



## wwPDB EM Validation Summary Report ⓘ

May 20, 2025 – 03:19 AM EDT

PDB ID : 9EAN / pdb\_00009ean  
EMDB ID : EMD-47837  
Title : Murine norovirus allosteric escape mutant D348E  
Authors : Smith, T.J.; Sherman, M.  
Deposited on : 2024-11-11  
Resolution : 2.40 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](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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

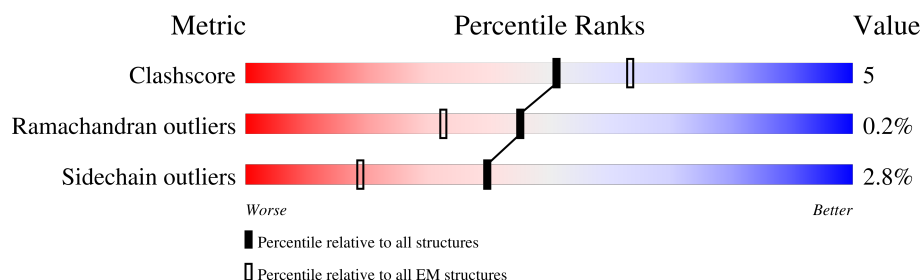
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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	A	540	<div> <div>84%</div> <div> <div></div> <div>10%</div> <div>5%</div> </div> </div>
1	B	540	<div> <div>85%</div> <div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>
1	C	540	<div> <div>83%</div> <div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11798 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total	C	N	O	S	0	0
			3953	2547	651	739	16		
1	B	516	Total	C	N	O	S	0	0
			3963	2553	652	742	16		
1	C	504	Total	C	N	O	S	0	0
			3882	2503	639	724	16		

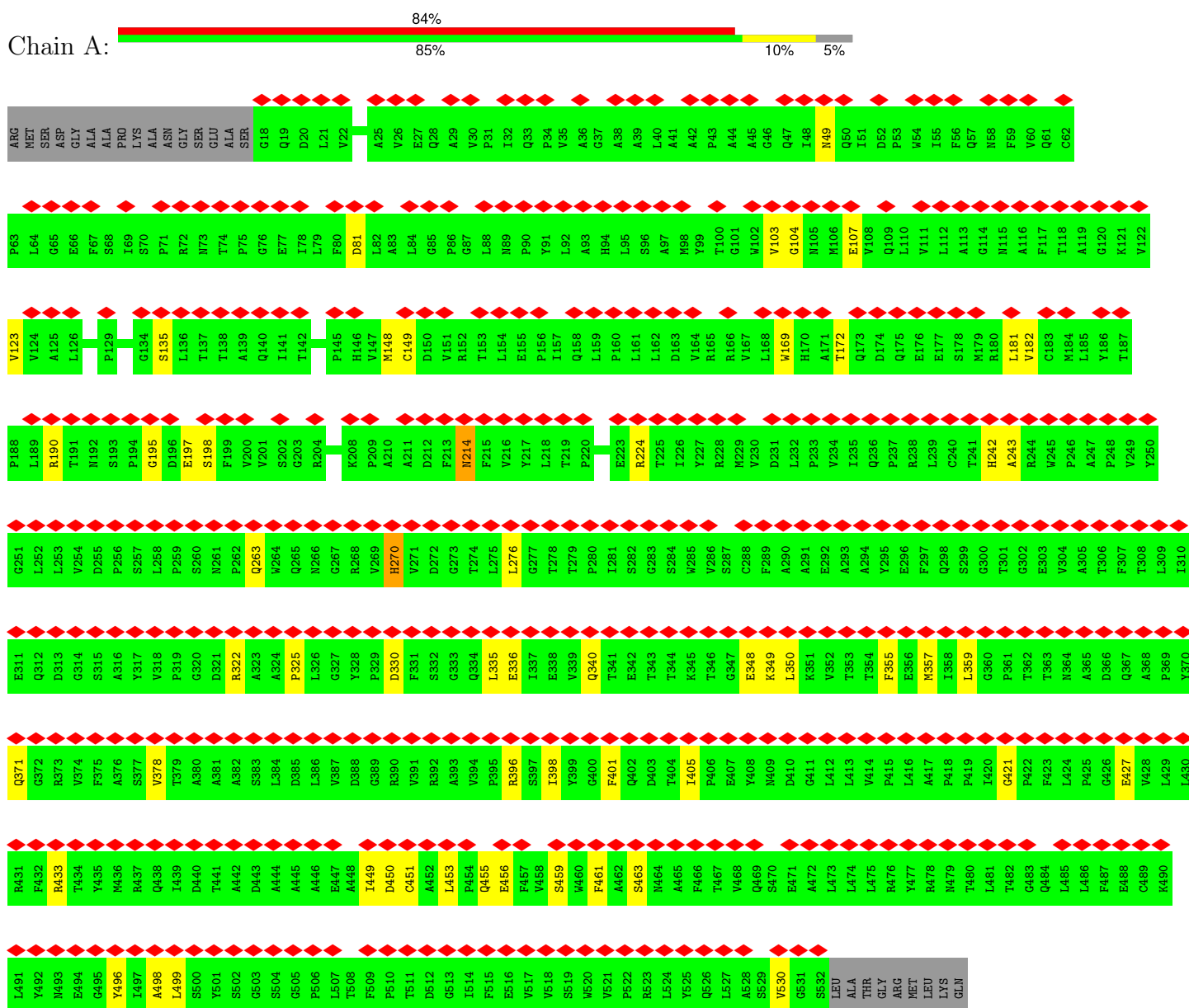
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLU	LYS	variant	UNP Q80J94
A	348	GLU	ASP	variant	UNP Q80J94
B	296	GLU	LYS	variant	UNP Q80J94
B	348	GLU	ASP	variant	UNP Q80J94
C	296	GLU	LYS	variant	UNP Q80J94
C	348	GLU	ASP	variant	UNP Q80J94


