Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:13 am GMT

PDB ID	:	6GV4
EMDB ID	:	EMD-0069
Title	:	High-resolution Cryo-EM of Fab-labeled human parechovirus 3
Authors	:	Domanska, A.; Flatt, J.W.; Jukonen, J.J.J.; Geraets, J.A.; Butcher, S.J.
Deposited on	:	2018-06-20
Resolution	:	2.80 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:

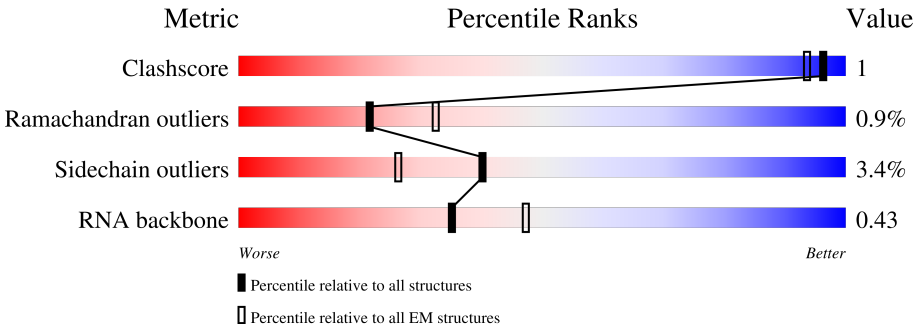
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.80 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
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	D	8	62% 25% 12%
2	A	289	86% • 11%
3	B	229	80% 5% 15%
4	C	256	90% • 6%
5	H	121	87% 10% ••
6	L	113	88% 8% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14001 atoms, of which 6653 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 RNA chain called RNA (5'-R(*UP*GP*GP*UP*AP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	8	Total	C	N	O	P	0	0
			156	70	25	54	7		

- Molecule 2 is a protein called VP0.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	256	Total	C	H	N	O	S	0	0
			3839	1259	1842	329	404	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	GLU	ASP	conflict	UNP Q8BES5

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	195	Total	C	H	N	O	S	0	0
			2978	996	1419	270	285	8		

- Molecule 4 is a protein called VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	241	Total	C	H	N	O	S	0	0
			3651	1202	1751	326	360	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	118	ASN	ILE	conflict	UNP Q8BES5
C	121	THR	ASN	conflict	UNP Q8BES5
C	123	ASP	ALA	conflict	UNP Q8BES5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ASN	THR	conflict	UNP Q8BES5
C	134	THR	SER	conflict	UNP Q8BES5
C	141	SER	PHE	conflict	UNP Q8BES5

- Molecule 5 is a protein called AT12-015 antibody variable heavy.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	118	Total	C	H	N	O	S	0	0
			1759	571	857	154	173	4		

- Molecule 6 is a protein called AT12-015 antibody variable light.

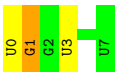
Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	108	Total	C	H	N	O	S	0	0
			1618	525	784	140	165	4		

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.

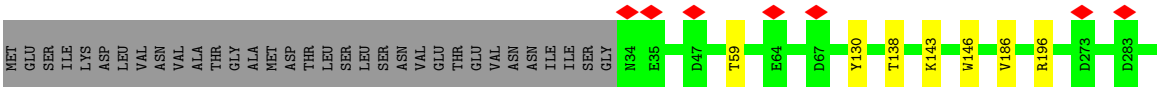
• Molecule 1: RNA (5'-R(*UP*GP*GP*UP*AP*UP*UP*U)-3')

Chain D:



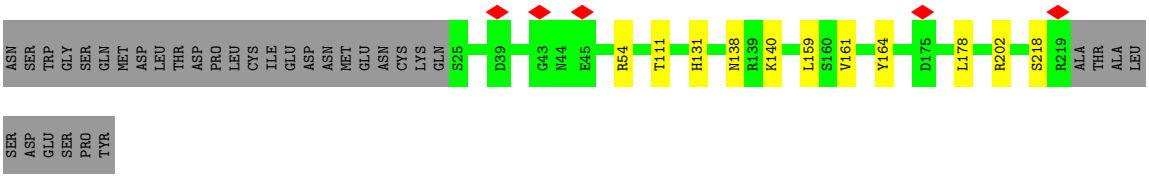
• Molecule 2: VP0

Chain A:



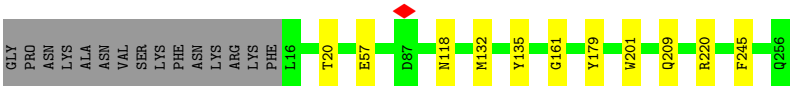
• Molecule 3: VP1

Chain B:



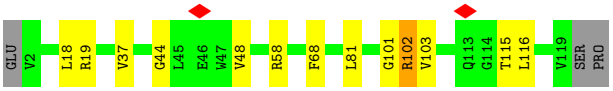
• Molecule 4: VP3

Chain C:



