



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 3JBA / pdb_00003jba
EMDB ID : EMD-6424
Title : The U4 antibody epitope on human papillomavirus 16 identified by cryo-EM
Authors : Guan, J.; Bywaters, S.M.; Brendle, S.A.; Lee, H.; Ashley, R.E.; Christensen, N.D.; Hafenstein, S.
Deposited on : 2015-08-11
Resolution : 12.00 Å(reported)
Based on initial model : 3J6R

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:

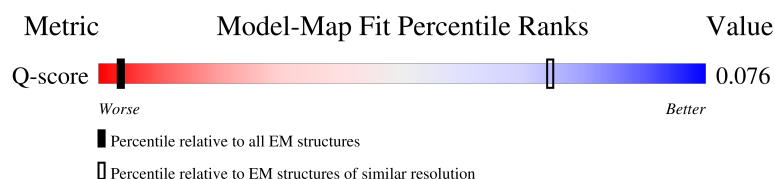
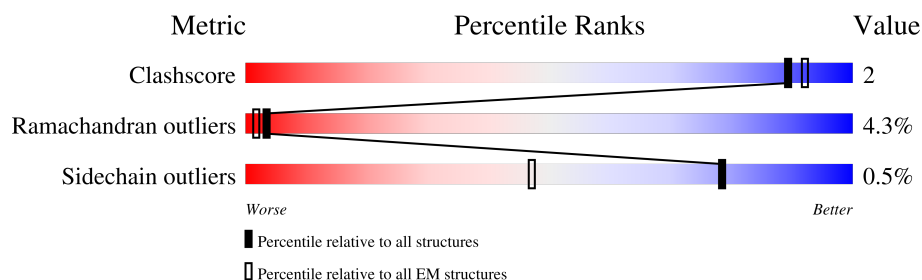
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 12.00 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	93 (11.50 - 12.50)

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	L	115	13% 92% 8%
2	H	115	87% 10% .
3	A	478	56% 40% .
3	B	478	54% 42% ..

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Mol	Chain	Length	Quality of chain
3	C	478	 53% 44% .
3	D	478	 55% 41% .
3	E	478	 54% 43% .
3	F	478	 58% 38% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20721 atoms, of which 7468 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 H16.U4 antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	115	Total	C	H	N	O	0	0
			1772	567	879	144	178		

- Molecule 2 is a protein called H16.U4 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	115	Total	C	H	N	O	0	0
			1735	560	841	151	178		

- Molecule 3 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	A	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	E	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	D	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	C	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	F	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLN	ASN	conflict	UNP C9E771
B	181	GLN	ASN	conflict	UNP C9E771
B	472	LEU	ALA	conflict	UNP C9E771
A	177	GLN	ASN	conflict	UNP C9E771
A	181	GLN	ASN	conflict	UNP C9E771

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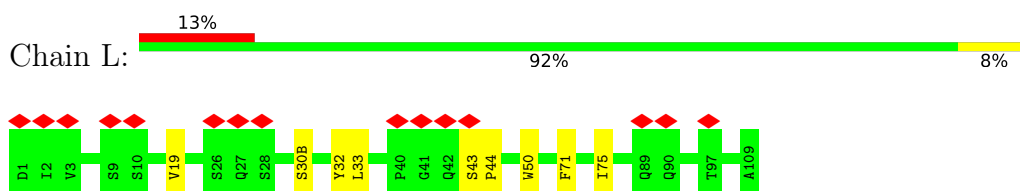
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Chain	Residue	Modelled	Actual	Comment	Reference
A	472	LEU	ALA	conflict	UNP C9E771
E	177	GLN	ASN	conflict	UNP C9E771
E	181	GLN	ASN	conflict	UNP C9E771
E	472	LEU	ALA	conflict	UNP C9E771
D	177	GLN	ASN	conflict	UNP C9E771
D	181	GLN	ASN	conflict	UNP C9E771
D	472	LEU	ALA	conflict	UNP C9E771
C	177	GLN	ASN	conflict	UNP C9E771
C	181	GLN	ASN	conflict	UNP C9E771
C	472	LEU	ALA	conflict	UNP C9E771
F	177	GLN	ASN	conflict	UNP C9E771
F	181	GLN	ASN	conflict	UNP C9E771
F	472	LEU	ALA	conflict	UNP C9E771

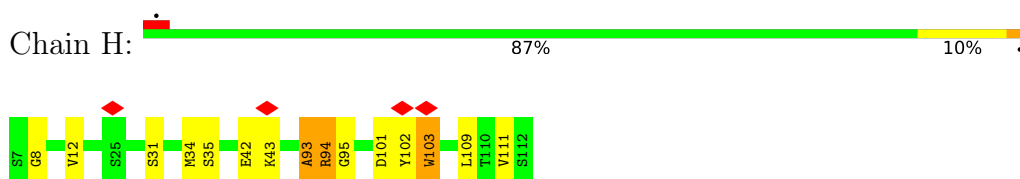
3 Residue-property plots [i](#)

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.

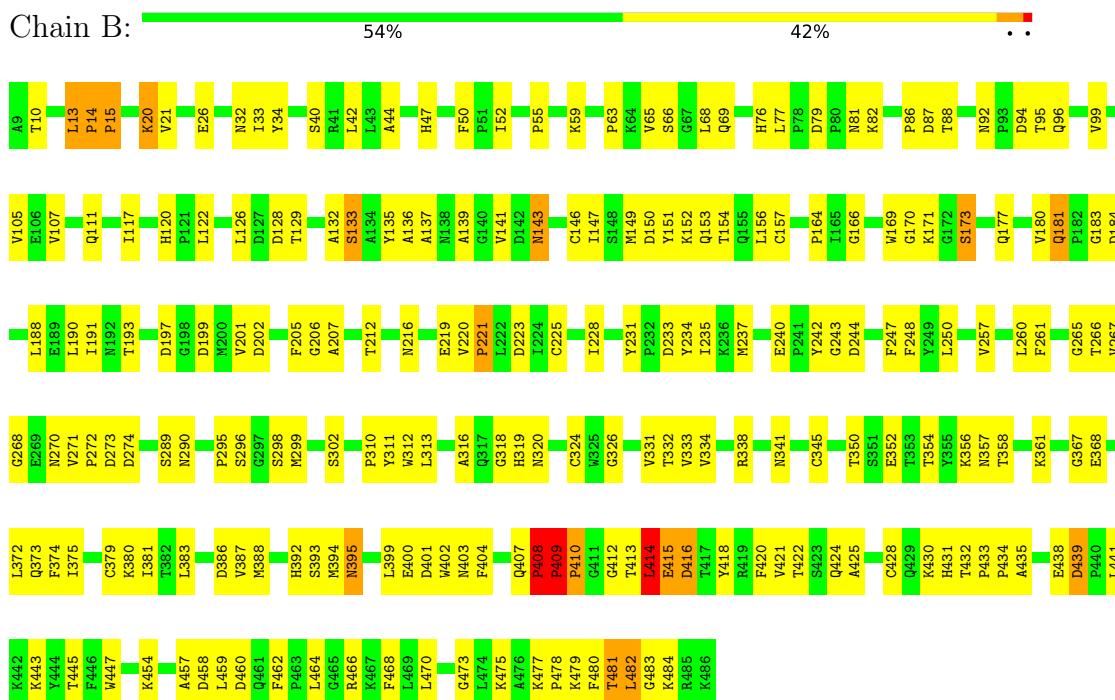
- Molecule 1: H16.U4 antibody light chain



