wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 03:09 PM EST

PDB ID	:	3JCX
EMDB ID	:	EMD-6629
Title	:	Canine Parvovirus complexed with Fab E
Authors	:	Organtini, L.J.; Iketani, S.; Huang, K.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Parrish, C.R.; Hafenstein, S.
Deposited on	:	2016-03-21
Resolution	:	4.10 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:

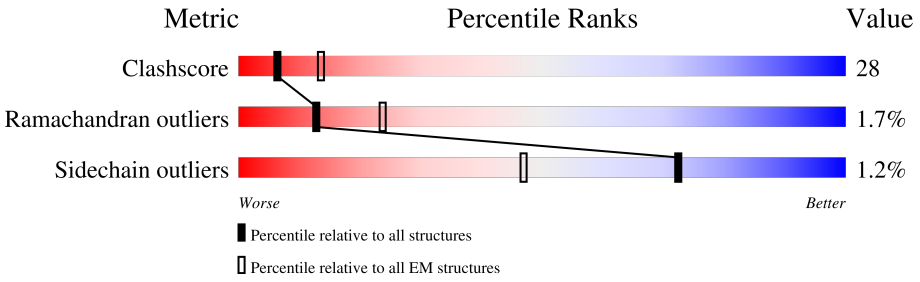
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.10 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	A	584	58% 33% • 6%
2	H	115	27% 23% 62% 12% •
3	L	107	17% 43% 55% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6072 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 Capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	548	4353	2765	742	830	16	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	TYR	GLU	CONFLICT	UNP B2ZG07
A	104	GLU	GLN	CONFLICT	UNP B2ZG07
A	300	ASP	ALA	CONFLICT	UNP B2ZG07
A	509	GLN	GLU	CONFLICT	UNP B2ZG07

- Molecule 2 is a protein called Fab E heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	115	899	575	148	172	4	0	0

- Molecule 3 is a protein called Fab E light chain.

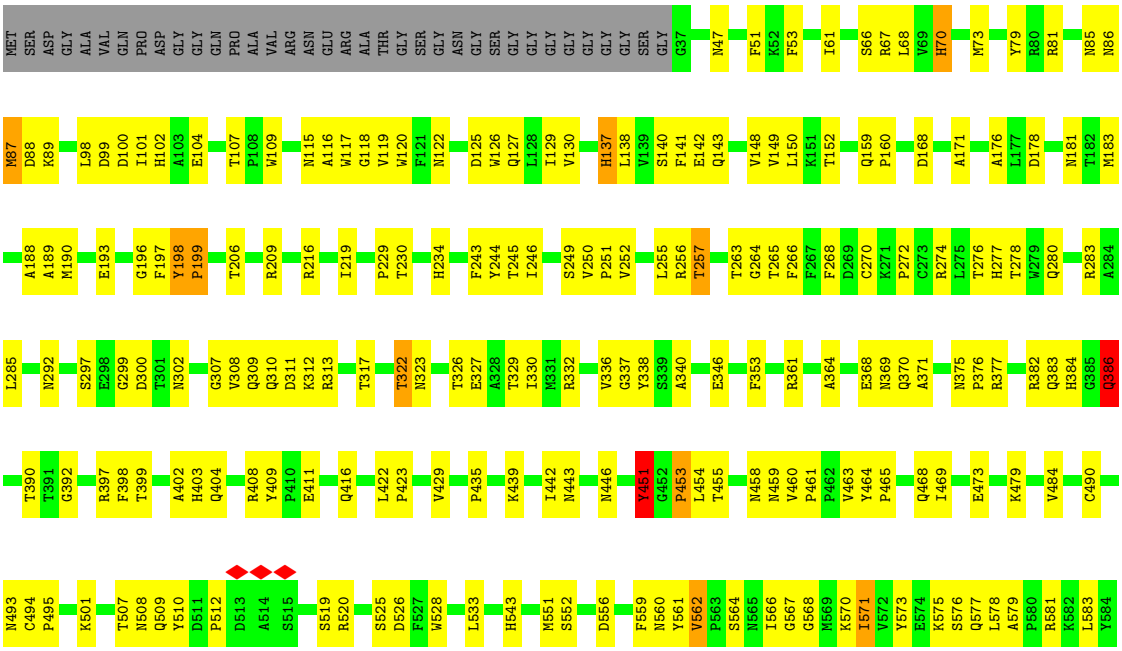
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	107	820	507	139	167	7	0	0

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.

