



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:00 AM UTC

PDB ID : 5JB1 / pdb_00005jb1
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:

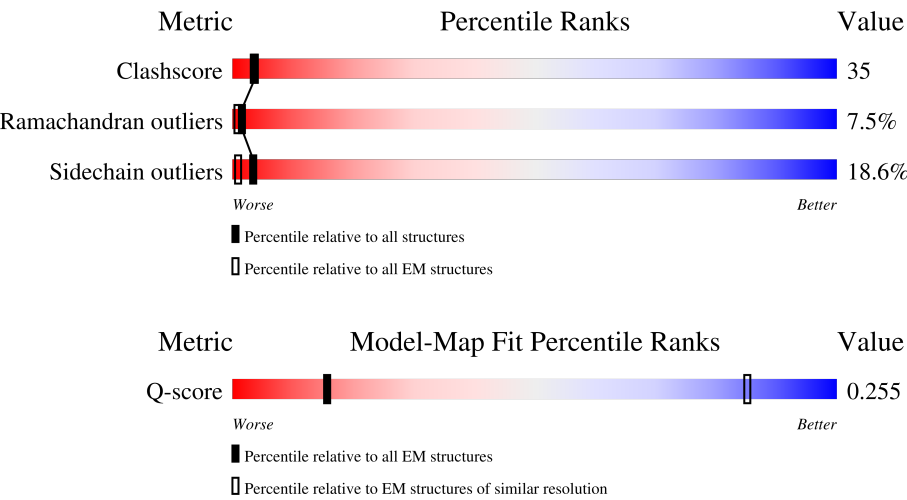
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

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	500	
1	B	500	
1	C	500	
1	D	500	

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Mol	Chain	Length	Quality of chain
1	E	500	13%16%30%33%12%9%
1	F	500	17%19%31%31%13%7%

2 Entry composition

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		

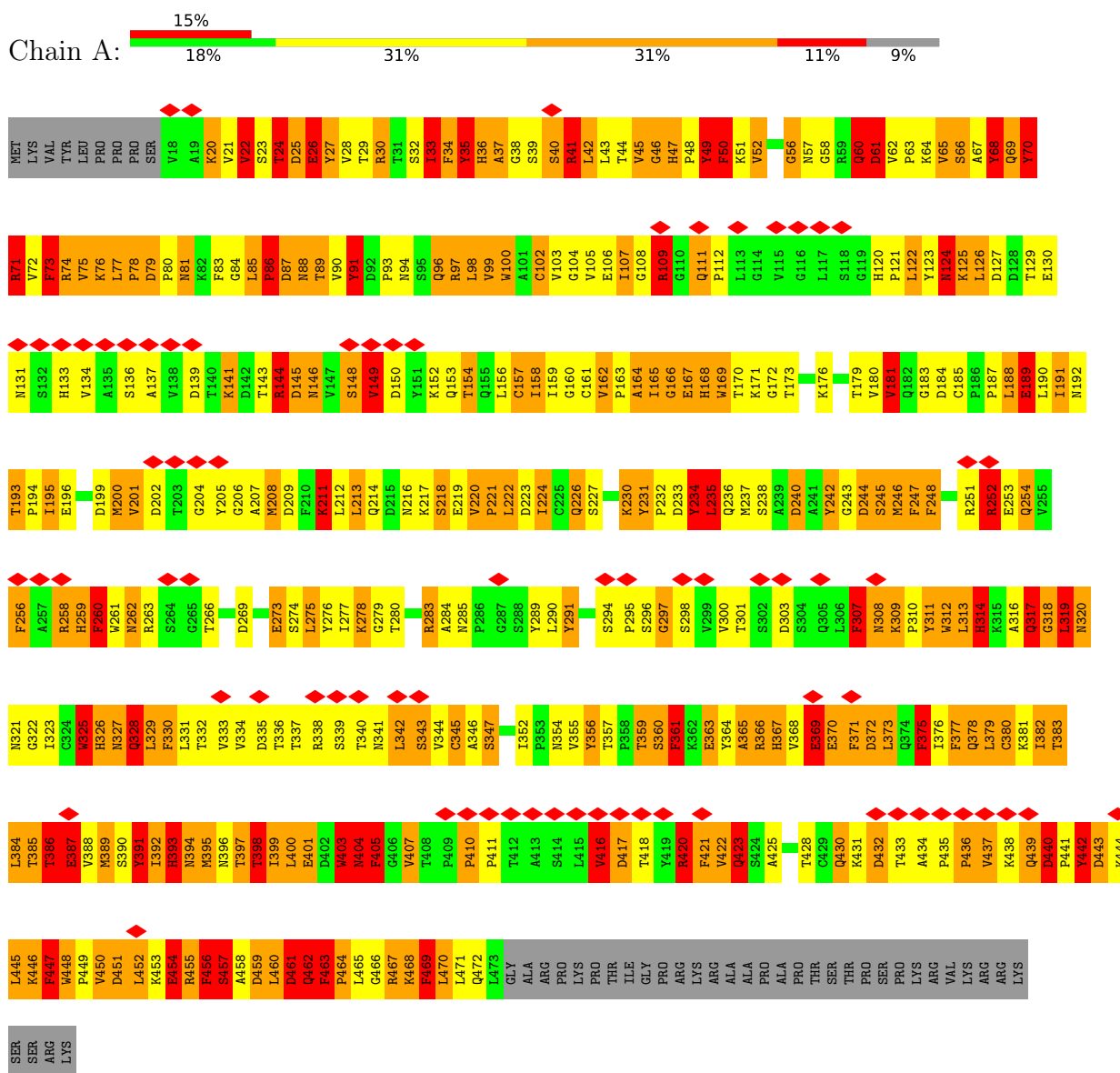
There are 6 discrepancies between the modelled and reference sequences:

