



Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 02:50 PM EST

PDB ID : 3IYK
EMDB ID : EMD-5147
Title : Bluetongue virus structure reveals a sialic acid binding domain, amphipathic helices and a central coiled coil in the outer capsid proteins
Authors : Zhang, X.; Boyce, M.; Bhattacharya, B.; Zhang, X.; Schein, S.; Roy, P.; Zhou, Z.H.
Deposited on : 2010-01-25
Resolution : 7.00 Å(reported)

This is a Full wwPDB EM Validation 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

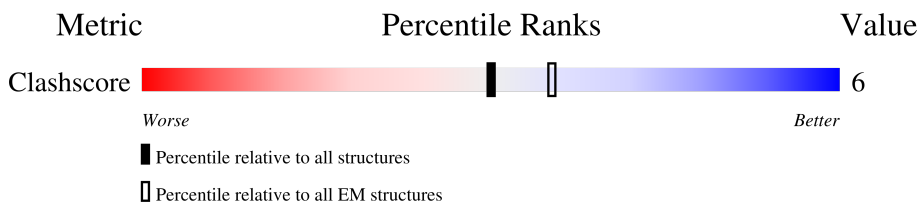
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 7.00 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	526	 58% 42%
1	B	526	 58% 42%
1	C	526	 58% 42%
1	D	526	 58% 42%
1	E	526	 58% 42%
1	F	526	 58% 42%
2	G	600	 23% 76%
2	I	600	 23% 76%
2	K	600	 23% 76%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2331 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.

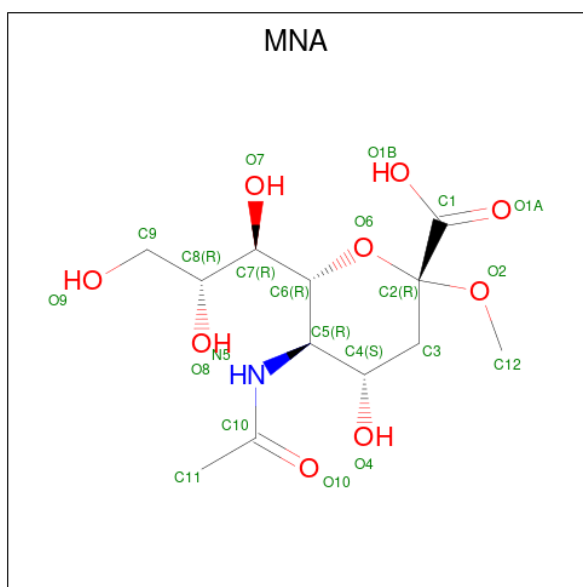
- Molecule 1 is a protein called VP5.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	307	Total C 307 307	0	307
1	B	307	Total C 307 307	0	307
1	C	307	Total C 307 307	0	307
1	D	307	Total C 307 307	0	307
1	E	307	Total C 307 307	0	307
1	F	307	Total C 307 307	0	307

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	G	141	Total C 141 141	0	141
2	I	141	Total C 141 141	0	141
2	K	141	Total C 141 141	0	141

- Molecule 3 is 2-O-methyl-5-N-acetyl-alpha-D-neuraminic acid (three-letter code: MNA) (formula: C₁₂H₂₁NO₉).

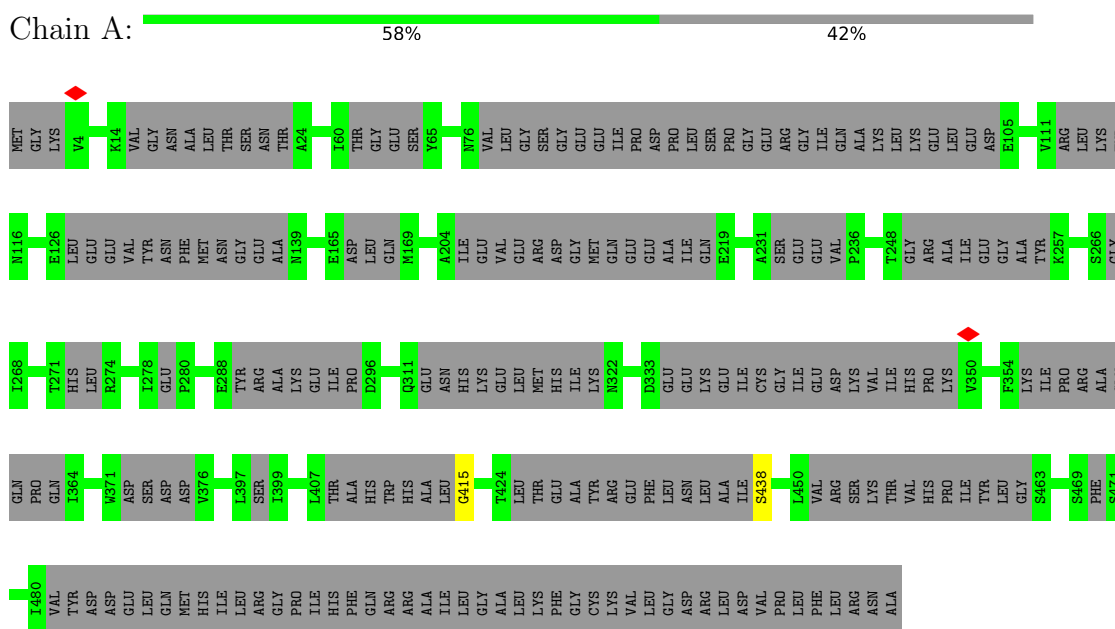


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	G	1	22	12	1	9	1
3	I	1	22	12	1	9	1
3	K	1	22	12	1	9	1

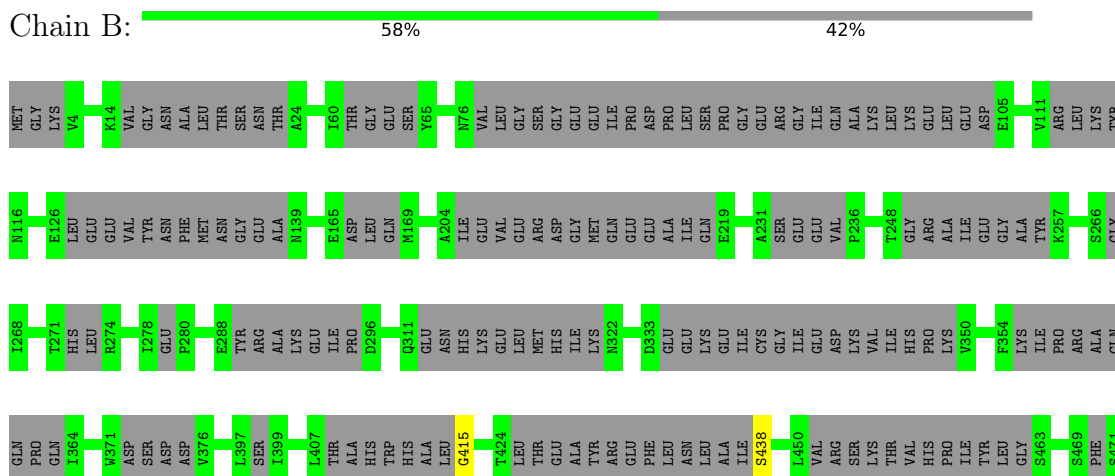
3 Residue-property plots [i](#)

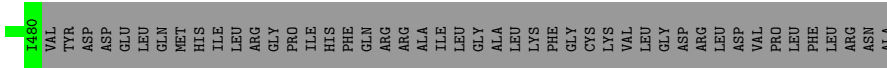
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: VP5

