



## wwPDB EM Validation Summary Report ⓘ

Oct 23, 2024 – 12:36 AM EDT

PDB ID : 3J8W  
EMDB ID : EMD-6184  
Title : Cryo-EM reconstruction of quasi-HPV16 complex with H263.A2 Fab  
Authors : Guan, J.; Hafenstein, S.  
Deposited on : 2014-11-19  
Resolution : 13.00 Å (reported)  
Based on initial model : 3OAE

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

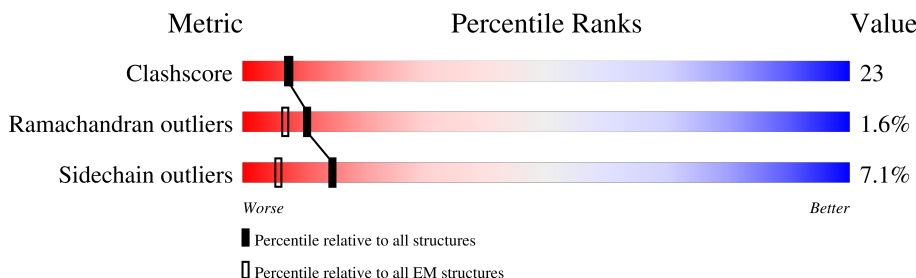
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	J	109	
1	K	109	
1	L	109	
1	M	109	
2	F	118	
2	G	118	
2	H	118	
2	I	118	

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Mol	Chain	Length	Quality of chain
3	A	455	
3	B	455	
3	C	455	
3	D	455	
3	E	455	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 30478 atoms, of which 6800 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 H263.A2 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	109	Total	C	H	N	O	S	0	0
			1656	530	815	141	167	3		
1	J	109	Total	C	H	N	O	S	0	0
			1656	530	815	141	167	3		
1	K	109	Total	C	H	N	O	S	0	0
			1656	530	815	141	167	3		
1	M	109	Total	C	H	N	O	S	0	0
			1656	530	815	141	167	3		

- Molecule 2 is a protein called H263.A2 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	118	Total	C	H	N	O	S	0	0
			1811	594	885	150	178	4		
2	F	118	Total	C	H	N	O	S	0	0
			1811	594	885	150	178	4		
2	G	118	Total	C	H	N	O	S	0	0
			1811	594	885	150	178	4		
2	I	118	Total	C	H	N	O	S	0	0
			1811	594	885	150	178	4		

- Molecule 3 is a protein called L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
3	B	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
3	C	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
3	D	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
3	E	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q4VRM0
A	177	GLN	ASN	conflict	UNP Q4VRM0
A	181	GLN	ASN	conflict	UNP Q4VRM0
A	472	LEU	ALA	conflict	UNP Q4VRM0
B	20	ALA	-	expression tag	UNP Q4VRM0
B	177	GLN	ASN	conflict	UNP Q4VRM0
B	181	GLN	ASN	conflict	UNP Q4VRM0
B	472	LEU	ALA	conflict	UNP Q4VRM0
C	20	ALA	-	expression tag	UNP Q4VRM0
C	177	GLN	ASN	conflict	UNP Q4VRM0
C	181	GLN	ASN	conflict	UNP Q4VRM0
C	472	LEU	ALA	conflict	UNP Q4VRM0
D	20	ALA	-	expression tag	UNP Q4VRM0
D	177	GLN	ASN	conflict	UNP Q4VRM0
D	181	GLN	ASN	conflict	UNP Q4VRM0
D	472	LEU	ALA	conflict	UNP Q4VRM0
E	20	ALA	-	expression tag	UNP Q4VRM0
E	177	GLN	ASN	conflict	UNP Q4VRM0
E	181	GLN	ASN	conflict	UNP Q4VRM0
E	472	LEU	ALA	conflict	UNP Q4VRM0

### 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.

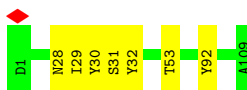
- Molecule 1: H263.A2 light chain

Chain L:  94% 5%



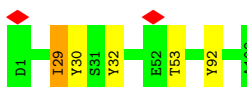
- Molecule 1: H263.A2 light chain

Chain J:  94% 6%



- Molecule 1: H263.A2 light chain

Chain K:  95%




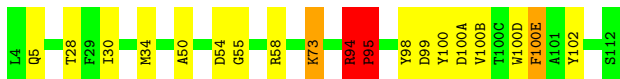
- Molecule 1: H263.A2 light chain

Chain M:  93% 6%



- Molecule 2: H263.A2 heavy chain

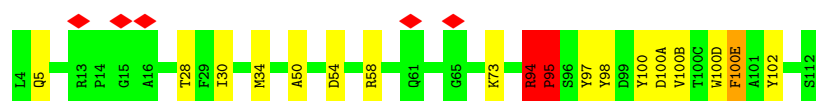
Chain H:  84% 13%



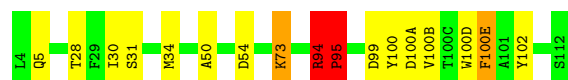
- Molecule 2: H263.A2 heavy chain

L4	Q5	T28	M34	A50	D54	R58	K73	R94	P95	S96	Y97	Y98	D99	Y100	D100A	V100B	T100C	W100D	F100E	A101	Y102	S112
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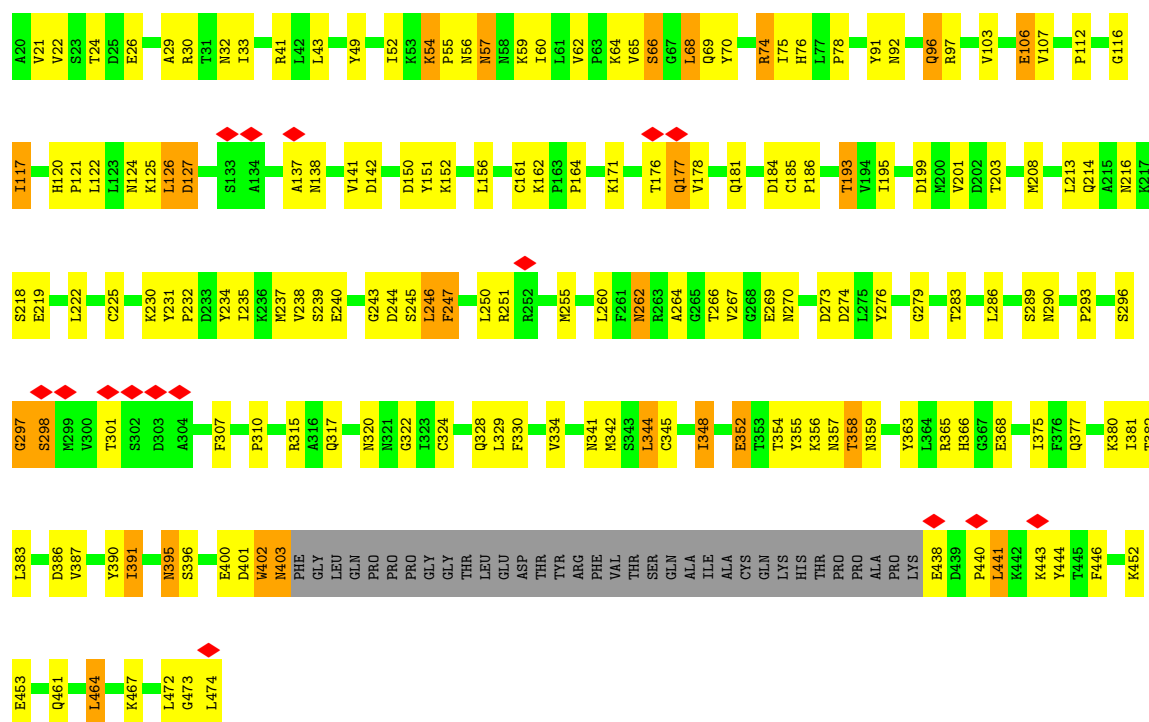
- Chain G:  85% 13% ..



