wwPDB EM Validation Summary Report (i)

May 14, 2024 – 12:16 am BST

PDB ID	:	6THN
EMDB ID	:	EMD-10506
Title	:	Multiple Genomic RNA-Coat Protein Contacts Play Vital Roles in the Assembly of Infectious Enterovirus-E symmetry expansion+2fold focused classification
Authors	:	Chandler-Bostock, R.; Mata, C.P.; Bingham, R.; Dykeman, E.J.; Meng, B.; Tuthill, T.J.; Rowlands, D.J.; Ranson, N.A.; Twarock, R.; Stockley, P.G.
Deposited on	:	2019-11-20
Resolution	:	2.60 Å(reported)
Based on initial model	:	1BEV

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:

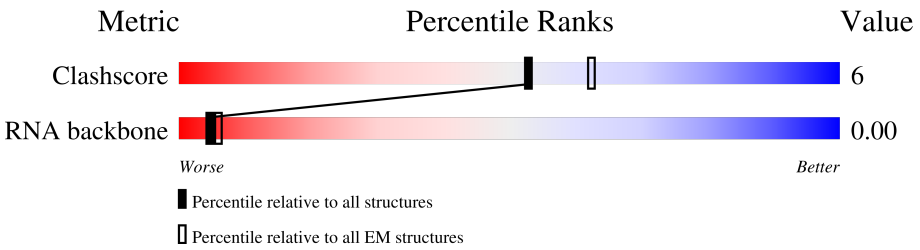
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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
RNA backbone	4643	859

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	1	281	88% 11%
2	2	248	83% 13%
3	3	242	88% 12%
4	4	52	10% 79% 21%
5	A	11	18% 18% 82%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6503 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	278	2178	1374	374	418	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	94	HIS	ASN	conflict	UNP P12915
1	237	TYR	CYS	conflict	UNP P12915

- Molecule 2 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	240	1878	1196	321	354	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	62	ARG	ALA	conflict	UNP P12915

- Molecule 3 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	242	1870	1195	306	357	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	32	PRO	LEU	conflict	UNP P12915
3	154	ILE	VAL	conflict	UNP P12915

- Molecule 4 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	52	396	247	68	81	0	0

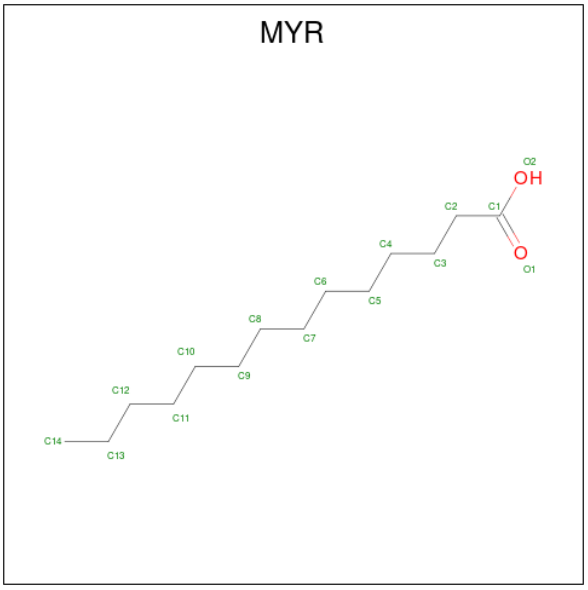
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	2	GLY	TYR	conflict	UNP P12915
4	4	GLN	THR	conflict	UNP P12915

- Molecule 5 is a RNA chain called RNA Peak 9 Bernoulli Plot.

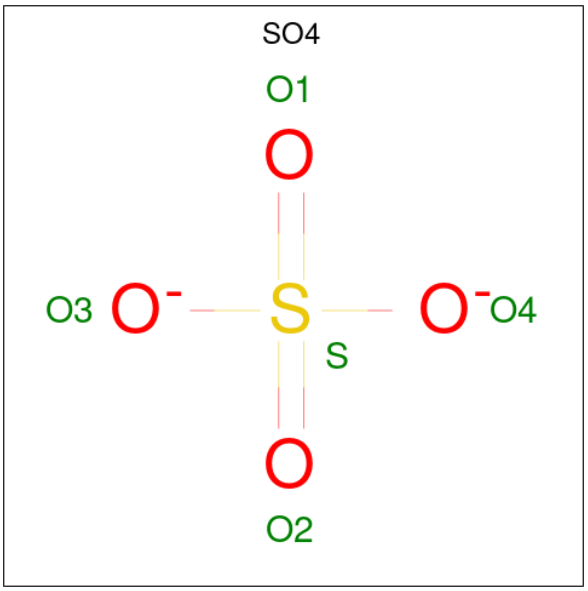
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2	42	19	7	14	2	0	0

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	1	1	16	14	2	0
6	4	1	16	14	2	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
7	1	1	5	4	1	0
			Total	O	S	
7	2	1	5	4	1	0

- Molecule 8 is water.