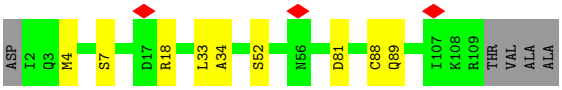
• Molecule 5: AT12-015 antibody variable heavy

Chain H:



• Molecule 6: AT12-015 antibody variable light

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	74927	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; GCTF was used to estimate ctf	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.419	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.65	0/172	0.80	0/265
2	A	0.88	0/2045	1.02	2/2801 (0.1%)
3	B	0.92	0/1605	1.06	1/2180 (0.0%)
4	C	0.91	0/1945	1.02	0/2636
5	H	0.94	0/922	1.08	2/1246 (0.2%)
6	L	0.89	0/852	1.08	1/1156 (0.1%)
All	All	0.90	0/7541	1.04	6/10284 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	4	MET	CG-SD-CE	-6.77	89.36	100.20
5	H	68	PHE	CB-CG-CD1	6.67	125.47	120.80
2	A	130	TYR	CB-CG-CD2	-6.09	117.34	121.00
5	H	68	PHE	CB-CG-CD2	-5.98	116.62	120.80
3	B	164	TYR	CB-CG-CD2	-5.54	117.67	121.00
2	A	130	TYR	CB-CG-CD1	5.41	124.24	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	196	ARG	Sidechain

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	D	156	0	74	2	0
2	A	1997	1842	1915	0	0
3	B	1559	1419	1508	1	0
4	C	1900	1751	1846	4	0
5	H	902	857	867	5	0
6	L	834	784	814	2	0
All	All	7348	6653	7024	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 1.

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)
5:H:102:ARG:H	5:H:102:ARG:HD3	1.11	1.08
1:D:1:G:H1'	4:C:20:THR:HG21	1.52	0.91
5:H:102:ARG:HD3	5:H:102:ARG:N	1.93	0.82
1:D:1:G:H1'	4:C:20:THR:CG2	2.13	0.79
5:H:102:ARG:HG2	5:H:102:ARG:O	2.06	0.55
3:B:131:HIS:CD2	3:B:161:VAL:HG11	2.44	0.52
5:H:102:ARG:O	5:H:103:VAL:HG13	2.10	0.51
5:H:102:ARG:H	5:H:102:ARG:CD	1.99	0.46
6:L:33:LEU:HD13	6:L:34:ALA:N	2.32	0.44
4:C:161:GLY:HA2	4:C:179:TYR:HA	2.02	0.42
4:C:135:TYR:CG	4:C:245:PHE:HB3	2.56	0.41
6:L:33:LEU:HD11	6:L:88:CYS:HB2	2.02	0.41

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
2	A	254/289 (88%)	228 (90%)	26 (10%)	0	100 100
3	B	193/229 (84%)	181 (94%)	10 (5%)	2 (1%)	15 44
4	C	239/256 (93%)	223 (93%)	15 (6%)	1 (0%)	34 66
5	H	116/121 (96%)	103 (89%)	11 (10%)	2 (2%)	9 29
6	L	106/113 (94%)	96 (91%)	7 (7%)	3 (3%)	5 17
All	All	908/1008 (90%)	831 (92%)	69 (8%)	8 (1%)	21 46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	81	ASP
4	C	220	ARG
5	H	101	GLY
5	H	44	GLY
3	B	138	ASN
3	B	218	SER
6	L	52	SER
6	L	7	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
2	A	225/254 (89%)	220 (98%)	5 (2%)	52 83
3	B	173/204 (85%)	167 (96%)	6 (4%)	36 70
4	C	211/224 (94%)	206 (98%)	5 (2%)	49 81
5	H	92/95 (97%)	83 (90%)	9 (10%)	8 24
6	L	93/96 (97%)	91 (98%)	2 (2%)	52 83
All	All	794/873 (91%)	767 (97%)	27 (3%)	40 71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	59	THR
2	A	138	THR
2	A	143	LYS
2	A	146	TRP
2	A	186	VAL
3	B	54	ARG
3	B	111	THR
3	B	140	LYS
3	B	159	LEU
3	B	178	LEU
3	B	202	ARG
4	C	57	GLU
4	C	118	ASN
4	C	132	MET
4	C	201	TRP
4	C	209	GLN
5	H	18	LEU
5	H	19	ARG
5	H	37	VAL
5	H	48	VAL
5	H	58	ARG
5	H	81	LEU
5	H	102	ARG
5	H	115	THR
5	H	116	LEU
6	L	18	ARG
6	L	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	37	GLN
3	B	131	HIS
4	C	116	HIS
4	C	118	ASN
4	C	209	GLN
4	C	256	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	7/8 (87%)	2 (28%)	2 (28%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	1	G
1	D	3	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	0	U
1	D	1	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

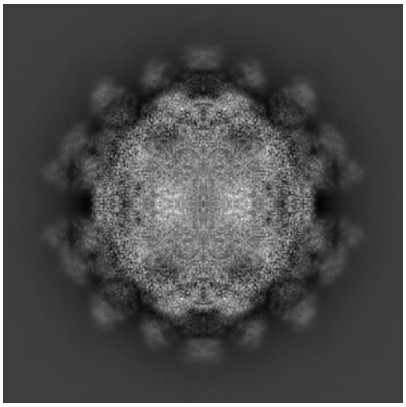
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0069. These allow visual inspection of the internal detail of the map and identification of artifacts.