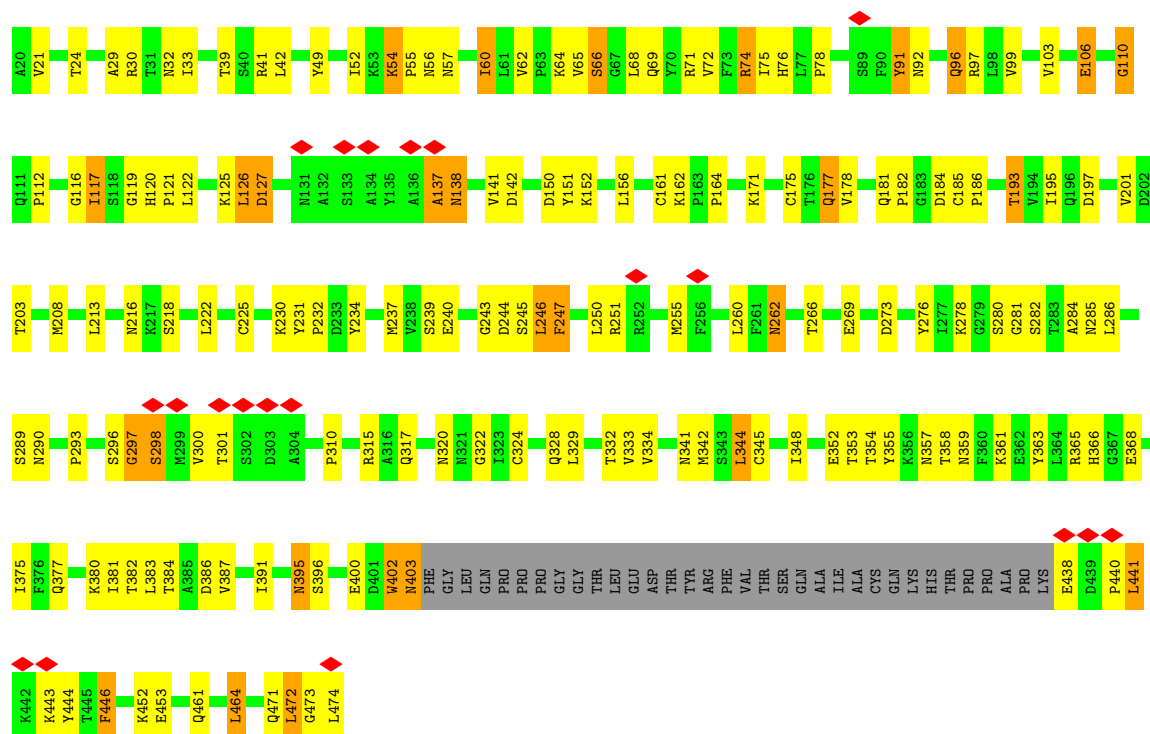
- Chain I:  86% 11% ..