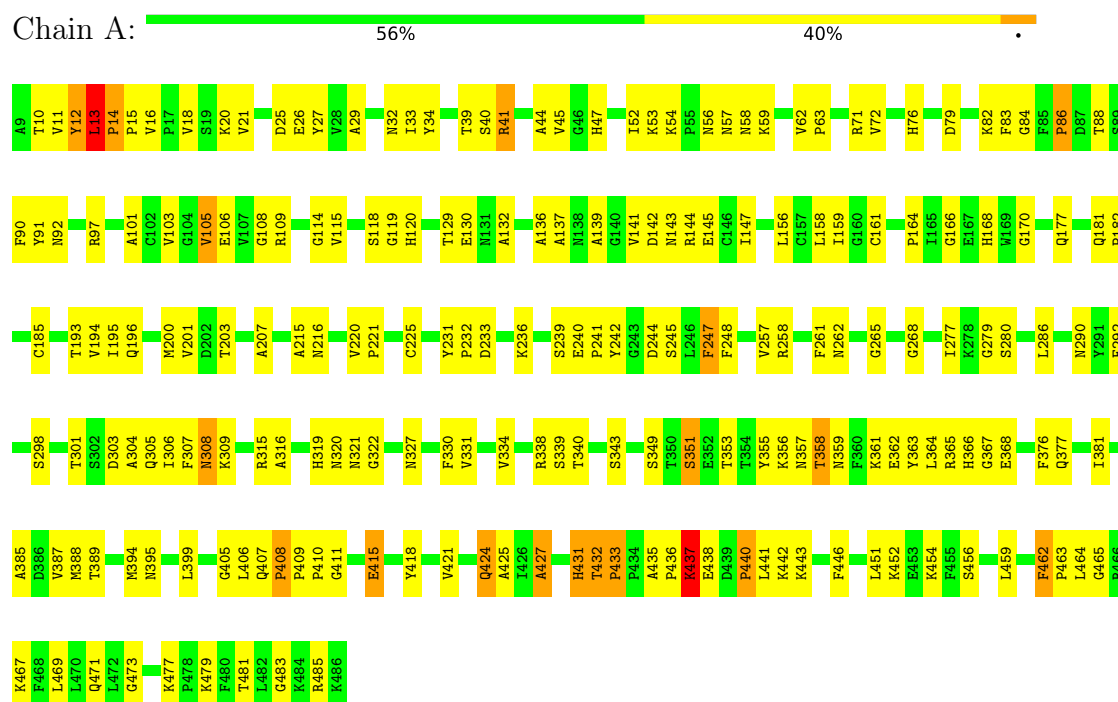
- Molecule 2: H16.U4 antibody heavy chain