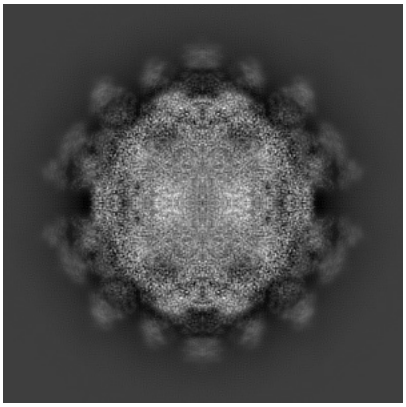
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

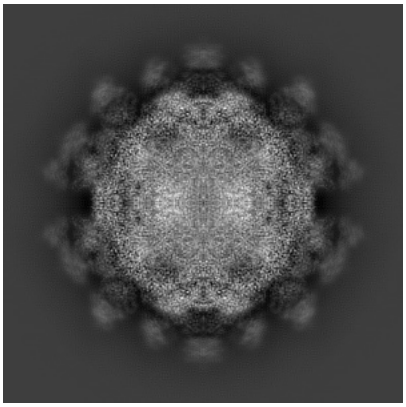
6.1.1 Primary map



X



Y

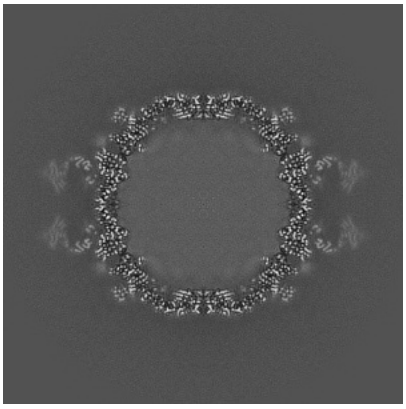


Z

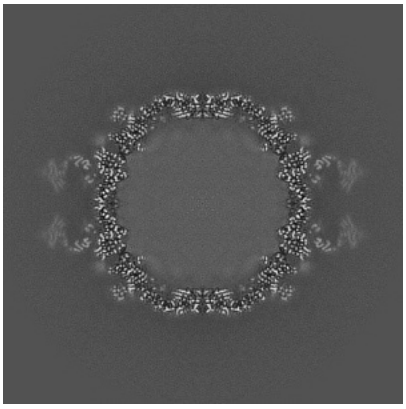
The images above show the map projected in three orthogonal directions.

6.2 Central slices

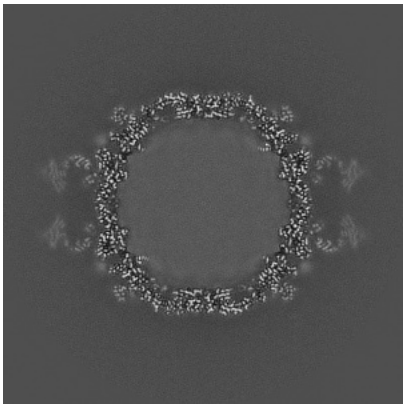
6.2.1 Primary map



X Index: 240



Y Index: 240

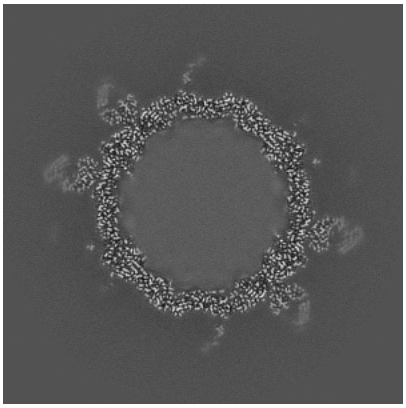


Z Index: 240

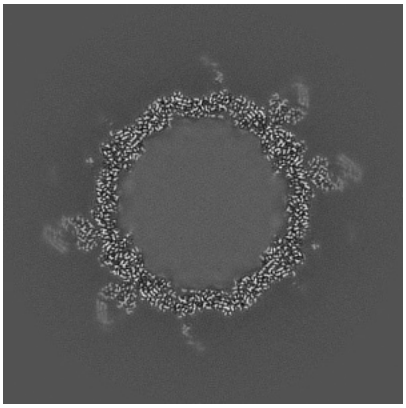
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

