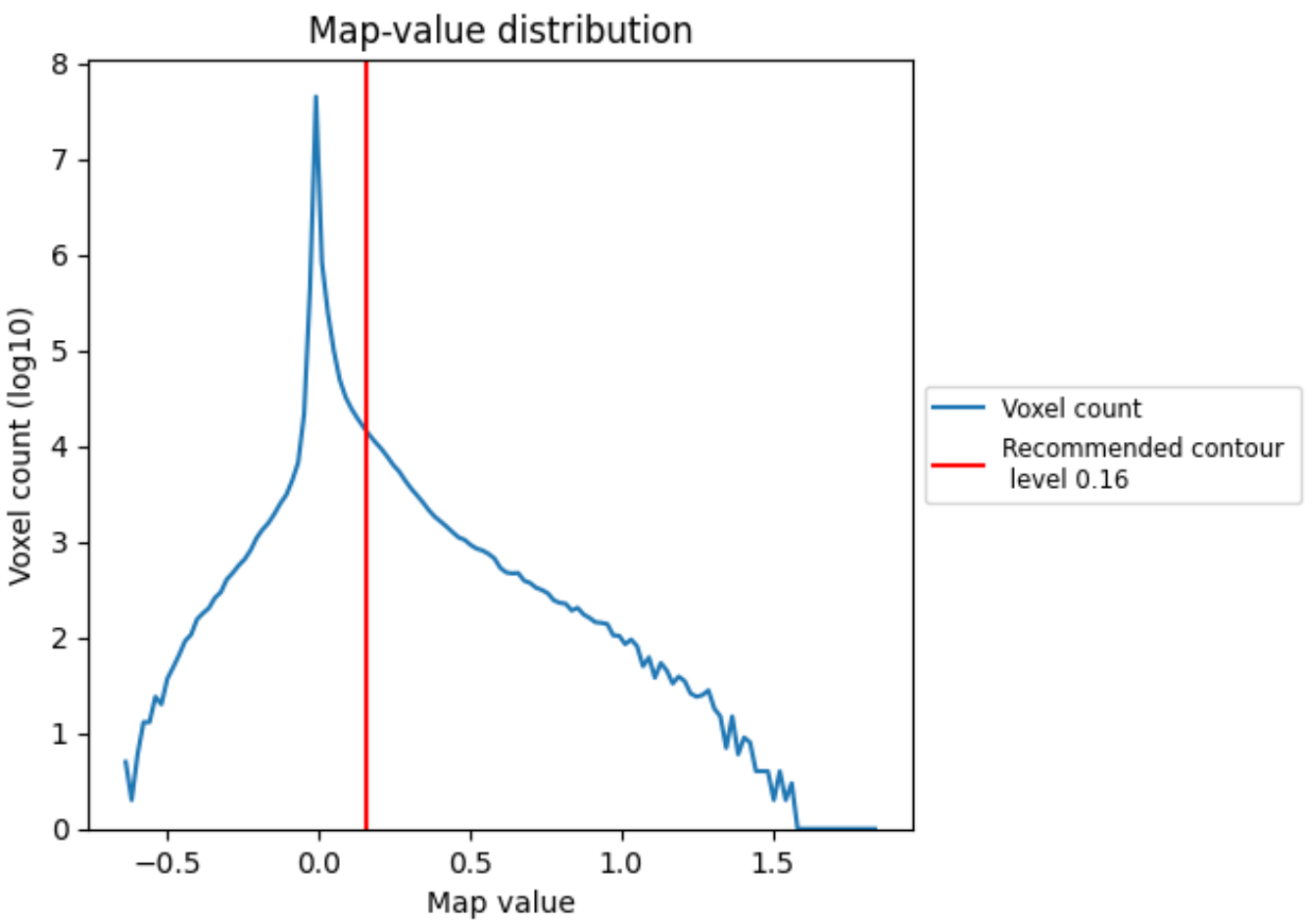
6.5 Mask visualisation (i)