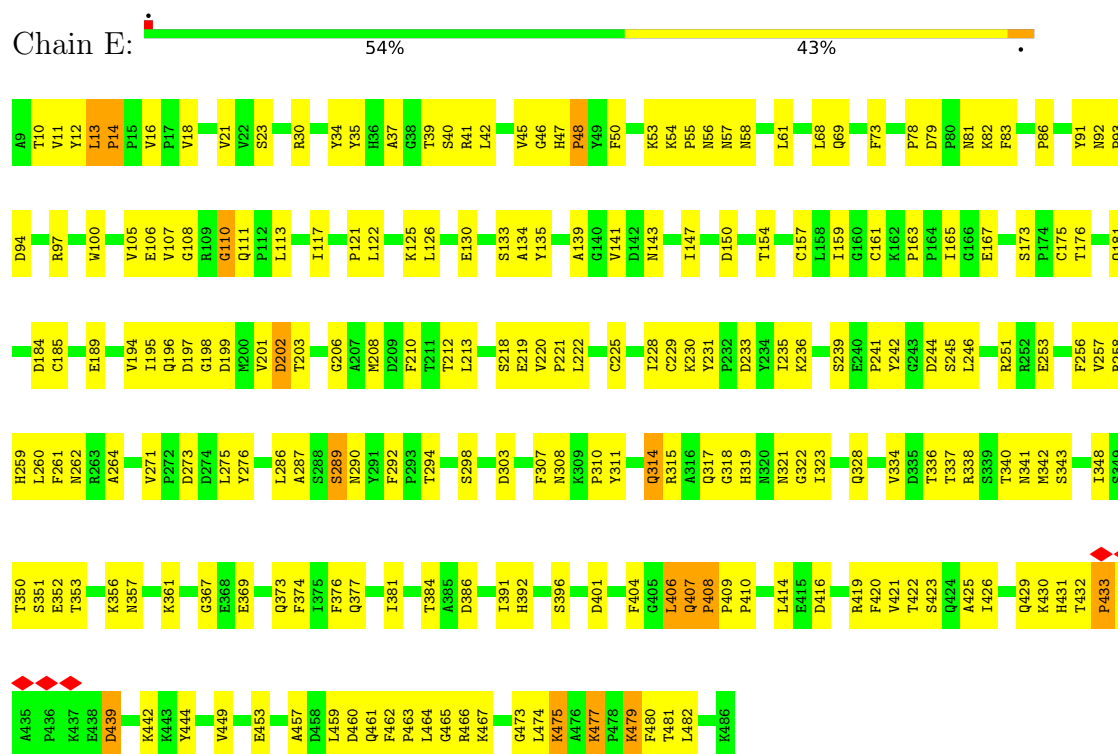
- Molecule 3: Major capsid protein L1



- Molecule 3: Major capsid protein L1

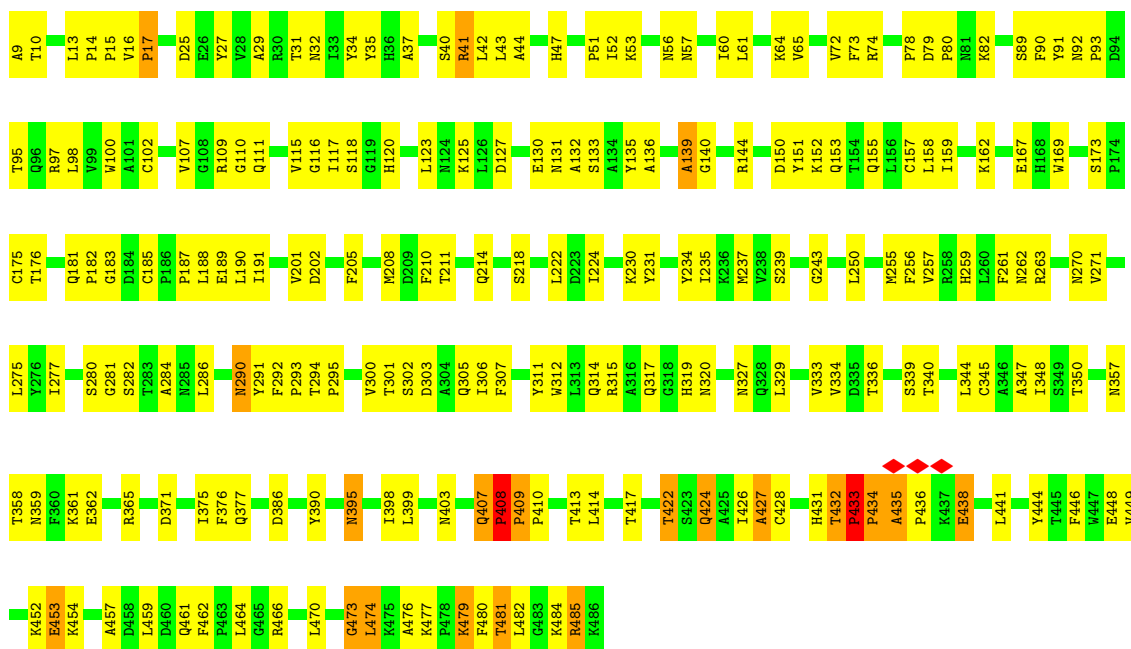


- Molecule 3: Major capsid protein L1



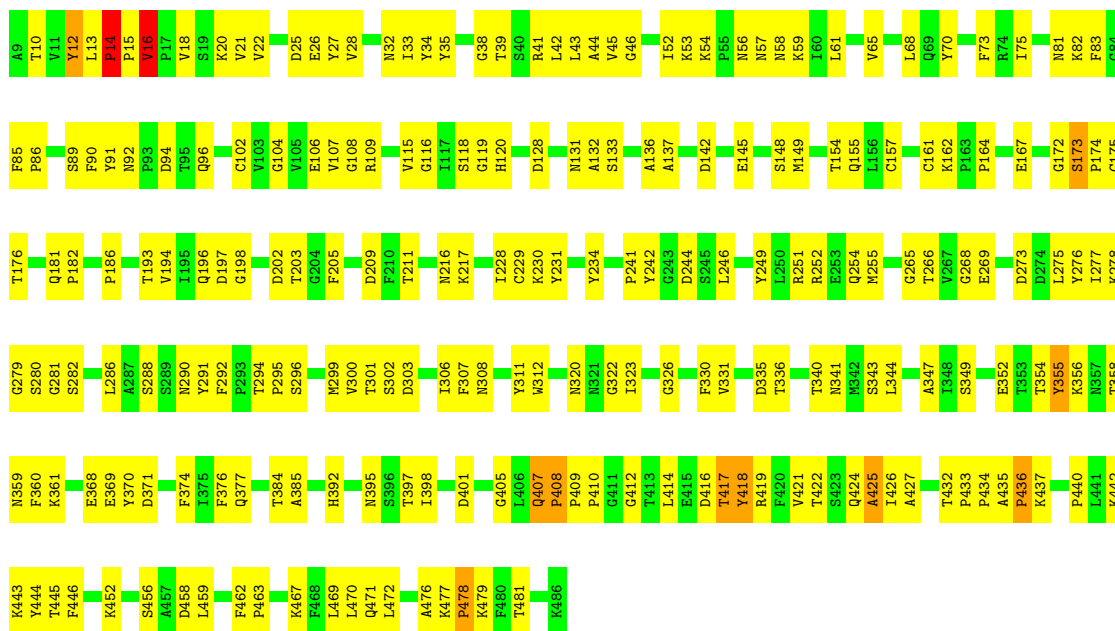
- Molecule 3: Major capsid protein L1





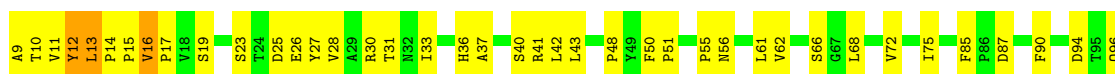
• Molecule 3: Major capsid protein L1

Chain C: 53% 44%



• Molecule 3: Major capsid protein L1

Chain F: 58% 38%



A476	K477	P478	K479	F480	T481	L482	G483	K484	R485	K486	N395	S396	T397	I398	D401	K402	N403	P404	G405	L406	G407	P408	P409	L414	E415	D416	T417	F420	V421	T422	S423	Q424	A425	I426	A427	C428	Q429	Q430	K431	A435	P436	K437	F438	D439	P440	L441	W447	N450	F455	S456	L459	F462	R466	L470	G471	L472	G473	L474	K475
Q314	R315	A316	H319	N320	N321	G322	L329	F330	V331	T332	V333	T336	T337	R338	S339	T340	N341	M342	S343	L344	A347	E352	T353	T354	Y355	T358	N359	F360	K361	E362	Y363	L364	R365	H366	G367	E368	E369	Y370	D371	I375	F376	K380	T384	V387	K388	T389	H392												
R97	C102	G103	G104	V105	E106	V107	G108	R109	G110	Q111	P112	L113	G114	V115	P121	L122	L123	N124	N131	A132	A137	M138	A139	D142	M143	R144	E145	C146	C157	L158	I159	K162	P163	P164	I165	W169	G170	K171	C175	T176	V178	A179	V180	Q181	C185	P186	T193												
V194	D197	G198	D199	T212	S218	E219	V220	P221	I228	M237	P241	Y242	G243	D244	S245	L246	F247	F248	R252	F256	V257	R258	H259	L260	F261	G265	V271	P272	D273	D274	L275	Y276	I277	S288	S289	N290	Y291	V300	T301	A304	Q305	I306	P310	Y311															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5806	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	JEOL 2100	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	5430	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	6.050	Depositor
Minimum map value	-2.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	894.72, 894.72, 894.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.33, 2.33, 2.33	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	L	0.72	1/913 (0.1%)	0.81	0/1236
2	H	1.29	3/916 (0.3%)	1.28	11/1236 (0.9%)
3	A	2.50	94/1910 (4.9%)	2.91	199/2386 (8.3%)
3	B	2.55	101/1910 (5.3%)	2.93	205/2386 (8.6%)
3	C	2.58	111/1910 (5.8%)	2.81	194/2386 (8.1%)
3	D	2.62	124/1910 (6.5%)	2.83	174/2386 (7.3%)
3	E	2.64	114/1910 (6.0%)	2.88	210/2386 (8.8%)
3	F	2.52	102/1910 (5.3%)	2.85	180/2386 (7.5%)
All	All	2.42	650/13289 (4.9%)	2.68	1173/16788 (7.0%)