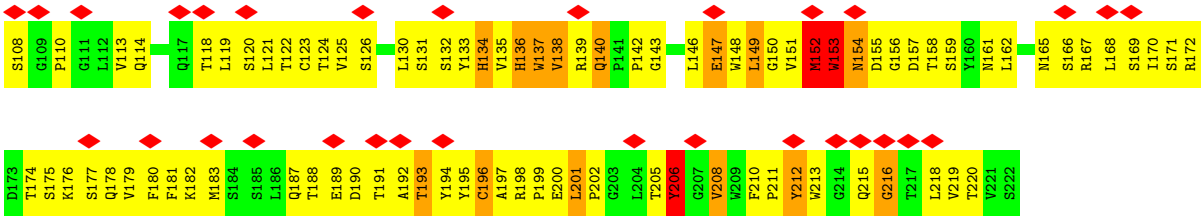
• Molecule 1: Capsid protein 2

Chain A: 58% 33% 6%



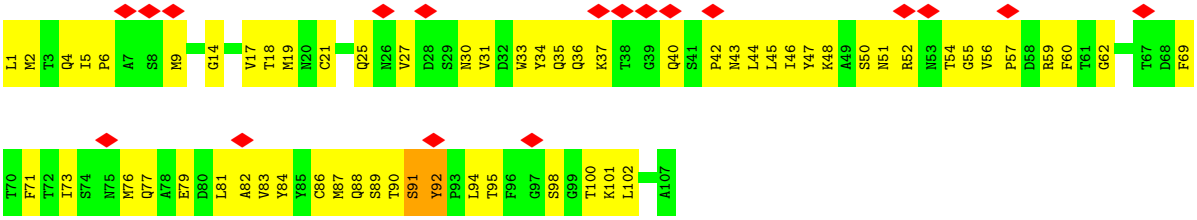
• Molecule 2: Fab E heavy chain

Chain H: 27% 23% 62% 12%



• Molecule 3: Fab E light chain

Chain L: 17% 43% 55%


L1 M2 T3 Q4 I5 P6 A7 S8 M9 G14 V17 T18 M19 N20 C21 Q25 N26 V27 D28 S29 N30 V31 D32 W33 Y34 Q35 Q36 K37 T38 G39 Q40 S41 P42 N43 L44 L45 I46 Y47 K48 A49 S50 N51 R52 N53 T54 G55 V56 P57 D58 R59 F60 T61 G62 T67 D68 F69
T70 F71 T72 I73 S74 N75 M76 Q77 A78 E79 D80 L81 A82 V83 Y84 Y85 C86 M87 Q88 S89 T90 S91 Y92 P93 L94 T95 P96 G97 S98 G99 T100 K101 L102 A107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	47563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.665	Depositor
Minimum map value	-14.584	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	479.5, 479.5, 479.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	0/4483	0.65	2/6133 (0.0%)
2	H	3.45	18/927 (1.9%)	1.91	26/1266 (2.1%)
3	L	0.79	4/834 (0.5%)	0.89	5/1127 (0.4%)
All	All	1.43	22/6244 (0.4%)	0.97	33/8526 (0.4%)

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
1	A	0	13
2	H	0	10
3	L	0	2
All	All	0	25

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	153	TRP	CB-CG	88.39	3.09	1.50
2	H	153	TRP	CG-CD1	26.65	1.74	1.36
2	H	206	TYR	CD1-CE1	-21.78	1.06	1.39
2	H	153	TRP	CA-CB	19.93	1.97	1.53
2	H	206	TYR	CD2-CE2	-15.23	1.16	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	153	TRP	N-CA-CB	21.15	148.68	110.60
2	H	153	TRP	CA-CB-CG	21.06	153.72	113.70
2	H	153	TRP	CD1-CG-CD2	-19.65	90.58	106.30
2	H	153	TRP	N-CA-C	-17.26	64.40	111.00
2	H	152	MET	CB-CG-SD	12.82	150.87	112.40

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ALA	Peptide
1	A	189	ALA	Peptide
1	A	255	LEU	Peptide
1	A	257	THR	Peptide
1	A	87	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4353	0	4144	146	0
2	H	899	0	861	143	0
3	L	820	0	798	69	0
All	All	6072	0	5803	338	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 28.

The worst 5 of 338 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)
2:H:153:TRP:CB	2:H:153:TRP:CA	1.97	1.40
2:H:153:TRP:CB	2:H:153:TRP:HA	1.77	1.11
1:A:87:MET:O	2:H:206:TYR:CE1	2.13	1.01
3:L:1:LEU:HD22	3:L:88:GLN:HE22	1.30	0.96
1:A:81:ARG:NH2	2:H:155:ASP:OD1	2.04	0.91

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	A	546/584 (94%)	472 (86%)	66 (12%)	8 (2%)	10 44
2	H	113/115 (98%)	80 (71%)	28 (25%)	5 (4%)	2 24
3	L	105/107 (98%)	89 (85%)	16 (15%)	0	100 100
All	All	764/806 (95%)	641 (84%)	110 (14%)	13 (2%)	13 42

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	152	MET
2	H	212	TYR
2	H	153	TRP
1	A	199	PRO
1	A	451	TYR

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	A	477/496 (96%)	470 (98%)	7 (2%)	65 79
2	H	101/101 (100%)	100 (99%)	1 (1%)	76 85
3	L	93/93 (100%)	93 (100%)	0	100 100
All	All	671/690 (97%)	663 (99%)	8 (1%)	72 83