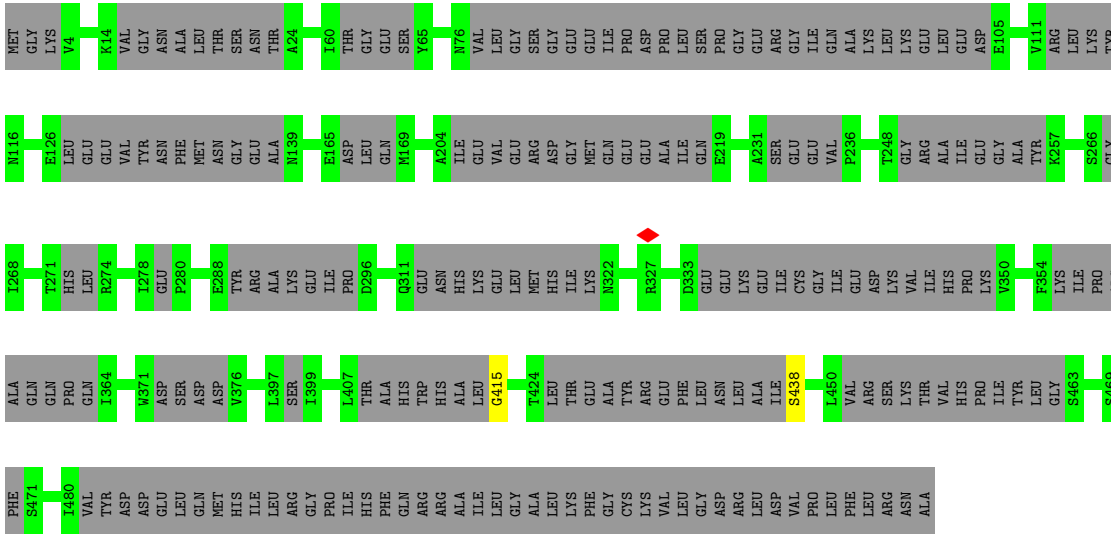


- Molecule 1: VP5

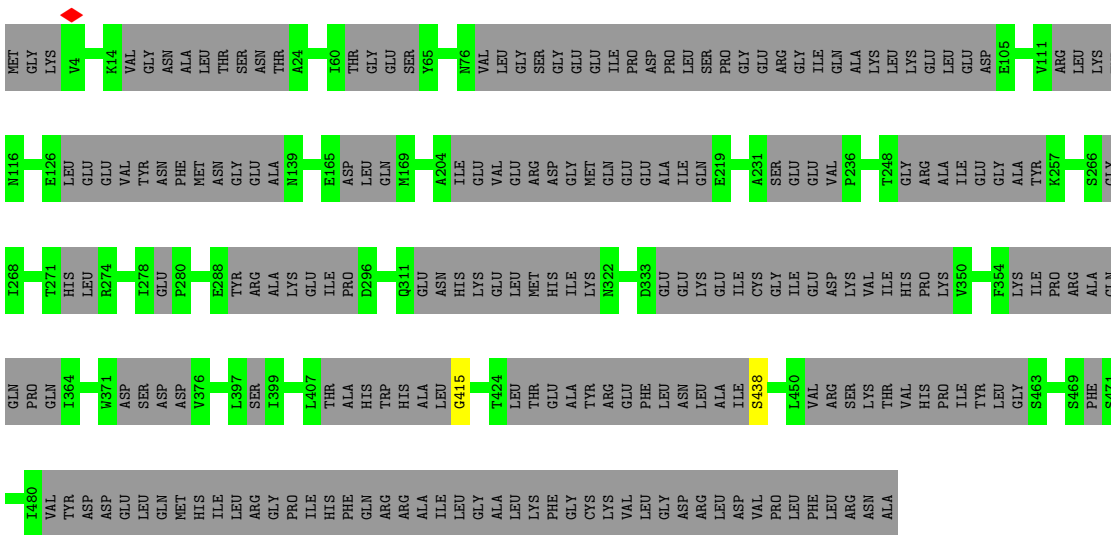




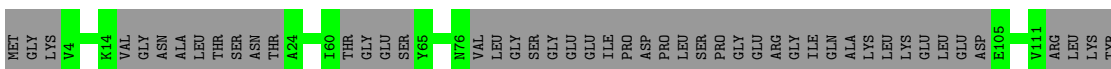
• Molecule 1: VP5



• Molecule 1: VP5



• Molecule 1: VP5



TYR ARG
LEU LEU
ASN HIS
SER SER
THR THR
ARG ARG
GLU GLU
THR THR
THR THR
TYR TYR
ALA ALA
GLN GLN
GLY GLY
ASN ASN
PRO PRO
CYS CYS
ASP ASP
LEU LEU
TYR TYR
PRO PRO
GLY GLY
GLU GLU
ASP ASP
ASP ASP
VAL VAL
LEU LEU
PHE PHE
THR THR
LYS LYS
PHE PHE
ASP ASP
ASP ASP
VAL VAL
ALA ALA
TYR TYR
GLY GLY
GLN GLN
MET MET
ASN ASN
LEU LEU
ILE ILE
MET MET
PRO PRO
GLU GLU
TYR TYR
PHE PHE
VAL VAL
ASN ASN
THR THR
LYS LYS
TRP TRP
ILE ILE
ILE ILE
ASP ASP
ARG ARG
GLU GLU
MET MET
ILE ILE
LYS LYS
HIS HIS
GLU GLU
GLY GLY
TRP TRP
ILE ILE
ALA ALA
ASN ASN
GLN GLN
ARG ARG
GLN GLN
PHE PHE
SER SER
LYS LYS
ASP ASP
MET MET
HIS HIS
LYS LYS
ILE ILE
LEU LEU

LYS SER
SER SER
GLY GLY
ASN ASN
VAL VAL
LEU LEU
THR THR
THR THR
ILE ILE
ASP ASP
PHE PHE
GLU GLU
LYS LYS
ASP ASP
ALA ALA
LYS LYS
LEU LEU
THR THR
THR THR
ASN ASN
GLU GLU
GLY GLY
VAL VAL
THR THR
MET MET
PRO PRO
GLU GLU
TYR TYR
PHE PHE
VAL VAL
ASN ASN
THR THR
LYS LYS
TRP TRP
ILE ILE
ILE ILE
ALA ALA
VAL VAL
PRO PRO
MET MET
PHE PHE
ASN ASN
ALA ALA
LYS LYS
LEU LEU
ARG ARG
ILE ILE
LYS LYS
HIS HIS
GLU GLU
GLY GLY
TRP TRP
ILE ILE
ALA ALA
GLN GLN
ARG ARG
GLN GLN
PHE PHE
SER SER
LYS LYS
ASP ASP
MET MET
HIS HIS
LYS LYS
VAL VAL
LEU LEU

ARG THR
THR THR
LEU LEU
SER SER
PRO PRO
ILE ILE
THR THR
ALA ALA
ASP ASP
PRO PRO
ILE ILE
GLU GLU
LEU LEU
GLN GLN
ARG ARG
LEU LEU
THR THR
LEU LEU
ALA ALA
ARG ARG
PHE PHE
TYR TYR
ASP ASP
ILE ILE
ARG ARG
PRO PRO
ALA ALA
LEU LEU
ARG ARG
GLY GLY
GLN GLN
ALA ALA
LEU LEU
SER SER
ARG ARG
GLN GLN
ALA ALA
GLN GLN
SER SER
THR THR
TYR TYR
ASP ASP
GLU GLU
GLU GLU
ILE ILE
SER SER
LYS LYS
GLN GLN
ARG ARG
ASP ASP
TYR TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	79787	Depositor
Image detector	GENERIC CCD	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.019	Depositor
Map size (\AA)	940.0, 940.0, 940.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.88, 1.88, 1.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MNA

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

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	307	0	0	1	0
1	B	307	0	0	1	0
1	C	307	0	0	1	0
1	D	307	0	0	1	0
1	E	307	0	0	1	0
1	F	307	0	0	1	0
2	G	141	0	0	3	0
2	I	141	0	0	3	0
2	K	141	0	0	3	0
3	G	22	0	20	0	0
3	I	22	0	20	0	0
3	K	22	0	20	0	0
All	All	2331	0	60	12	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.