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
3	A	0	12
3	B	0	10
3	C	0	13
3	D	0	15
3	E	0	9
3	F	0	11
All	All	0	70

The worst 5 of 650 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	94	ARG	C-N	30.52	1.75	1.33
3	C	85	PHE	CA-C	-18.55	1.37	1.52
3	A	143	ASN	CA-C	-10.85	1.40	1.53
3	C	149	MET	CA-C	-10.37	1.39	1.52
3	A	305	GLN	C-N	9.93	1.44	1.33

The worst 5 of 1173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	ARG	CA-C-N	-17.29	105.71	122.66
2	H	94	ARG	C-N-CA	-17.29	105.71	122.66
3	C	306	ILE	N-CA-C	-13.18	101.23	111.90
3	F	220	VAL	N-CA-C	-12.95	98.57	109.19
3	C	409	PRO	CA-C-O	-12.80	111.69	120.90

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	13	LEU	Peptide
3	B	14	PRO	Peptide
3	B	181	GLN	Peptide
3	B	408	PRO	Peptide
3	B	409	PRO	Peptide

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	L	893	879	879	8	0
2	H	894	841	837	22	0
3	A	1911	958	512	2	0
3	B	1911	958	512	1	0
3	C	1911	958	512	0	0
3	D	1911	958	512	0	0
3	E	1911	958	512	0	0
3	F	1911	958	512	2	0
All	All	13253	7468	4788	33	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 2.

The worst 5 of 33 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:94:ARG:C	2:H:95:GLY:N	1.75	1.43
2:H:94:ARG:CA	2:H:95:GLY:N	1.92	1.30
2:H:94:ARG:HA	2:H:95:GLY:N	1.70	1.04
2:H:103:TRP:HE3	2:H:103:TRP:H	1.02	0.98
2:H:103:TRP:O	2:H:103:TRP:CE3	2.17	0.96

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	L	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	H	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
3	A	476/478 (100%)	403 (85%)	55 (12%)	18 (4%)	2	19
3	B	476/478 (100%)	395 (83%)	50 (10%)	31 (6%)	1	12
3	C	476/478 (100%)	402 (84%)	52 (11%)	22 (5%)	2	17
3	D	476/478 (100%)	404 (85%)	47 (10%)	25 (5%)	1	15
3	E	476/478 (100%)	417 (88%)	43 (9%)	16 (3%)	3	21
3	F	476/478 (100%)	405 (85%)	52 (11%)	19 (4%)	2	18
All	All	3082/3098 (100%)	2646 (86%)	305 (10%)	131 (4%)	3	17

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	15	PRO
3	B	87	ASP
3	B	133	SER
3	B	395	ASN
3	B	408	PRO

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	L	100/100 (100%)	100 (100%)	0	100	100
2	H	95/95 (100%)	94 (99%)	1 (1%)	65	76
All	All	195/195 (100%)	194 (100%)	1 (0%)	78	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	103	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	76	ASN

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	94:ARG	C	95:GLY	N	1.75

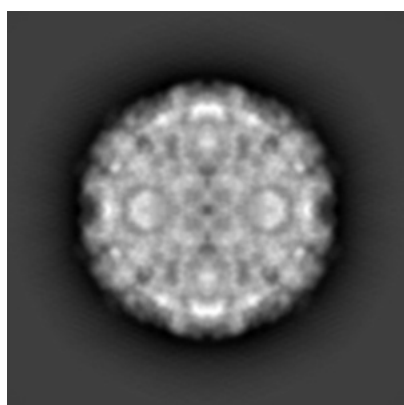
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6424. These allow visual inspection of the internal detail of the map and identification of artifacts.

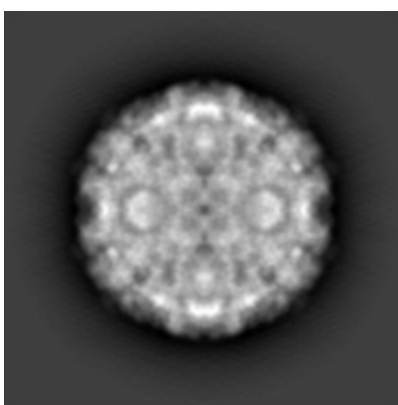
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

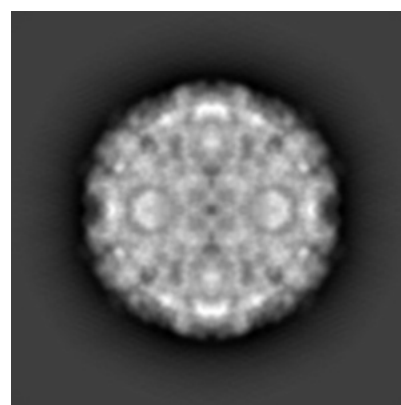
6.1.1 Primary map



X



Y

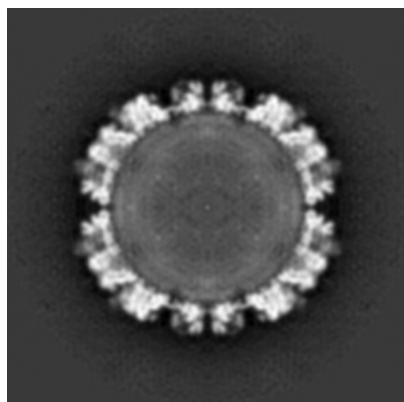


Z

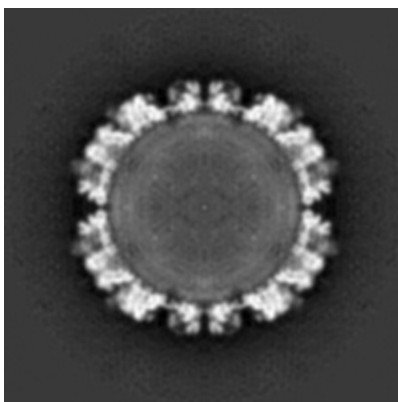
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