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

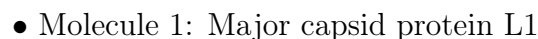
3 Residue-property plots

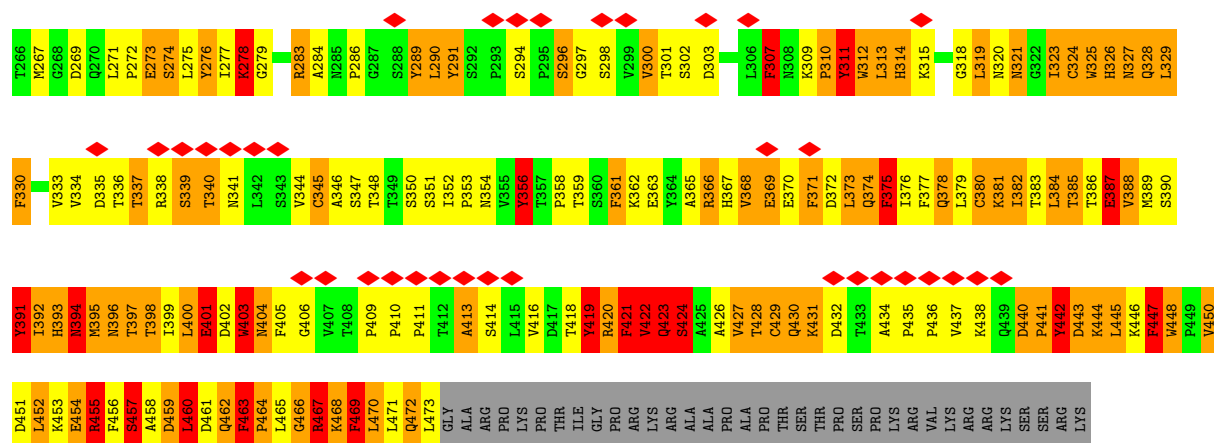
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