All (12) 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:C:415:GLY:CA	1:C:438:SER:CA	2.38	1.02
1:D:415:GLY:CA	1:D:438:SER:CA	2.38	1.02
1:E:415:GLY:CA	1:E:438:SER:CA	2.38	1.02
1:B:415:GLY:CA	1:B:438:SER:CA	2.38	1.01
1:A:415:GLY:CA	1:A:438:SER:CA	2.38	1.01
1:F:415:GLY:CA	1:F:438:SER:CA	2.38	1.00
2:G:271:ASP:CA	2:K:209:ARG:CA	2.50	0.89
2:I:209:ARG:CA	2:K:271:ASP:CA	2.62	0.78
2:G:209:ARG:CA	2:I:271:ASP:CA	2.64	0.75
2:G:156:GLU:CA	2:G:157:ASP:CA	2.97	0.43
2:K:156:GLU:CA	2:K:157:ASP:CA	2.97	0.43
2:I:156:GLU:CA	2:I:157:ASP:CA	2.97	0.42

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

3 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
3	MNA	I	1000[B]	-	22,22,22	0.86	2 (9%)	27,32,32	0.76	0
3	MNA	K	1000[C]	-	22,22,22	0.87	2 (9%)	27,32,32	0.77	0
3	MNA	G	1000[A]	-	22,22,22	0.85	2 (9%)	27,32,32	0.77	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
3	MNA	I	1000[B]	-	-	3/23/41/41	0/1/1/1
3	MNA	K	1000[C]	-	-	3/23/41/41	0/1/1/1
3	MNA	G	1000[A]	-	-	3/23/41/41	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1000[C]	MNA	C4-C5	2.29	1.55	1.53
3	G	1000[A]	MNA	C4-C5	2.24	1.55	1.53
3	I	1000[B]	MNA	C4-C5	2.24	1.55	1.53
3	I	1000[B]	MNA	C3-C2	2.15	1.55	1.52
3	K	1000[C]	MNA	C3-C2	2.13	1.55	1.52
3	G	1000[A]	MNA	C3-C2	2.10	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

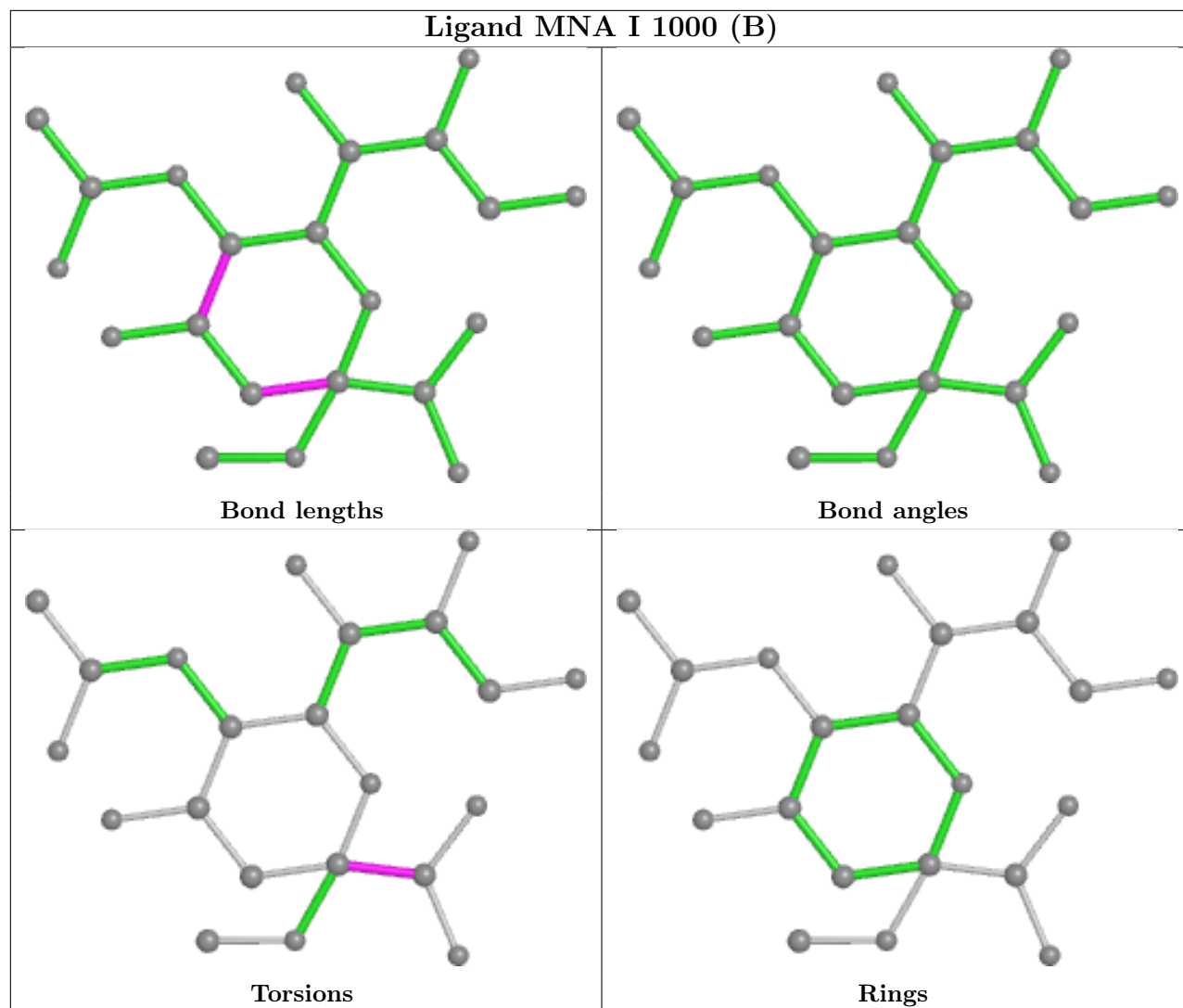
All (9) torsion outliers are listed below:

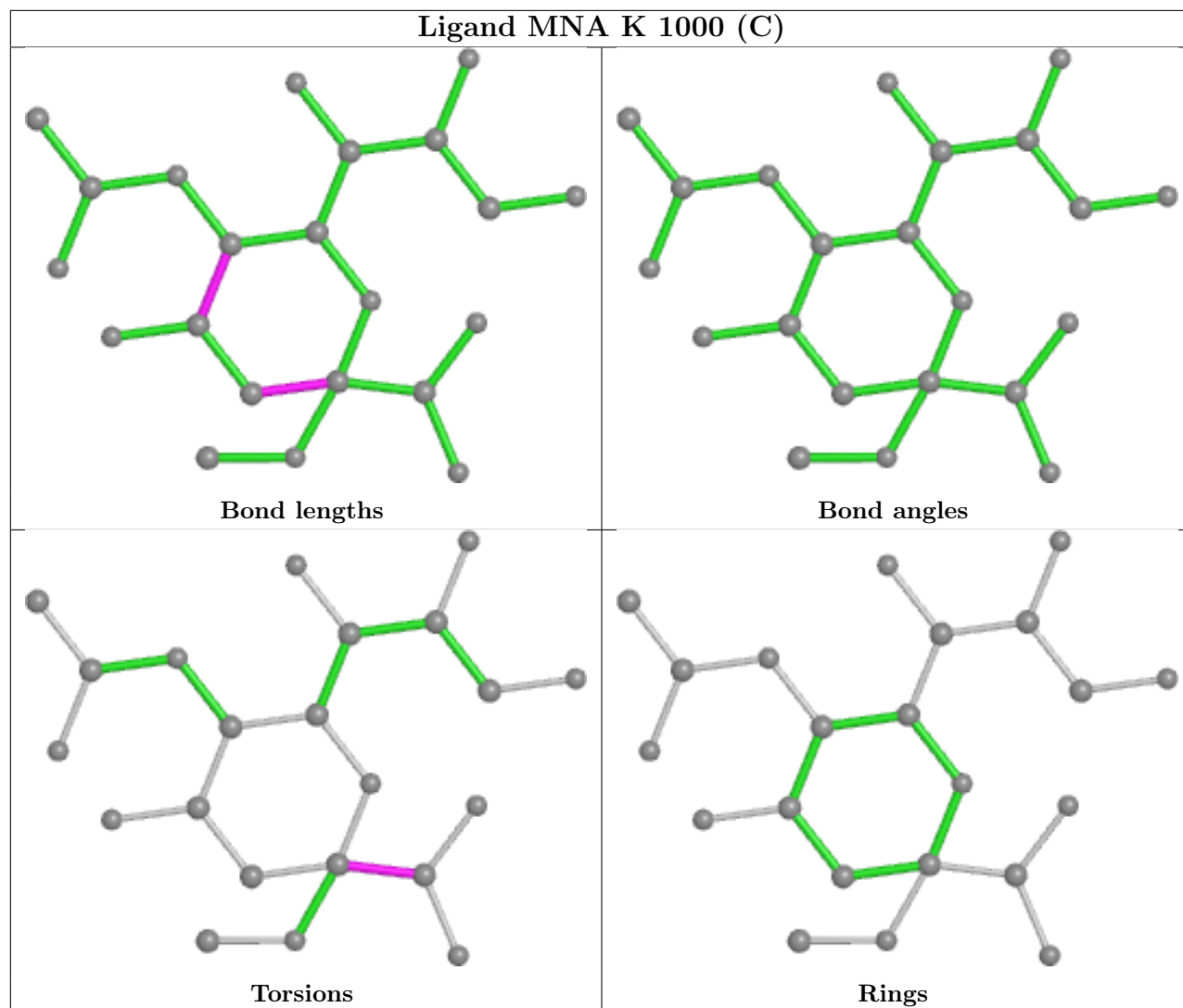
Mol	Chain	Res	Type	Atoms
3	G	1000[A]	MNA	O1B-C1-C2-O2
3	G	1000[A]	MNA	O1B-C1-C2-O6
3	I	1000[B]	MNA	O1B-C1-C2-O2
3	I	1000[B]	MNA	O1B-C1-C2-O6
3	K	1000[C]	MNA	O1B-C1-C2-O2
3	K	1000[C]	MNA	O1B-C1-C2-O6
3	G	1000[A]	MNA	O1A-C1-C2-O2
3	I	1000[B]	MNA	O1A-C1-C2-O2
3	K	1000[C]	MNA	O1A-C1-C2-O2