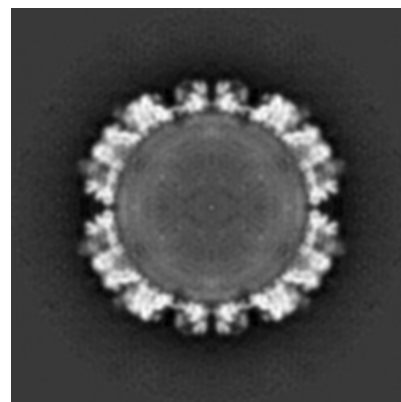
6.2.1 Primary map



X Index: 192



Y Index: 192

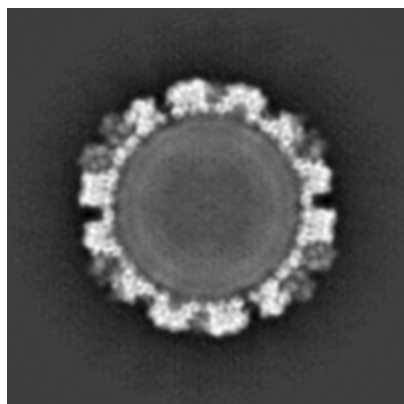


Z Index: 192

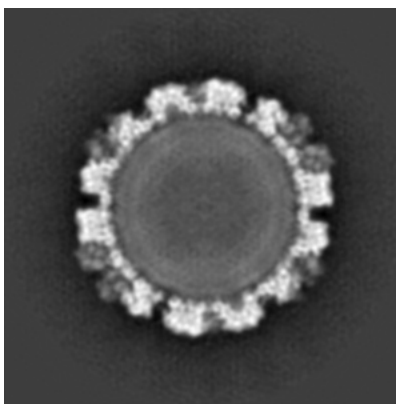
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

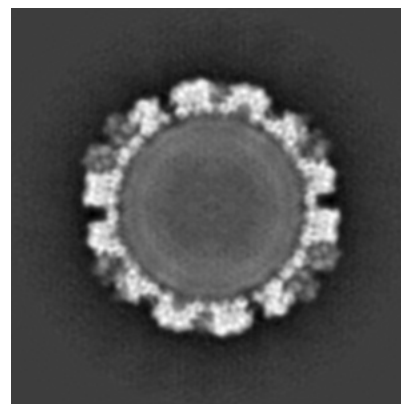
6.3.1 Primary map



X Index: 217



Y Index: 167

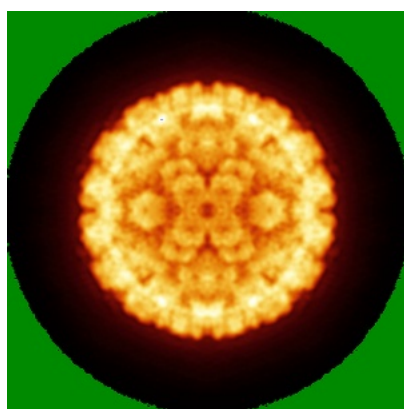


Z Index: 217

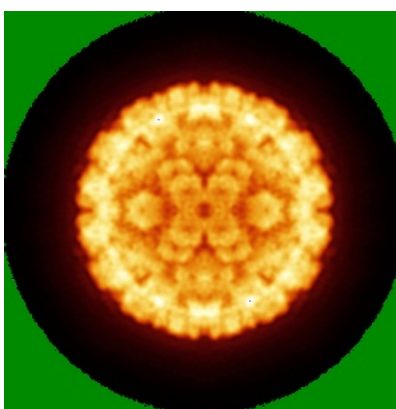
The images above show the largest variance slices of the map in three orthogonal directions.

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

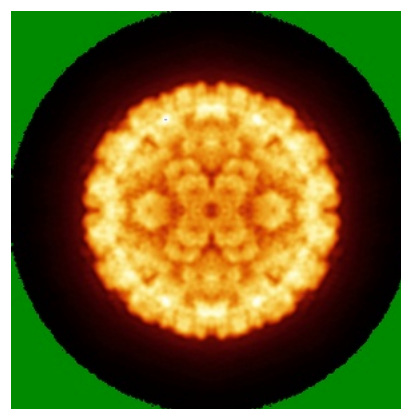
6.4.1 Primary map



X



Y

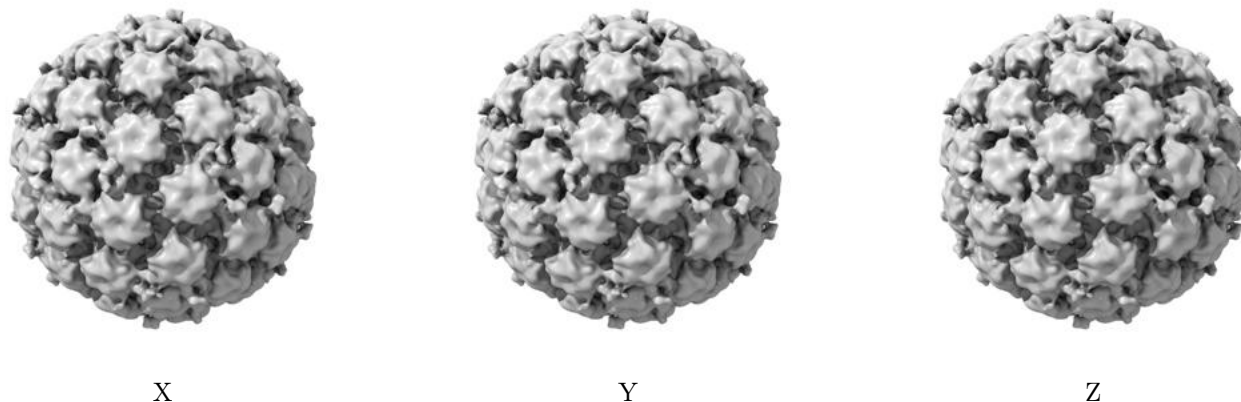


Z

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



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.