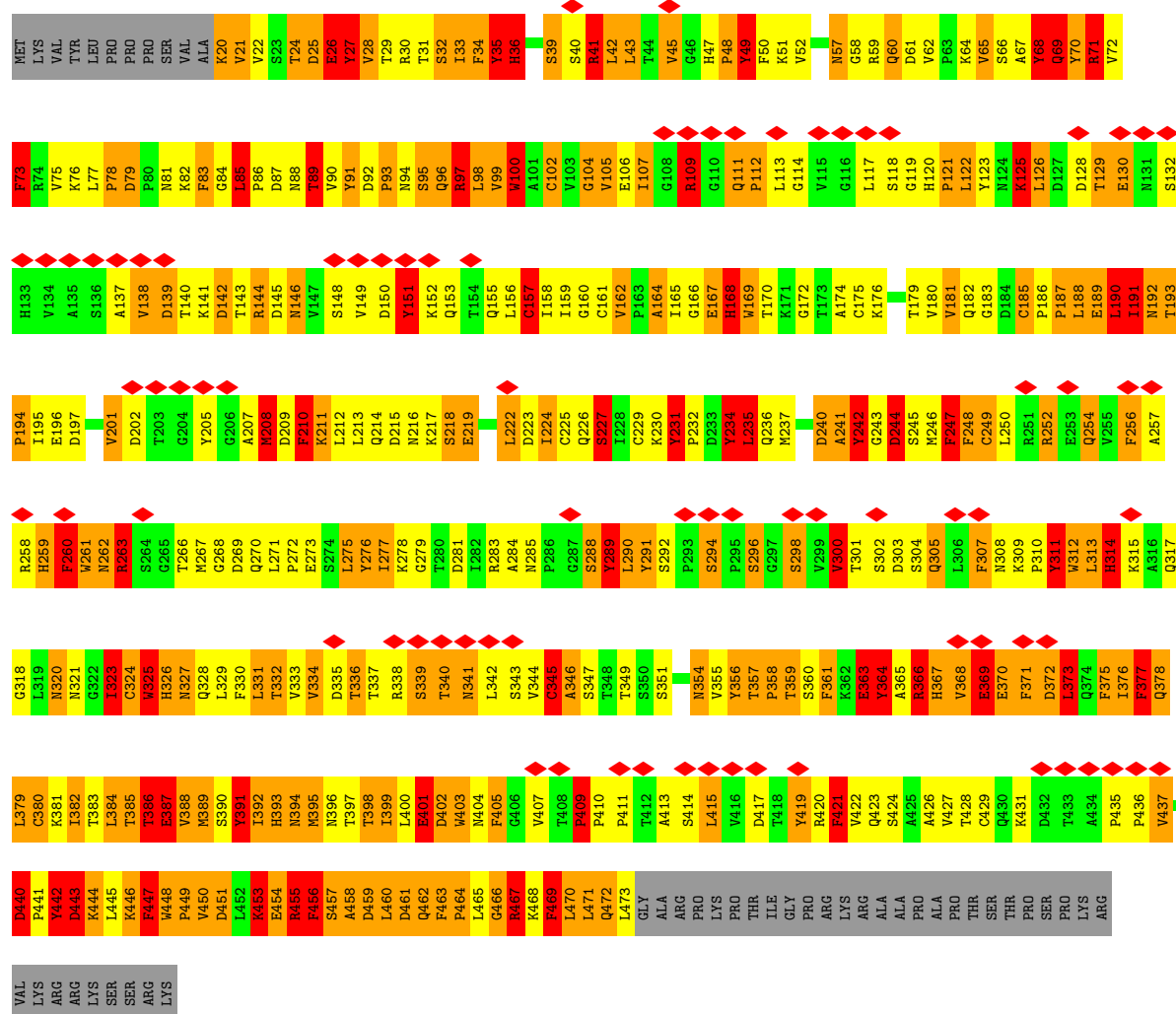


• Molecule 1: Major capsid protein L1

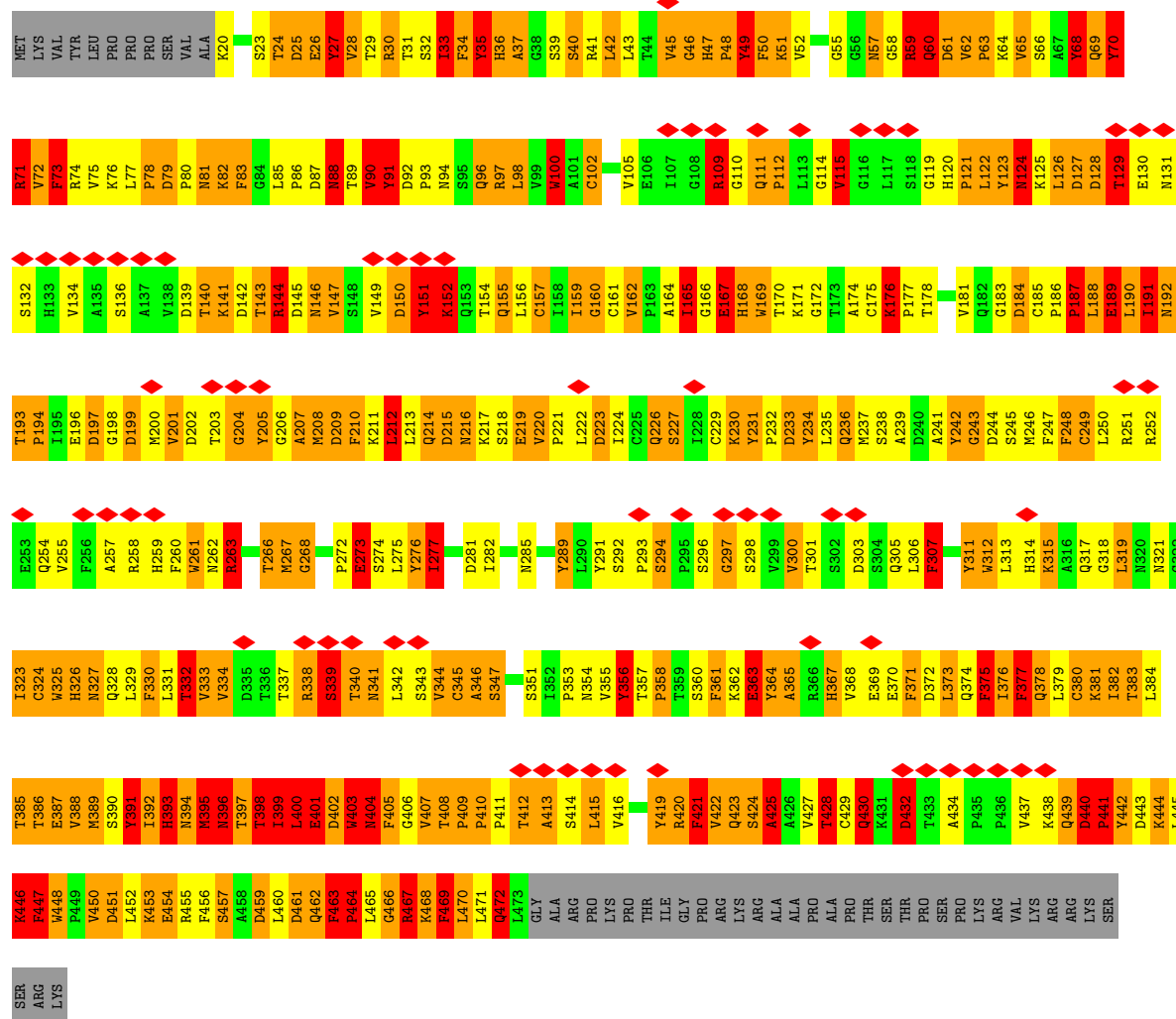




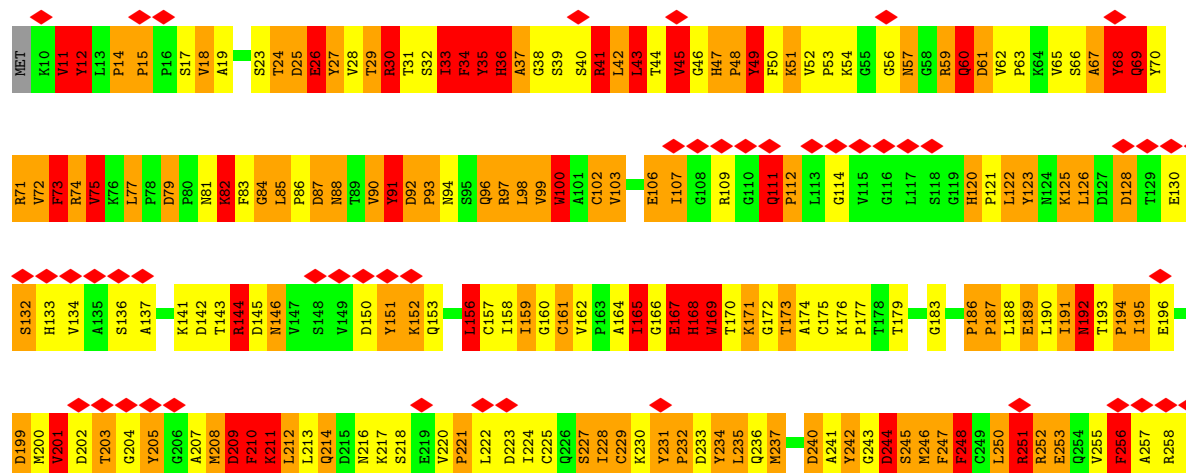
• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



R453	E454	R455	F456	S457	A458	D459	L460	D461	Q462	F463	P464	L465	G466	R467	K468	R469	L470	L471	Q472	L473	GLY	ALA	ARG	PRO	LYS	PRO	THR	THR	ILE	GLY	PRO	ARG	LYS	ARG	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
R393	N394	N395	N396	T397	T398	T399	L400	E401	D402	W403	N404	F405	G406	V407	T408	P409	P410	P411	T412	A413	S414	L415	V416	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				
F330	L331	T332	V333	V334	D335	T336	T337	R338	S339	T340	N341	L342	S343	V344	C345	A346	S347	I352	P353	N354	V355	Y356	T357	P358	T359	S360	F361	K362	E363	Y364	A365	R366	H367	V368	E369	E370	F371	D372	L373	Q374	F375	I376	F377	Q378	L379	C380	K381	I382	T383	L384	T385	T386	E387	V388	M389	S390	Y391	I392					
F260	W261	N262	R263	S264	G265	T266	E273	S274	L275	Y276	I277	K278	G279	T280	D281	T282	R283	Y289	L290	Y291	S292	P293	S294	P295	S296	G297	S298	V299	V300	T301	S302	D303	S304	Q305	L306	F307	N308	K309	P310	Y311	H312	L313	H314	K315	A316	Q317	G318	L319	N320	I323	C324	H325	H326	N327	Q328	L329							

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	910.2, 910.2, 910.2	wwPDB
Map dimensions	820, 820, 820	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	2.31	192/3694 (5.2%)	2.49	258/5036 (5.1%)
1	B	2.25	178/3761 (4.7%)	2.41	241/5130 (4.7%)
1	C	2.31	193/3700 (5.2%)	2.46	246/5044 (4.9%)
1	D	2.34	193/3682 (5.2%)	2.41	245/5019 (4.9%)
1	E	3.01	195/3682 (5.3%)	2.48	267/5019 (5.3%)
1	F	2.32	215/3761 (5.7%)	2.41	265/5130 (5.2%)
All	All	2.44	1166/22280 (5.2%)	2.44	1522/30378 (5.0%)

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 1166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	PHE	N-CA	119.81	3.00	1.46
1	A	219	GLU	CA-C	-17.43	1.44	1.52
1	A	463	PHE	CA-C	-14.09	1.41	1.52
1	F	463	PHE	CA-C	-13.77	1.37	1.52
1	A	447	PHE	CA-C	-12.69	1.36	1.52

The worst 5 of 1522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	THR	N-CA-C	27.06	146.38	111.75
1	F	463	PHE	CA-CB-CG	-17.36	96.44	113.80
1	A	447	PHE	CA-CB-CG	-16.38	97.42	113.80
1	D	447	PHE	CA-CB-CG	-16.17	97.63	113.80
1	B	447	PHE	CA-CB-CG	-16.00	97.80	113.80

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 ⓘ

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	288	0
1	B	3661	0	3571	254	0
1	C	3604	0	3508	242	0
1	D	3586	0	3489	252	0
1	E	3586	0	3489	271	0
1	F	3661	0	3571	249	0
All	All	21696	0	21131	1494	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 35.