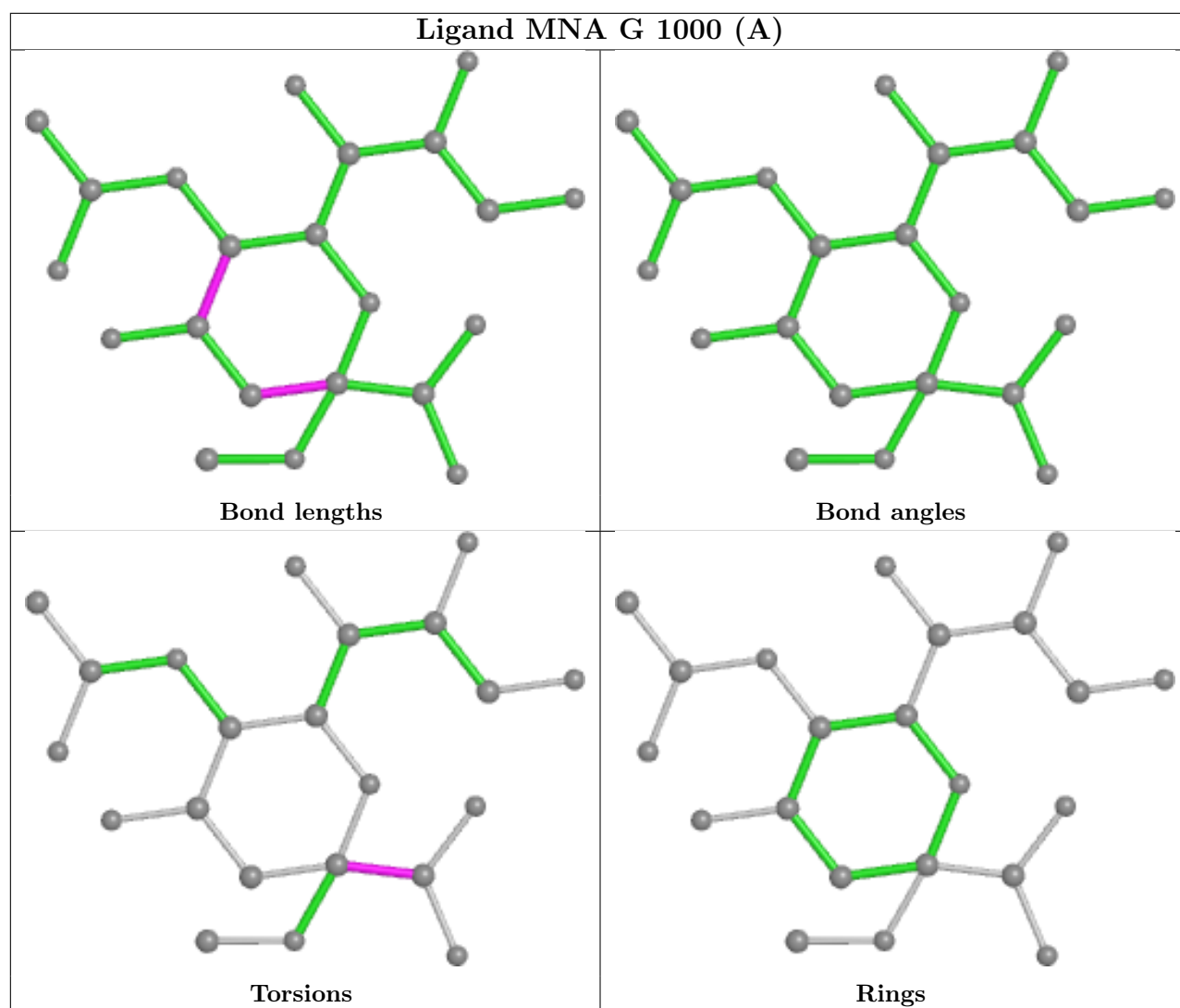
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

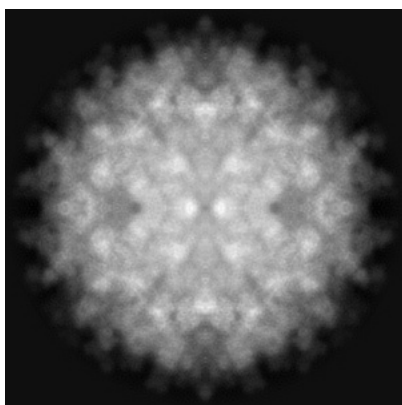
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5147. These allow visual inspection of the internal detail of the map and identification of artifacts.

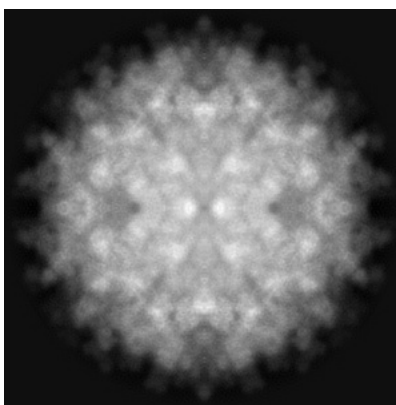
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

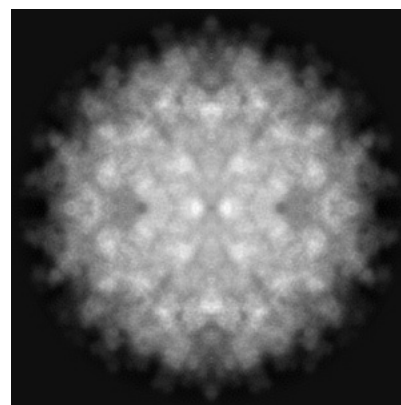
6.1.1 Primary map



X



Y

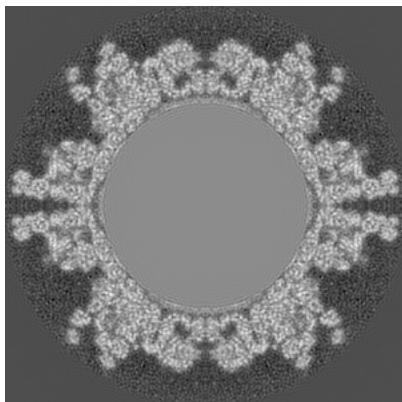


Z

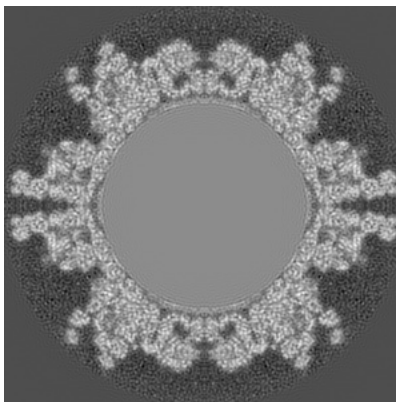
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