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

7 Map analysis (i)

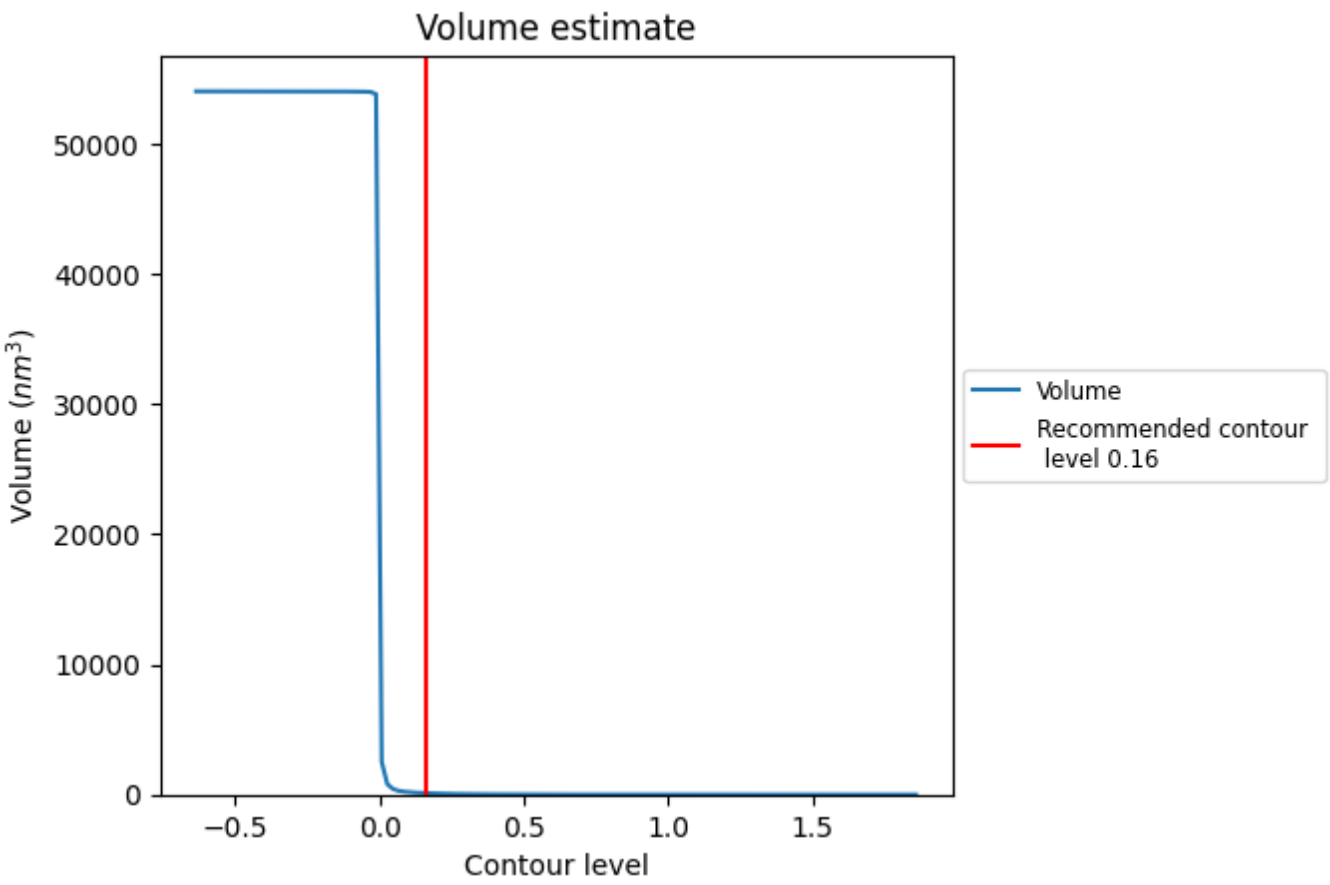
This section contains the results of statistical analysis of the map.

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.