### 3 Residue-property plots

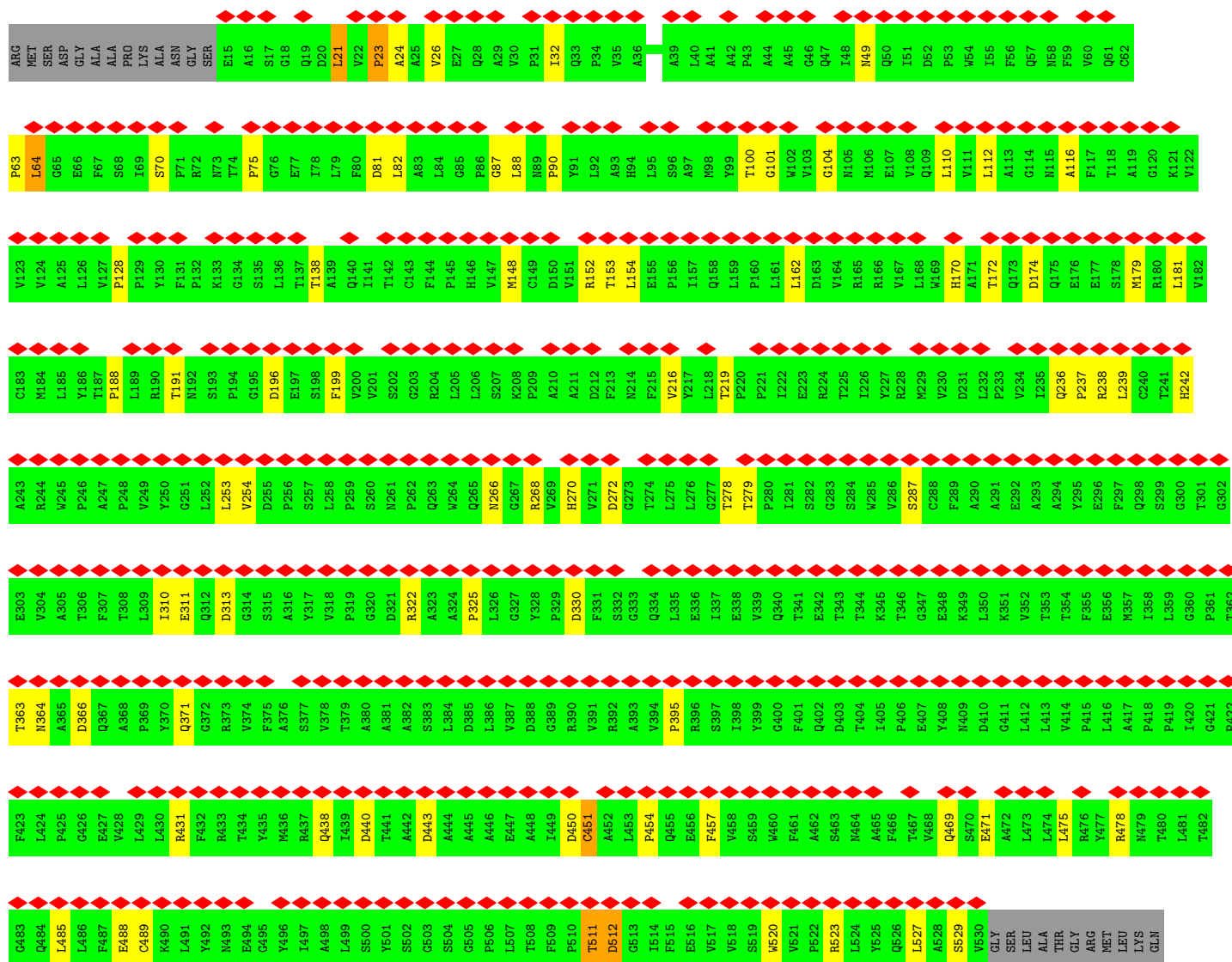
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Capsid protein VP1




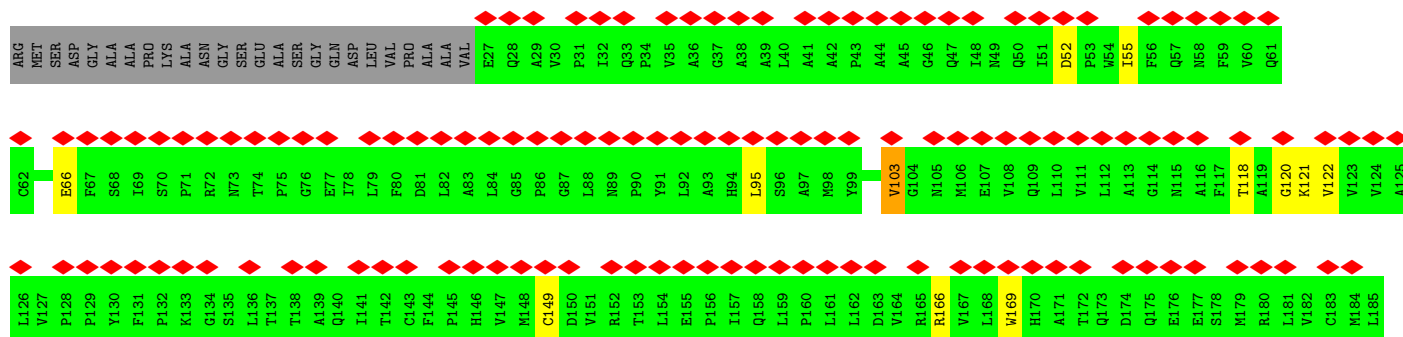
#### • Molecule 1: Capsid protein VP1

Chain B: 