The worst 5 of 1494 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	9
1	B	462/500 (92%)	356 (77%)	65 (14%)	41 (9%)	0	8
1	C	455/500 (91%)	363 (80%)	57 (12%)	35 (8%)	1	9
1	D	452/500 (90%)	370 (82%)	53 (12%)	29 (6%)	1	12
1	E	452/500 (90%)	351 (78%)	70 (16%)	31 (7%)	1	11
1	F	462/500 (92%)	367 (79%)	62 (13%)	33 (7%)	1	10
All	All	2737/3000 (91%)	2166 (79%)	366 (13%)	205 (8%)	1	10

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 ⓘ

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%)	336 (83%)	70 (17%)	2	10
1	B	414/444 (93%)	350 (84%)	64 (16%)	2	12
1	C	407/444 (92%)	339 (83%)	68 (17%)	2	10
1	D	405/444 (91%)	323 (80%)	82 (20%)	1	7
1	E	405/444 (91%)	320 (79%)	85 (21%)	1	6
1	F	414/444 (93%)	328 (79%)	86 (21%)	1	6
All	All	2451/2664 (92%)	1996 (81%)	455 (19%)	3	8

5 of 455 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	ILE
1	F	436	PRO
1	E	57	ASN
1	F	419	TYR
1	F	208	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	326	HIS
1	E	226	GLN
1	D	327	ASN
1	E	133	HIS
1	E	354	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

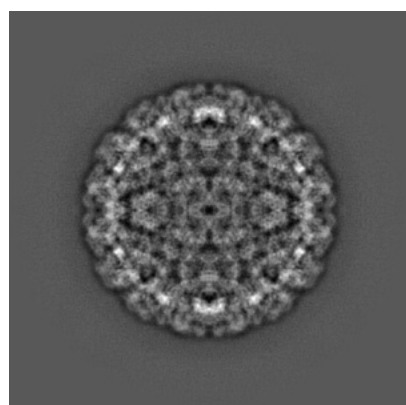
6 Map visualisation [i](#)

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

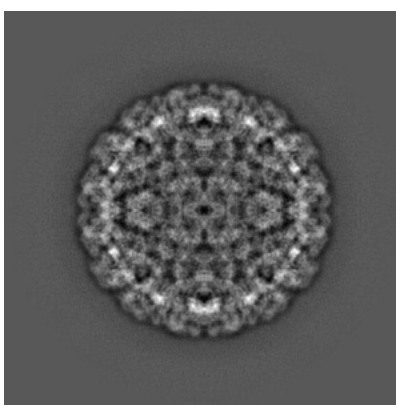
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

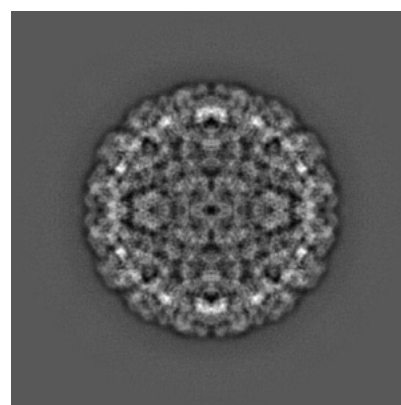
6.1.1 Primary map



X



Y

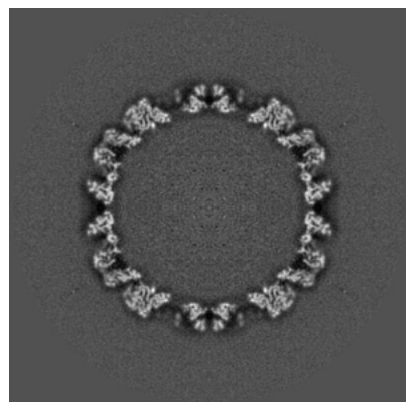


Z

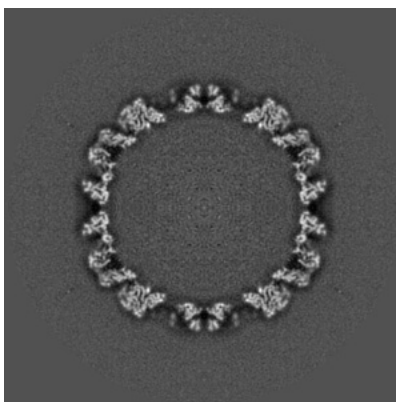
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

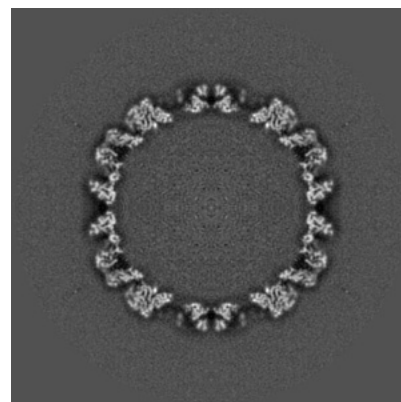
6.2.1 Primary map



X Index: 410



Y Index: 410

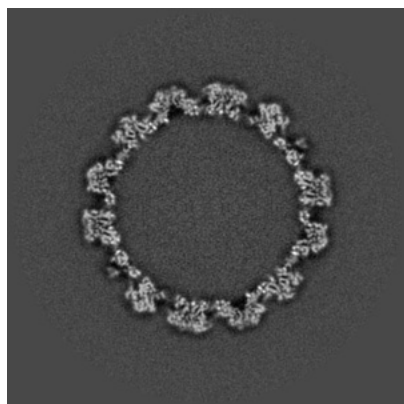


Z Index: 410

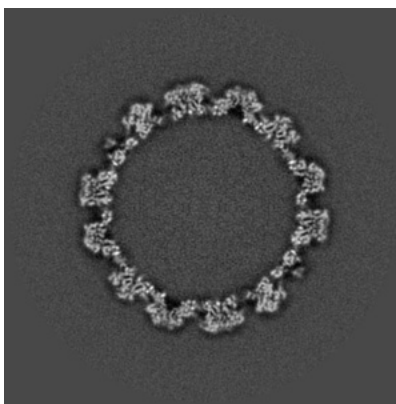
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