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	136	HIS
1	A	543	HIS
1	A	277	HIS
1	A	234	HIS
1	A	403	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	134	HIS
2	H	140	GLN
3	L	88	GLN
3	L	35	GLN
3	L	40	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

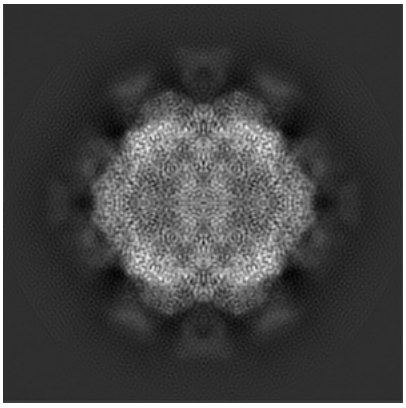
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6629. These allow visual inspection of the internal detail of the map and identification of artifacts.

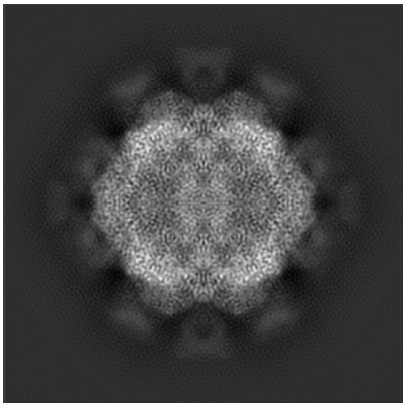
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

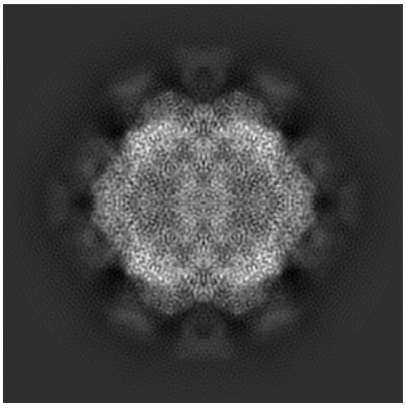
6.1.1 Primary map



X



Y

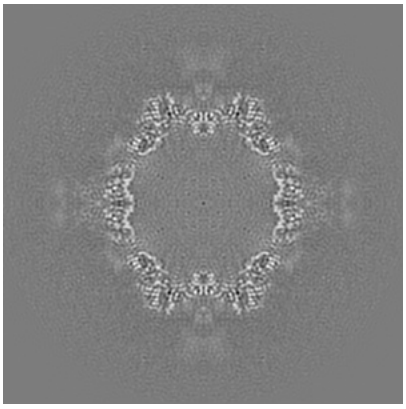


Z

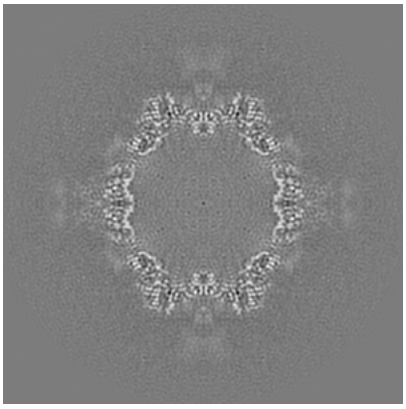
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

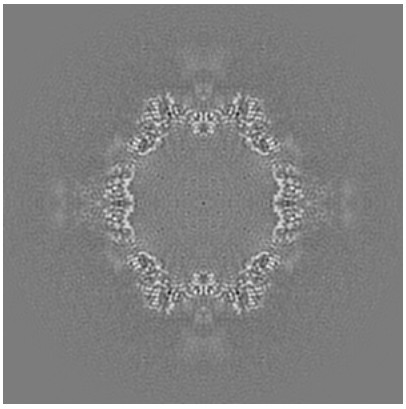
6.2.1 Primary map



X Index: 175



Y Index: 175

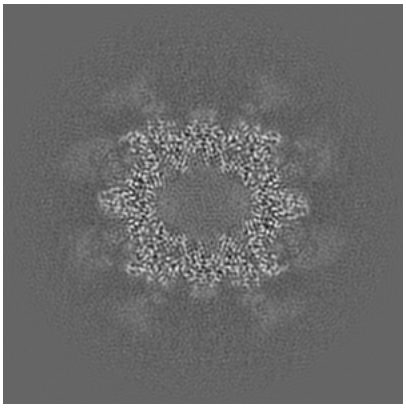


Z Index: 175

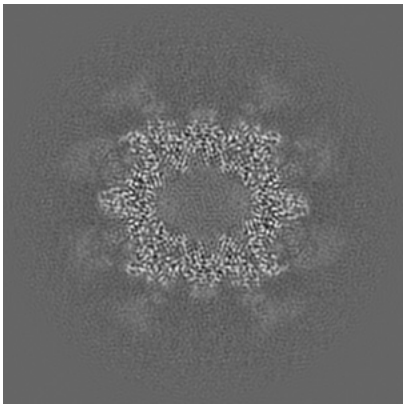
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