• Molecule 1: Capsid protein VP1

Chain C: 



C489	C490	L491	Y492	M493	E494	G495	Y496	I497	A498	L499	S500	Y501	S502	G503	S504	G505	P506	L507	T508	F509	P510	T511	D512	G513	I514	F515	E516	V517	V518	S519	W520	V521	P522	R523	L524	Y525	Q526	L527	A528	S529	V530	GLY	SER	LEU	ALA	THR	GLY	ARG	MET	LEU	LYS	GLN							
V428	L429	L430	R431	F432	R433	T434	Y435	M436	R437	Q438	I439	D440	T441	A442	D443	A444	A445	A446	E447	A448	I449	D450	C451	A452	L453	P454	Q455	E456	F457	W460	F461	A462	S463	M464	A465	F466	T467	V468	Q469	S470	E471	A472	L473	L474	L475	R476	Y477	R478	N479	T480	L481	T482	G483	Q484	L485	L486	F487	E488	
A368	P369	Y370	Q371	G372	R373	V374	F375	A376	S377	V378	T379	A380	A381	A382	S383	L384	D385	L386	V387	D388	G389	R390	V391	R392	A393	V394	P395	R396	S397	I398	V399	G400	F401	Q402	D403	T404	I405	F406	E407	Y408	N409	D410	G411	L412	L413	V414	P415	L416	A417	F418	P419	I420	G421	F422	F423	L424	P425	G426	E427
T308	L309	I310	E311	Q312	D313	G314	S315	A316	Y317	V318	P319	G320	D321	R322	A323	A324	P325	L326	G327	Y328	P329	D330	F331	S332	G333	Q334	L335	E336	I337	E338	V339	Q340	T341	E342	T343	T344	K345	T346	G347	E348	K349	L350	K351	V352	T353	T354	F355	E356	K357	I358	L359	G360	P361	T362	T363	N364	A365	D366	Q367
Y186	T187	P188	L189	R190	T191	N192	S193	P194	G195	D196	E197	S198	F199	V200	V201	S202	G203	R204	L205	L206	S207	A210	A211	D212	F213	N214	F215	V216	Y217	L218	T219	P220	P221	I222	E223	R224	T225	I226	Y227	R228	W229	V230	D231	L232	P233	V234	I235	Q236	P237	R238	L239	C240	T241	H242	A243	R244	W245	P246	
	V249	Y250	G251	L252	L253	V254	D255	P256	S257	L258	P259	S260	N261	P262	Q263	W264	Q265	N266	G267	R268	V269	H270	V271	D272	G273	T274	L275	L276	G277	T278	T279	P280	I281	S282	G283	S284	W285	V286	S287	C288	F289	A290	A291	E292	A293	A294	Y295	E296	F297	Q298	S299	G300	T301	G302	E303	V304	A305	T306	F307

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.844	Depositor
Minimum map value	-2.220	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.154	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.24	0/4062	0.47	1/5570 (0.0%)
1	B	0.26	0/4072	0.51	1/5584 (0.0%)
1	C	0.25	0/3990	0.48	0/5470
All	All	0.25	0/12124	0.49	2/16624 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	N-CA-C	6.09	118.63	111.63
1	B	104	GLY	N-CA-C	5.52	117.98	111.63

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	A	3953	0	3899	30	0
1	B	3963	0	3907	48	0
1	C	3882	0	3826	50	0
All	All	11798	0	11632	125	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 5.

The worst 5 of 125 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:B:49:ASN:ND2	1:B:216:VAL:O	2.09	0.85
1:C:225:THR:HG22	1:C:227:TYR:H	1.42	0.84
1:B:191:THR:HG21	1:B:199:PHE:H	1.50	0.74
1:C:268:ARG:H	1:C:279:THR:HG21	1.50	0.73
1:A:499:LEU:HD23	1:A:530:VAL:HG11	1.68	0.73

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	513/540 (95%)	488 (95%)	24 (5%)	1 (0%)	44	59
1	B	514/540 (95%)	484 (94%)	29 (6%)	1 (0%)	44	59
1	C	502/540 (93%)	470 (94%)	31 (6%)	1 (0%)	44	59
All	All	1529/1620 (94%)	1442 (94%)	84 (6%)	3 (0%)	45	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	PRO
1	C	348	GLU
1	A	348	GLU

### 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	426/443 (96%)	416 (98%)	10 (2%)	45	66
1	B	427/443 (96%)	415 (97%)	12 (3%)	38	59
1	C	418/443 (94%)	405 (97%)	13 (3%)	35	56
All	All	1271/1329 (96%)	1236 (97%)	35 (3%)	40	59

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	THR
1	C	344	THR
1	C	388	ASP
1	B	70	SER
1	B	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	89	ASN
1	C	469	GLN
1	A	340	GLN
1	B	236	GLN
1	B	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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.