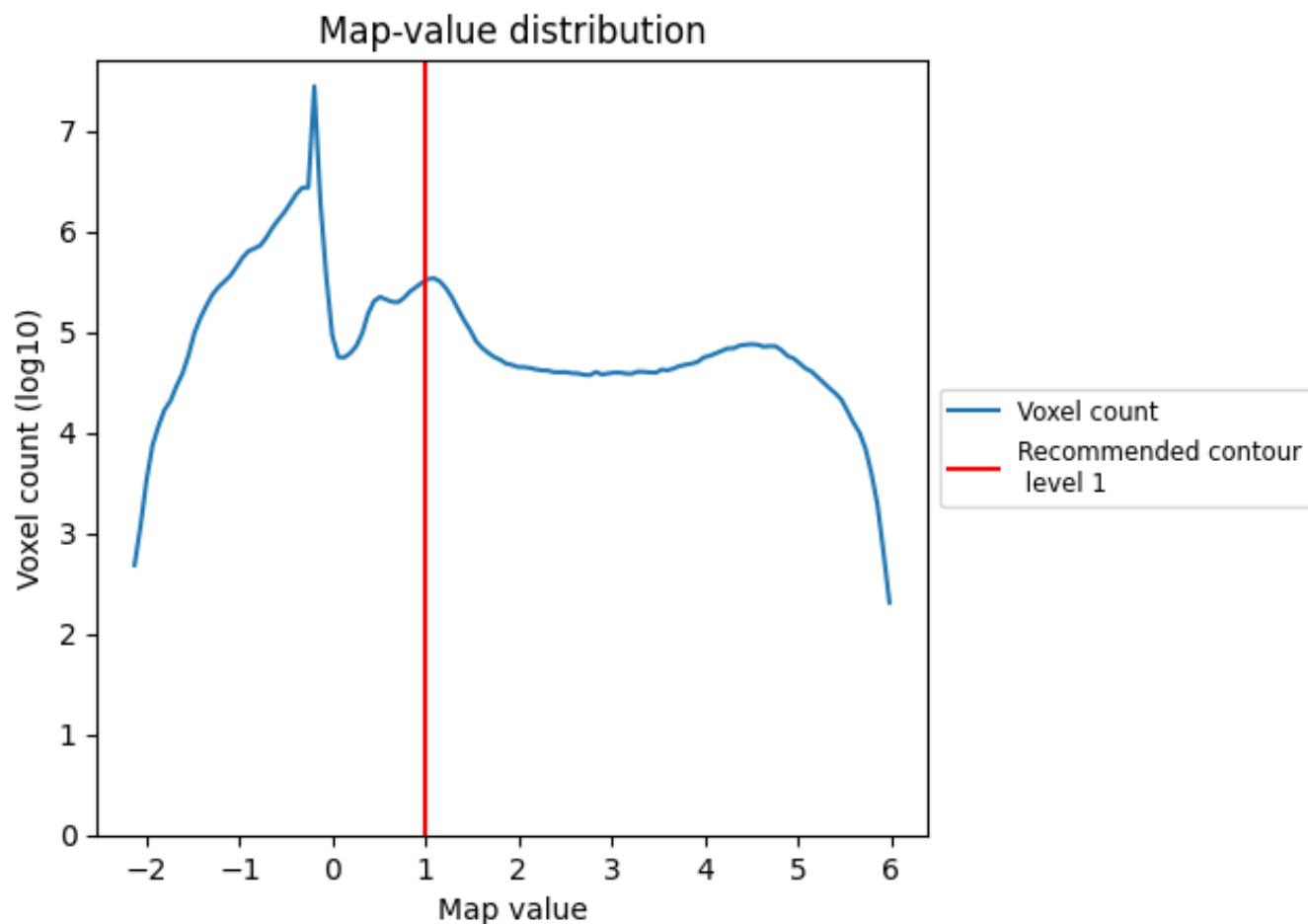
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

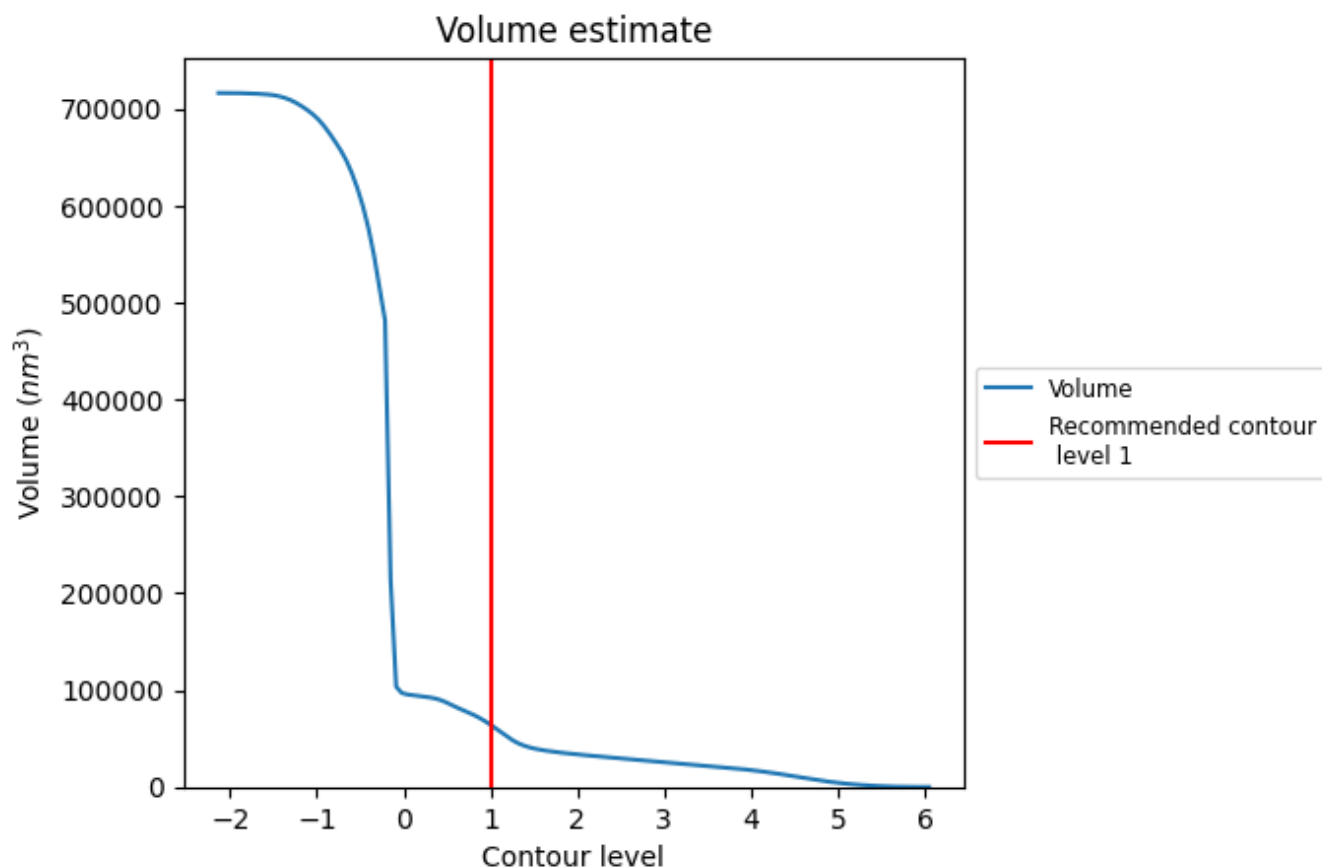
This section contains the results of statistical analysis of the map.