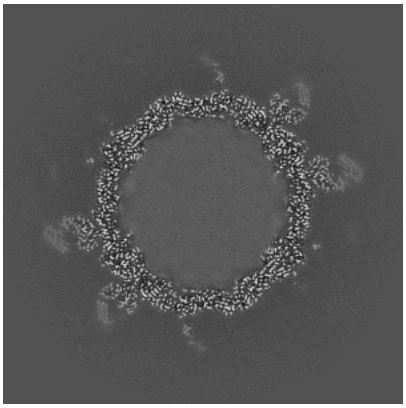
6.3.1 Primary map



X Index: 256



Y Index: 224

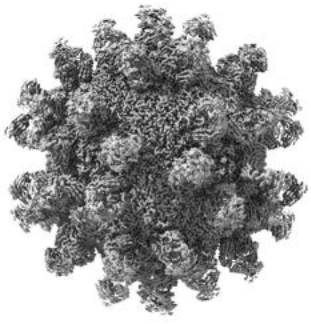


Z Index: 223

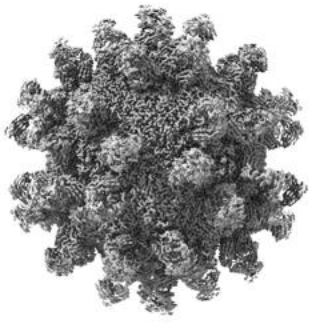
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

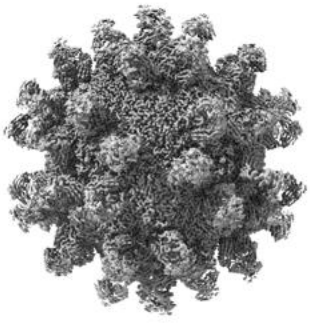
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

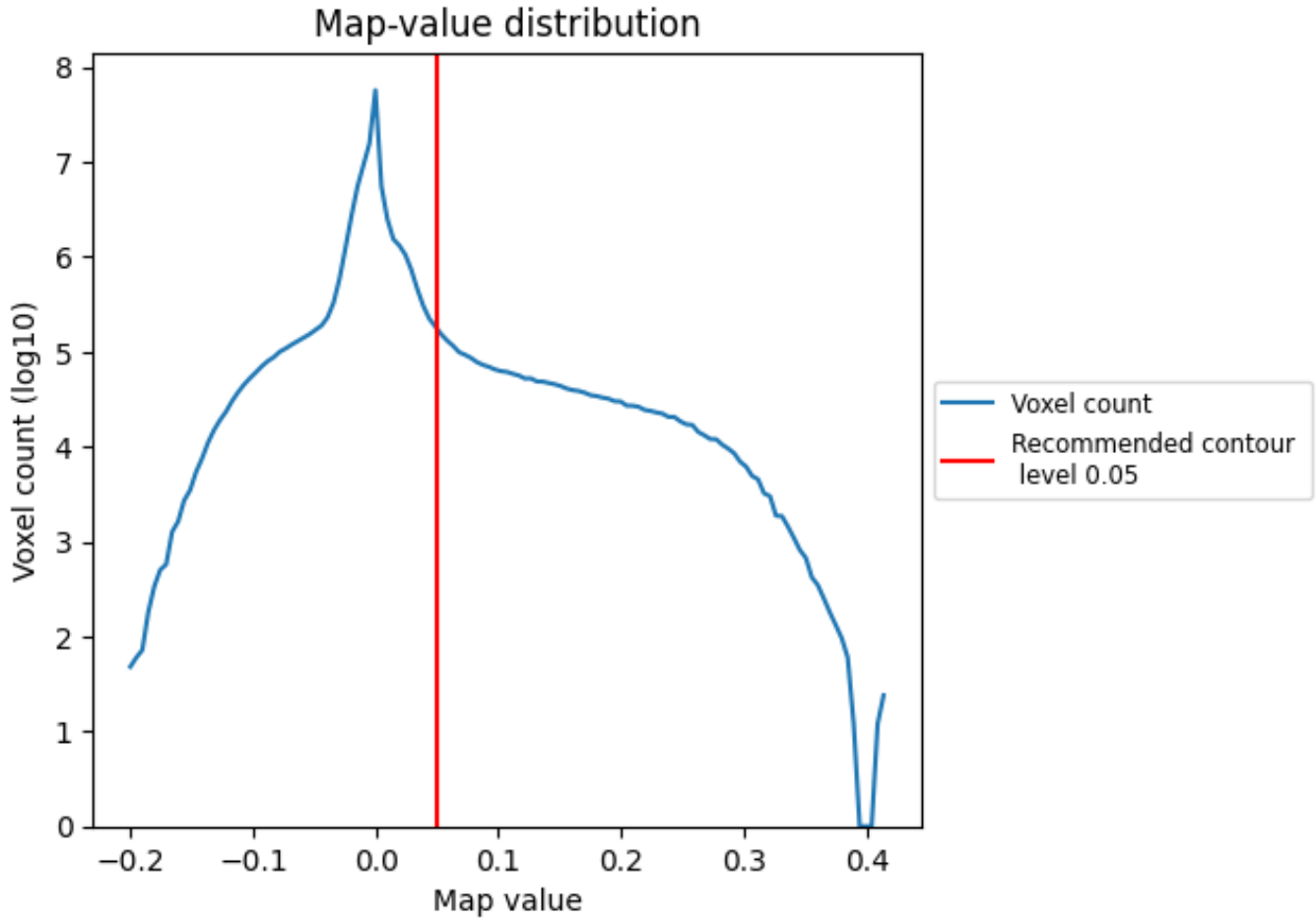
6.5 Mask visualisation (i)