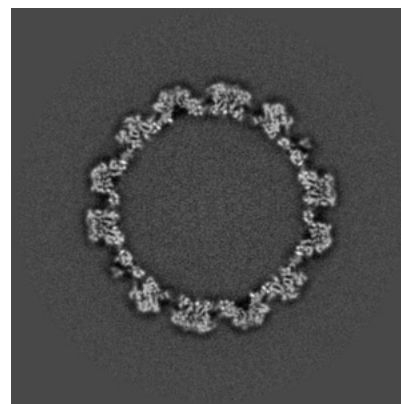
6.3.1 Primary map



X Index: 356



Y Index: 464

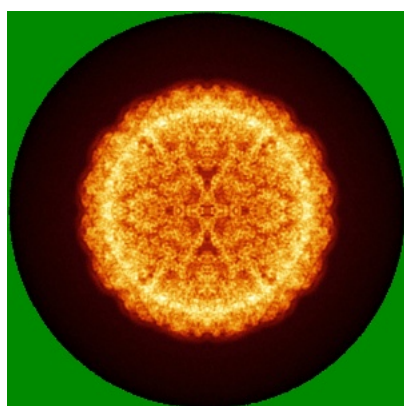


Z Index: 356

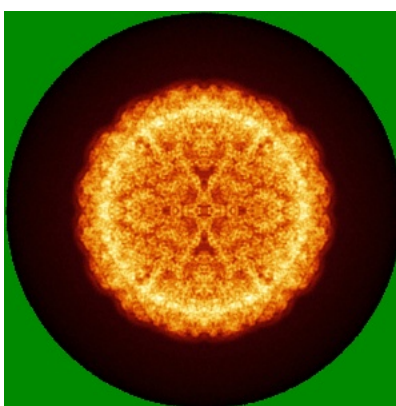
The images above show the largest variance slices of the map in three orthogonal directions.

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

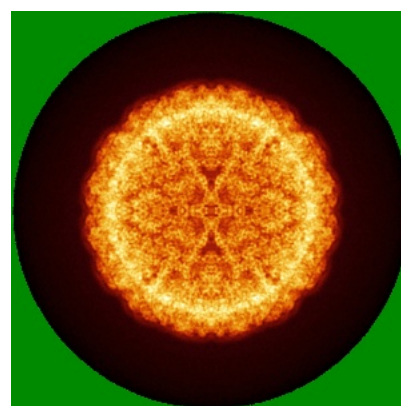
6.4.1 Primary map



X



Y

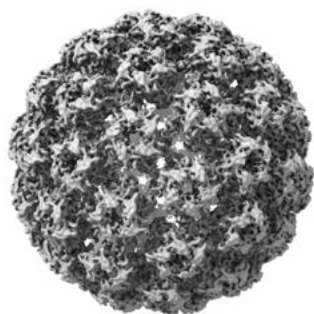


Z

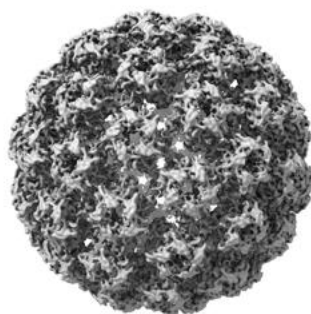
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

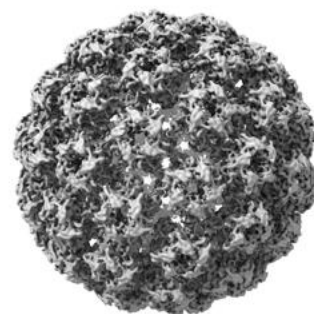
6.5.1 Primary map



X



Y



Z

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

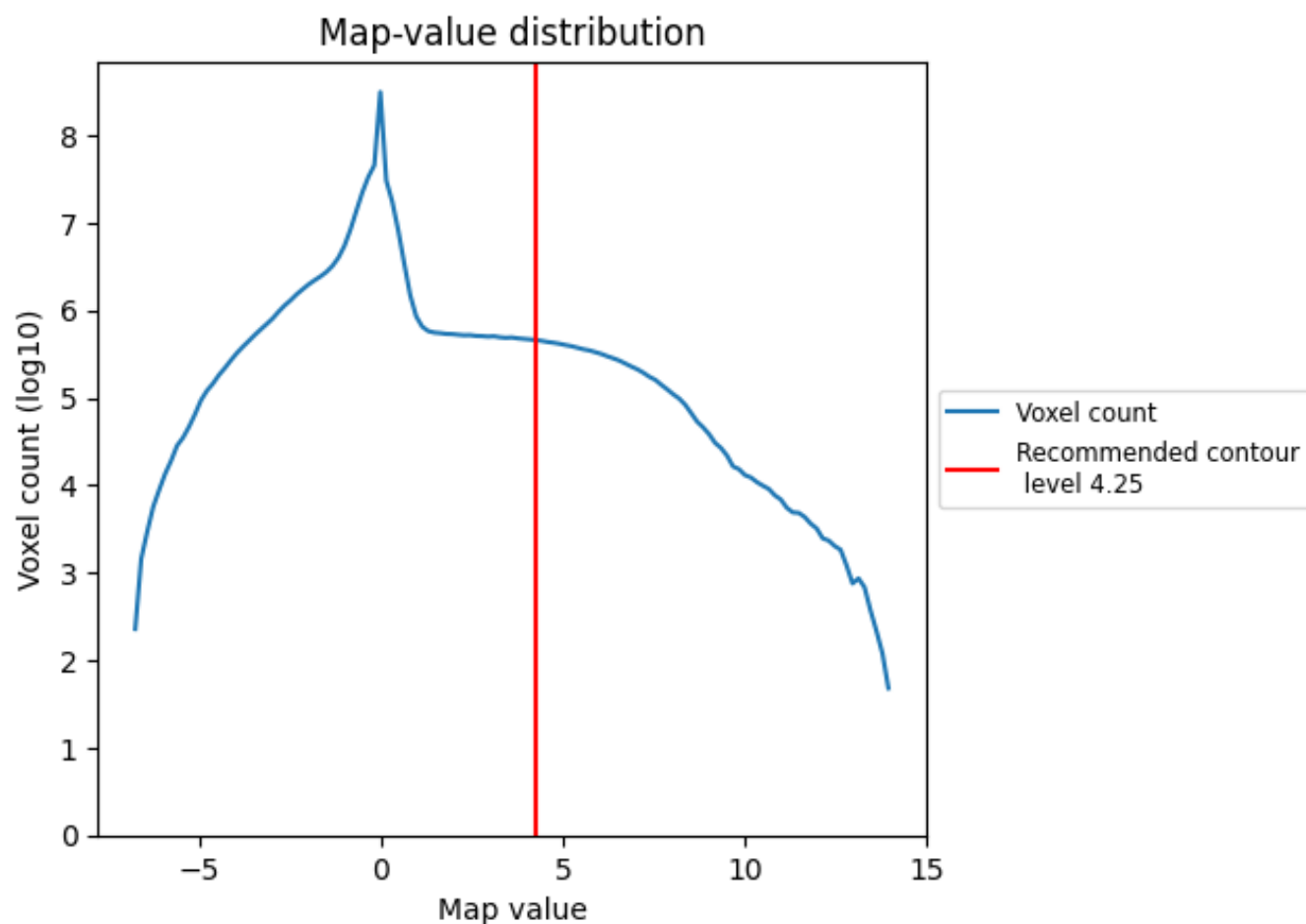
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