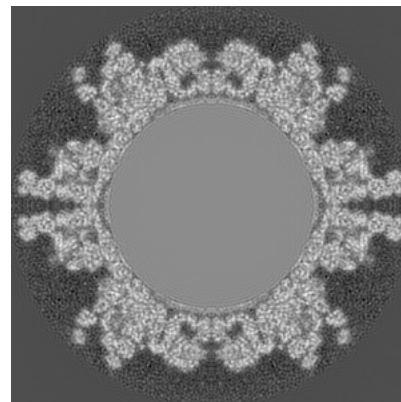
6.2.1 Primary map



X Index: 250



Y Index: 250

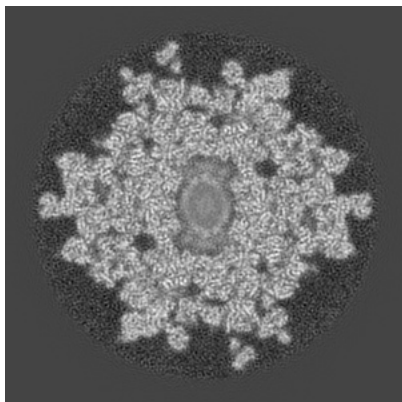


Z Index: 250

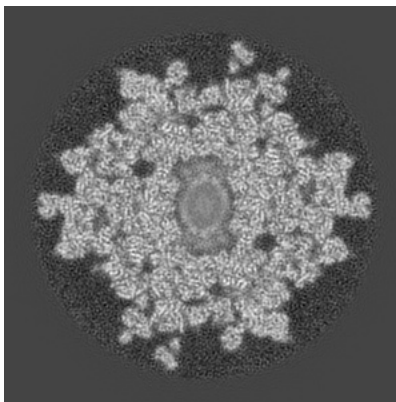
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

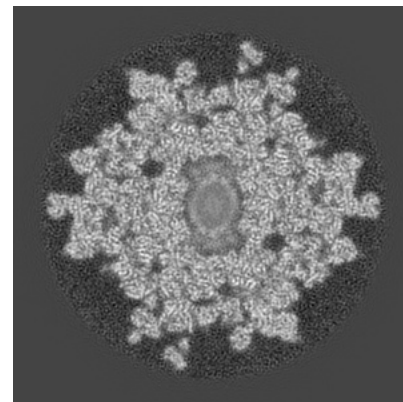
6.3.1 Primary map



X Index: 375



Y Index: 125

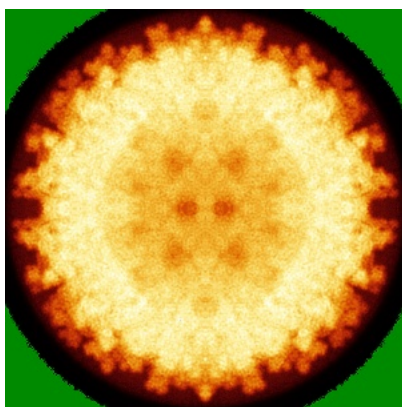


Z Index: 125

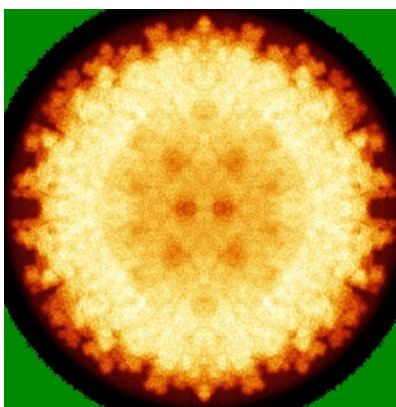
The images above show the largest variance slices of the map in three orthogonal directions.

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

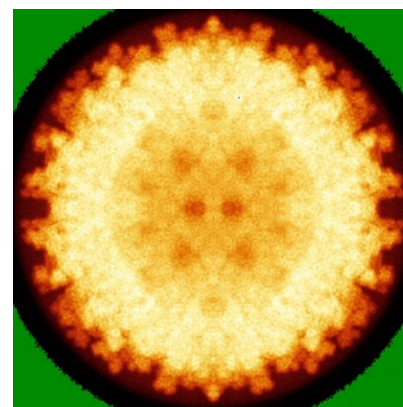
6.4.1 Primary map



X



Y

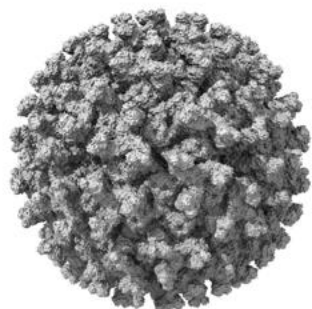


Z

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

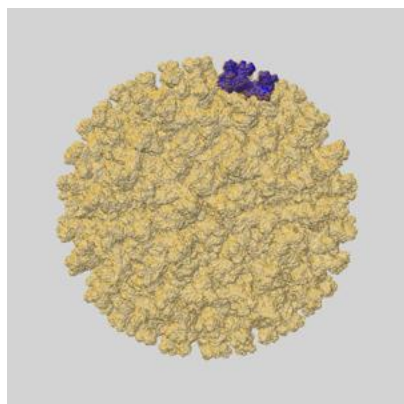
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

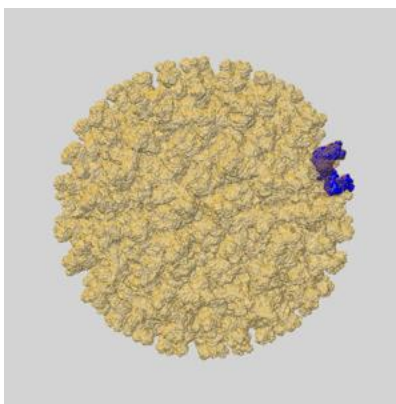
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

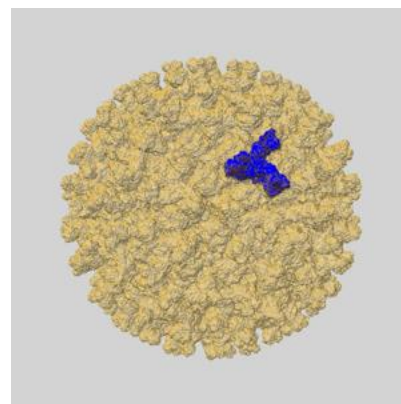
6.6.1 emd_5147_msk_1.map [i](#)



X

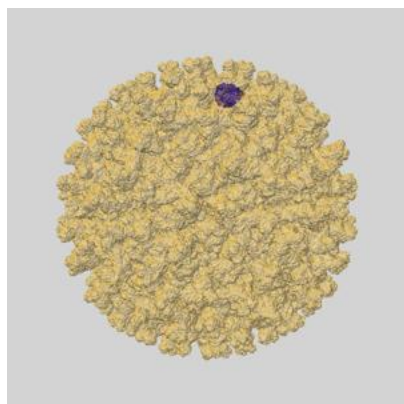


Y

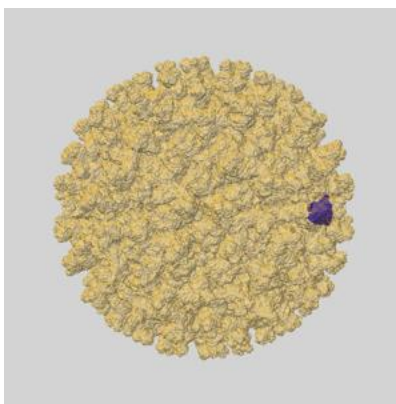


Z

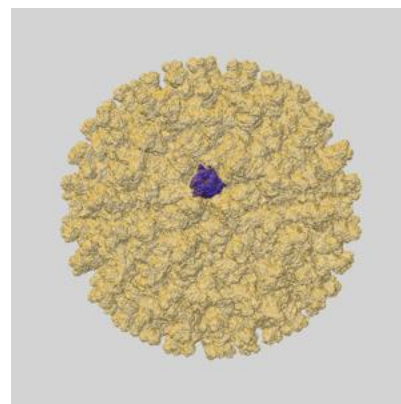
6.6.2 emd_5147_msk_2.map [i](#)