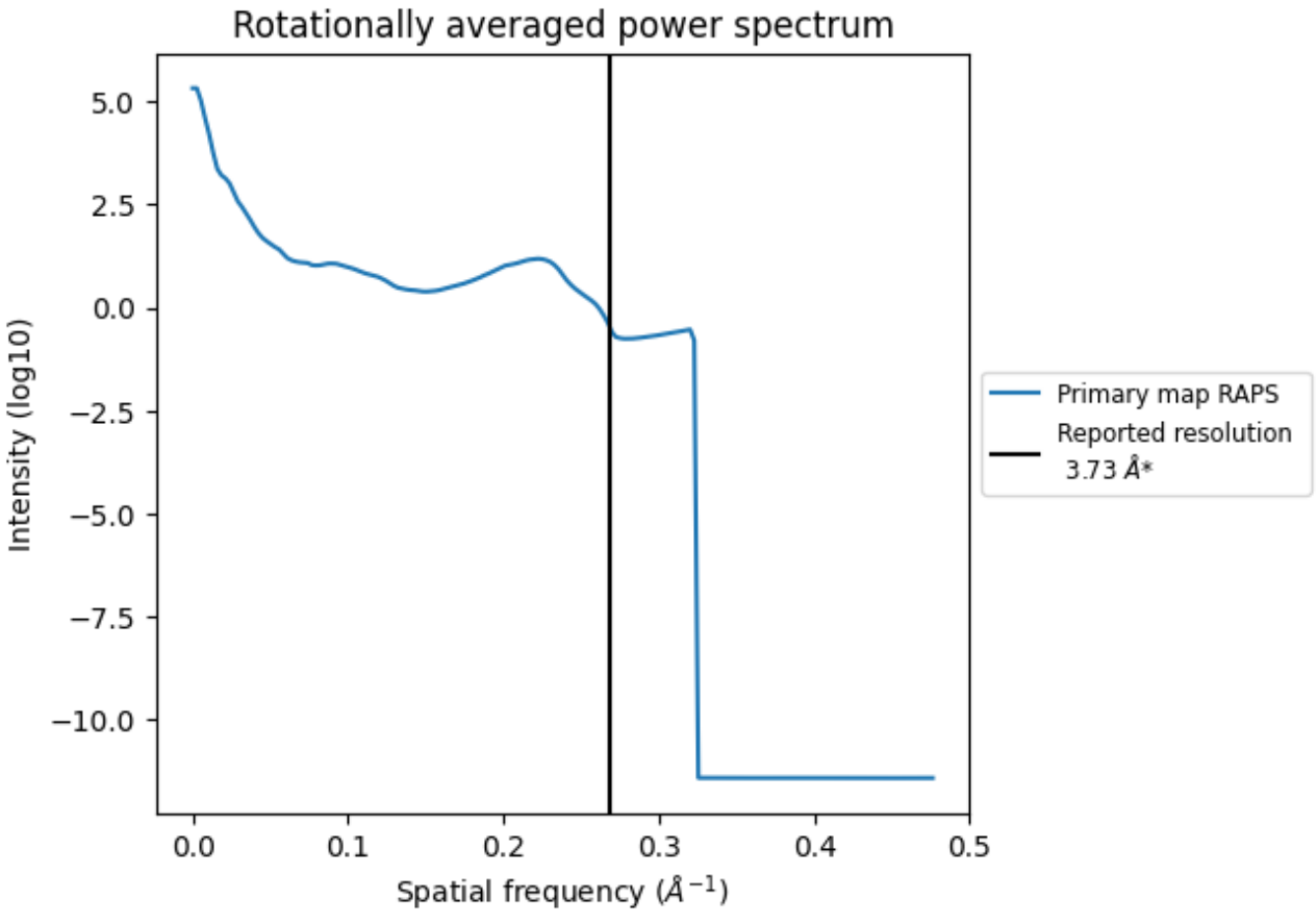
7.2 Volume estimate (i)



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 99 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 0.268 Å^{-1}

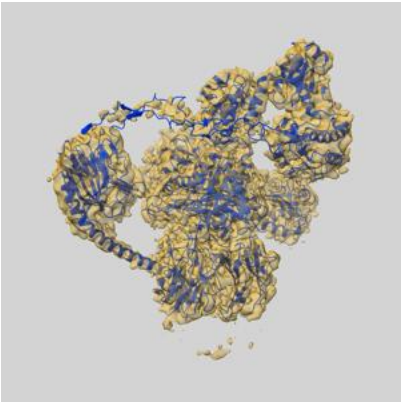
8 Fourier-Shell correlation (i)

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

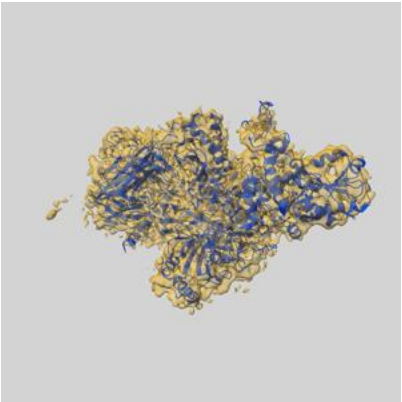
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14119 and PDB model 7QPD. Per-residue inclusion information can be found in section 3 on page 5.

