wwPDB EM Validation Summary Report

Nov 7, 2022 – 09:42 AM JST

PDB ID	:	5JB1
EMDB ID	:	EMD-8147
Title	:	Pseudo-atomic structure of Human Papillomavirus Type 59 L1 Virus-like Particle
Authors	:	Li, Z.H.; Yan, X.D.; Yu, H.; Zheng, Q.B.; Gu, Y.; Li, S.W.
Deposited on	:	2016-04-13
Resolution	:	6.00 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 ⓘ 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:

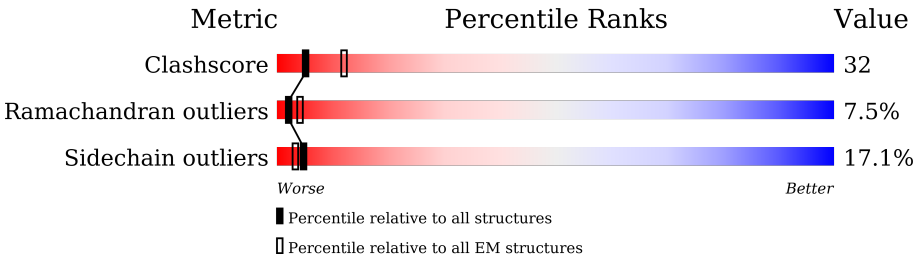
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.00 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
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	500	15% 32% 38% 13% 7% 9%
1	B	500	16% 33% 37% 16% 7% 7%
1	C	500	17% 33% 37% 15% 6% 9%
1	D	500	15% 31% 38% 14% 8% 9%
1	E	500	13% 30% 38% 16% 6% 9%
1	F	500	17% 33% 38% 15% 6% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21696 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	456	Total	C	N	O	S	0	0
			3598	2289	604	686	19		
1	B	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		
1	C	457	Total	C	N	O	S	0	0
			3604	2292	605	688	19		
1	D	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	E	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	F	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		

There are 6 discrepancies between the modelled and reference sequences:

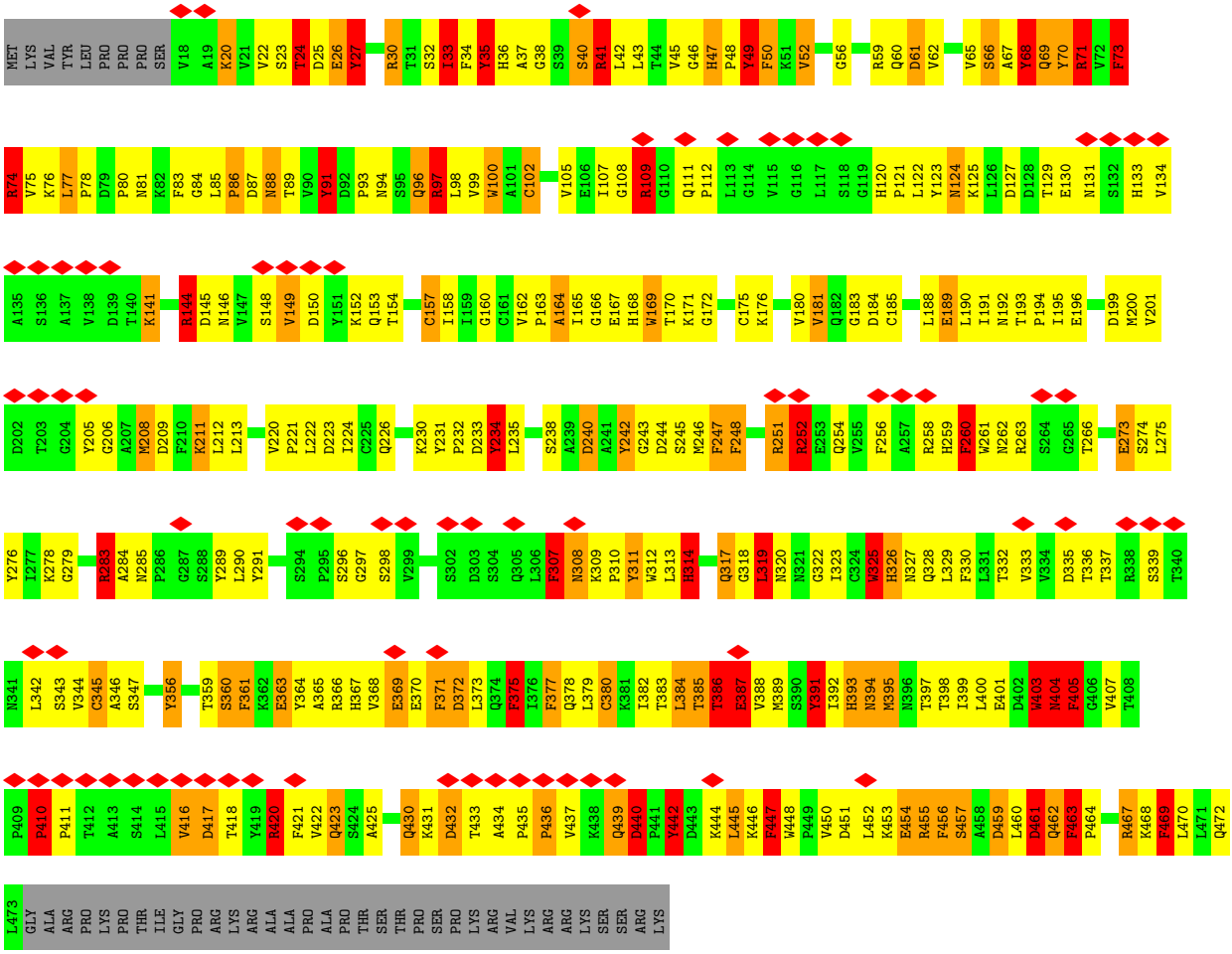
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971

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.