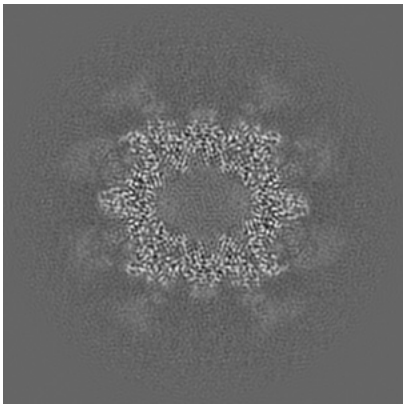
6.3.1 Primary map



X Index: 125



Y Index: 125

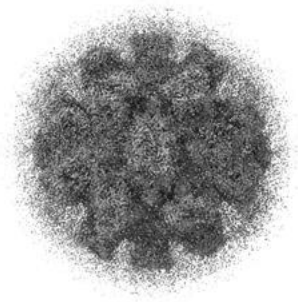


Z Index: 125

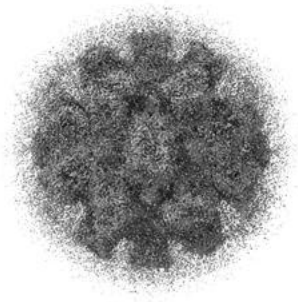
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

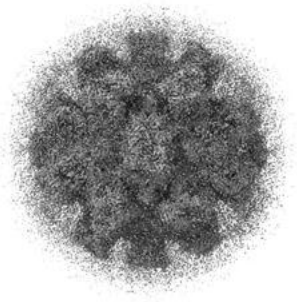
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

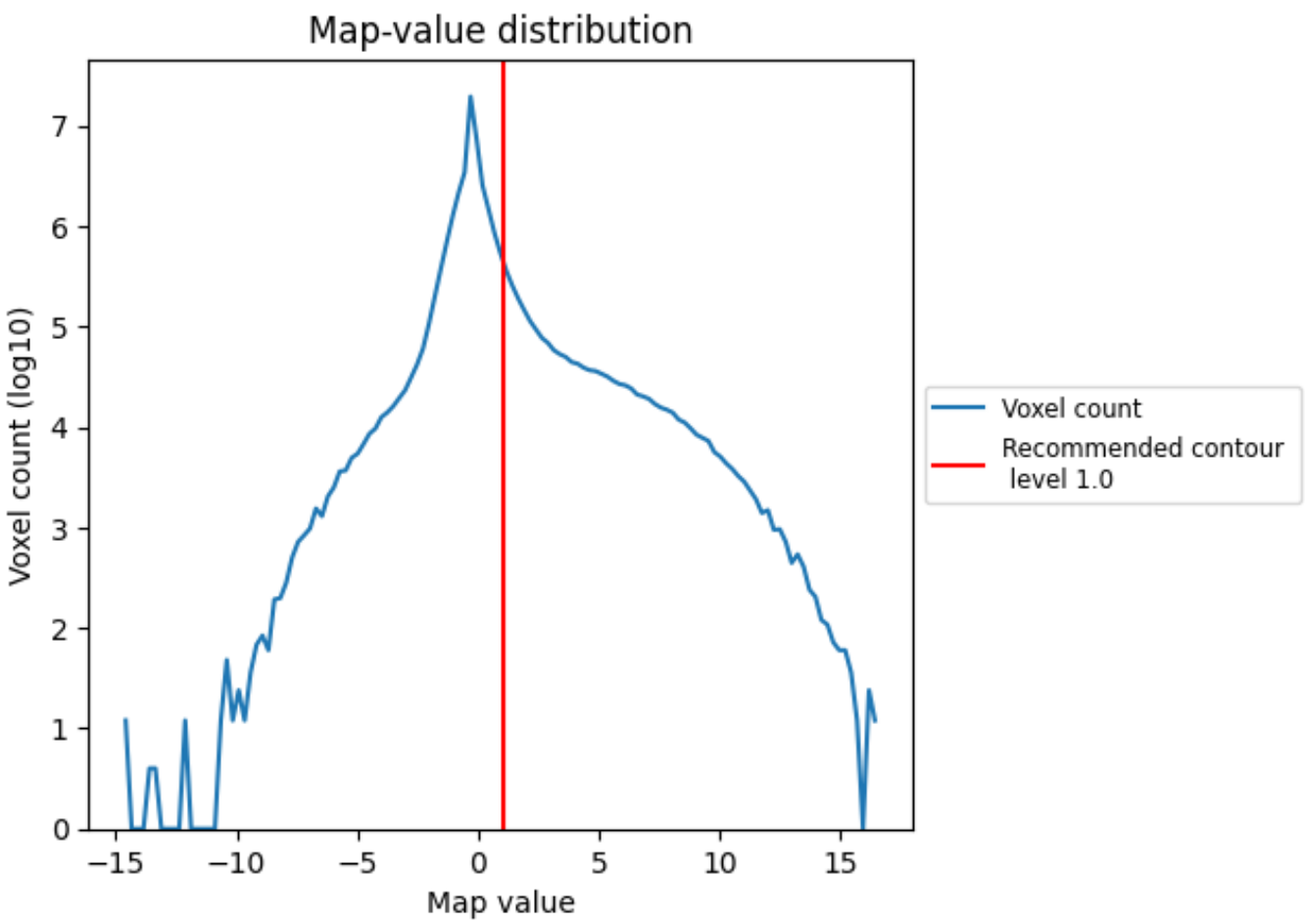
6.5 Mask visualisation (i)