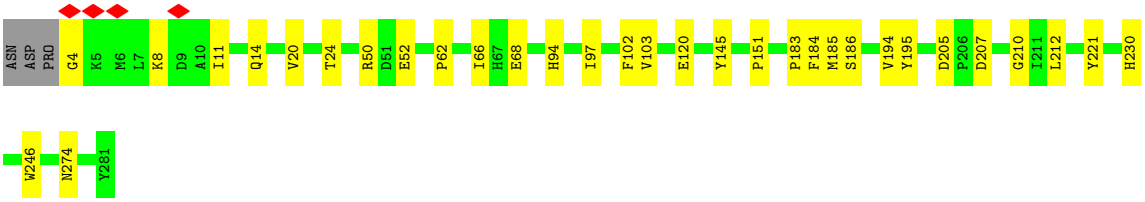
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	1	34	34	34	0
			Total	O	
8	2	36	36	36	0
			Total	O	
8	3	27	27	27	0

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.

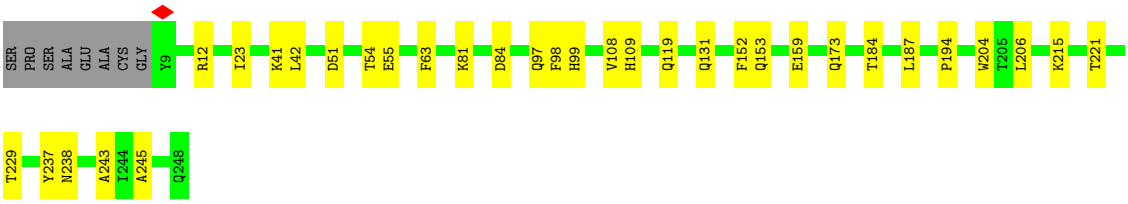
- Molecule 1: Genome polyprotein

Chain 1:



- Molecule 2: Genome polyprotein

Chain 2:

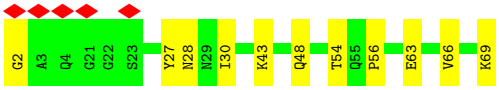


- Molecule 3: Genome polyprotein

Chain 3:

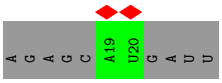
- Molecule 4: Genome polyprotein

Chain 4:



- Molecule 5: RNA Peak 9 Bernoulli Plot

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	946982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.353	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.052	Depositor
Map size (Å)	498.42, 498.42, 498.42	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: SO4, MYR

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	1	0.50	0/2237	0.58	0/3043
2	2	0.49	0/1933	0.64	0/2650
3	3	0.50	0/1918	0.63	0/2618
4	4	0.50	0/403	0.54	0/546
5	A	0.16	0/46	0.60	0/69
All	All	0.50	0/6537	0.61	0/8926

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	1	2178	0	2089	28	0
2	2	1878	0	1814	23	0
3	3	1870	0	1833	23	0
4	4	396	0	376	13	0
5	A	42	0	22	0	0
6	1	16	0	27	2	0
6	4	16	0	27	4	0
7	1	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2	5	0	0	0	0
8	1	34	0	0	3	0
8	2	36	0	0	0	0
8	3	27	0	0	1	0
All	All	6503	0	6188	70	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 6.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:274:ASN:HD21	3:3:66:ARG:HH12	1.16	0.90
1:1:195:TYR:H	2:2:131:GLN:HE21	1.29	0.80
1:1:68:GLU:OE1	8:1:401:HOH:O	2.03	0.76
1:1:230:HIS:ND1	7:1:302:SO4:O3	2.24	0.70
1:1:195:TYR:H	2:2:131:GLN:NE2	1.90	0.69

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)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	1/11 (9%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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)

4 ligands 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	MYR	1	301	-	15,15,15	0.63	1 (6%)	15,15,15	1.04	2 (13%)
6	MYR	4	101	-	15,15,15	0.56	0	15,15,15	1.03	0
7	SO4	1	302	-	4,4,4	0.17	0	6,6,6	0.24	0
7	SO4	2	301	-	4,4,4	0.10	0	6,6,6	0.29	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	MYR	1	301	-	-	5/13/13/13	-
6	MYR	4	101	-	-	9/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	301	MYR	O2-C1	-2.31	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1	301	MYR	O2-C1-O1	-2.40	117.31	123.30
6	1	301	MYR	O2-C1-C2	2.27	121.33	114.03