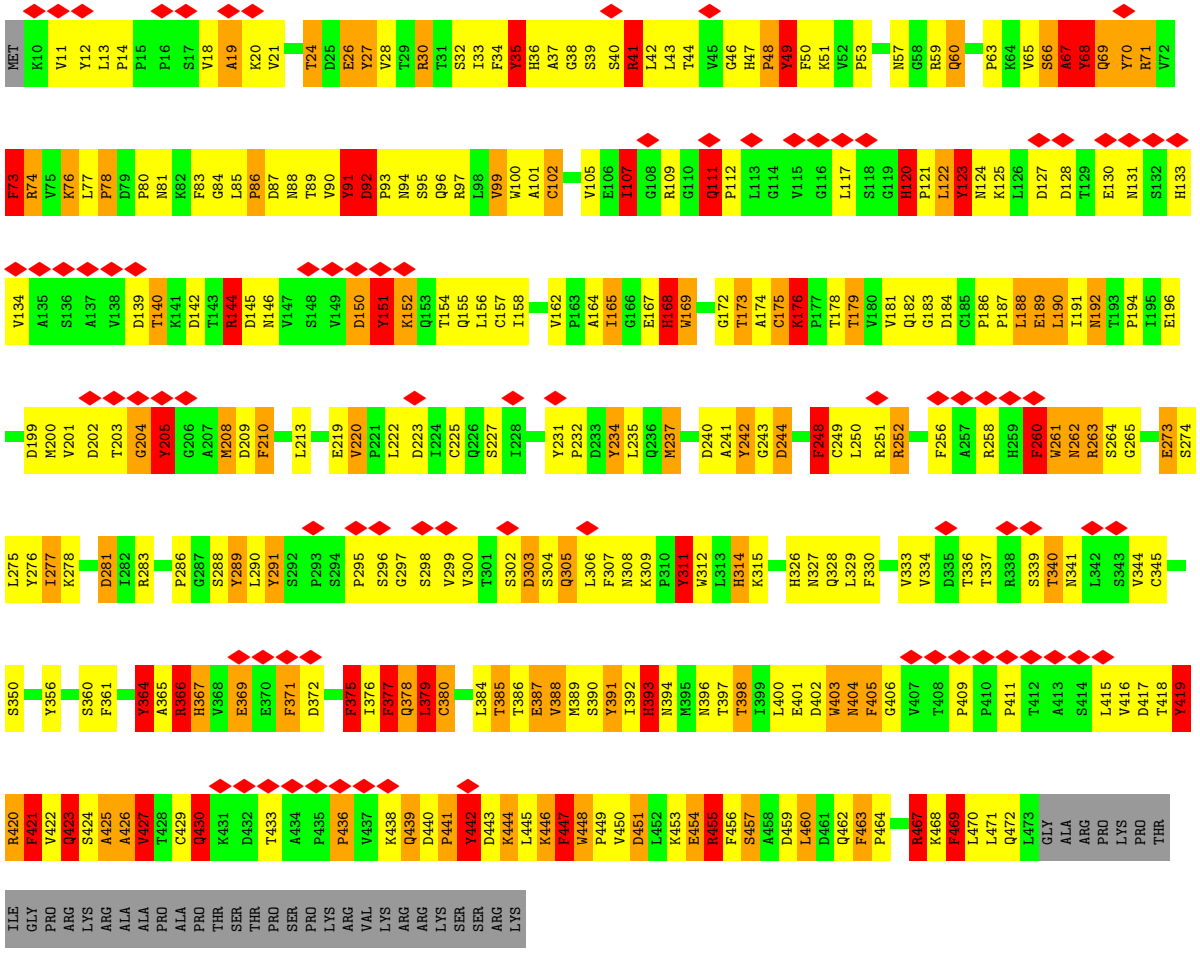
• Molecule 1: Major capsid protein L1

Chain A:



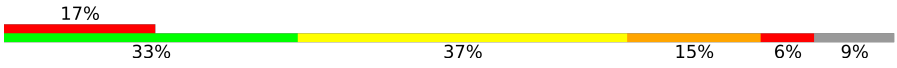
• Molecule 1: Major capsid protein L1

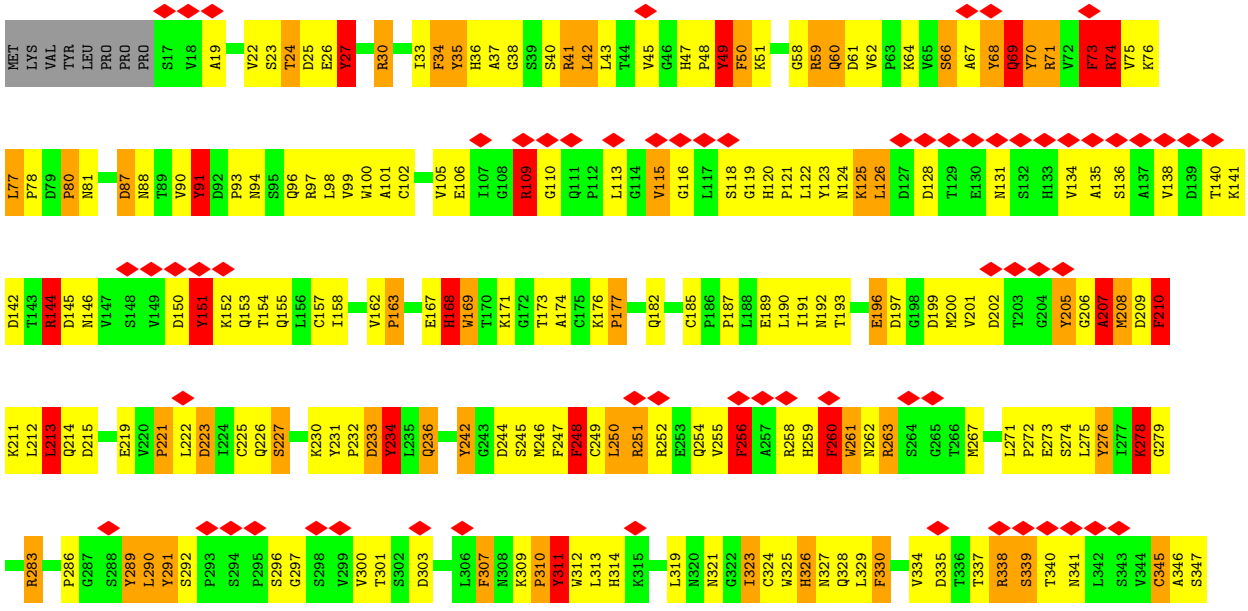
Chain B:

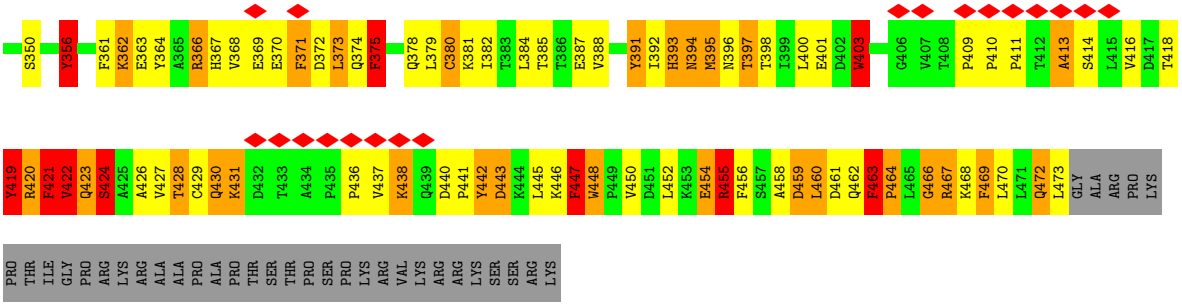


• Molecule 1: Major capsid protein L1

Chain C:

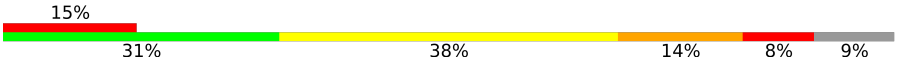


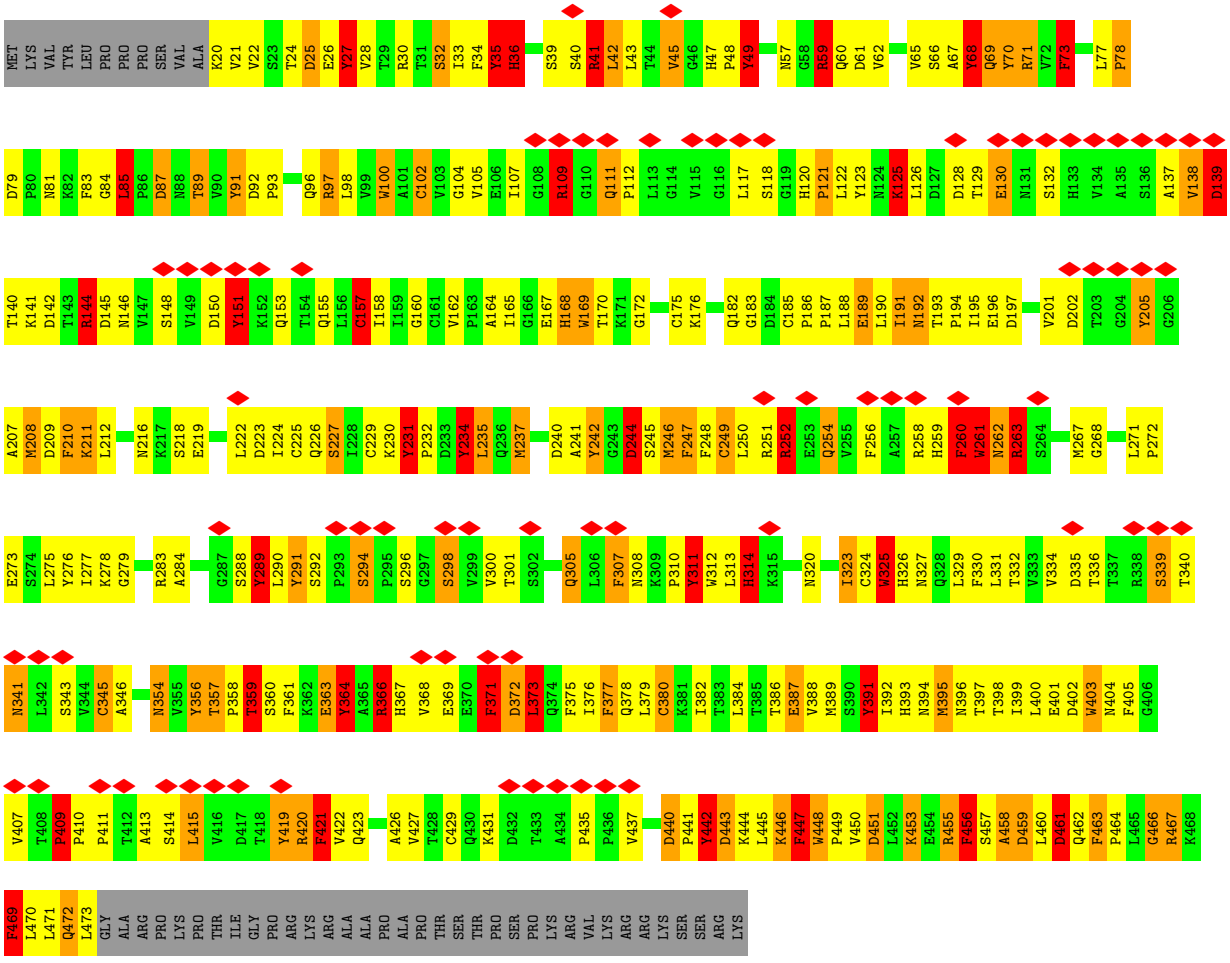




• Molecule 1: Major capsid protein L1

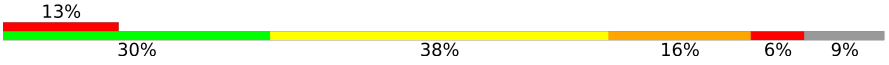
Chain D:

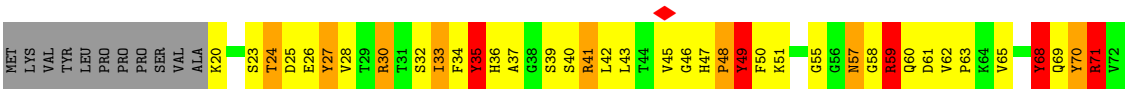


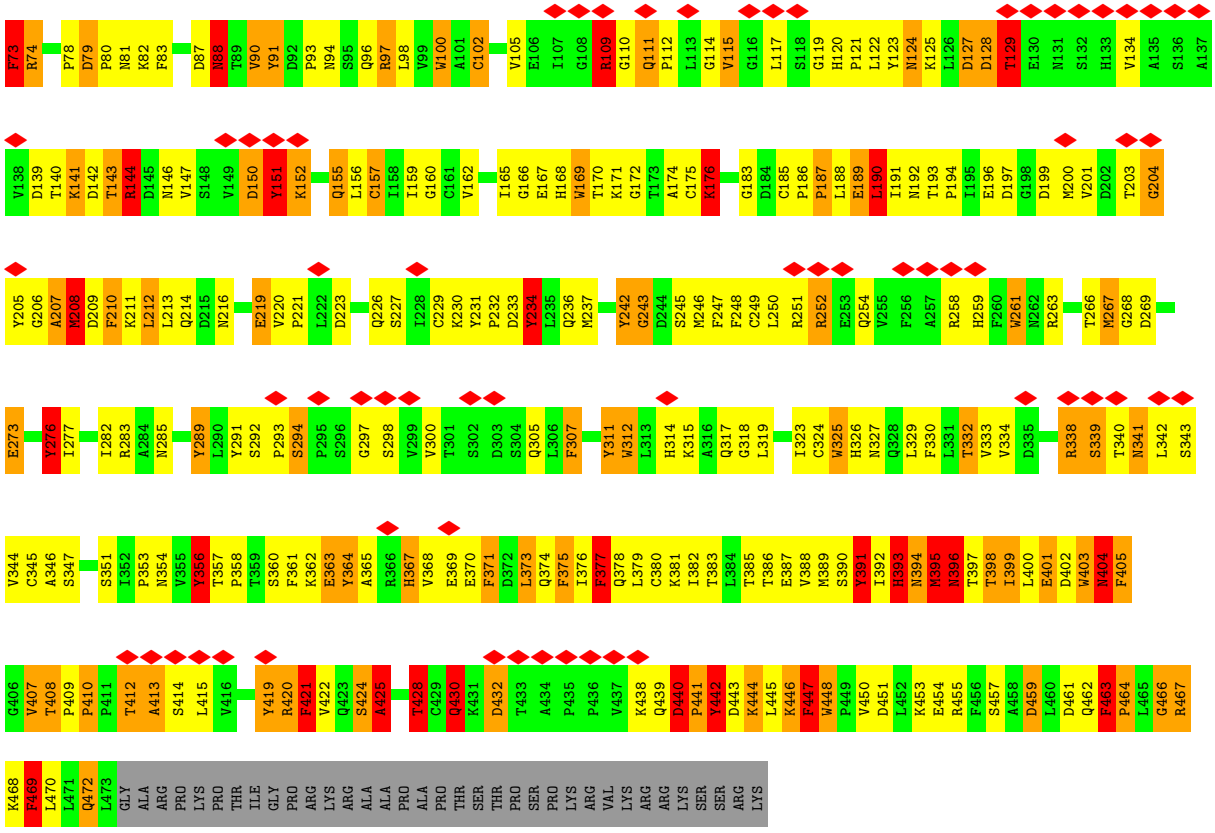


• Molecule 1: Major capsid protein L1

Chain E:

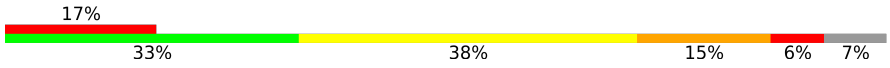


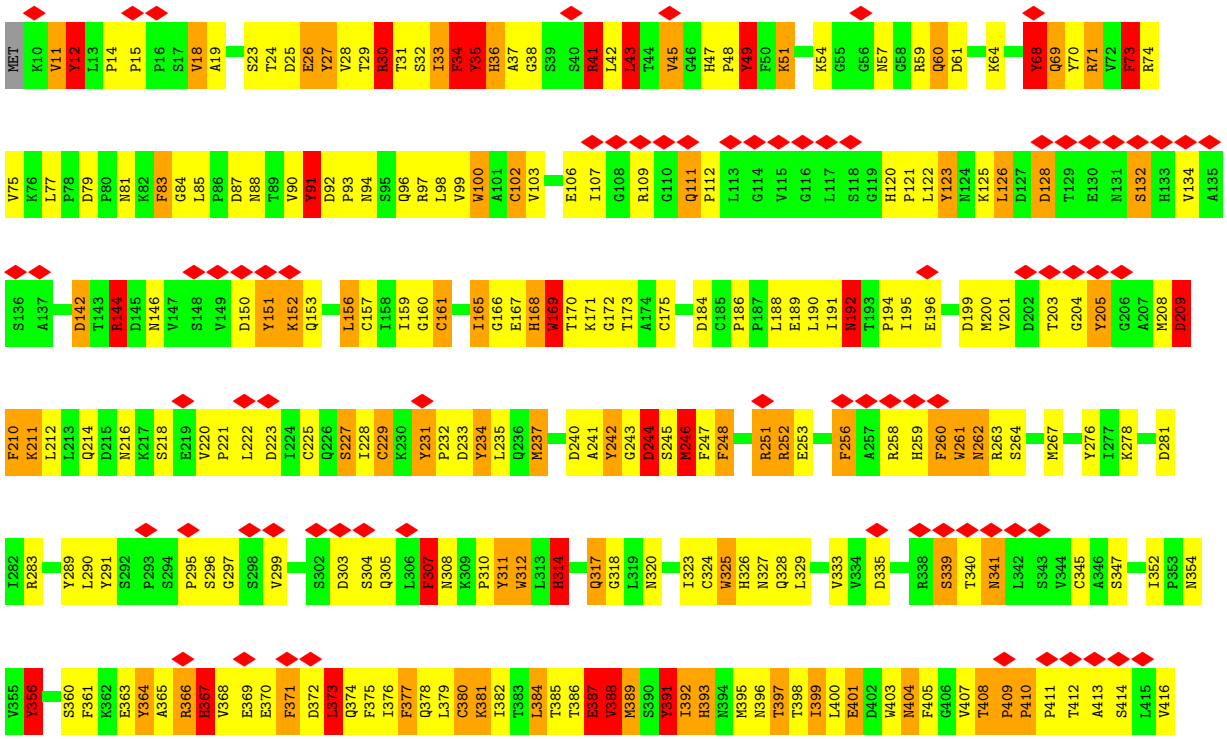


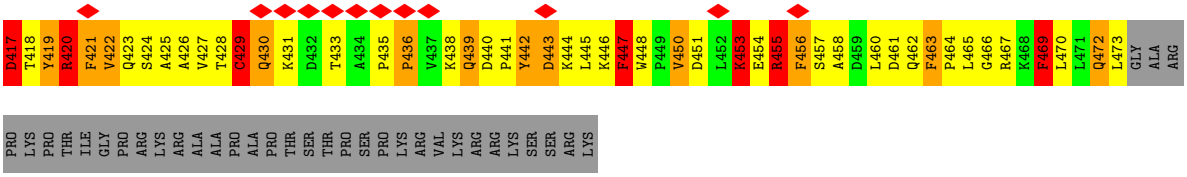


• Molecule 1: Major capsid protein L1

Chain F:






D417 T418 Y419 R420 F421 V422 Q423 S424 A425 A426 V427 T428 C429 Q430 K431 D432 T433 A434 P435 P436 V437 K438 Q439 D440 P441 Y442 D443 K444 L445 K446 F447 W448 P449 V450 D451 L452 K453 E454 R455 F456 S457 A458 D459 L460 D461 Q462 F463 P464 L465 G466 R467 K468 F469 L470 L471 Q472 L473 GLY ALA ARG
PRO LYS PRO THR ILE GLY PRO ARG LYS ARG ALA ALA PRO ALA PRO THR SER THR PRO SER PRO LYS ARG VAL LYS ARG ARG LYS SER SER ARG LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3100	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	14.133	Depositor
Minimum map value	-6.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.25	Depositor
Map size (Å)	910.2, 910.2, 910.2	wwPDB
Map dimensions	820, 820, 820	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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	A	1.47	8/3694 (0.2%)	1.88	94/5036 (1.9%)
1	B	1.45	7/3761 (0.2%)	1.89	110/5130 (2.1%)
1	C	1.48	5/3700 (0.1%)	1.91	107/5044 (2.1%)
1	D	1.49	11/3682 (0.3%)	1.87	97/5019 (1.9%)
1	E	1.94	8/3682 (0.2%)	1.89	100/5019 (2.0%)
1	F	1.49	11/3761 (0.3%)	1.88	88/5130 (1.7%)
All	All	1.56	50/22280 (0.2%)	1.89	596/30378 (2.0%)

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	35
1	B	0	45
1	C	0	46
1	D	0	43
1	E	0	37
1	F	0	47
All	All	0	253

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	PHE	N-CA	77.19	3.00	1.46
1	B	35	TYR	CB-CG	-7.31	1.40	1.51
1	E	469	PHE	CB-CG	-6.46	1.40	1.51
1	F	392	ILE	N-CA	-6.36	1.33	1.46
1	A	447	PHE	CA-C	-6.18	1.36	1.52

The worst 5 of 596 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	455	ARG	NE-CZ-NH1	13.91	127.26	120.30
1	B	91	TYR	CB-CG-CD2	-13.52	112.89	121.00
1	C	91	TYR	CB-CG-CD2	-13.48	112.91	121.00
1	C	420	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	A	386	THR	N-CA-C	13.11	146.38	111.00

There are no chirality outliers.

5 of 253 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	TYR	Sidechain
1	A	41	ARG	Sidechain
1	A	49	TYR	Sidechain
1	A	68	TYR	Sidechain
1	A	70	TYR	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	A	3598	0	3503	270	0
1	B	3661	0	3571	243	0
1	C	3604	0	3506	219	0
1	D	3586	0	3488	236	0
1	E	3586	0	3489	244	0
1	F	3661	0	3571	230	0
All	All	21696	0	21128	1384	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 32.

The worst 5 of 1384 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:A:386:THR:HG22	1:A:386:THR:O	1.56	1.06
1:D:169:TRP:CD1	1:D:190:LEU:HD13	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TRP:CE2	1:B:190:LEU:HD13	2.05	0.90
1:A:70:TYR:CD1	1:A:201:VAL:HG12	2.07	0.90
1:F:169:TRP:CD1	1:F:190:LEU:HD13	2.11	0.85

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	454/500 (91%)	359 (79%)	59 (13%)	36 (8%)	1	12
1	B	462/500 (92%)	356 (77%)	65 (14%)	41 (9%)	1	11
1	C	455/500 (91%)	363 (80%)	57 (12%)	35 (8%)	1	13
1	D	452/500 (90%)	370 (82%)	53 (12%)	29 (6%)	1	16
1	E	452/500 (90%)	351 (78%)	70 (16%)	31 (7%)	1	14
1	F	462/500 (92%)	367 (79%)	62 (13%)	33 (7%)	1	14
All	All	2737/3000 (91%)	2166 (79%)	366 (13%)	205 (8%)	2	13

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	50	PHE
1	A	67	ALA
1	A	86	PRO
1	A	404	ASN

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	406/444 (91%)	341 (84%)	65 (16%)	2 13
1	B	414/444 (93%)	353 (85%)	61 (15%)	3 15
1	C	407/444 (92%)	343 (84%)	64 (16%)	2 14
1	D	405/444 (91%)	328 (81%)	77 (19%)	1 8
1	E	405/444 (91%)	332 (82%)	73 (18%)	1 10
1	F	414/444 (93%)	334 (81%)	80 (19%)	1 8
All	All	2451/2664 (92%)	2031 (83%)	420 (17%)	5 11

5 of 420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	261	TRP
1	E	159	ILE
1	F	401	GLU
1	D	325	TRP
1	D	421	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	327	ASN
1	E	326	HIS
1	D	462	GLN
1	E	133	HIS
1	E	472	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.