- Chain A:  55% 32% 6% 7%

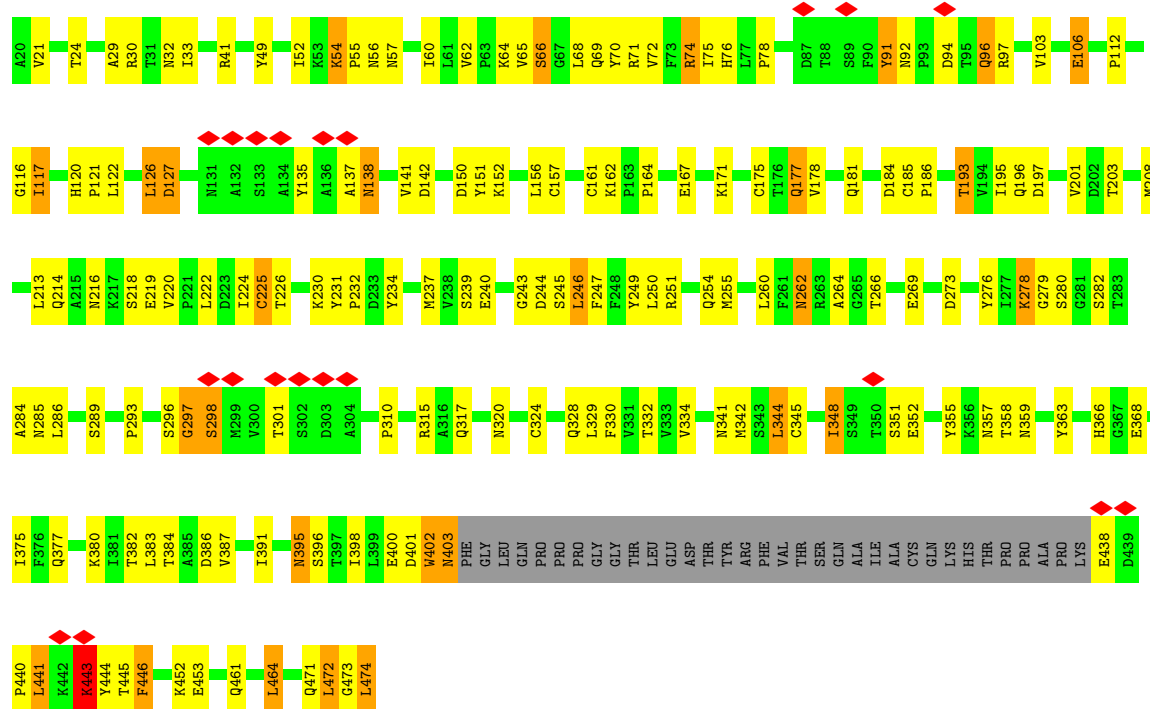


- Chain B:  55% 31% 6% 7%



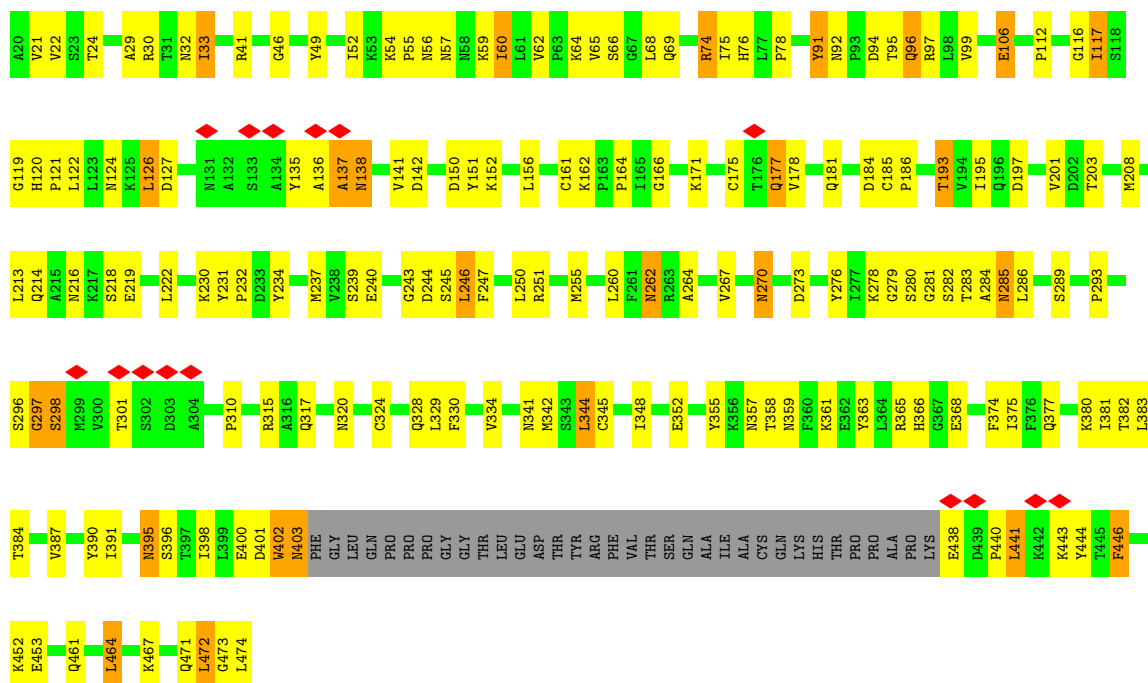
### • Molecule 3: L1

Chain C: 55% 32% 6% 7%

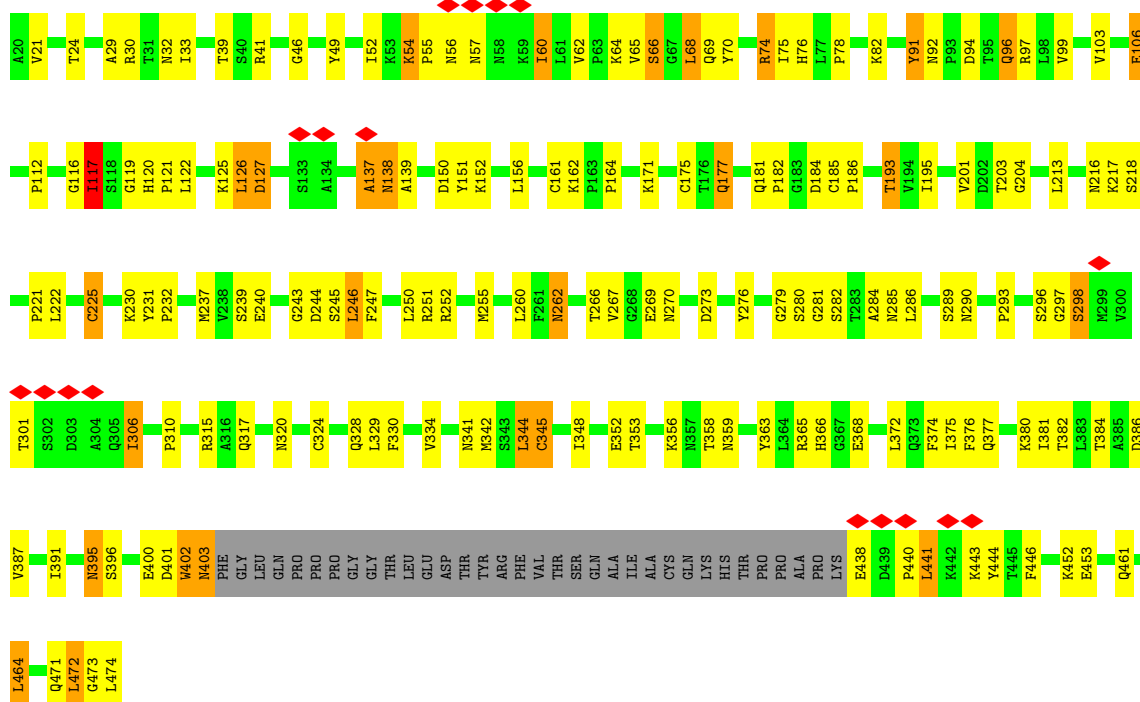


### • Molecule 3: L1

Chain D: 55% 32% 6% 7%



• Molecule 3: L1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8908	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)	1490	Depositor
Maximum defocus (nm)	5520	Depositor
Magnification	40000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	8.339	Depositor
Minimum map value	-9.356	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ( $\text{\AA}$ )	1152.58, 1152.58, 1152.58	wwPDB
Map dimensions	403, 403, 403	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.86, 2.86, 2.86	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	J	0.90	2/860 (0.2%)	0.79	0/1166
1	K	0.90	2/860 (0.2%)	0.79	0/1166
1	L	0.90	2/860 (0.2%)	0.79	0/1166
1	M	0.90	2/860 (0.2%)	0.79	0/1166
2	F	0.73	2/952 (0.2%)	0.98	8/1290 (0.6%)
2	G	0.73	2/952 (0.2%)	0.98	8/1290 (0.6%)
2	H	0.73	2/952 (0.2%)	0.98	8/1290 (0.6%)
2	I	0.73	2/952 (0.2%)	0.98	8/1290 (0.6%)
3	A	0.59	6/3407 (0.2%)	0.72	3/4632 (0.1%)
3	B	0.49	0/3407	0.70	2/4632 (0.0%)
3	C	0.53	2/3407 (0.1%)	0.71	1/4632 (0.0%)
3	D	0.55	3/3407 (0.1%)	0.71	3/4632 (0.1%)
3	E	0.53	1/3407 (0.0%)	0.72	0/4632
All	All	0.63	28/24283 (0.1%)	0.77	41/32984 (0.1%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	29	ILE	C-N	14.56	1.67	1.34
1	M	29	ILE	C-N	14.56	1.67	1.34
1	L	29	ILE	C-N	14.54	1.67	1.34
1	J	29	ILE	C-N	14.51	1.67	1.34
2	F	95	PRO	N-CD	12.41	1.65	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	95	PRO	CA-N-CD	-13.79	92.20	111.50
2	F	95	PRO	CA-N-CD	-13.79	92.20	111.50
2	H	95	PRO	CA-N-CD	-13.78	92.20	111.50
2	G	95	PRO	CA-N-CD	-13.77	92.22	111.50
2	G	5	GLN	O-C-N	6.91	133.75	122.70

There are no chirality outliers.