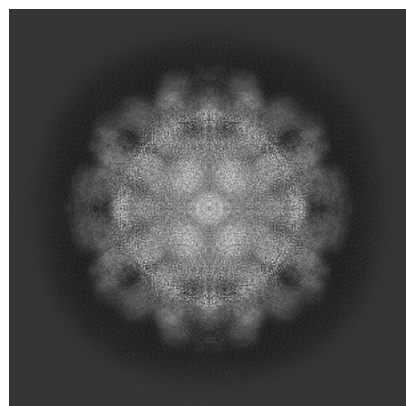
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47837. These allow visual inspection of the internal detail of the map and identification of artifacts.

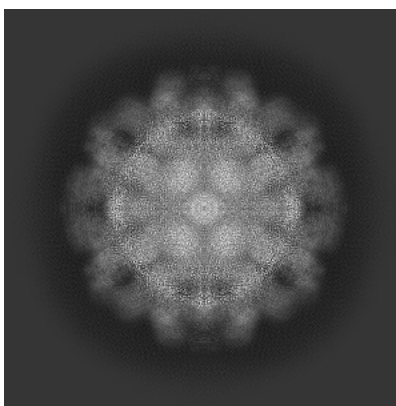
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

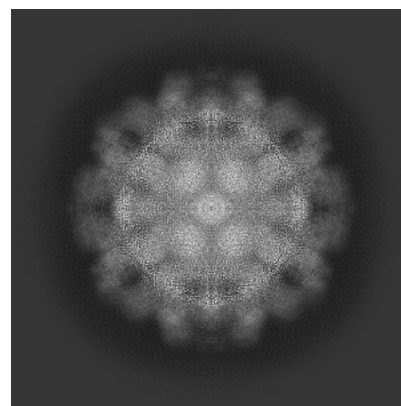
#### 6.1.1 Primary map



X

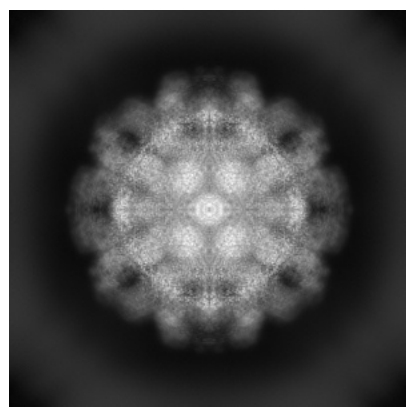


Y

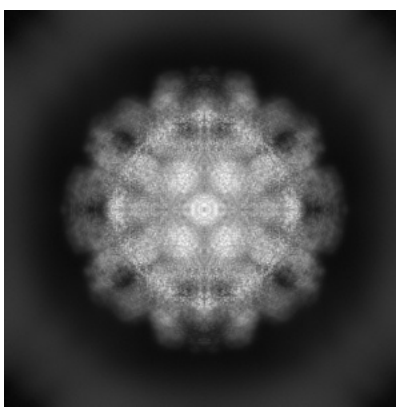


Z

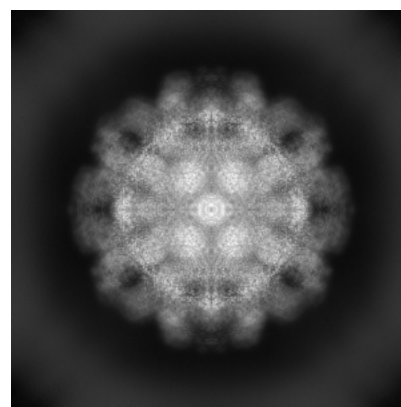
#### 6.1.2 Raw map



X



Y

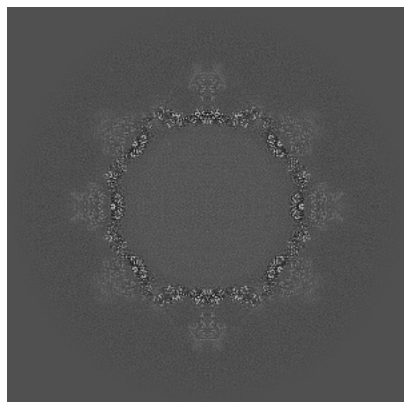


Z

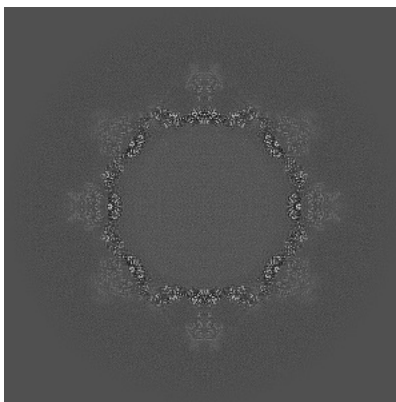
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