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

7 Map analysis

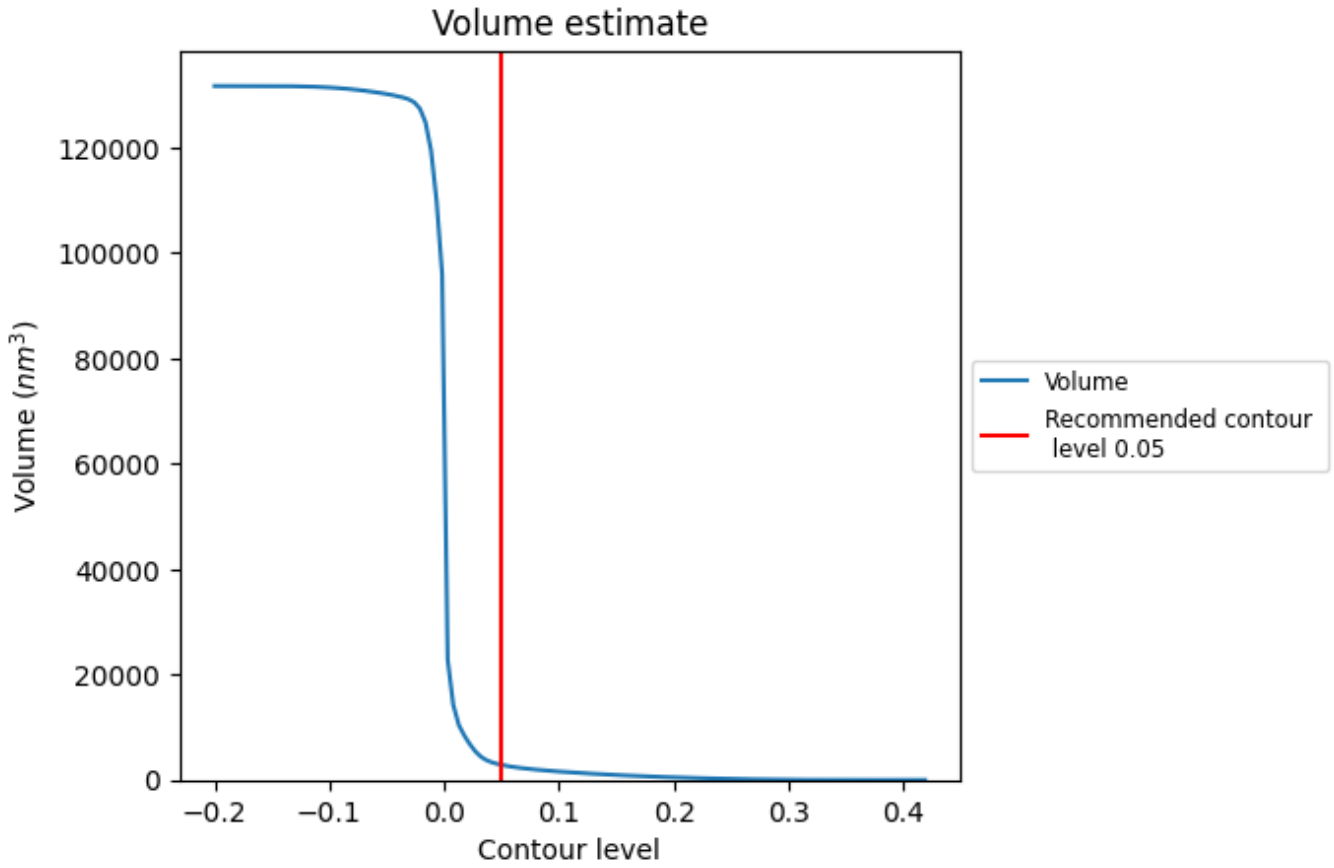
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