There are no planarity outliers.

## 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	J	841	815	814	41	0
1	K	841	815	813	29	0
1	L	841	815	814	42	0
1	M	841	815	814	32	0
2	F	926	885	881	83	0
2	G	926	885	880	77	0
2	H	926	885	879	88	0
2	I	926	885	879	60	0
3	A	3322	0	3227	160	0
3	B	3322	0	3226	221	0
3	C	3322	0	3224	224	0
3	D	3322	0	3227	251	0
3	E	3322	0	3227	212	0
All	All	23678	6800	22905	1055	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 23.

The worst 5 of 1055 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:98:TYR:CE2	3:D:358:THR:HG21	1.29	1.66
1:J:32:TYR:CE2	3:D:284:ALA:HB3	1.23	1.64
1:L:30:TYR:CB	3:E:281:GLY:HA3	1.25	1.64
2:F:100:TYR:HA	3:D:285:ASN:CB	1.21	1.63
2:F:100:TYR:CB	3:D:285:ASN:HB2	1.19	1.63

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	J	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
1	K	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
1	L	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
1	M	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	F	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	G	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	H	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	I	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
3	A	417/455 (92%)	378 (91%)	29 (7%)	10 (2%)	5	27
3	B	417/455 (92%)	378 (91%)	29 (7%)	10 (2%)	5	27
3	C	417/455 (92%)	376 (90%)	32 (8%)	9 (2%)	5	29
3	D	417/455 (92%)	377 (90%)	30 (7%)	10 (2%)	5	27
3	E	417/455 (92%)	377 (90%)	32 (8%)	8 (2%)	6	32
All	All	2969/3183 (93%)	2738 (92%)	184 (6%)	47 (2%)	10	38

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	137	ALA
3	A	298	SER
3	A	402	TRP
3	B	137	ALA
3	B	298	SER

### 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	J	92/92 (100%)	92 (100%)	0	100	100
1	K	92/92 (100%)	92 (100%)	0	100	100
1	L	92/92 (100%)	92 (100%)	0	100	100
1	M	92/92 (100%)	92 (100%)	0	100	100
2	F	95/95 (100%)	93 (98%)	2 (2%)	48	66
2	G	95/95 (100%)	93 (98%)	2 (2%)	48	66
2	H	95/95 (100%)	93 (98%)	2 (2%)	48	66
2	I	95/95 (100%)	93 (98%)	2 (2%)	48	66
3	A	368/396 (93%)	334 (91%)	34 (9%)	7	23
3	B	368/396 (93%)	335 (91%)	33 (9%)	8	24
3	C	368/396 (93%)	329 (89%)	39 (11%)	5	19
3	D	368/396 (93%)	335 (91%)	33 (9%)	8	24
3	E	368/396 (93%)	330 (90%)	38 (10%)	6	20
All	All	2588/2728 (95%)	2403 (93%)	185 (7%)	15	32

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	33	ILE
3	D	453	GLU
3	D	95	THR
3	D	270	ASN
3	E	60	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	153	GLN
3	E	262	ASN
3	C	395	ASN
3	E	153	GLN
3	E	377	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 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
2	F	1
2	G	1
2	I	1
1	L	1
1	J	1
1	K	1
1	M	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	94:ARG	C	95:PRO	N	2.22
1	F	94:ARG	C	95:PRO	N	2.22
1	G	94:ARG	C	95:PRO	N	2.22
1	I	94:ARG	C	95:PRO	N	2.22

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	29:ILE	C	30:TYR	N	1.67

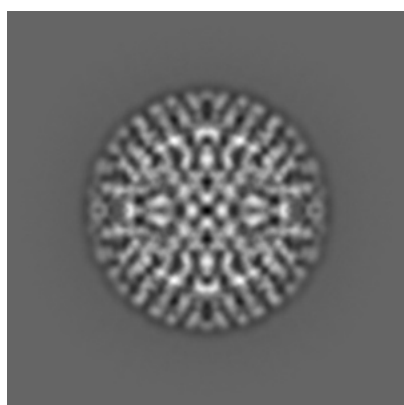
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6184. These allow visual inspection of the internal detail of the map and identification of artifacts.

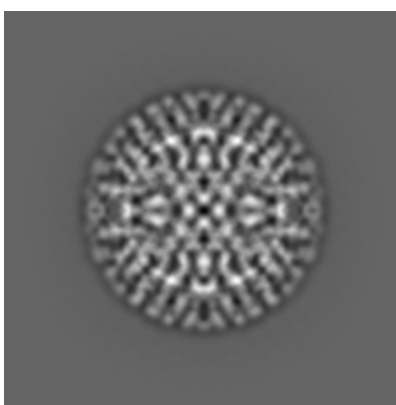
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

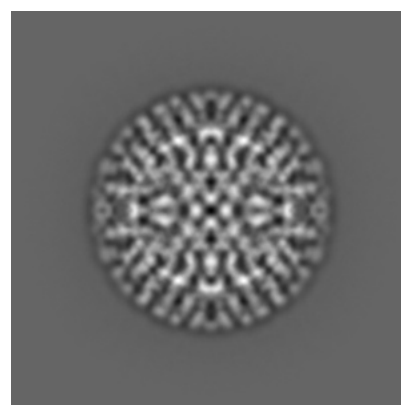
#### 6.1.1 Primary map



X



Y



Z

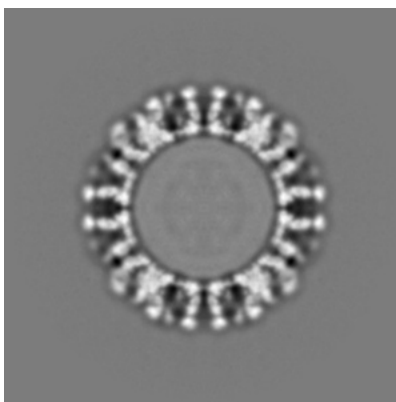
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

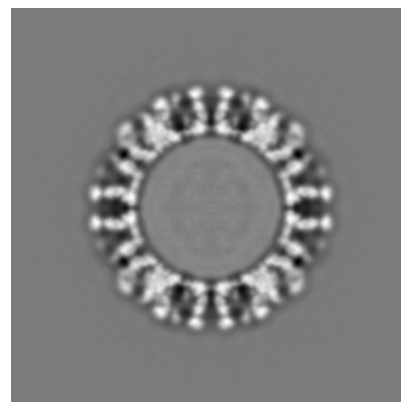
#### 6.2.1 Primary map



X Index: 201



Y Index: 201



Z Index: 201

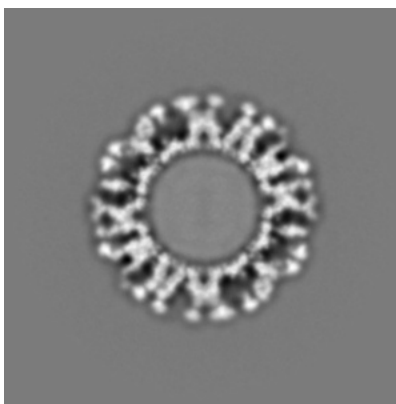
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