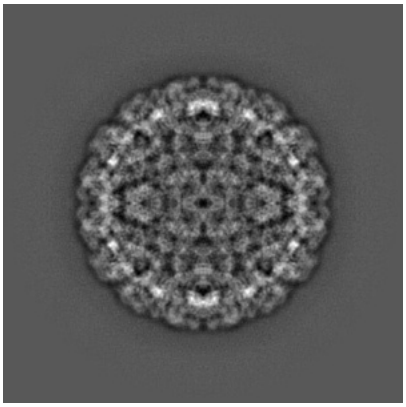
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8147. These allow visual inspection of the internal detail of the map and identification of artifacts.

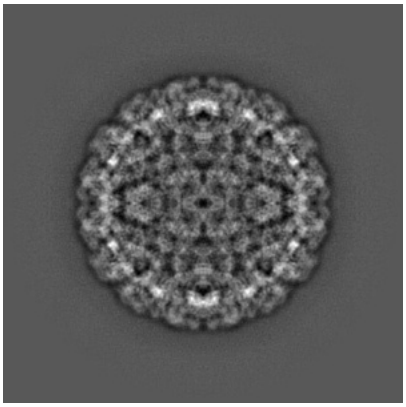
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

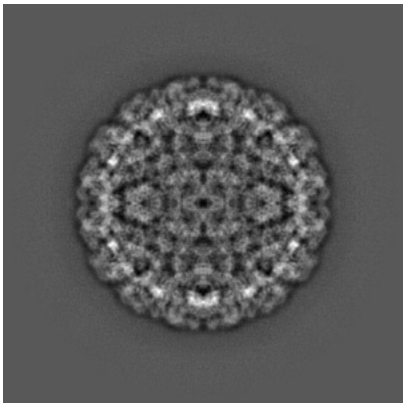
6.1.1 Primary map



X



Y

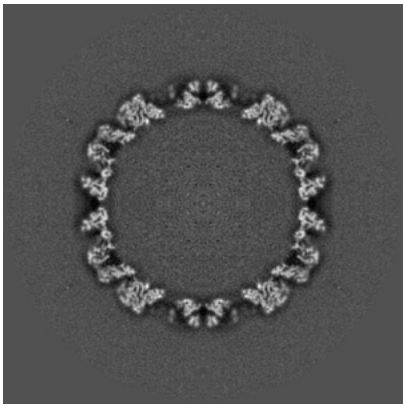


Z

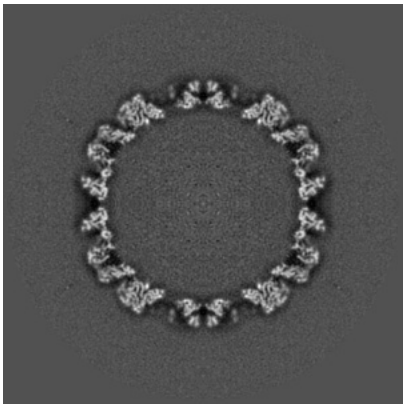
The images above show the map projected in three orthogonal directions.

6.2 Central slices

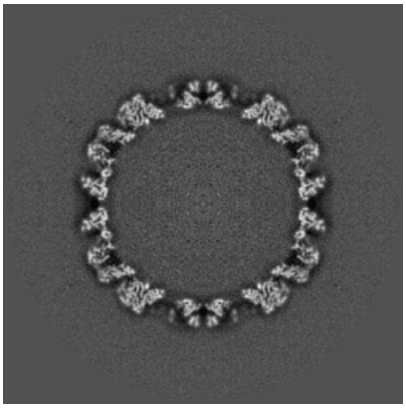
6.2.1 Primary map



X Index: 410



Y Index: 410

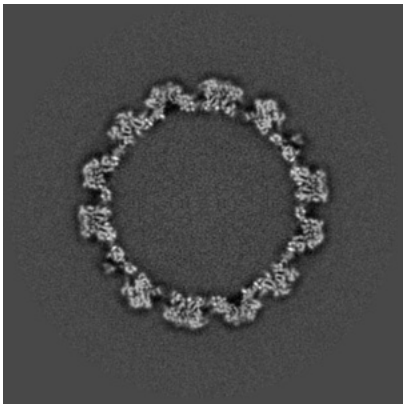


Z Index: 410

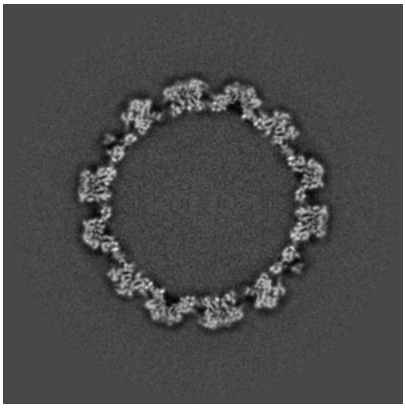
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

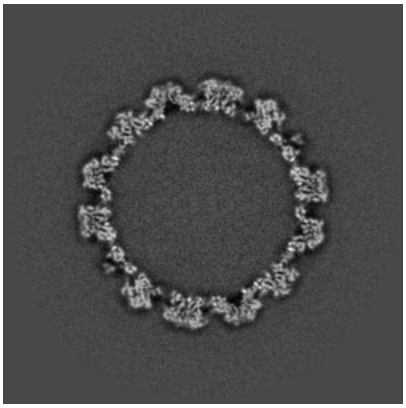
6.3.1 Primary map



X Index: 356



Y Index: 464

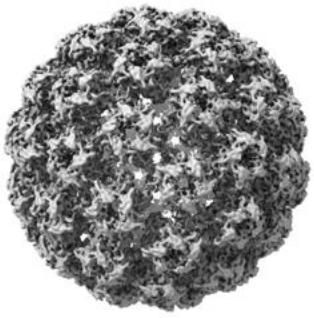


Z Index: 356

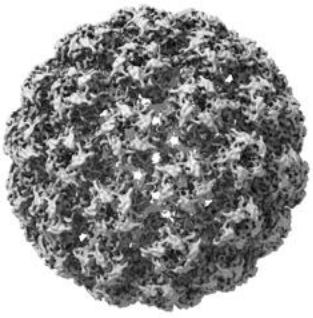
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

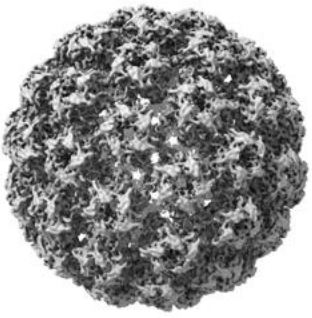
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