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	4	101	MYR	C1-C2-C3-C4
6	4	101	MYR	C5-C6-C7-C8
6	4	101	MYR	C9-C10-C11-C12
6	4	101	MYR	C6-C7-C8-C9
6	1	301	MYR	C10-C11-C12-C13

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	301	MYR	2	0
6	4	101	MYR	4	0
7	1	302	SO4	1	0

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
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	4:GLN	C	21:GLY	N	6.64

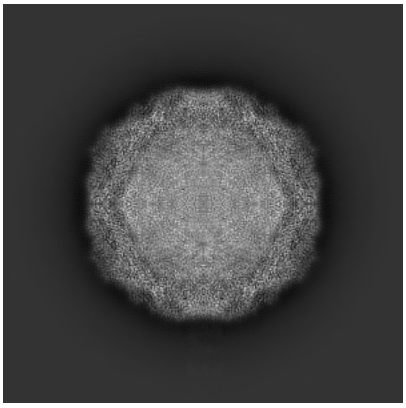
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10506. These allow visual inspection of the internal detail of the map and identification of artifacts.

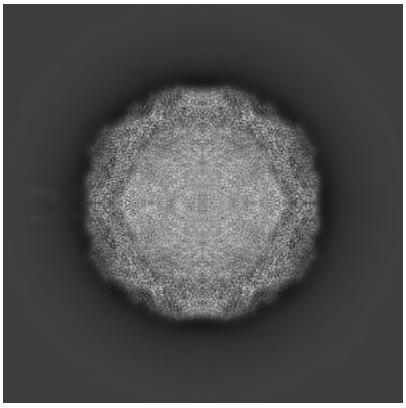
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

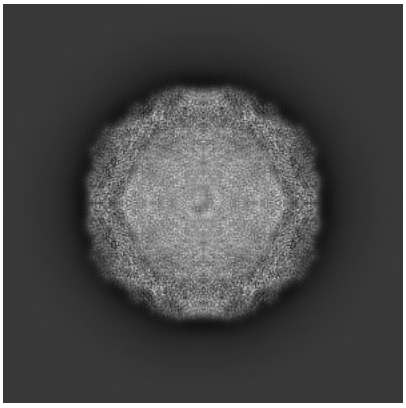
6.1.1 Primary map



X



Y

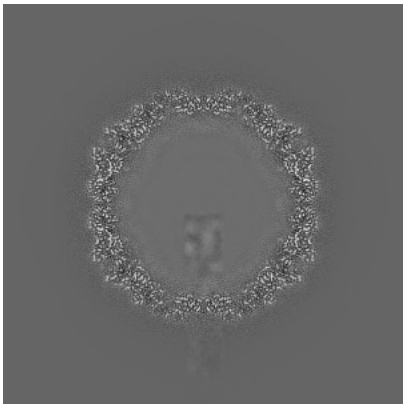


Z

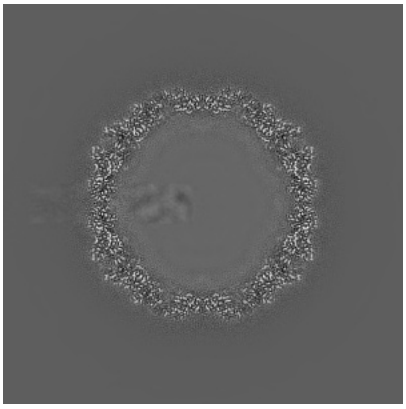
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