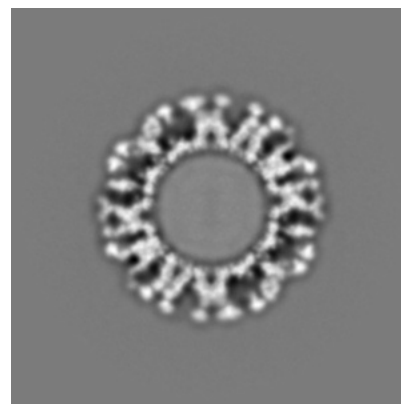
### 6.3.1 Primary map



X Index: 156



Y Index: 156

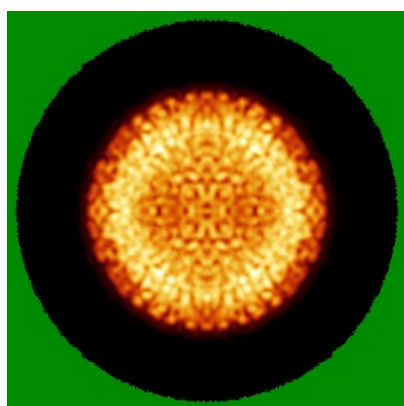


Z Index: 156

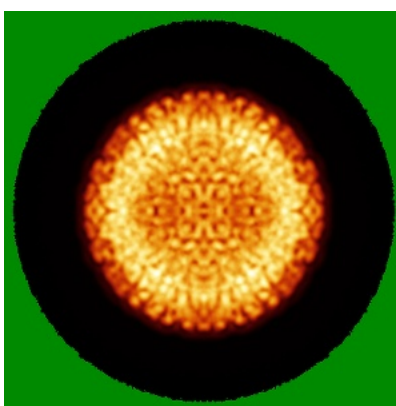
The images above show the largest variance slices of the map in three orthogonal directions.

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

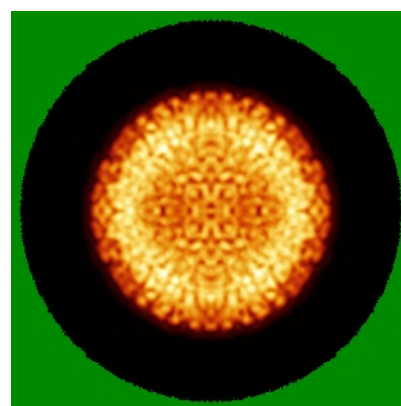
### 6.4.1 Primary map



X



Y

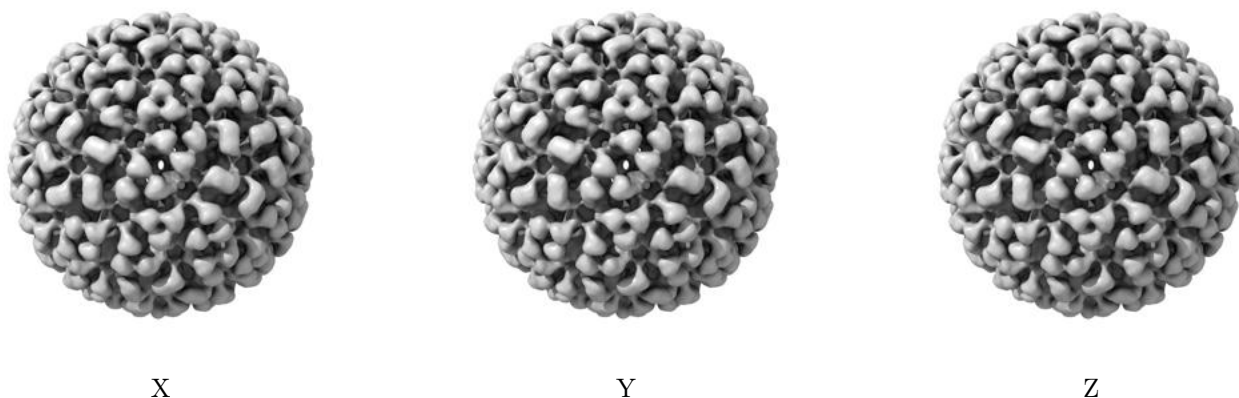


Z

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.

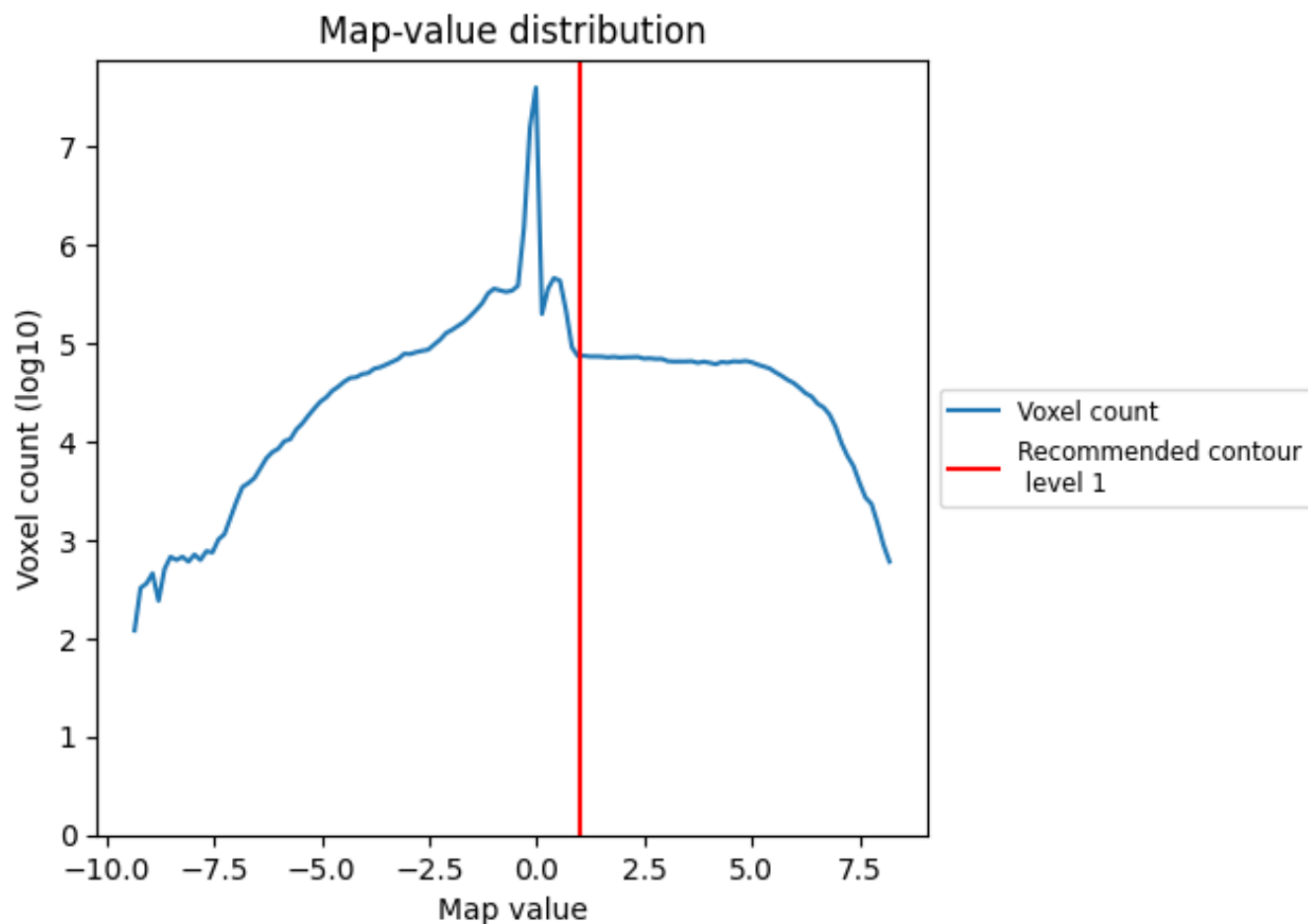
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