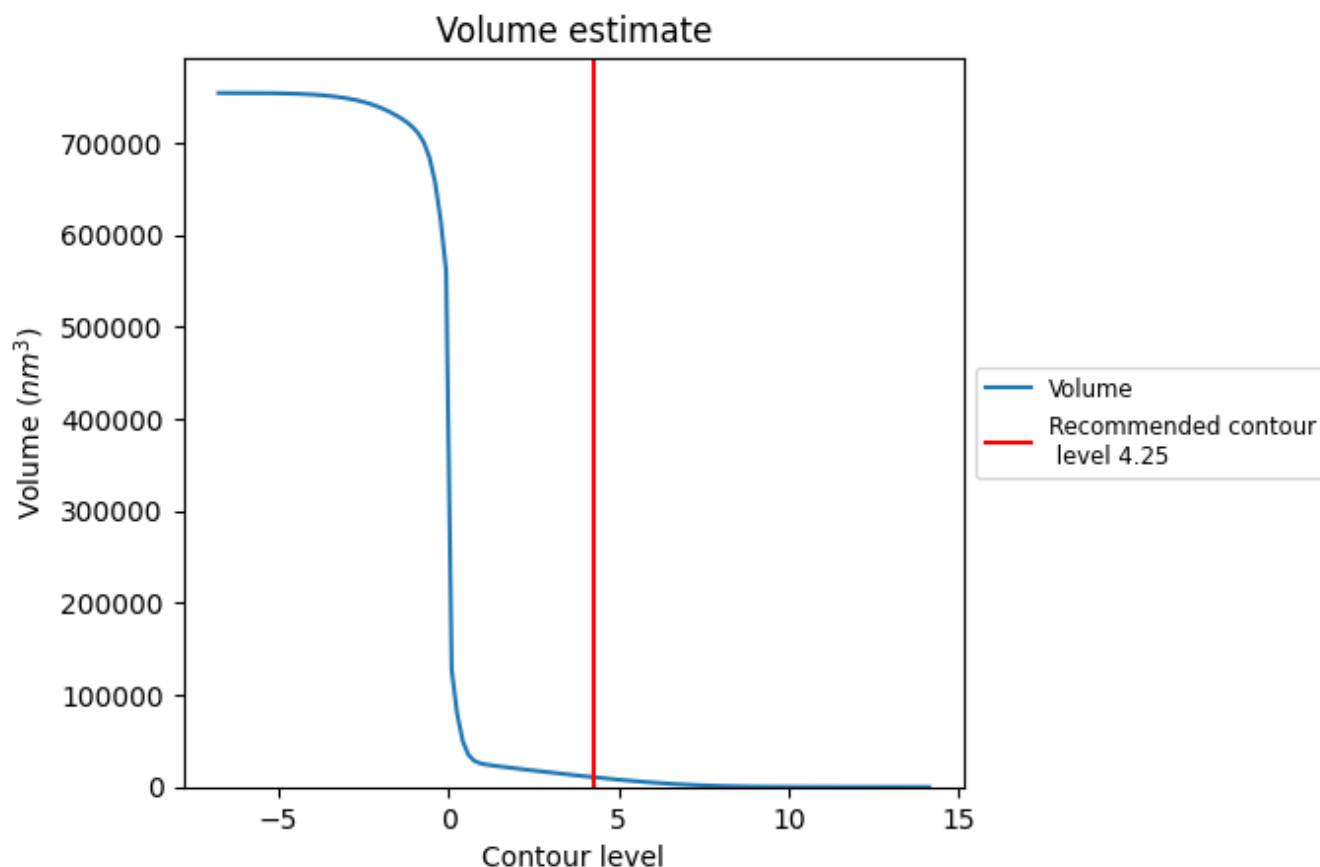
This section contains the results of statistical analysis of the map.

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.

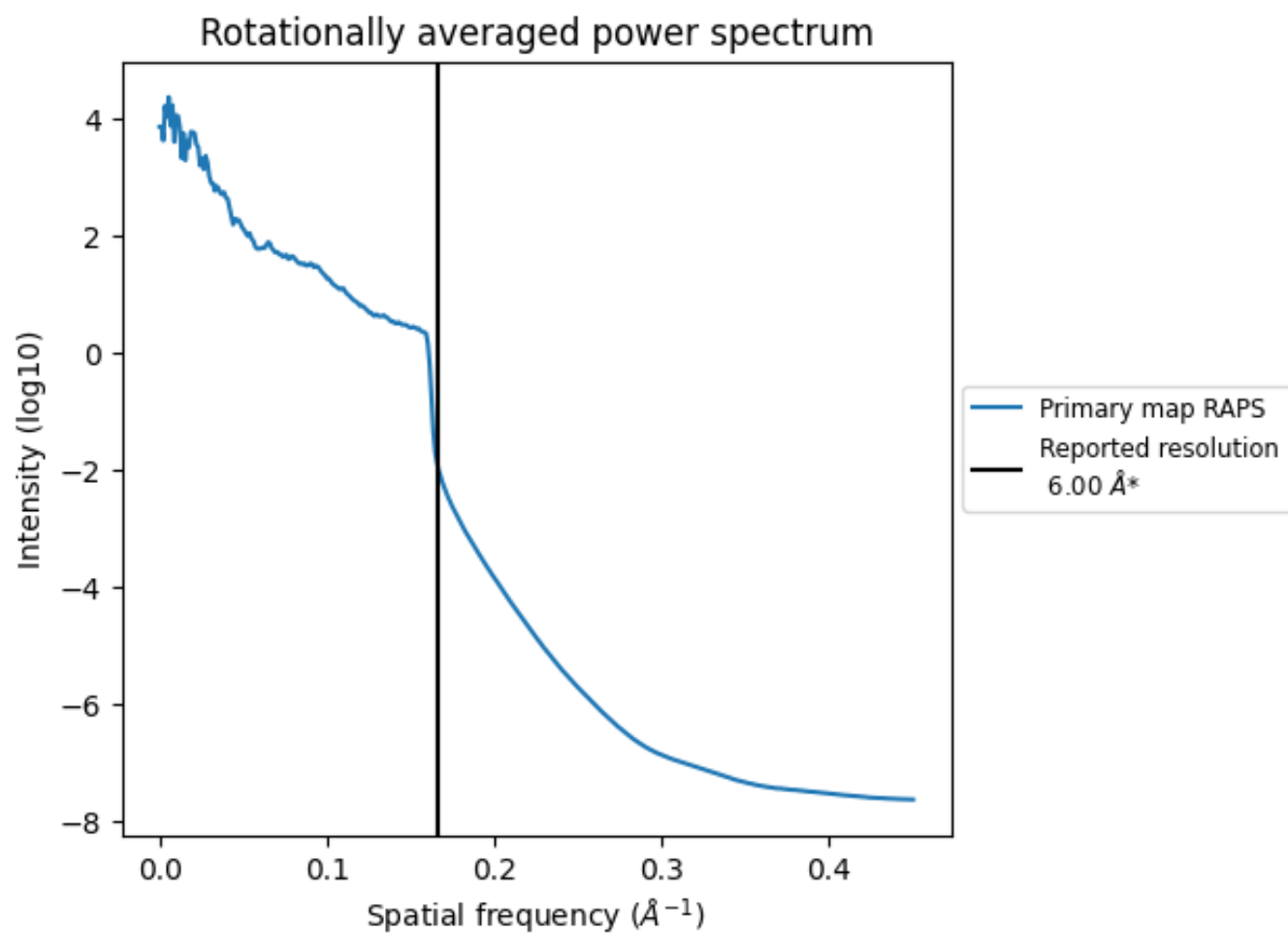
7.2 Volume estimate [i](#)