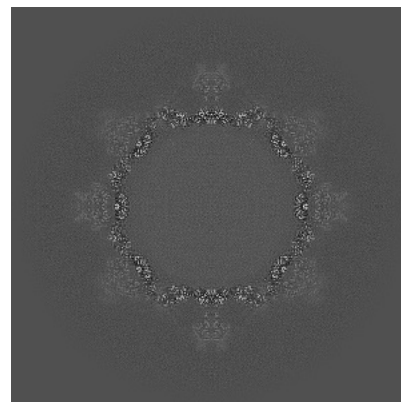
### 6.2.1 Primary map



X Index: 270

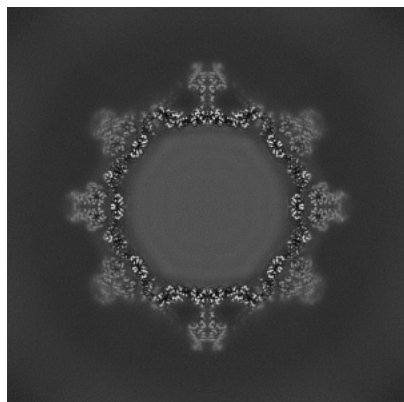


Y Index: 270

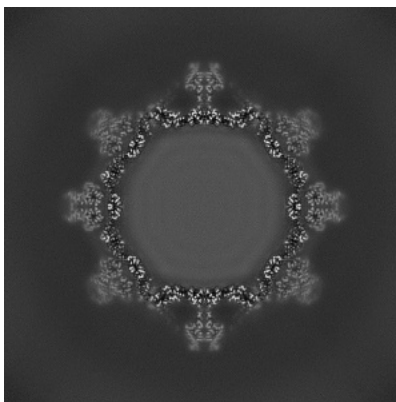


Z Index: 270

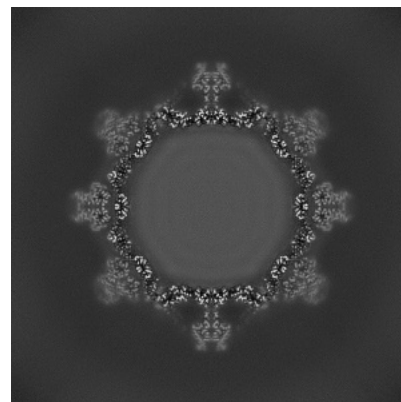
### 6.2.2 Raw map



X Index: 270



Y Index: 270

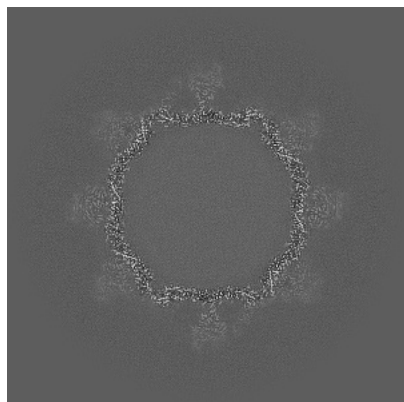


Z Index: 270

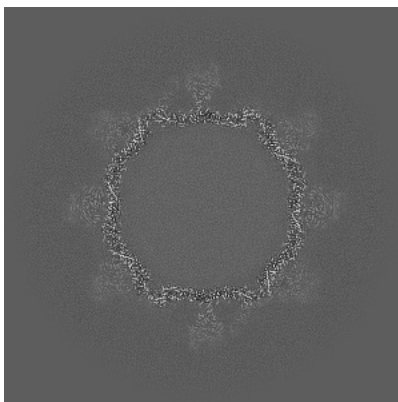
The images above show central slices of the map in three orthogonal directions.

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

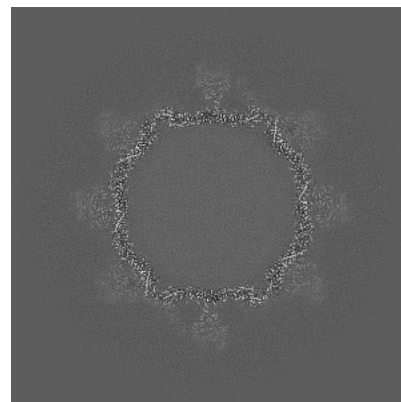
### 6.3.1 Primary map



X Index: 275

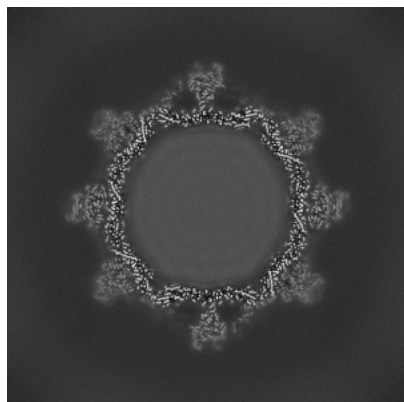


Y Index: 275

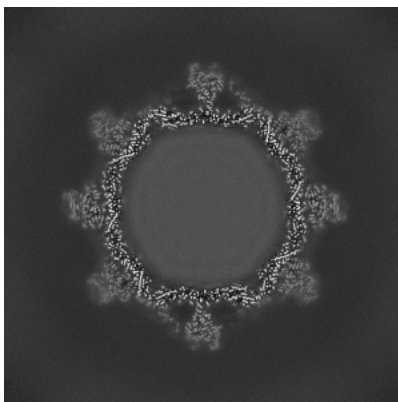


Z Index: 265

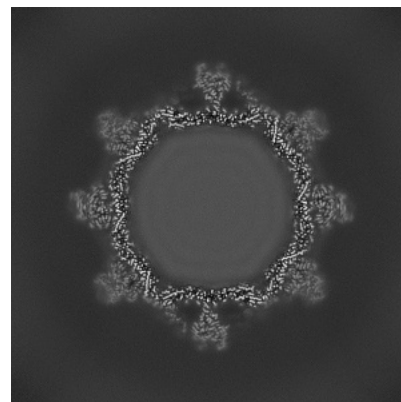
### 6.3.2 Raw map



X Index: 275



Y Index: 265

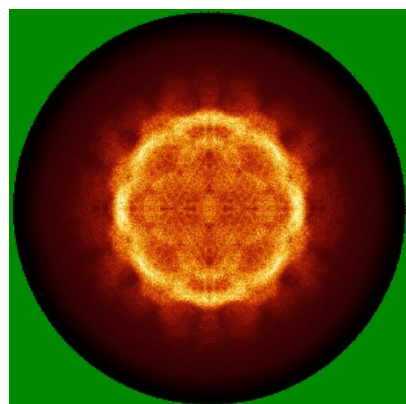


Z Index: 265

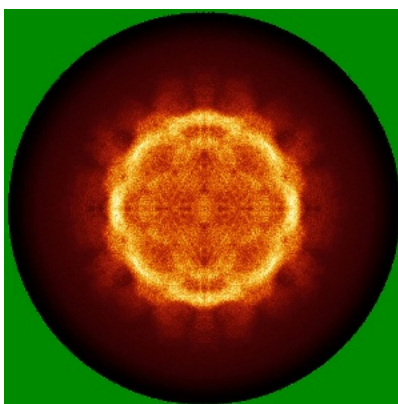
The images above show the largest variance slices of the map in three orthogonal directions.