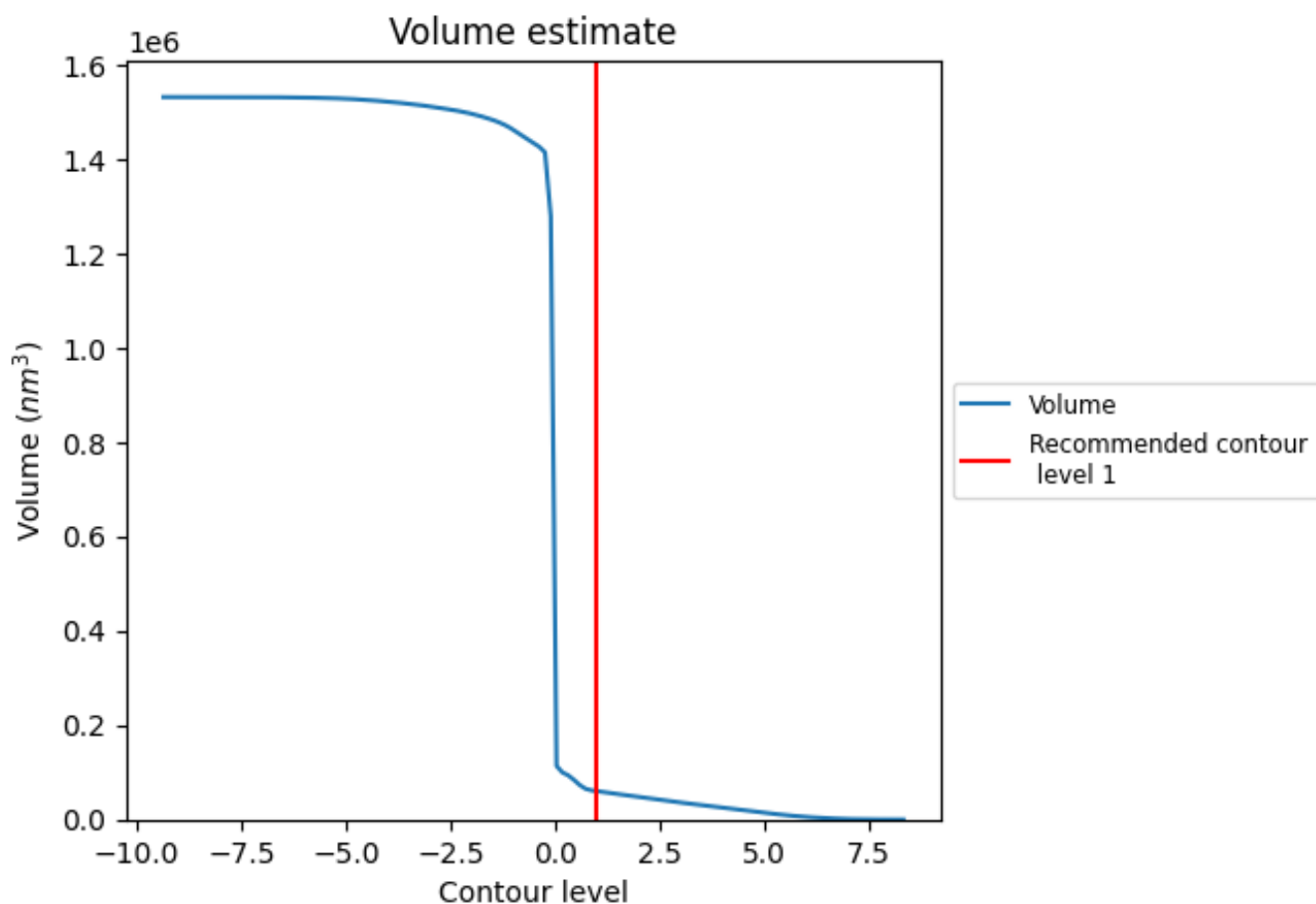
This section contains the results of statistical analysis of the map.