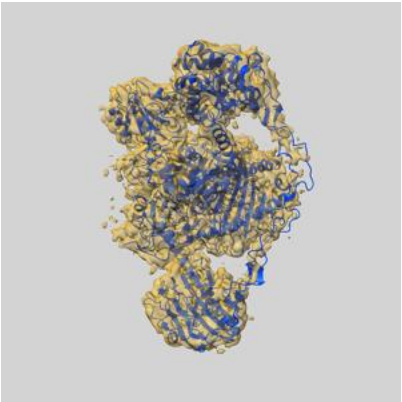
9.1 Map-model overlay (i)



X



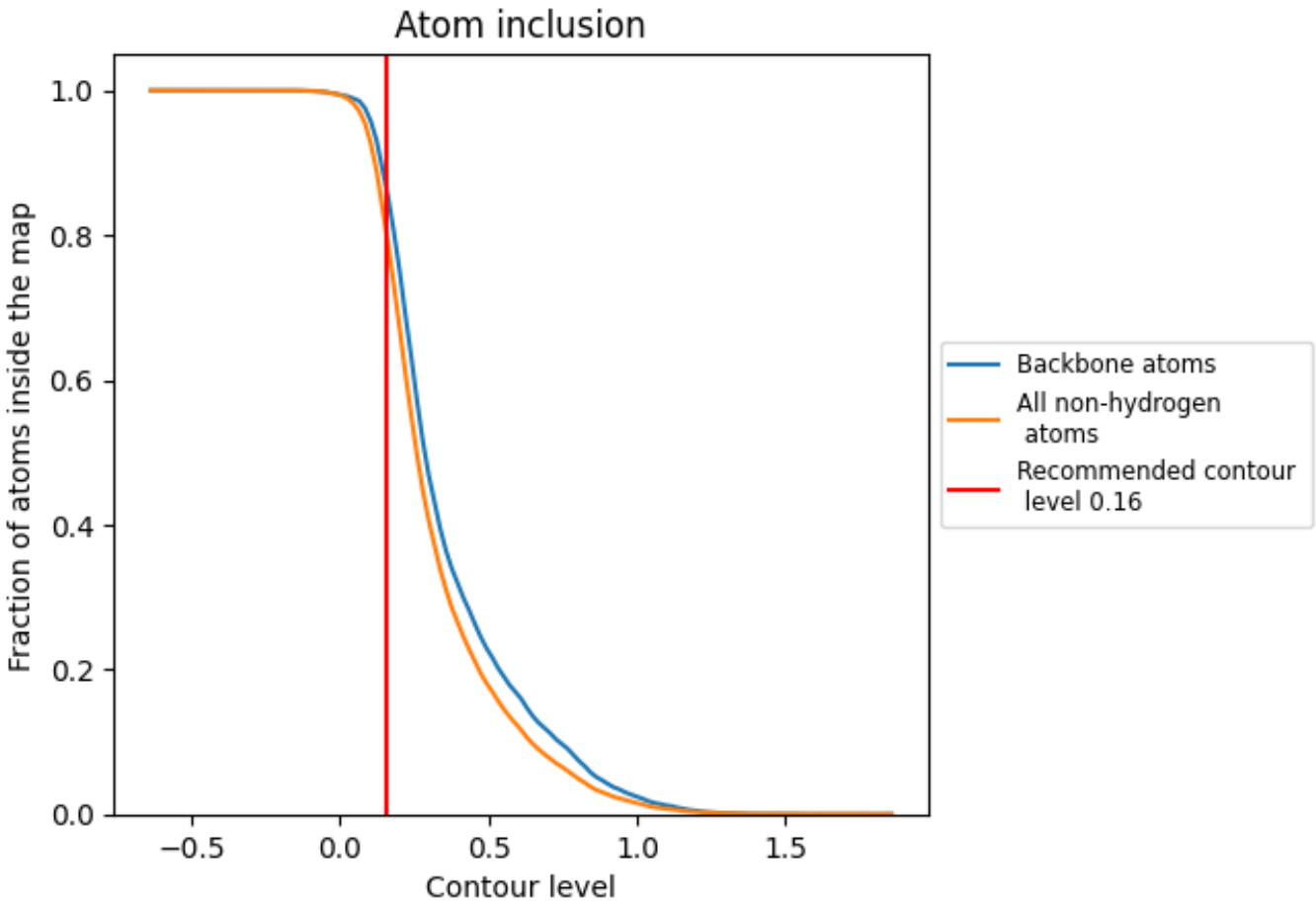
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.