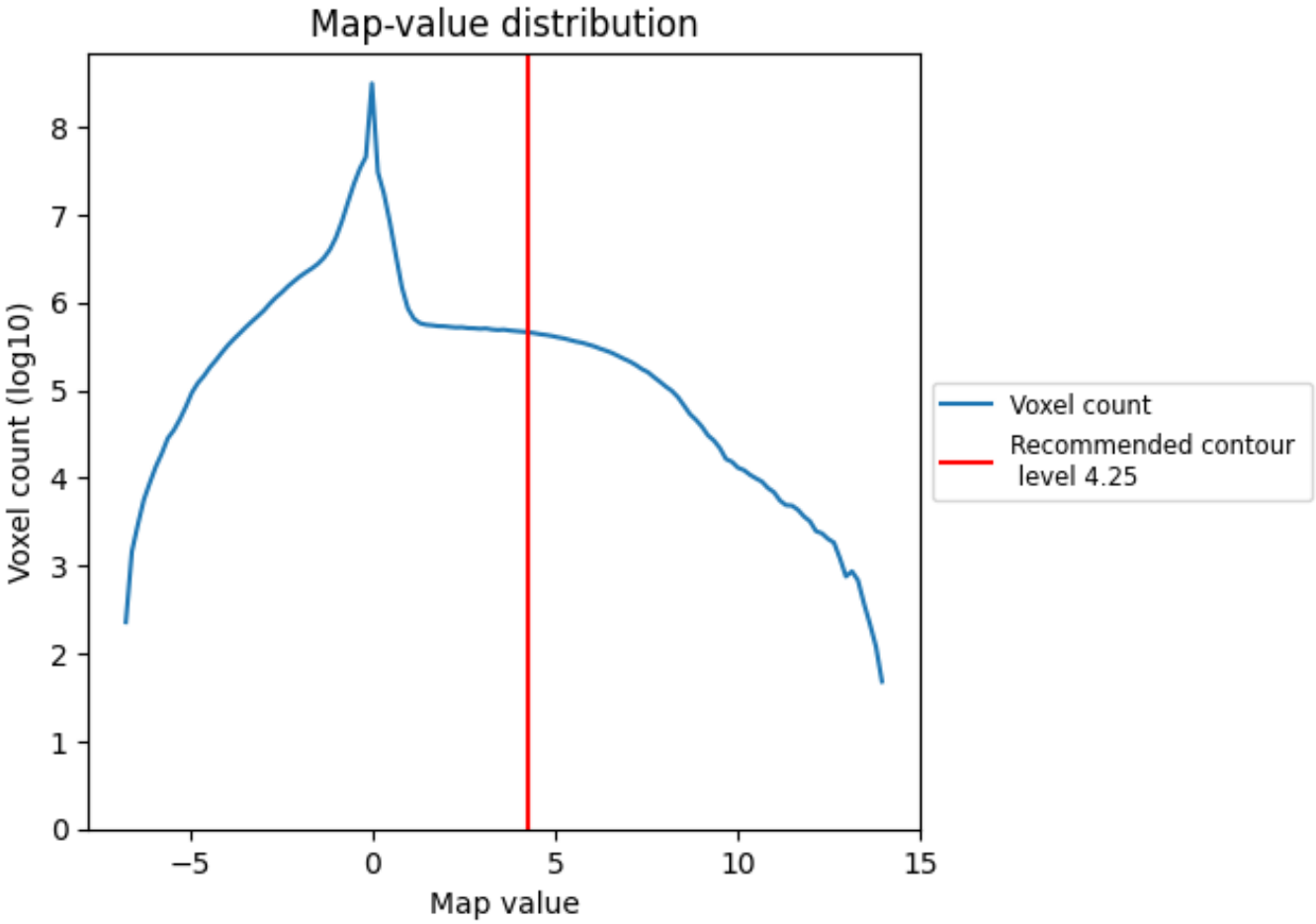
6.5 Mask visualisation (i)

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

7 Map analysis

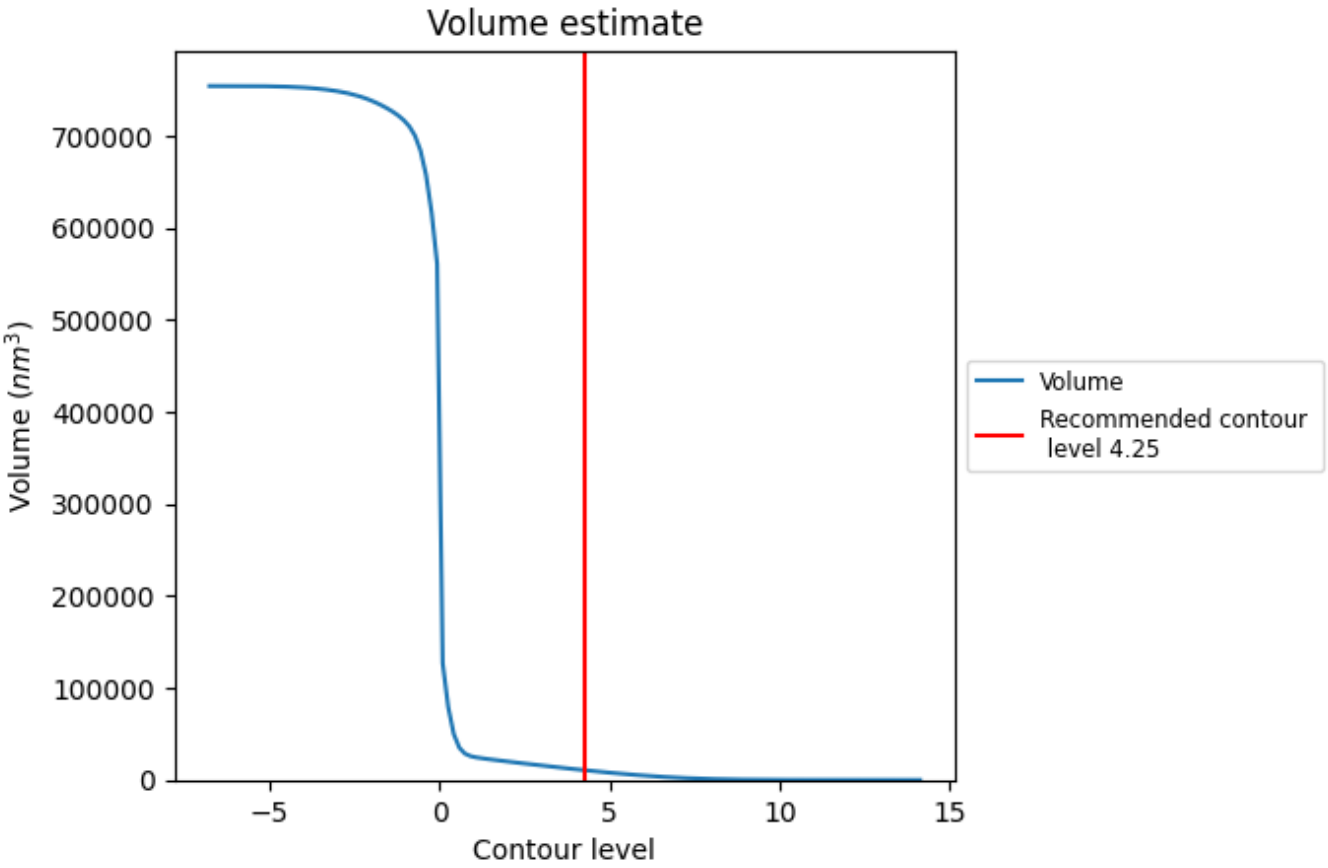
This section contains the results of statistical analysis of the map.