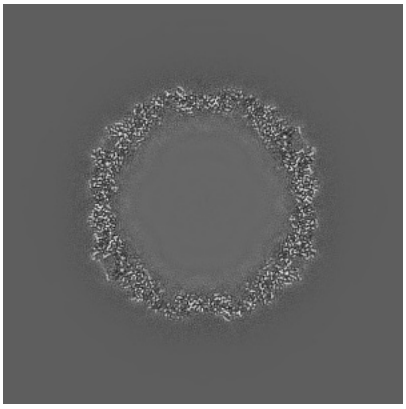
6.2.1 Primary map



X Index: 234



Y Index: 234

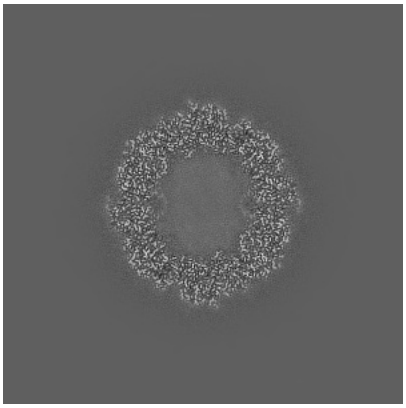


Z Index: 234

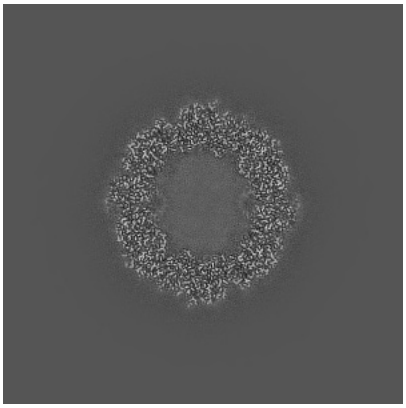
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

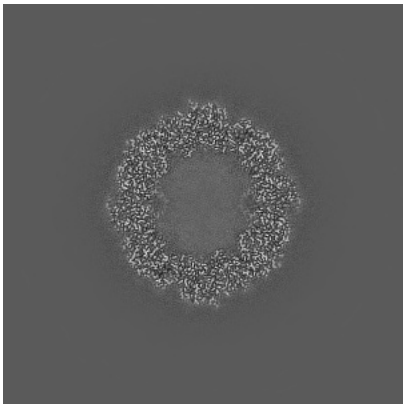
6.3.1 Primary map



X Index: 318



Y Index: 150

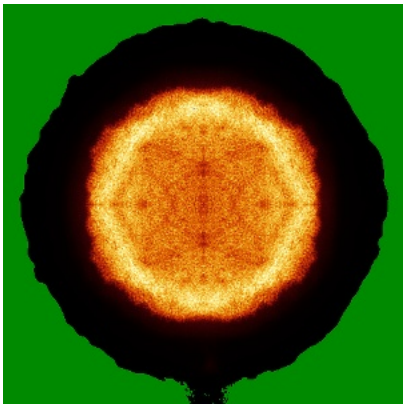


Z Index: 317

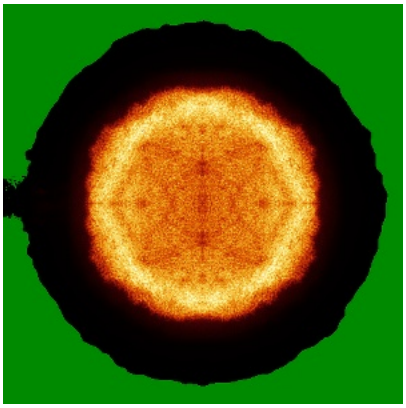
The images above show the largest variance slices of the map in three orthogonal directions.

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

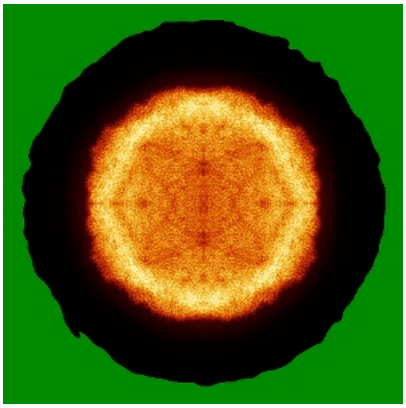
6.4.1 Primary map



X



Y

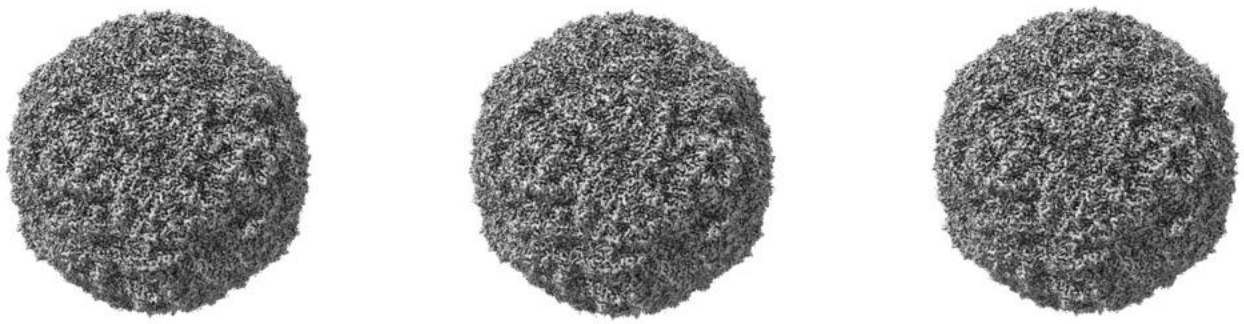


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.052. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