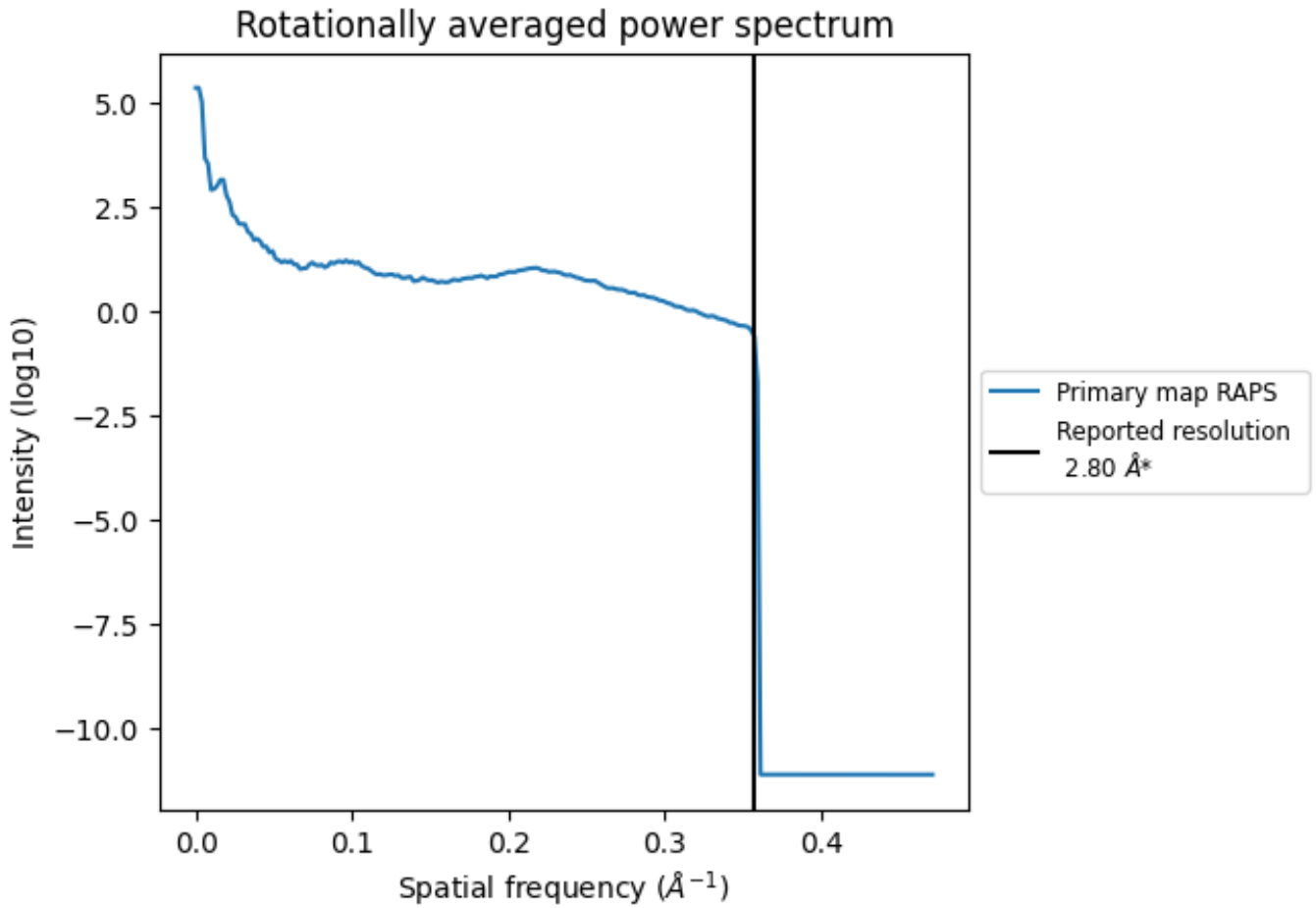
7.2 Volume estimate



The volume at the recommended contour level is 2868 nm^3; this corresponds to an approximate mass of 2590 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 0.357 $Å^{-1}$

8 Fourier-Shell correlation (i)

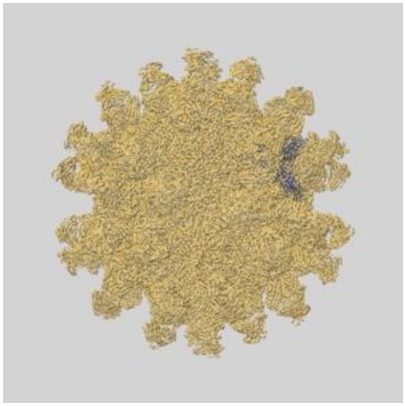
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

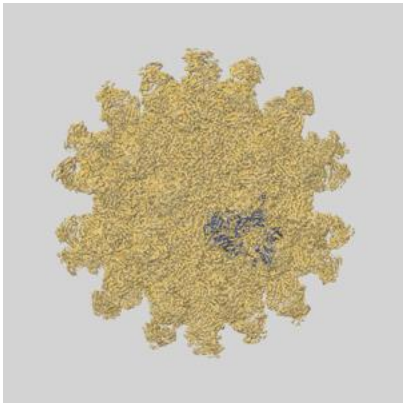
This section contains information regarding the fit between EMDB map EMD-0069 and PDB model 6GV4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