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.

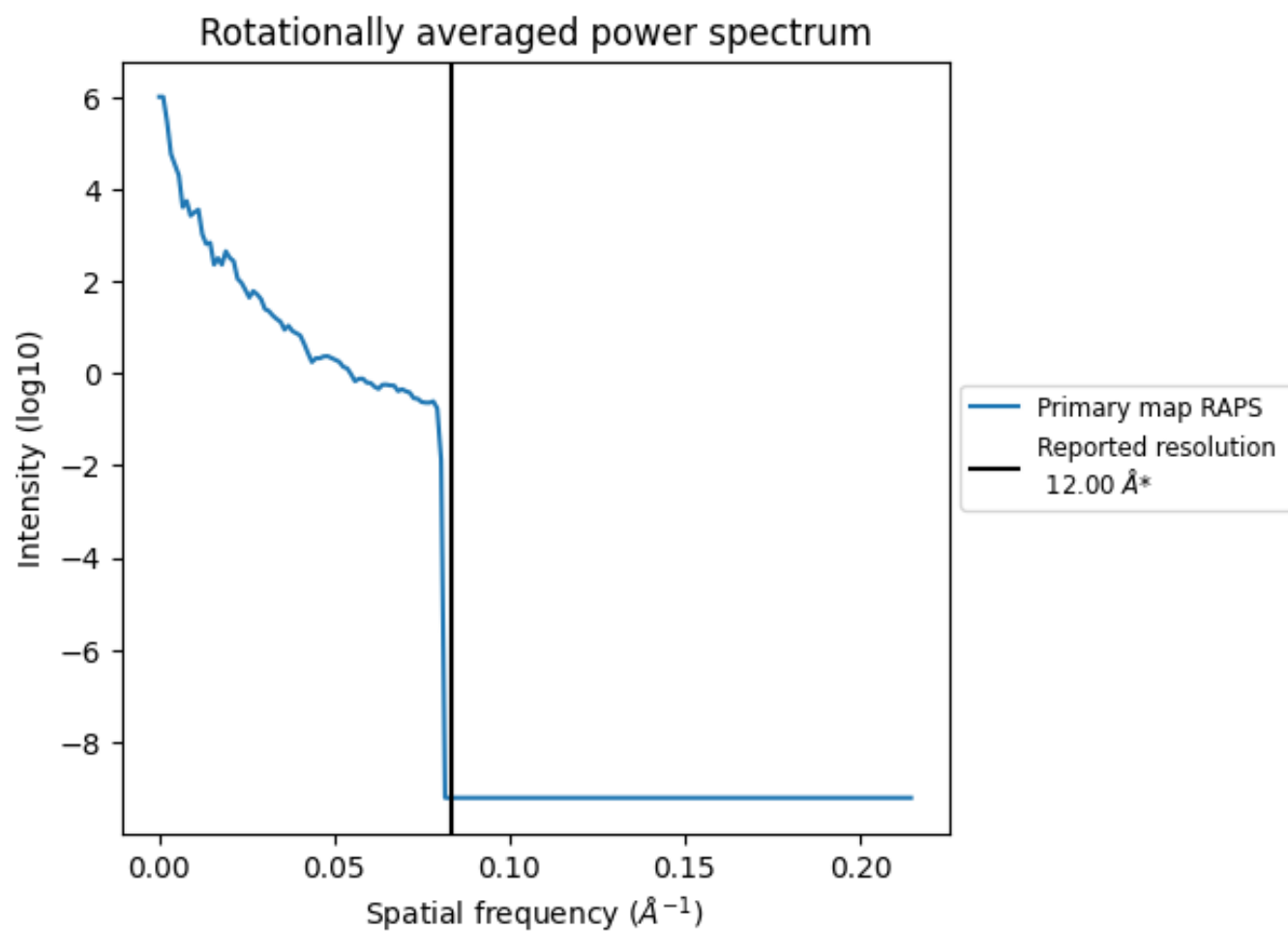
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64244 nm^3 ; this corresponds to an approximate mass of 58034 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 0.083 Å⁻¹

8 Fourier-Shell correlation

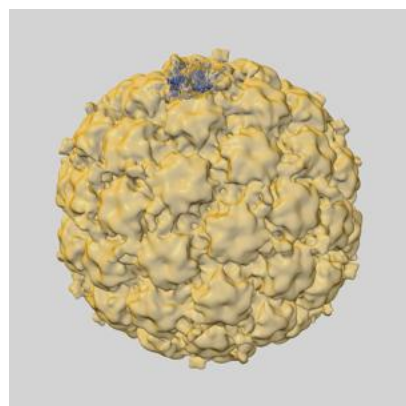
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

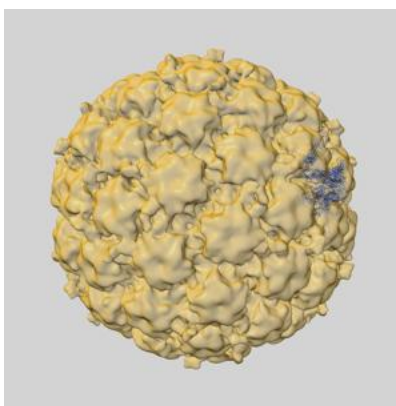
This section contains information regarding the fit between EMDB map EMD-6424 and PDB model 3JBA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