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

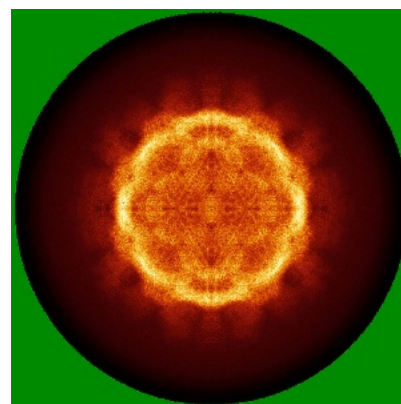
### 6.4.1 Primary map



X

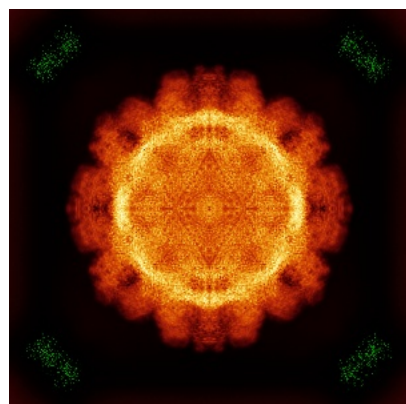


Y

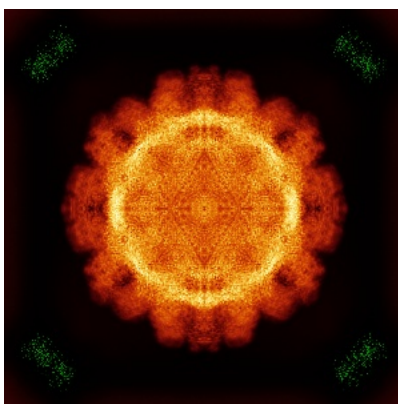


Z

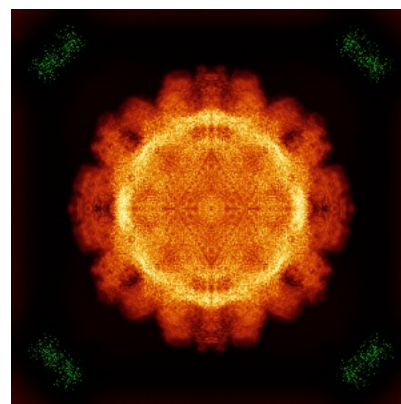
### 6.4.2 Raw map



X



Y



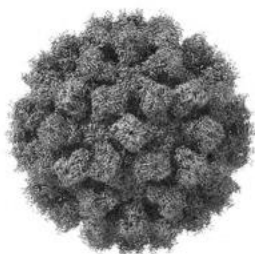
Z

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.

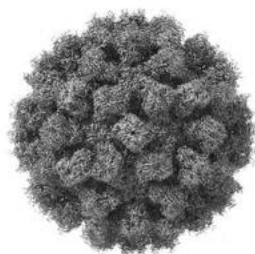


## 6.5 Orthogonal surface views [i](#)

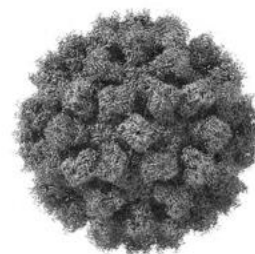
### 6.5.1 Primary map



X



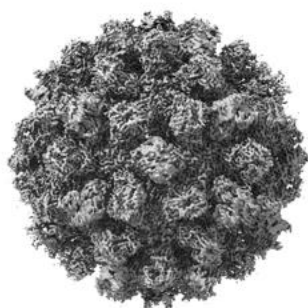
Y



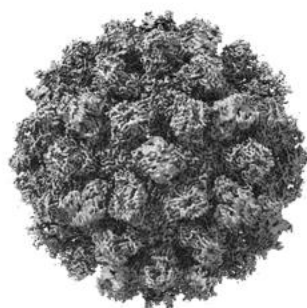
Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

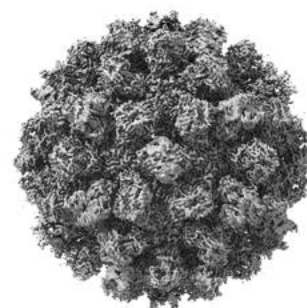
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