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.

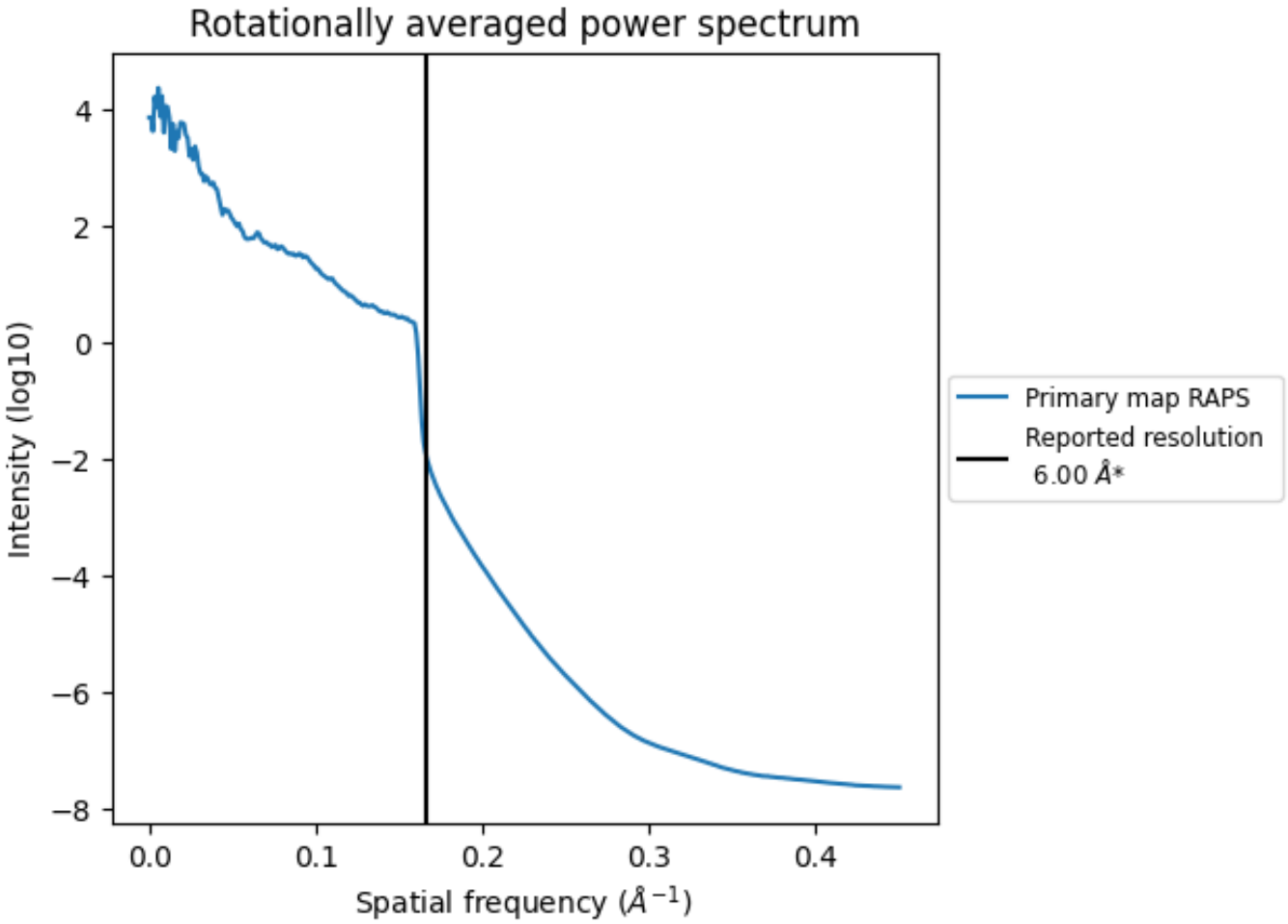
7.2 Volume estimate (i)



The volume at the recommended contour level is 10663 nm^3; this corresponds to an approximate mass of 9632 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 0.167 Å^{-1}

8 Fourier-Shell correlation (i)

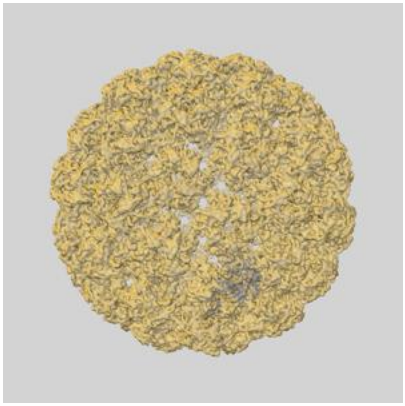
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

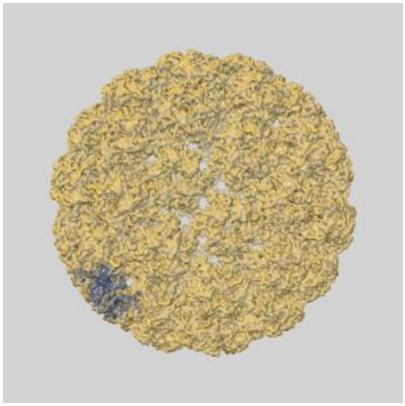
This section contains information regarding the fit between EMDB map EMD-8147 and PDB model 5JB1. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