X



Y

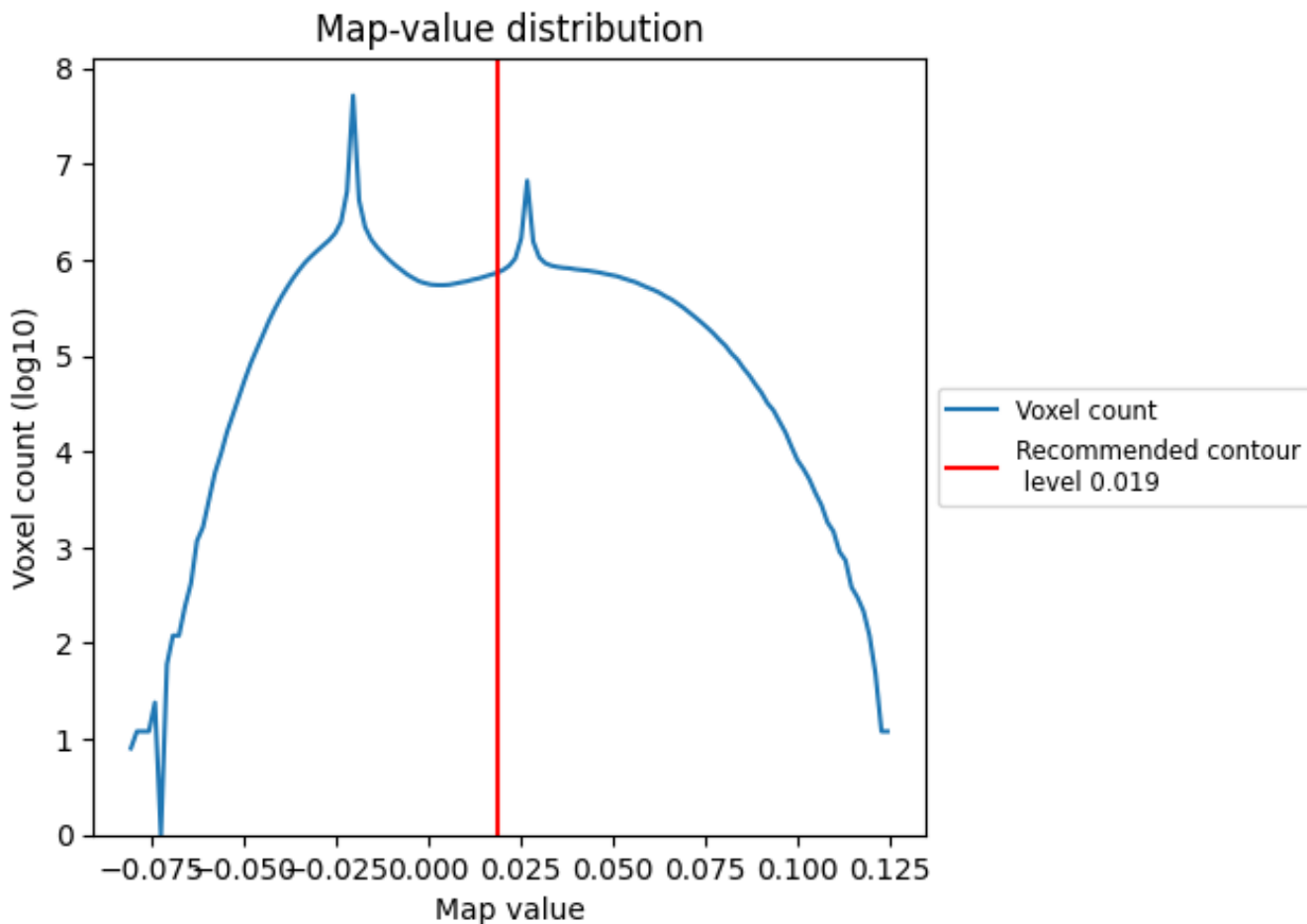


Z

7 Map analysis [i](#)

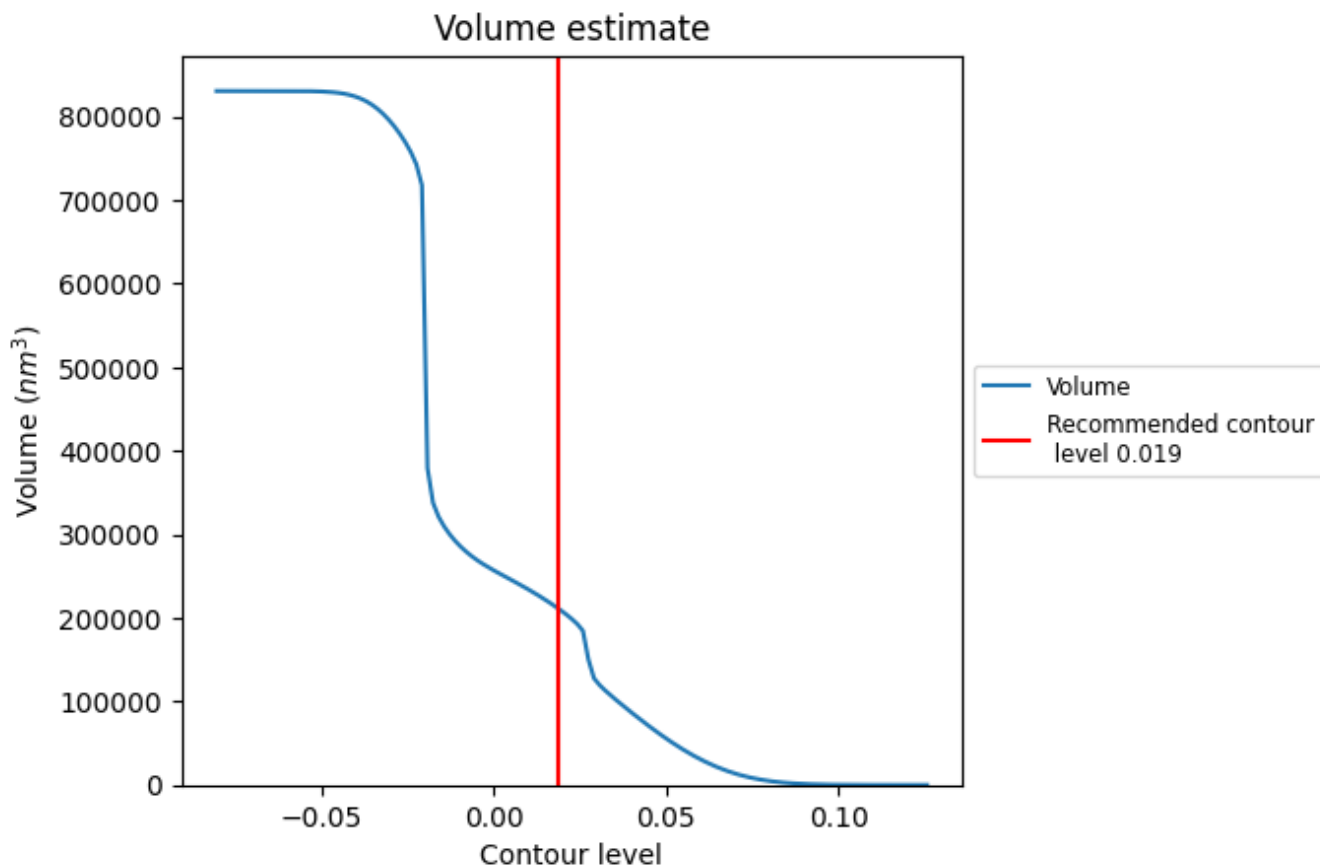
This section contains the results of statistical analysis of the map.