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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation ⓘ

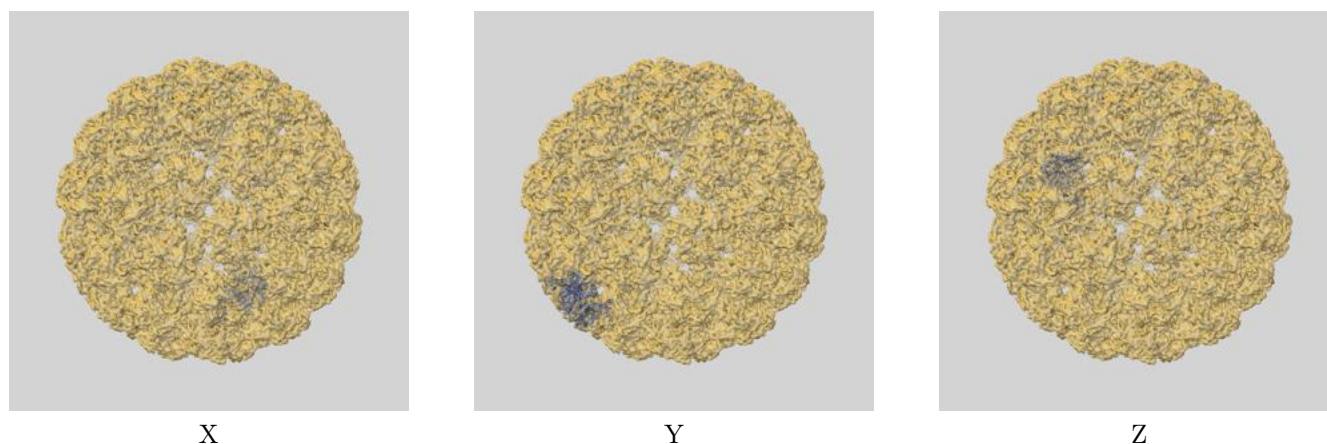
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

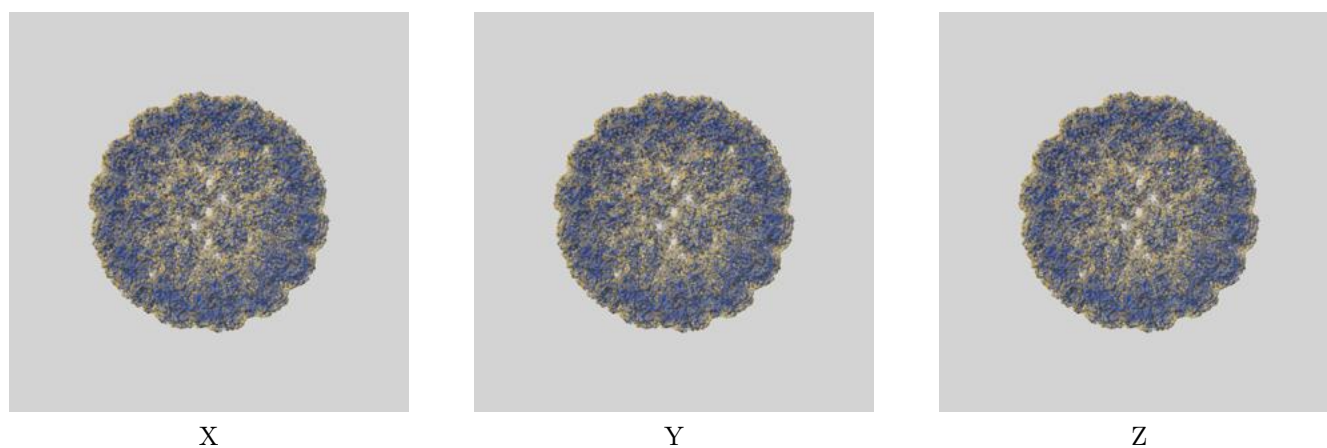
This section contains information regarding the fit between EMDB map EMD-8147 and PDB model 5JB1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