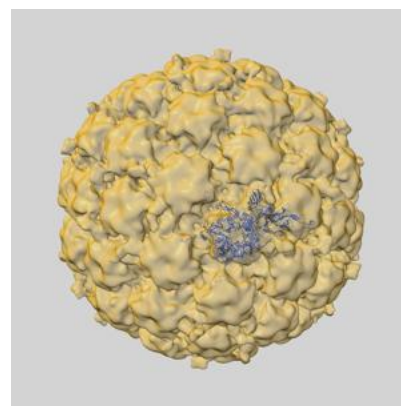
9.1.1 Map-model overlay [i](#)



X

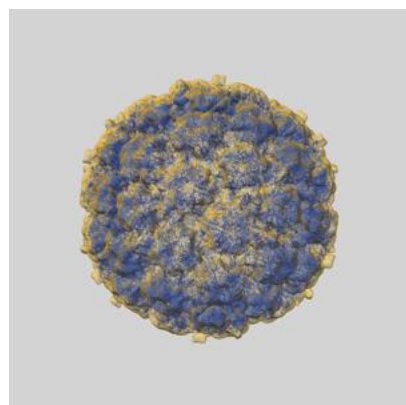


Y

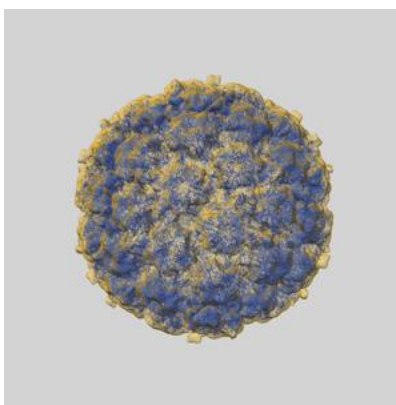


Z

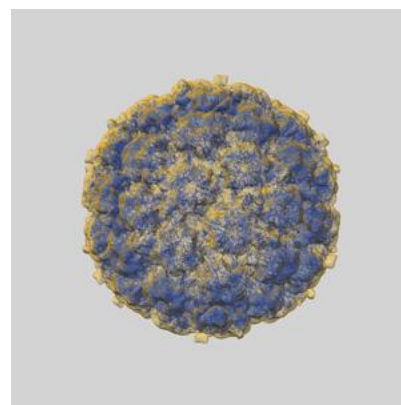
9.1.2 Map-model assembly overlay [i](#)



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](#)

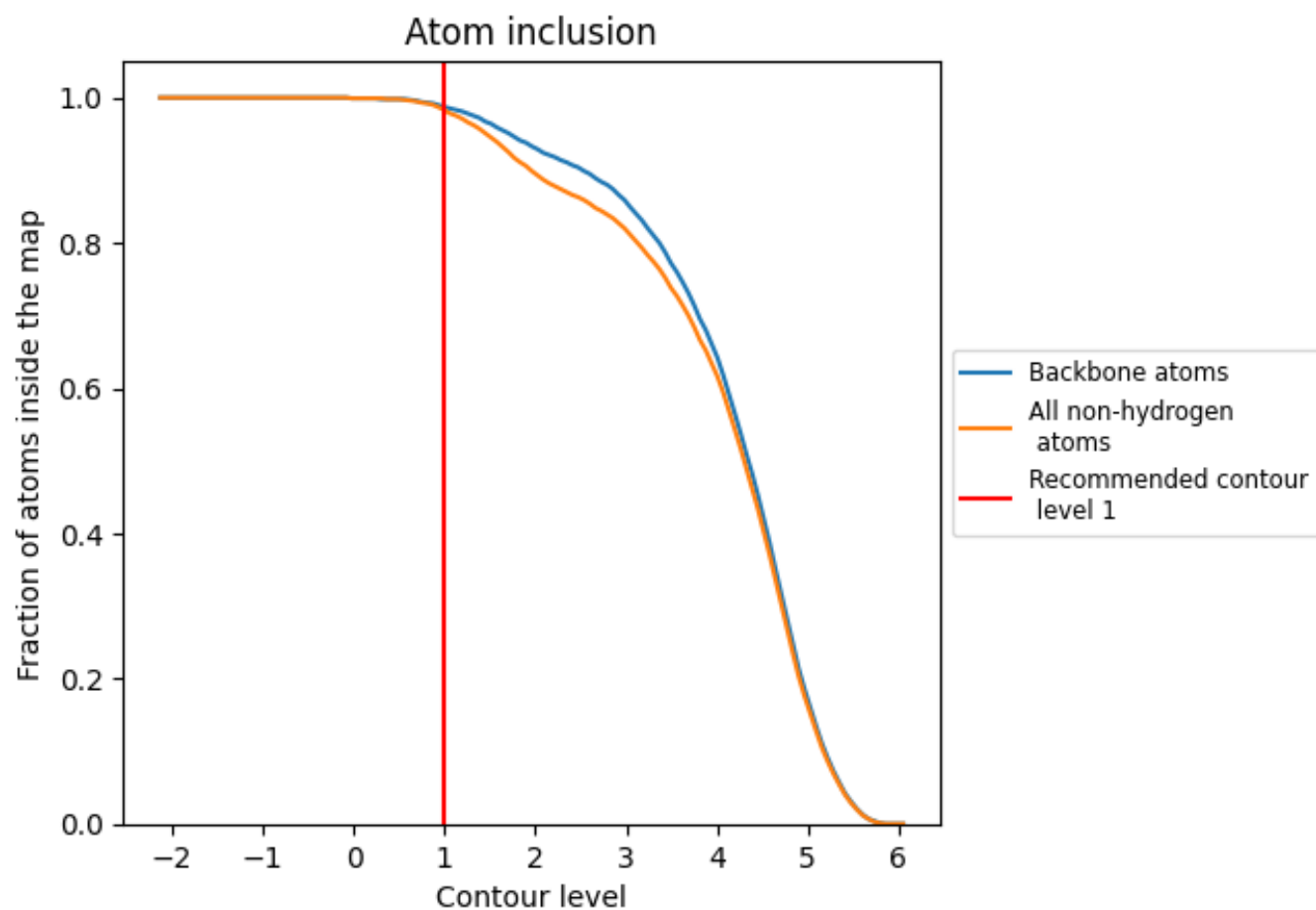


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.0760
A	1.0000	0.0880
B	1.0000	0.0830
C	0.9990	0.0880
D	0.9920	0.0830
E	0.9890	0.0860
F	1.0000	0.0810
H	0.9220	0.0260
L	0.8220	0.0090

1.0

0.0

<0.0