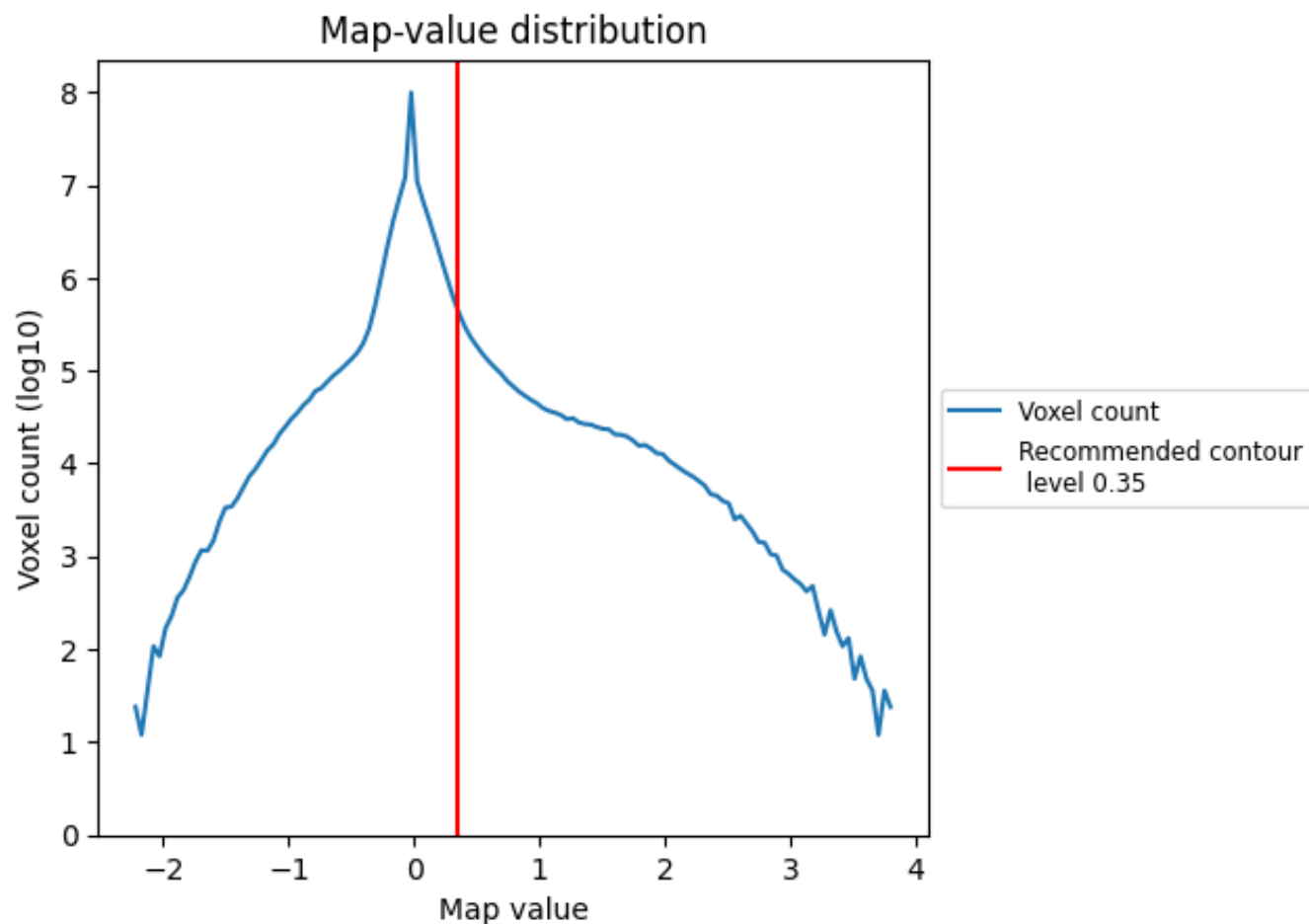
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

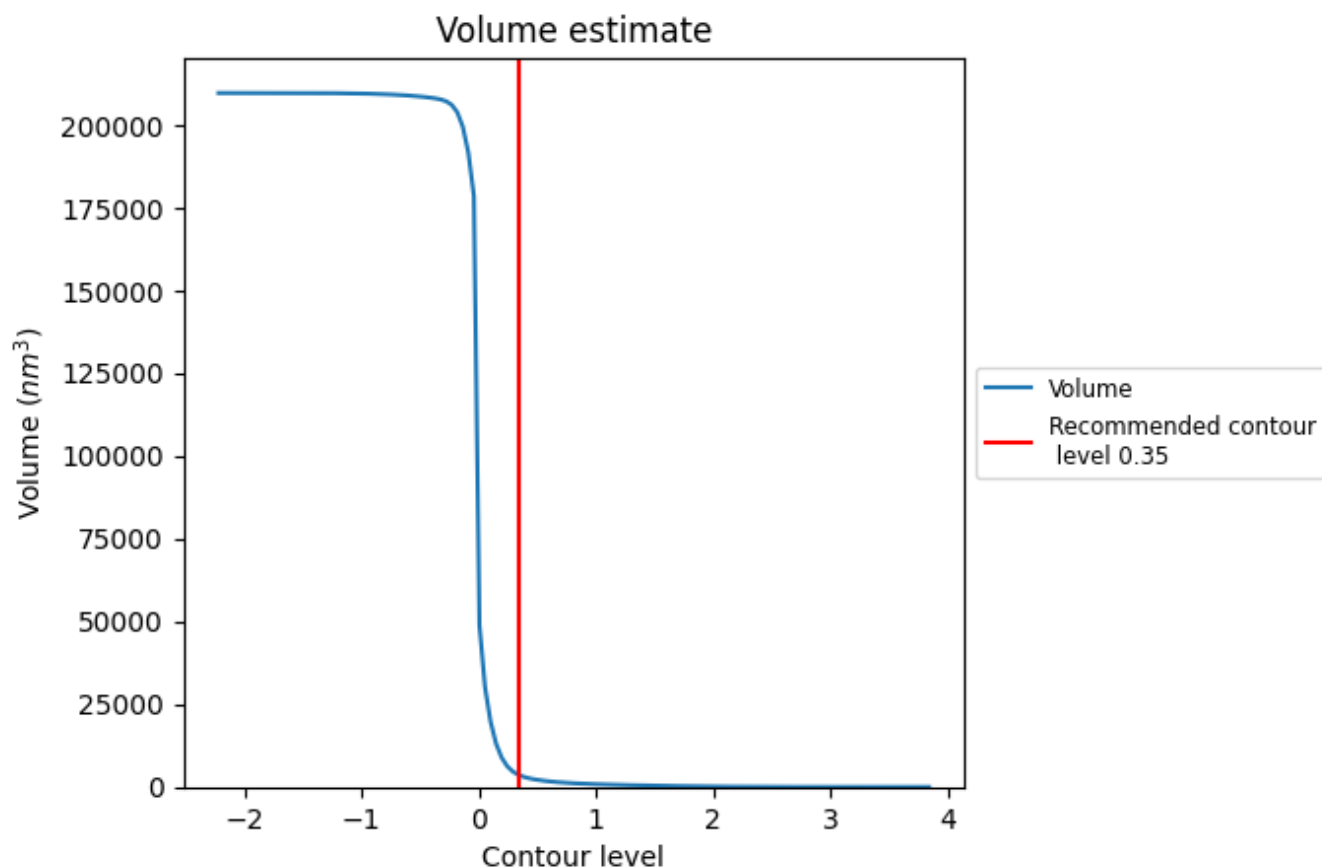
This section contains the results of statistical analysis of the map.