### 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.

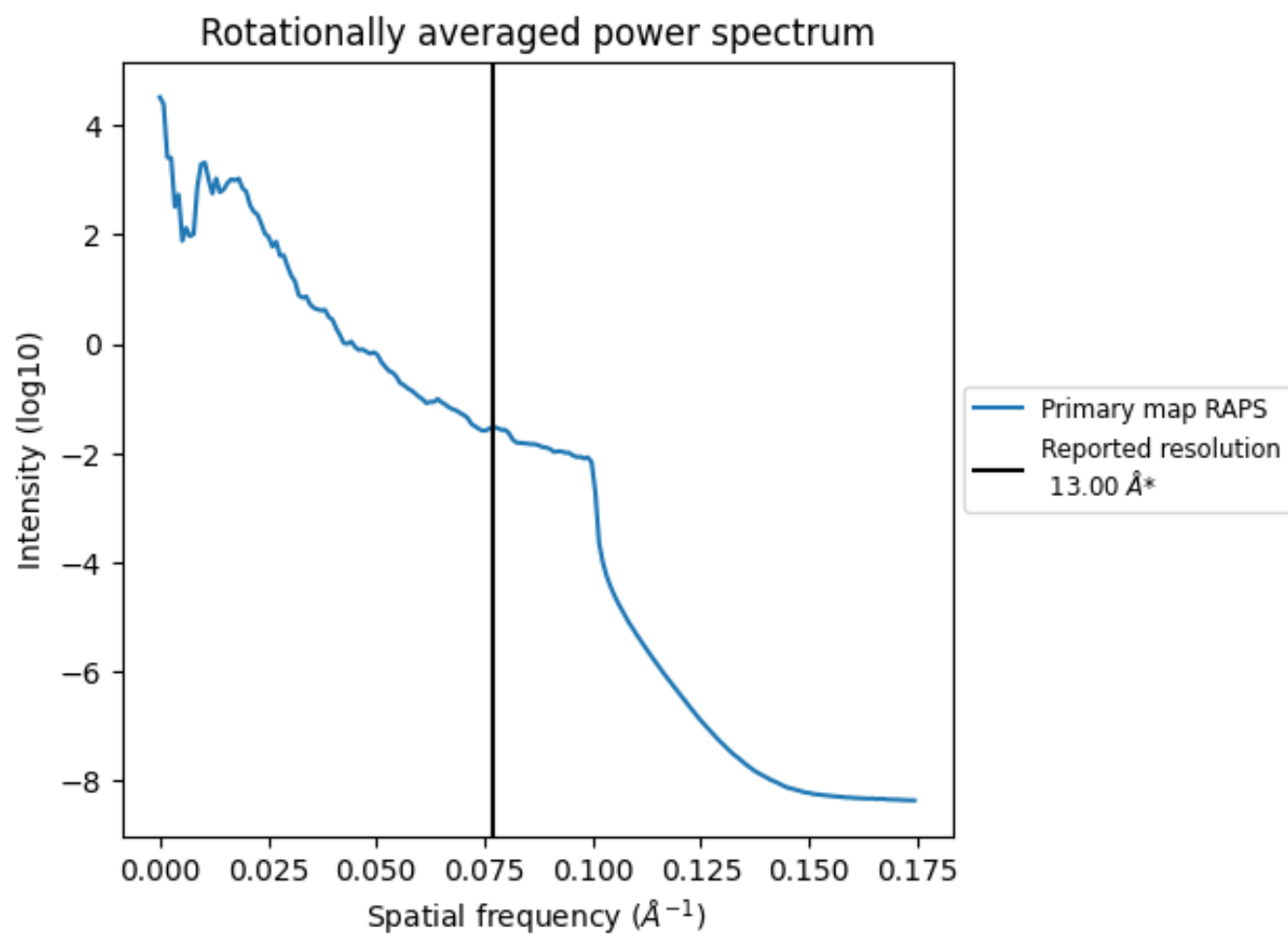
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60179 nm<sup>3</sup>; this corresponds to an approximate mass of 54361 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 0.077 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

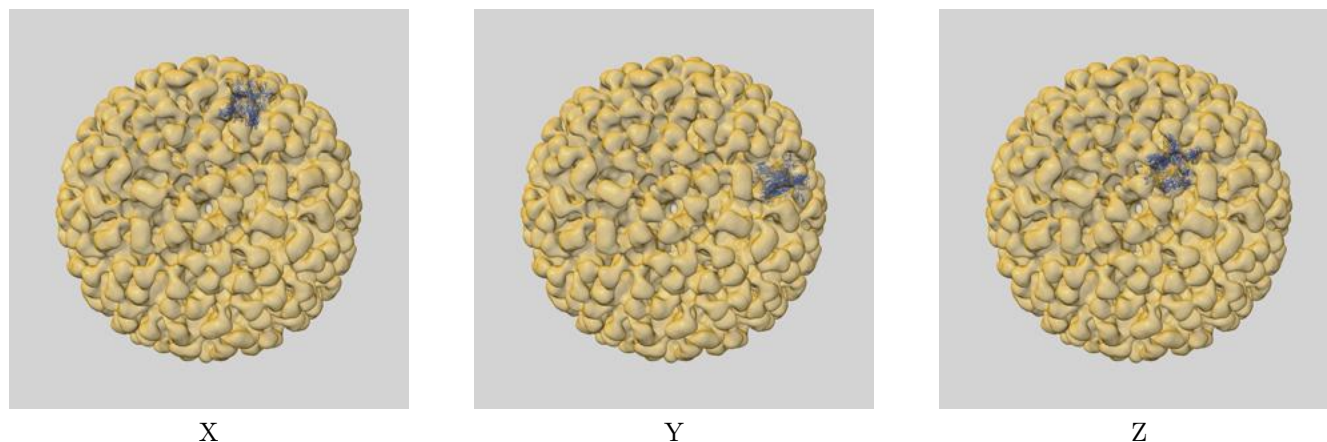
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

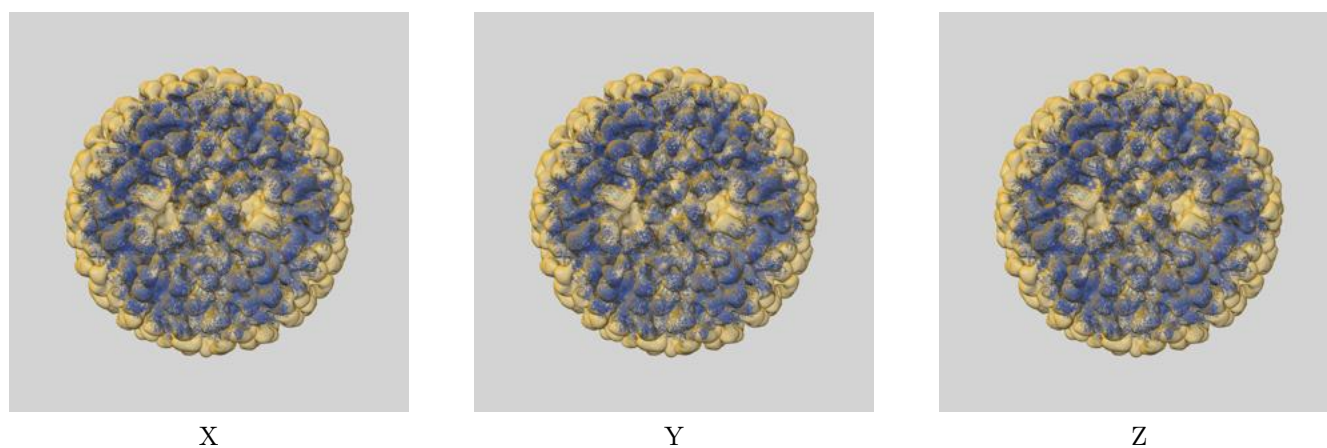
This section contains information regarding the fit between EMDB map EMD-6184 and PDB model 3J8W. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