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

7 Map analysis (i)

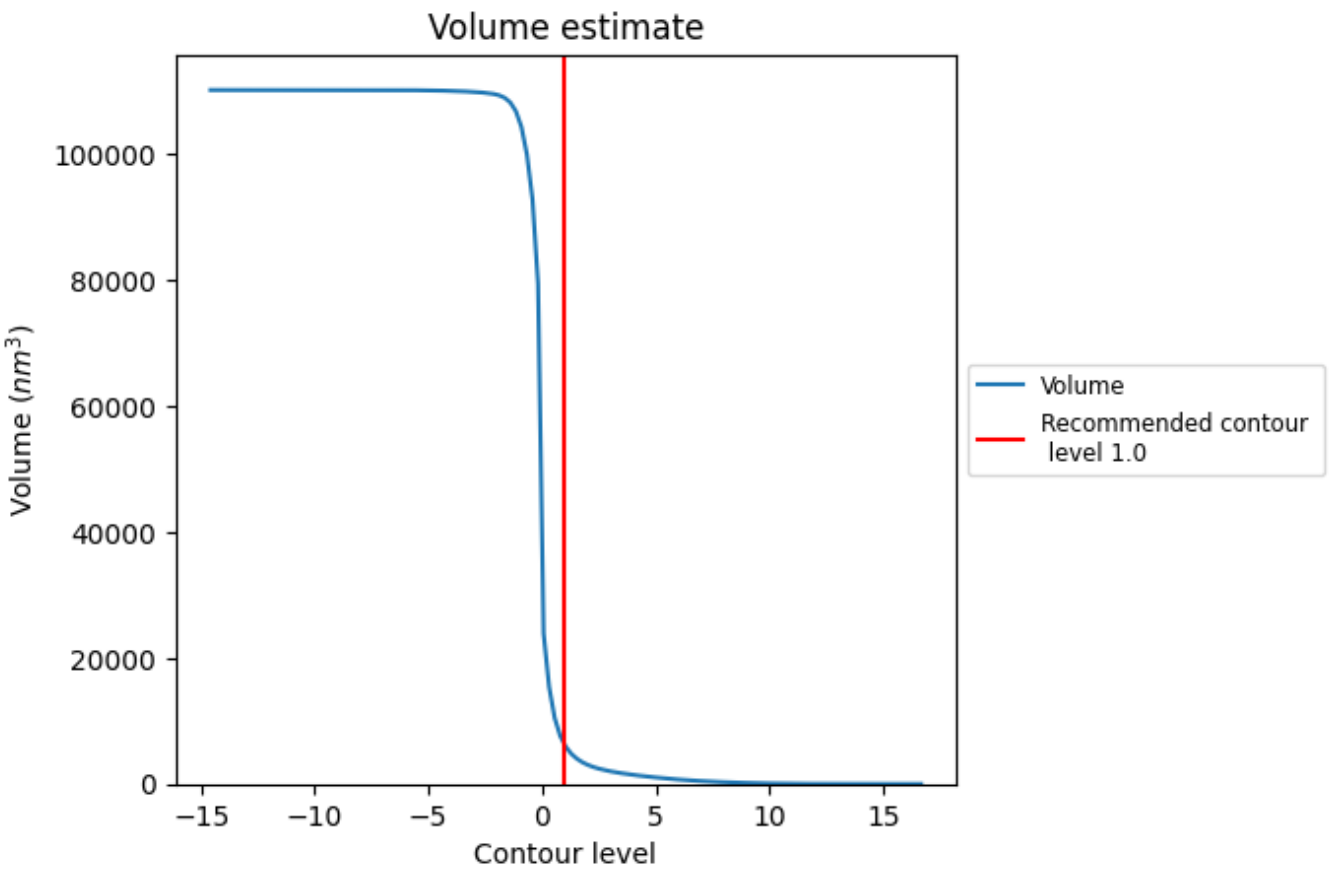
This section contains the results of statistical analysis of the map.

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.