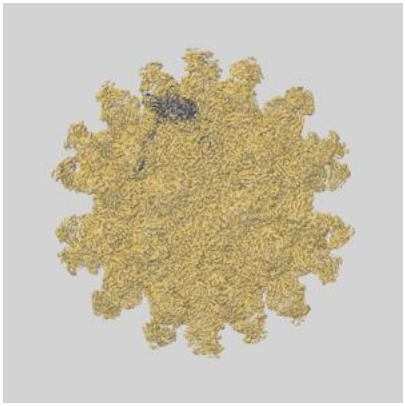
9.1.1 Map-model overlay



X

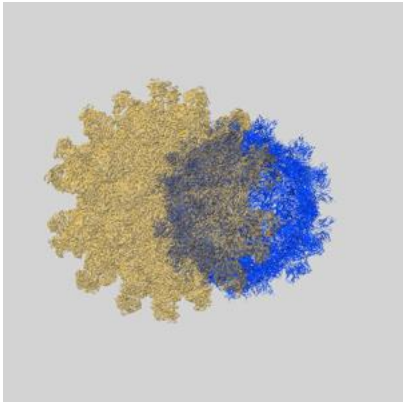


Y

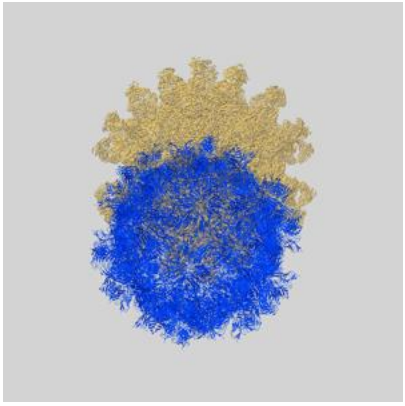


Z

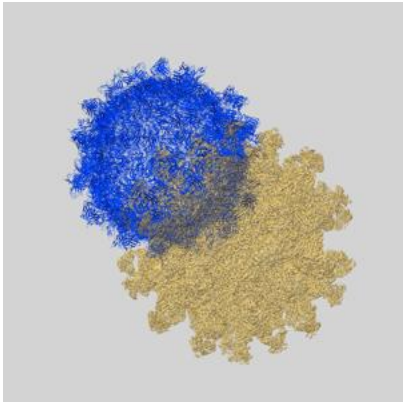
9.1.2 Map-model assembly overlay



X



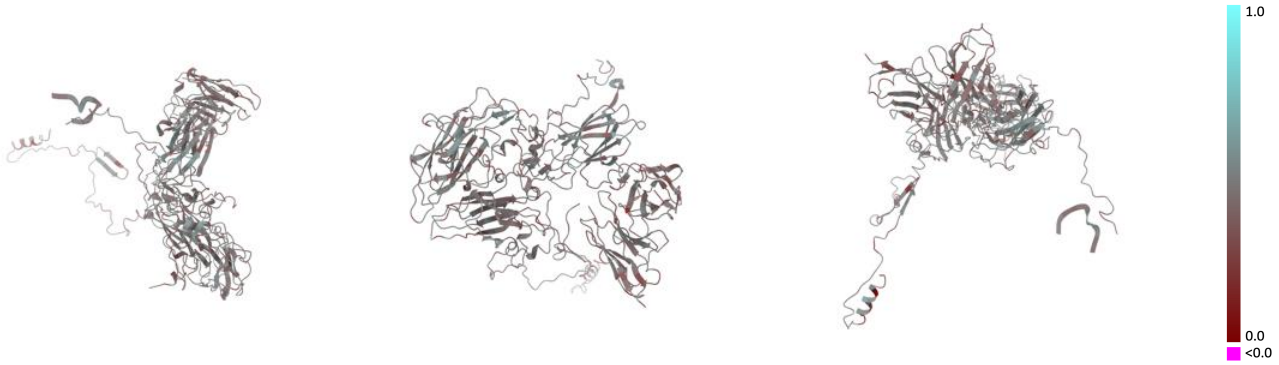
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