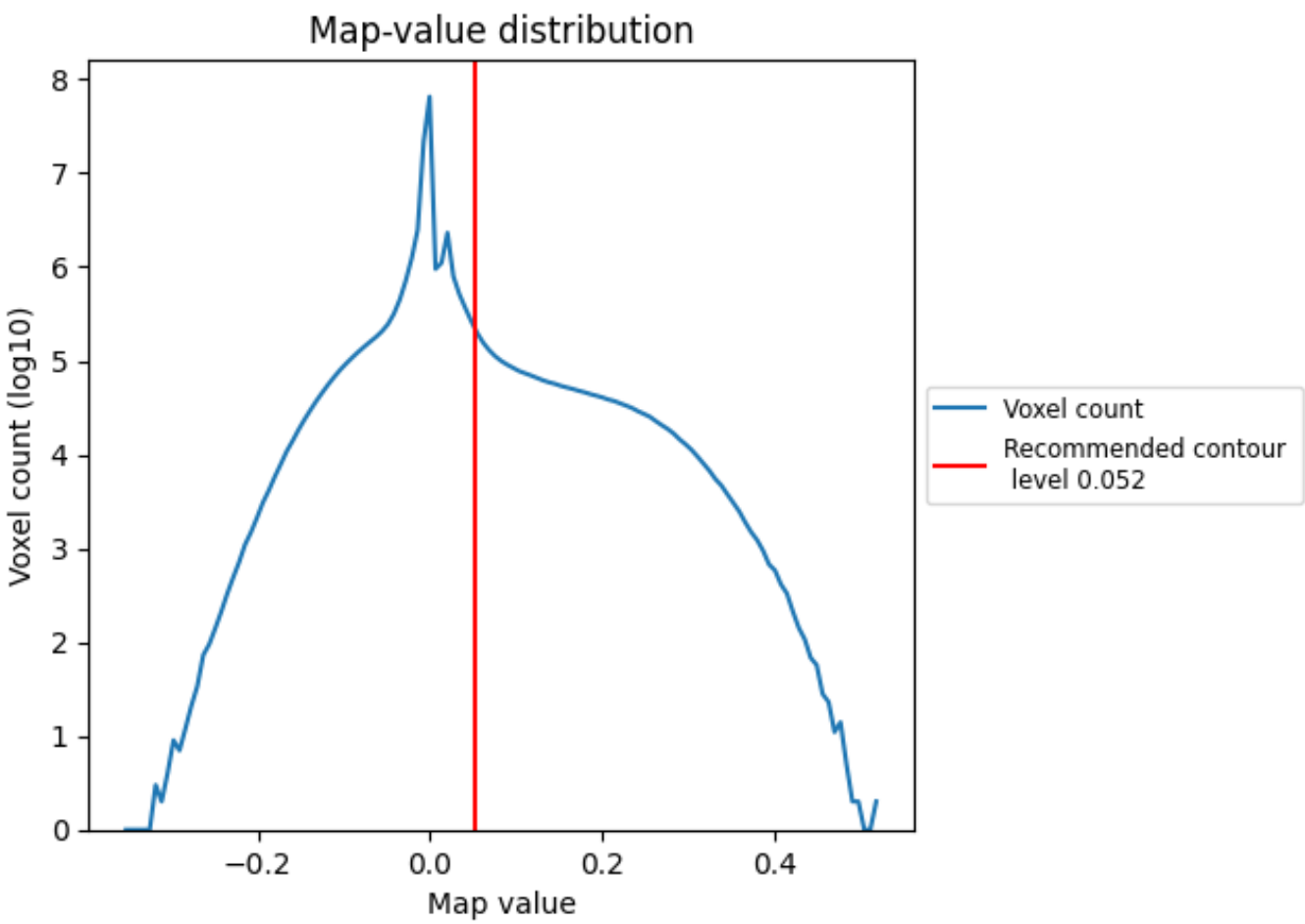
6.6 Mask visualisation (i)