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.

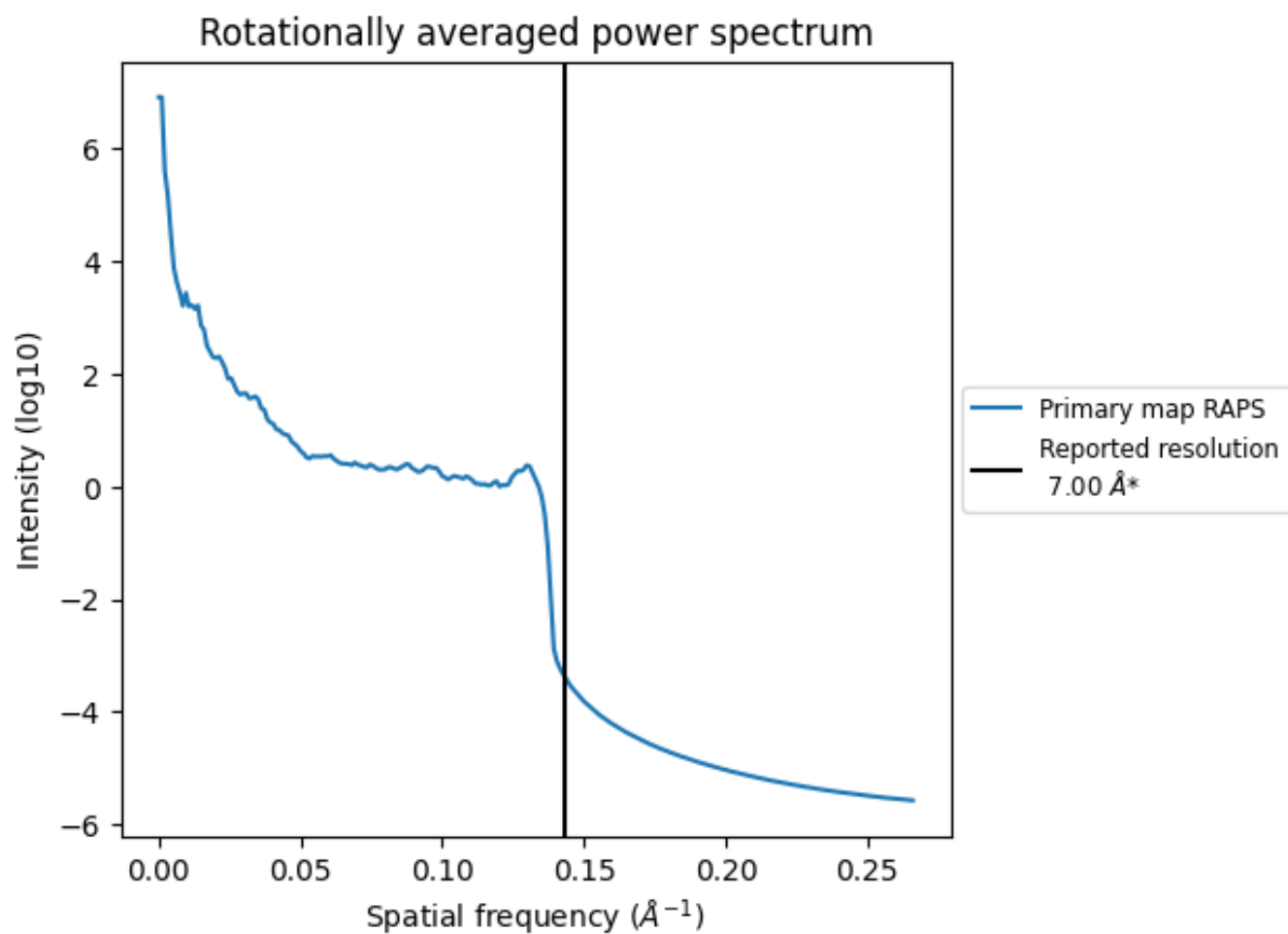
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210568 nm^3 ; this corresponds to an approximate mass of 190212 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 0.143 Å⁻¹

8 Fourier-Shell correlation

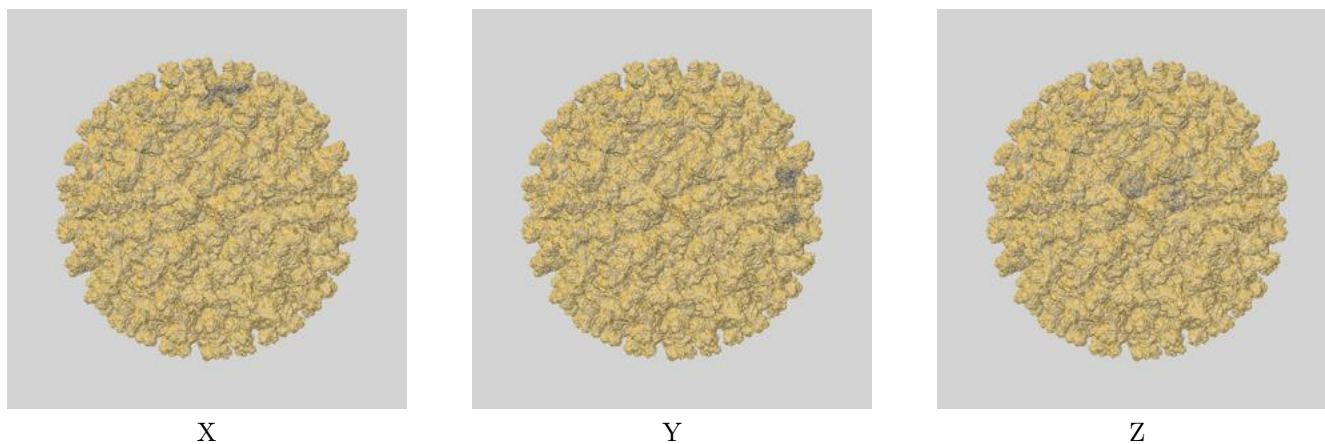
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

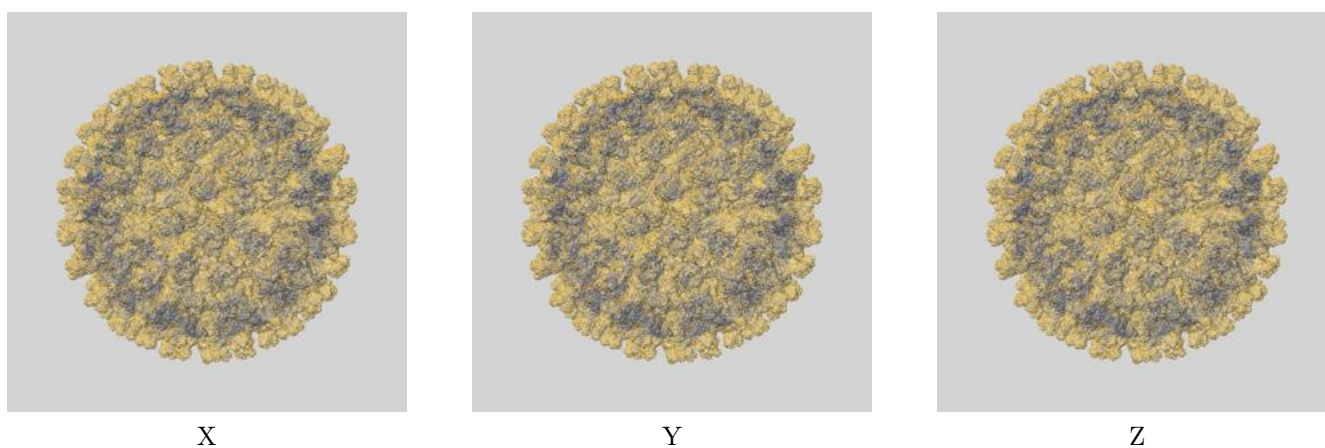
This section contains information regarding the fit between EMDB map EMD-5147 and PDB model 3IYK. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