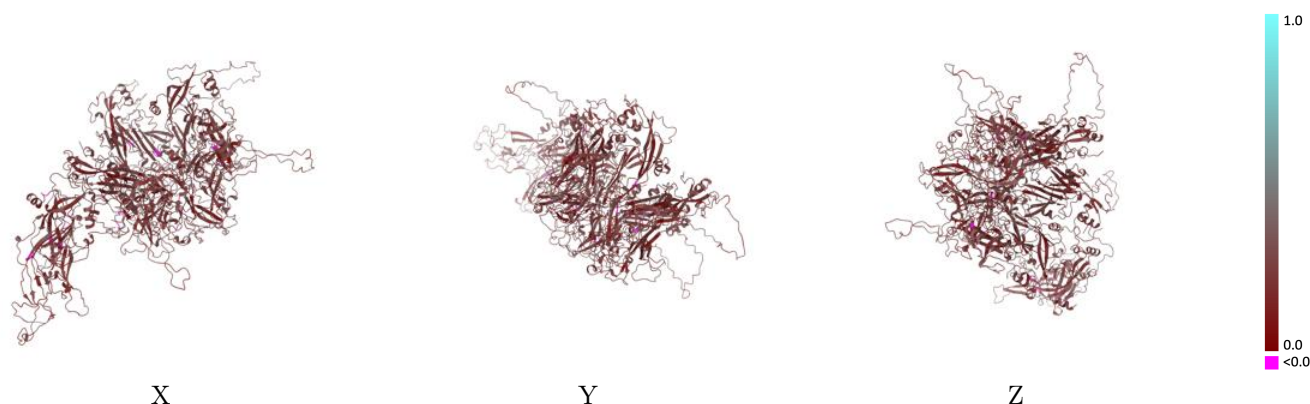


9.1.2 Map-model assembly overlay [i](#)



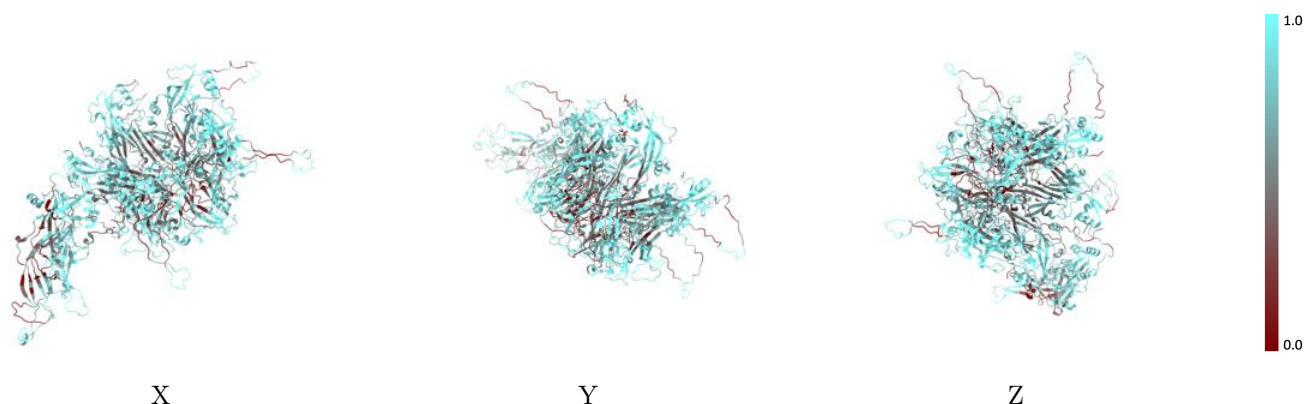
The images above show the 3D surface view of the map at the recommended contour level 4.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



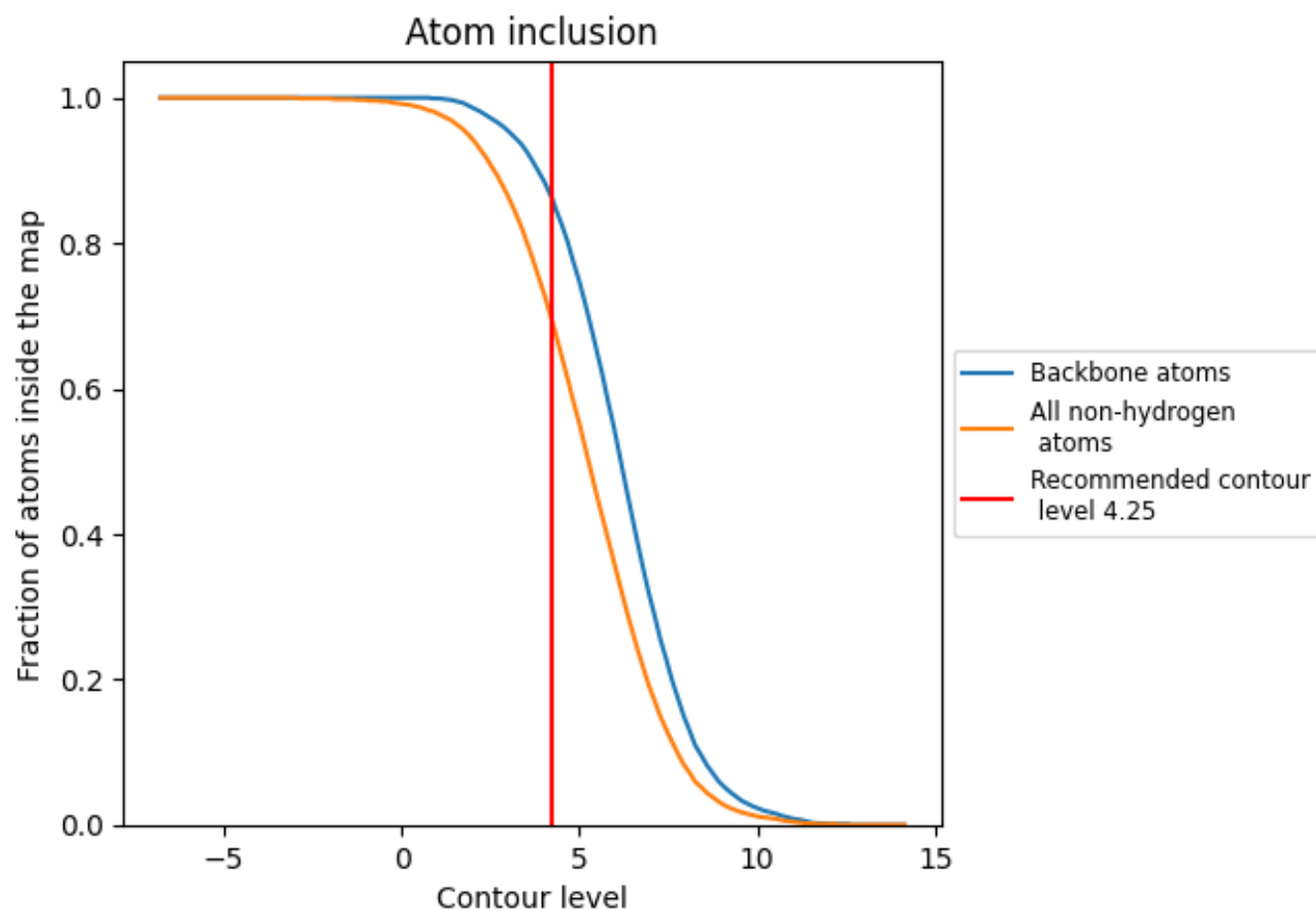
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	0.6910	0.2550
A	0.6750	0.2530
B	0.6960	0.2540
C	0.6910	0.2550
D	0.6980	0.2580
E	0.7170	0.2570
F	0.6670	0.2560

1.0

0.0

<0.0