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

7 Map analysis (i)

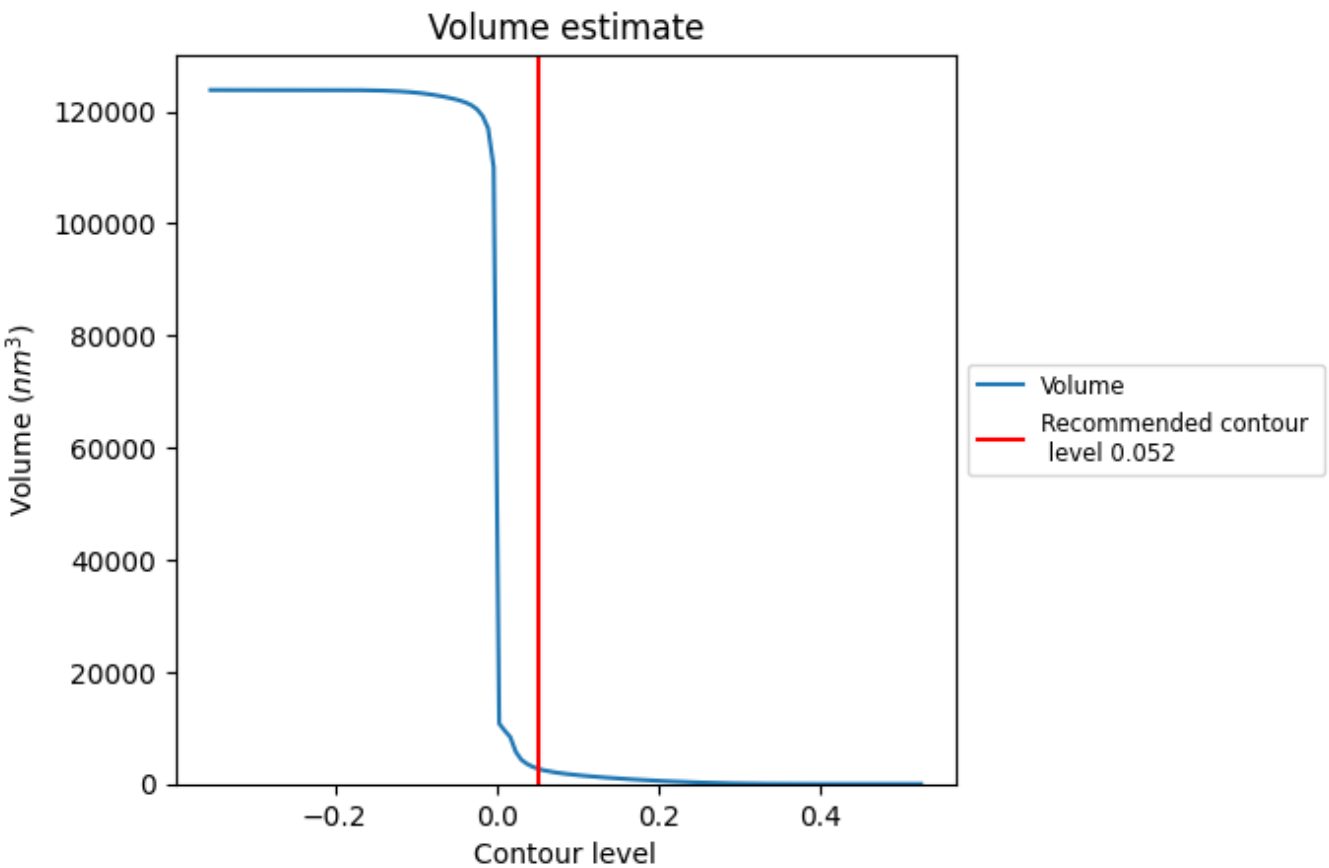
This section contains the results of statistical analysis of the map.

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.