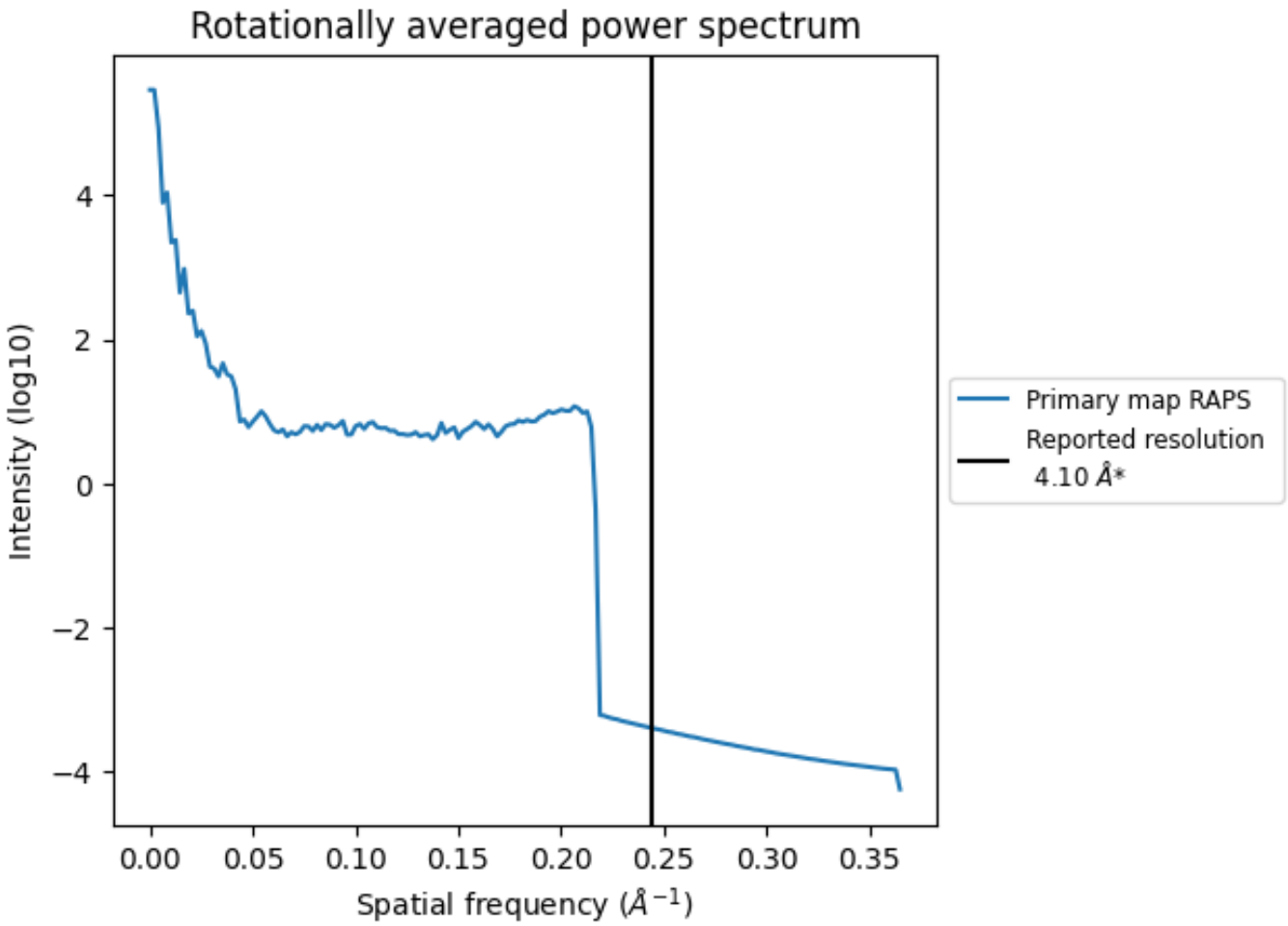
7.2 Volume estimate (i)



The volume at the recommended contour level is 6187 nm^3; this corresponds to an approximate mass of 5588 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 0.244 Å^{-1}

8 Fourier-Shell correlation (i)

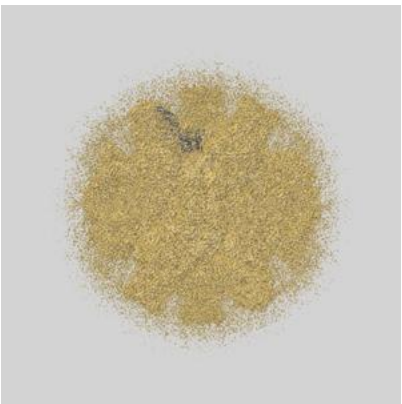
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

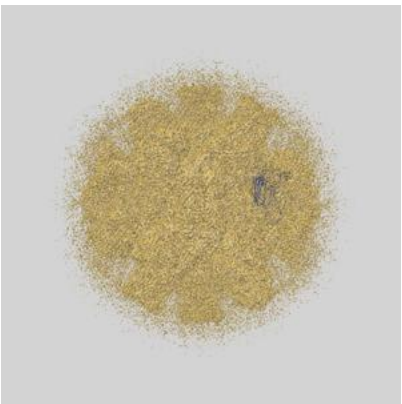
This section contains information regarding the fit between EMDB map EMD-6629 and PDB model 3JCX. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