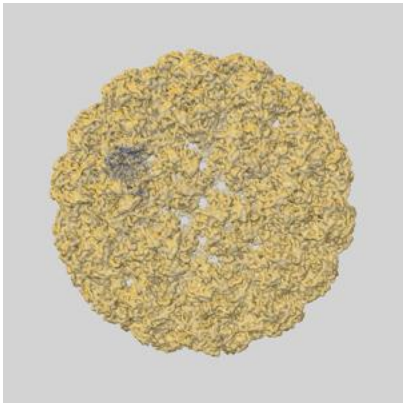
9.1.1 Map-model overlay



X

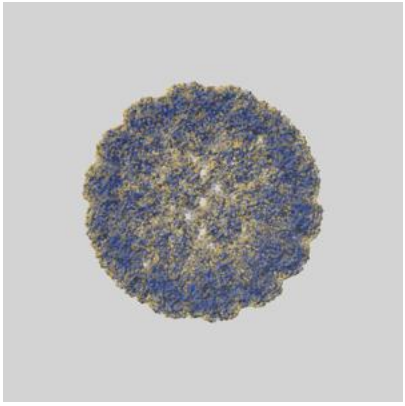


Y

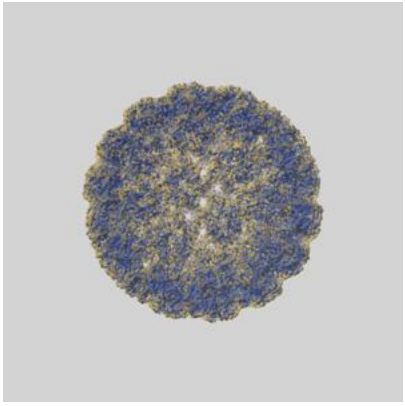


Z

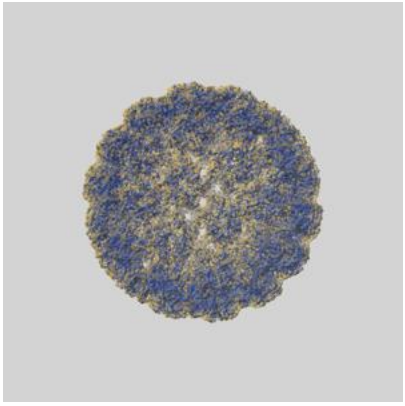
9.1.2 Map-model assembly overlay



X



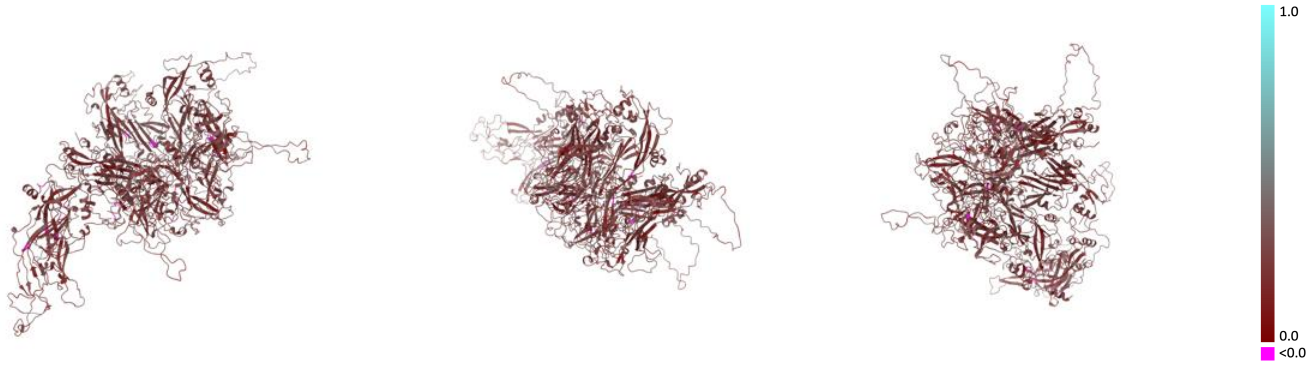
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.25 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.

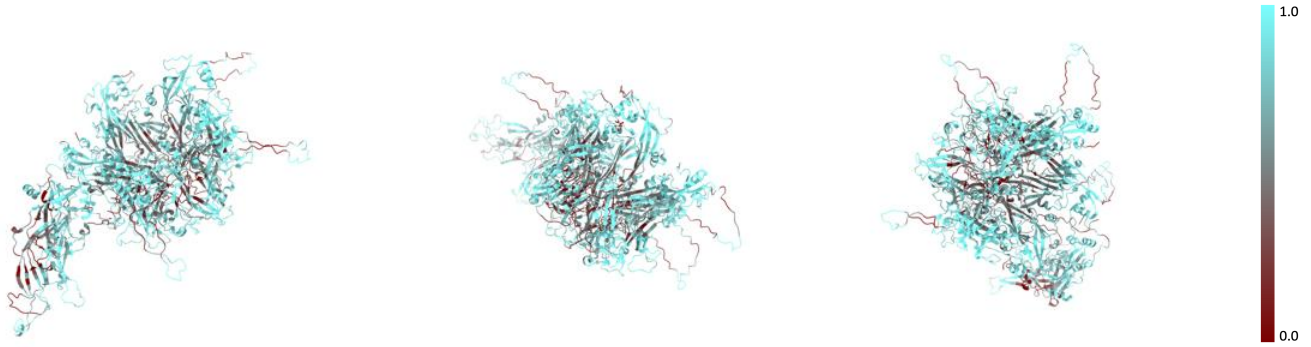
9.2 Q-score mapped to coordinate model (i)



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.

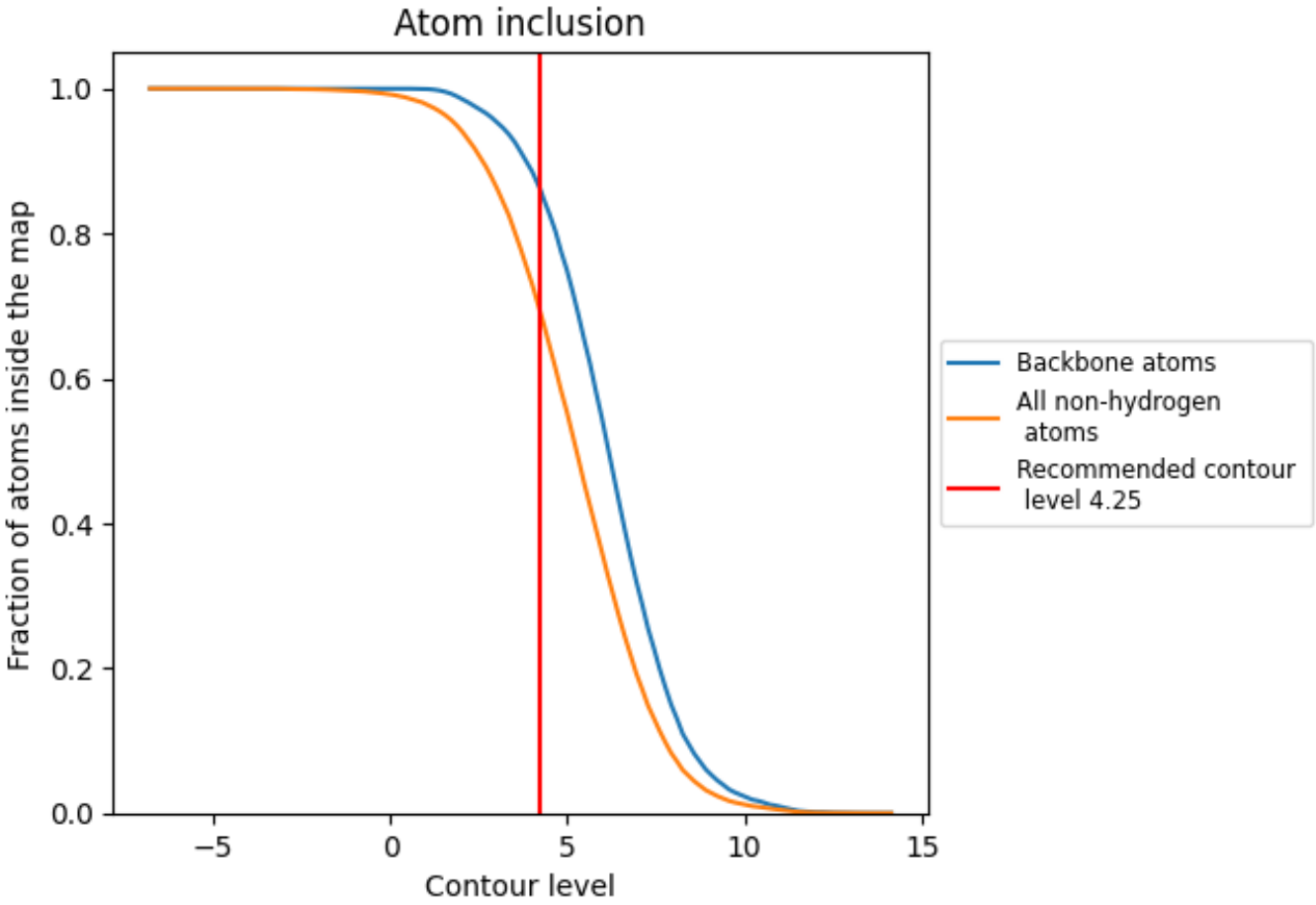
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.25).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (4.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6906	0.2550
A	0.6749	0.2530
B	0.6958	0.2540
C	0.6912	0.2550
D	0.6979	0.2580
E	0.7172	0.2570
F	0.6671	0.2560