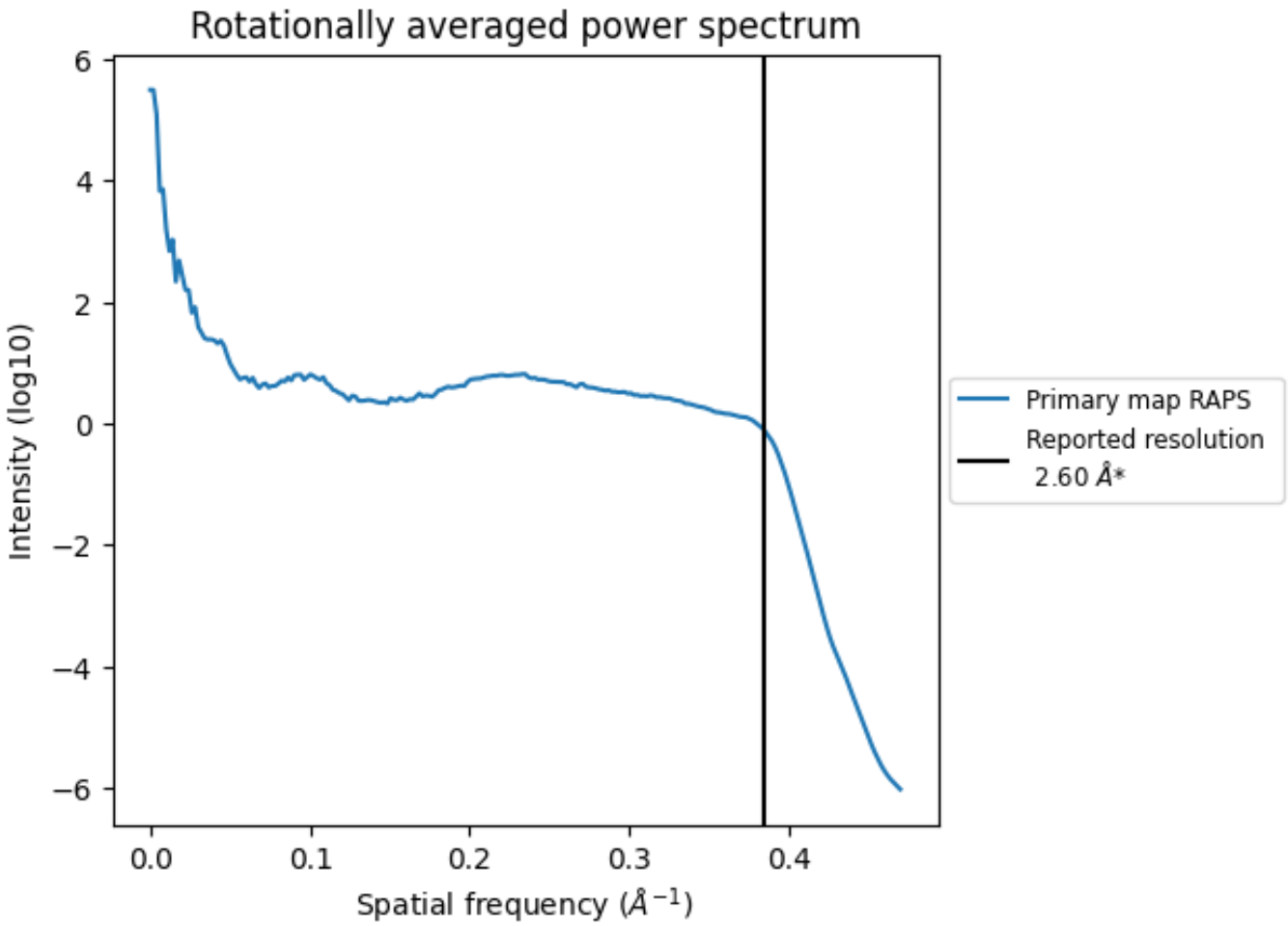
7.2 Volume estimate (i)



The volume at the recommended contour level is 2692 nm^3; this corresponds to an approximate mass of 2432 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 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

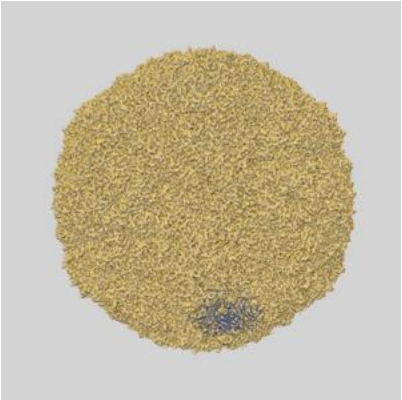
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

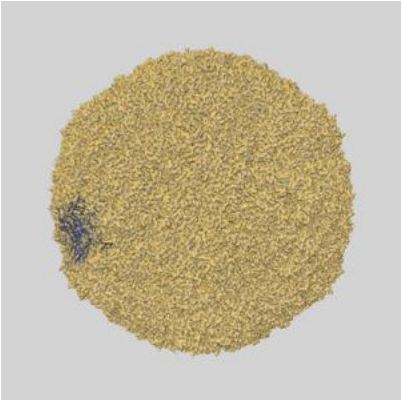
This section contains information regarding the fit between EMDB map EMD-10506 and PDB model 6THN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

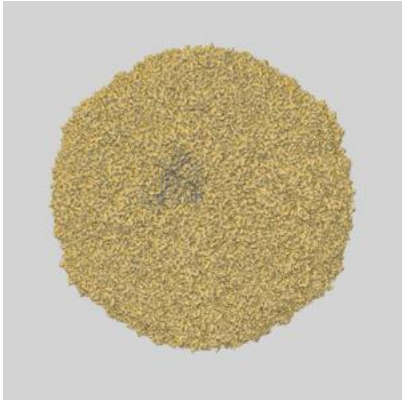
9.1.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.052 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.