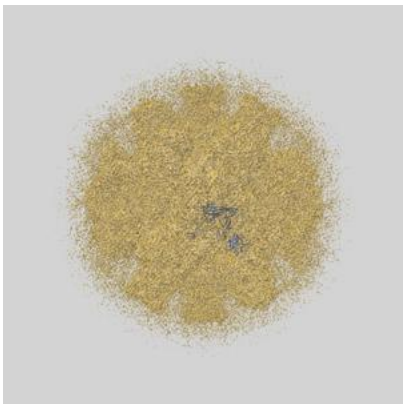
9.1.1 Map-model overlay (i)



X

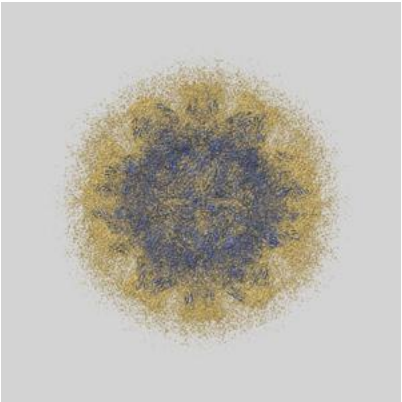


Y

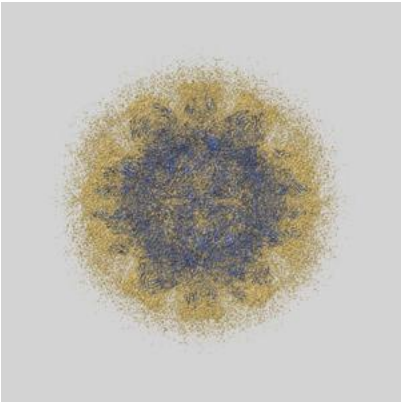


Z

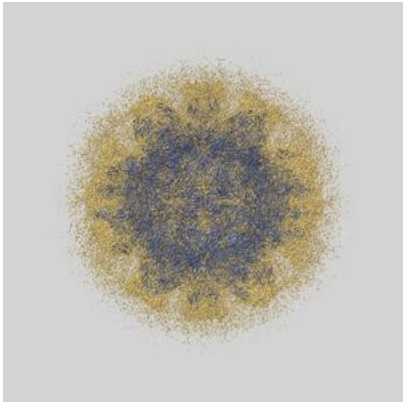
9.1.2 Map-model assembly overlay (i)



X



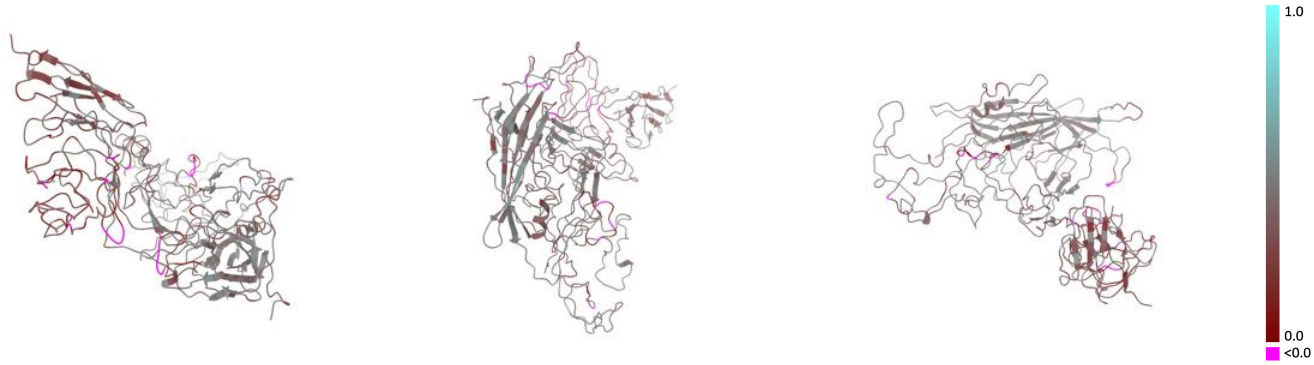
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