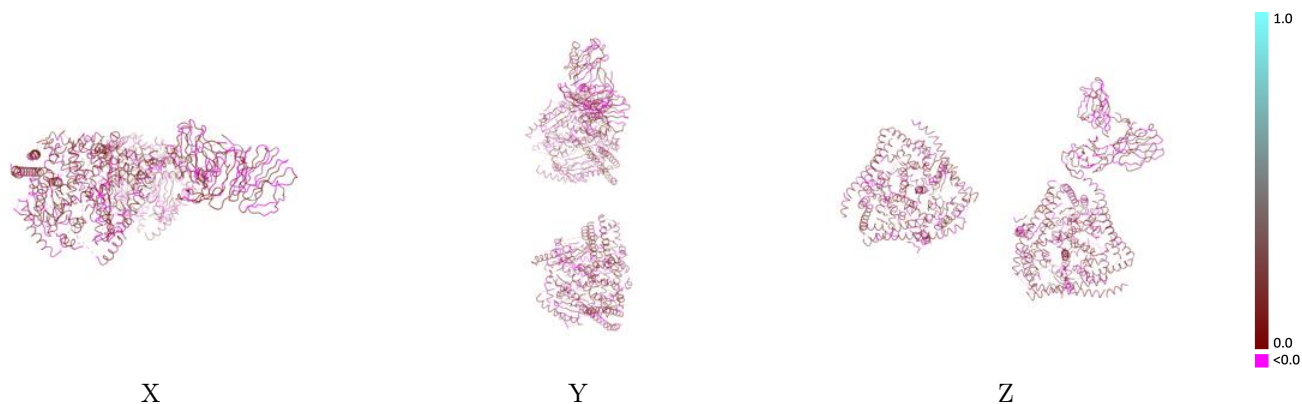


9.1.2 Map-model assembly overlay [i](#)



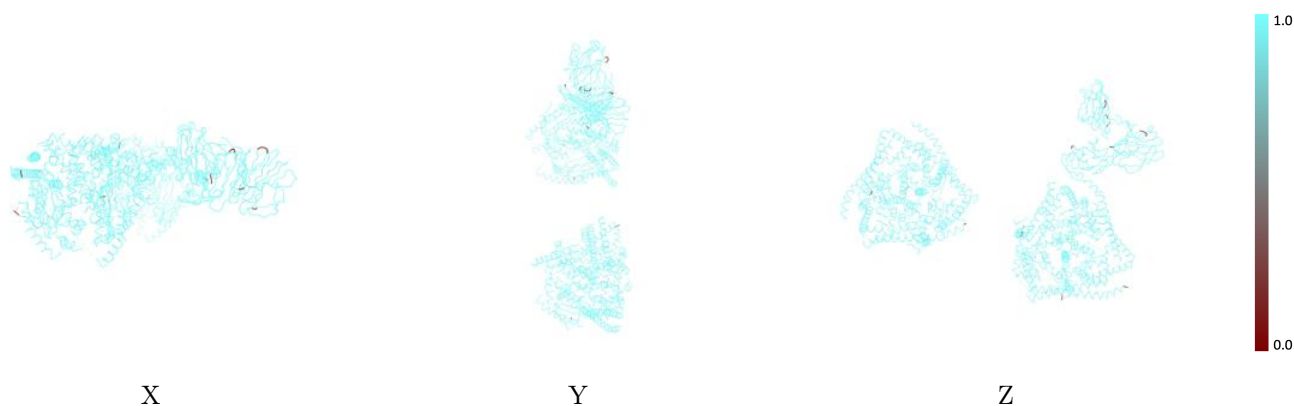
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



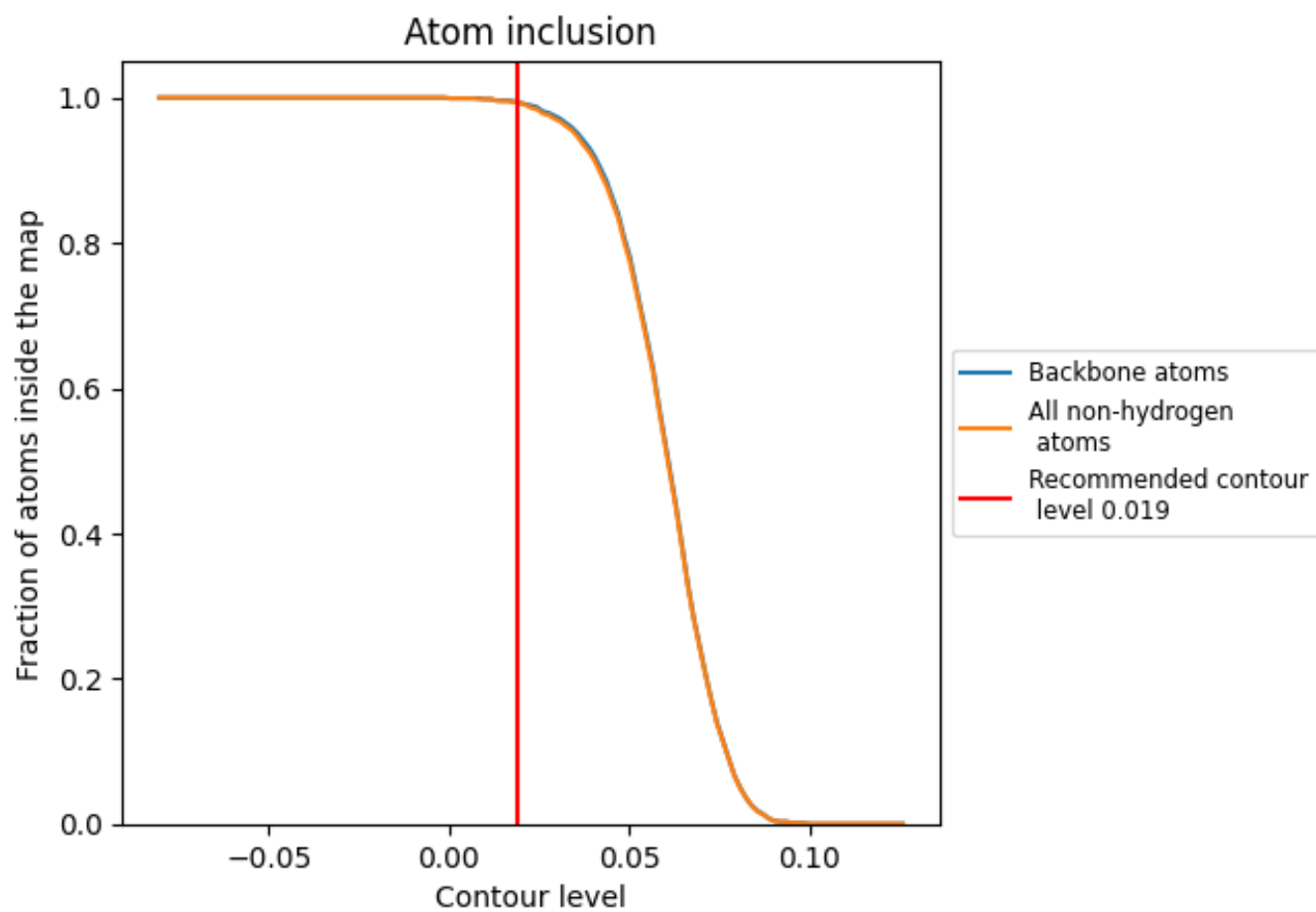
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9930	 0.0990
A	 0.9940	 0.1290
B	 1.0000	 0.1080
C	 0.9970	 0.1120
D	 0.9970	 0.1140
E	 1.0000	 0.1150
F	 0.9970	 0.1120
G	 0.9630	 0.0320
I	 0.9720	 0.0390
K	 0.9930	 0.0370