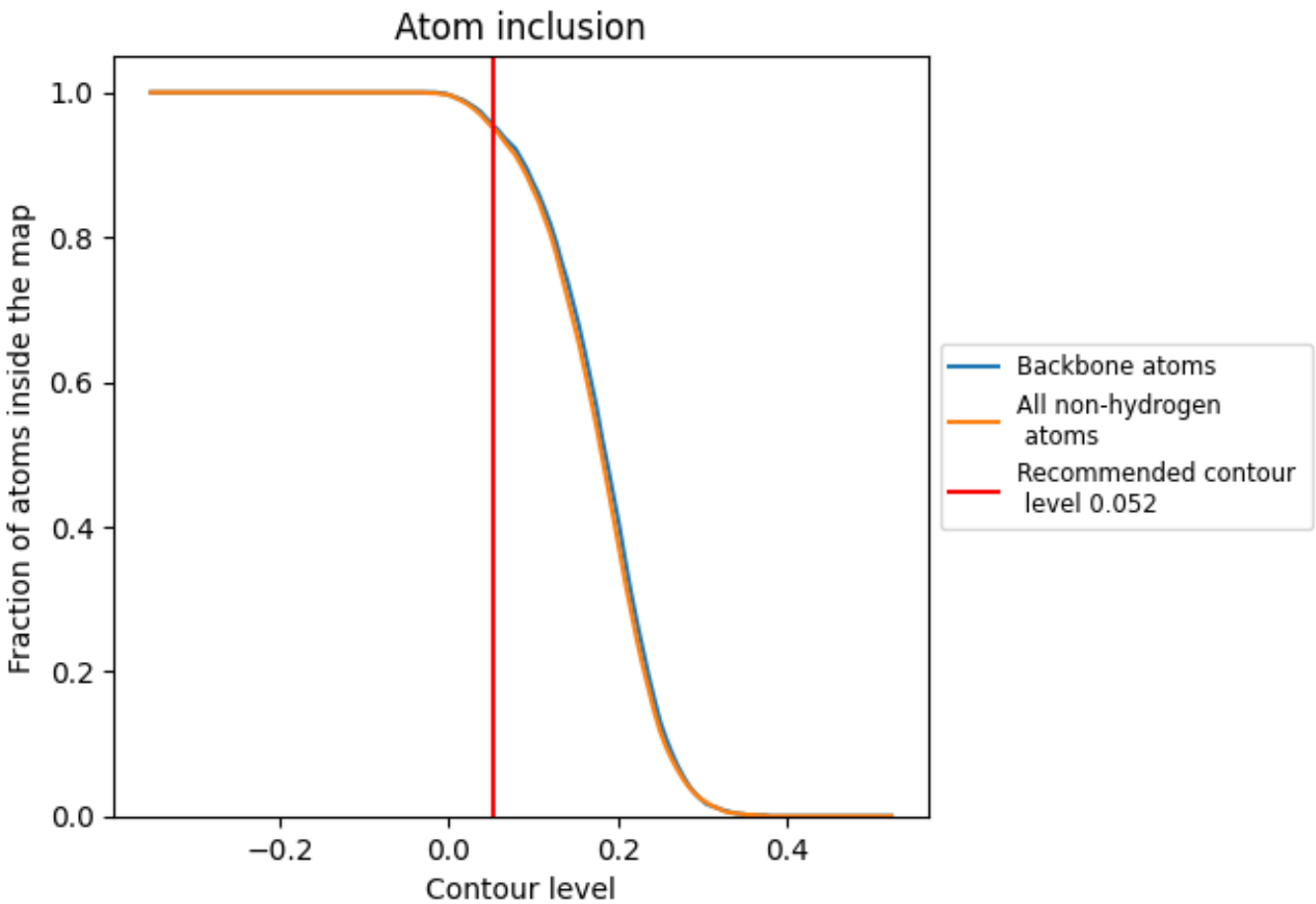
9.2 Q-score mapped to coordinate model (i)

This section was not generated.

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.052) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9510
1	0.9570
2	0.9700
3	0.9720
4	0.8190
A	0.2860