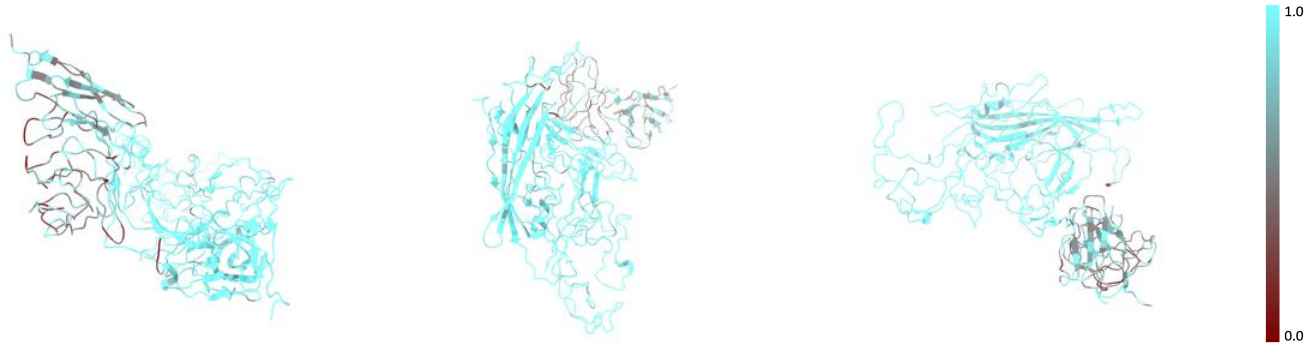
9.2 Q-score mapped to coordinate model (i)



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.

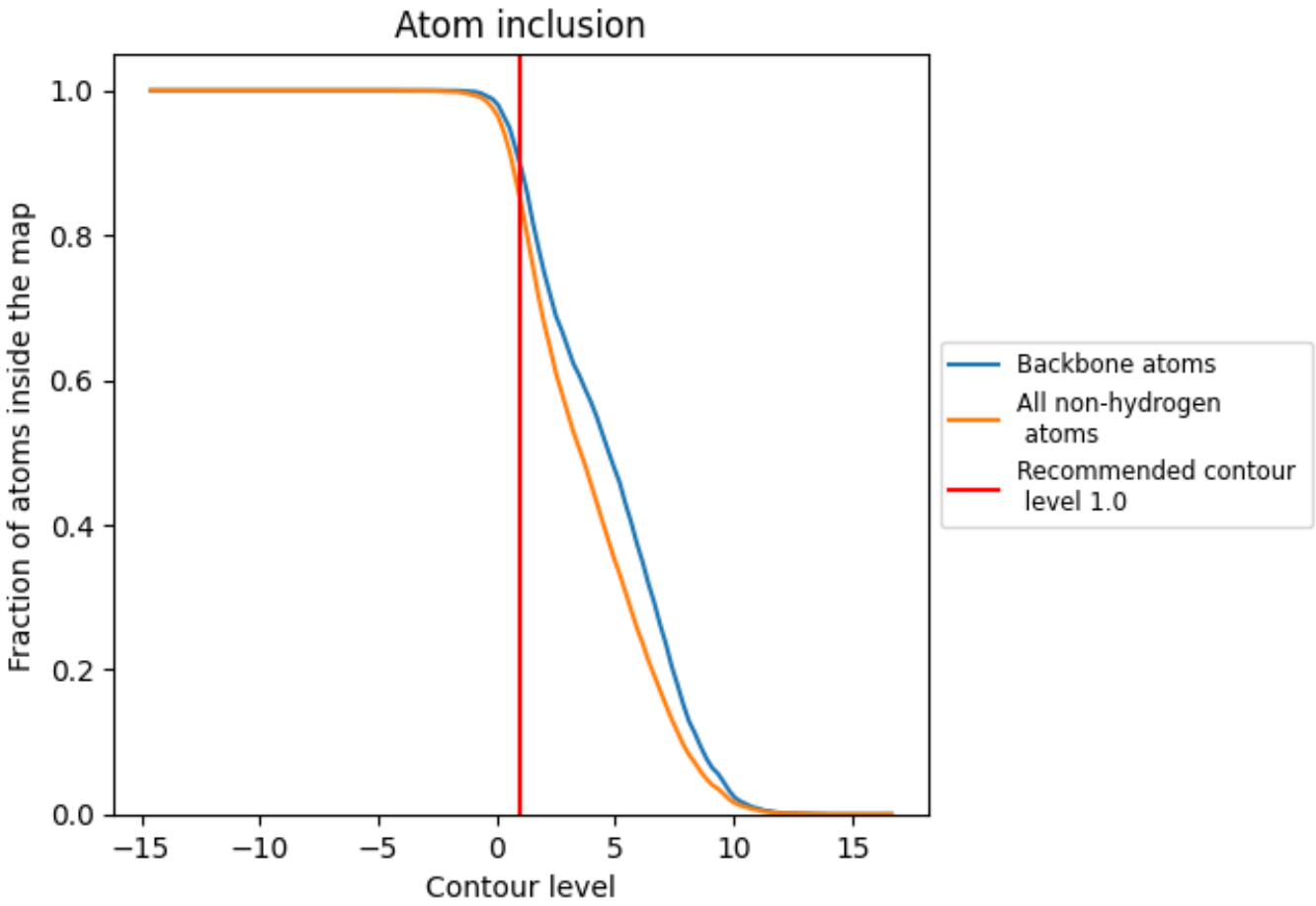
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8487	0.3680
A	0.9464	0.4000
H	0.5670	0.2430
L	0.6377	0.3360