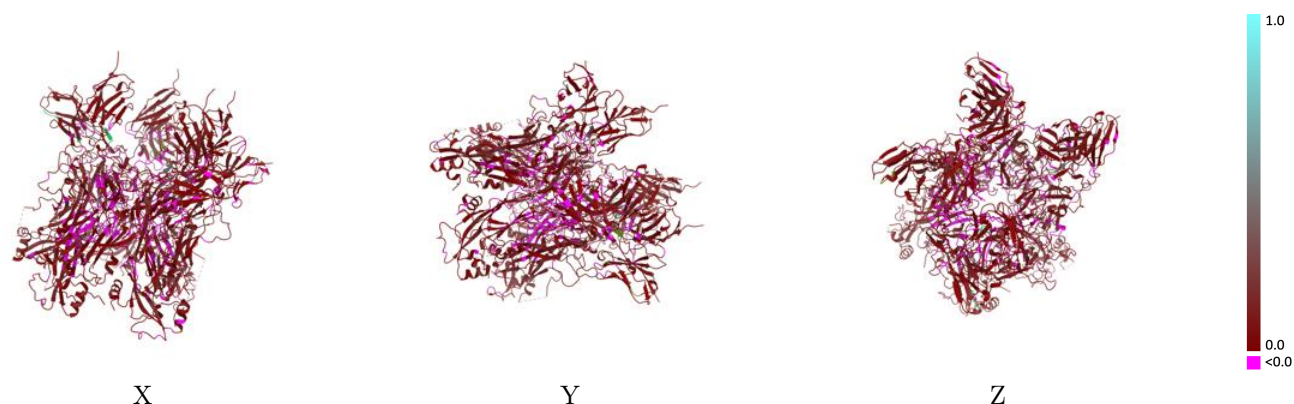


#### 9.1.2 Map-model assembly overlay [i](#)



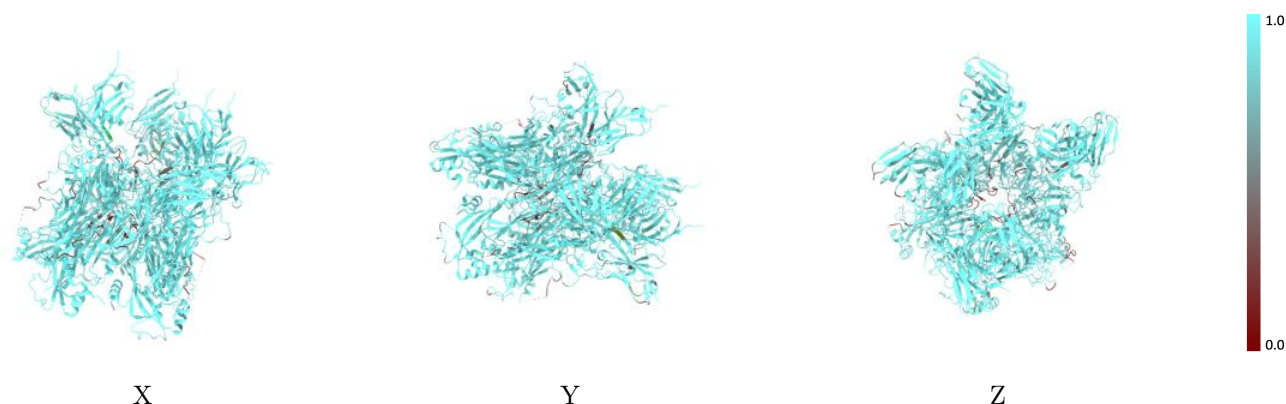
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



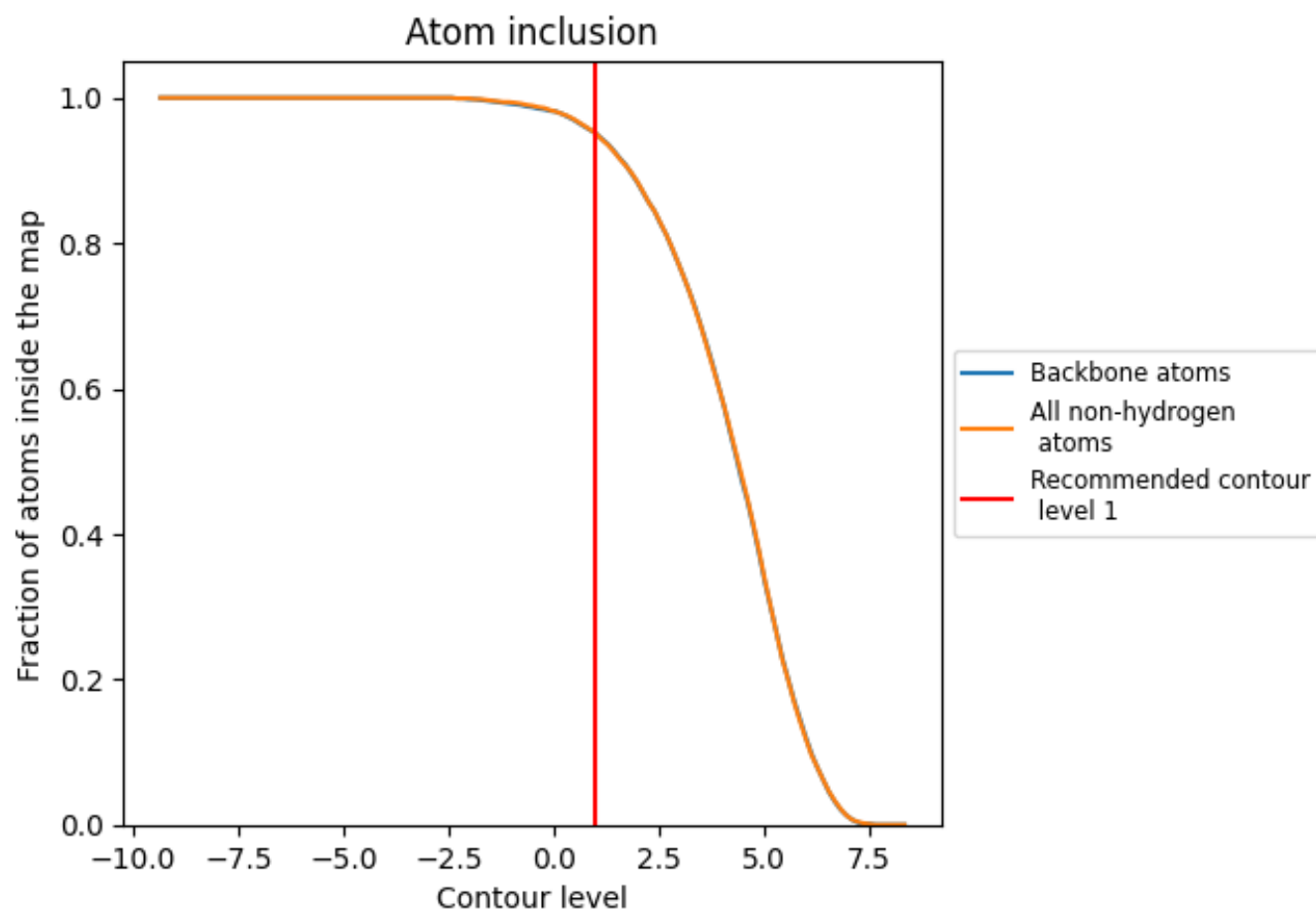
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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	 0.9510	 0.0670
A	 0.9500	 0.0650
B	 0.9420	 0.0610
C	 0.9420	 0.0650
D	 0.9540	 0.0670
E	 0.9460	 0.0690
F	 0.9800	 0.0740
G	 0.9310	 0.0800
H	 0.9670	 0.0650
I	 0.9780	 0.0770
J	 0.9780	 0.0670
K	 0.9590	 0.0640
L	 0.9770	 0.0770
M	 0.9840	 0.0650