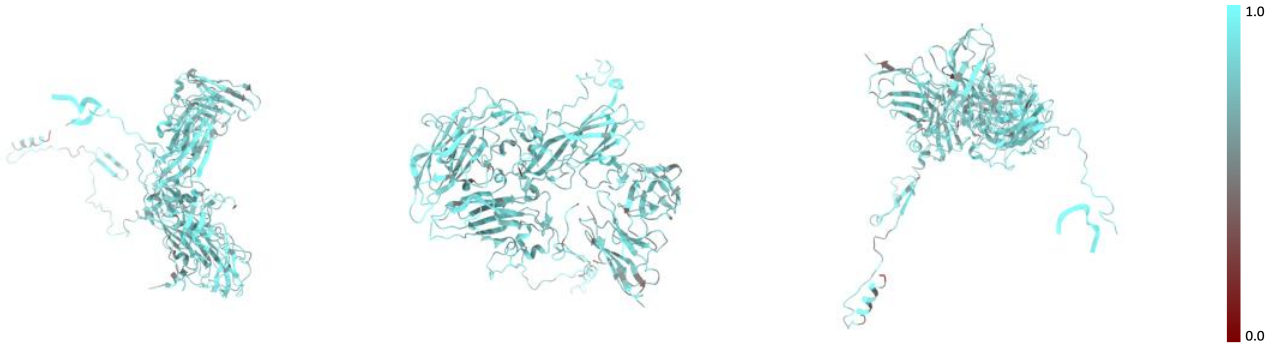
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

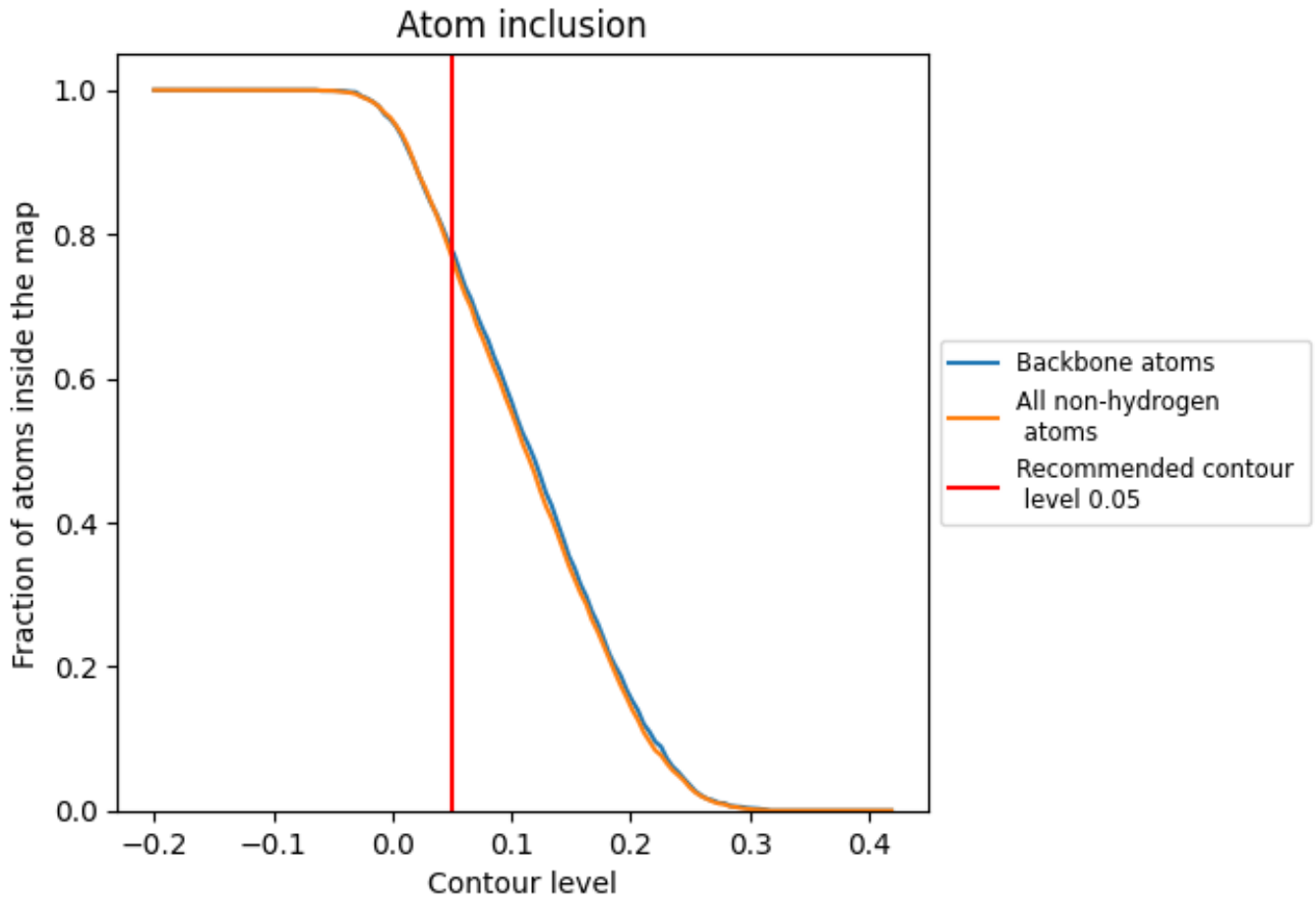
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7679	0.4340
A	0.7597	0.4300
B	0.7860	0.4460
C	0.7953	0.4470
D	0.8718	0.4660
H	0.7432	0.4130
L	0.7274	0.4130