### 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.

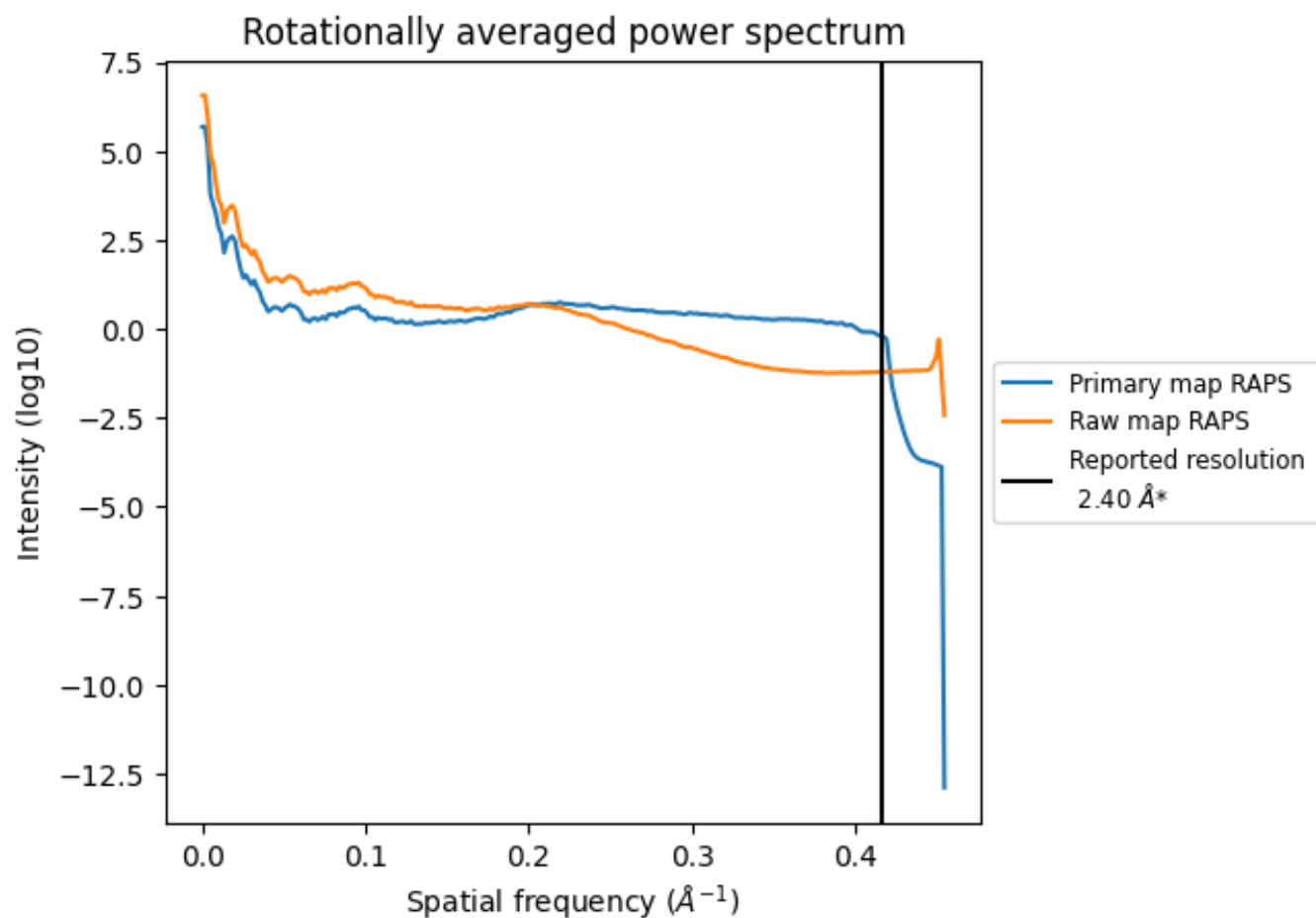
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3529  $\text{nm}^3$ ; this corresponds to an approximate mass of 3188 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 ⓘ

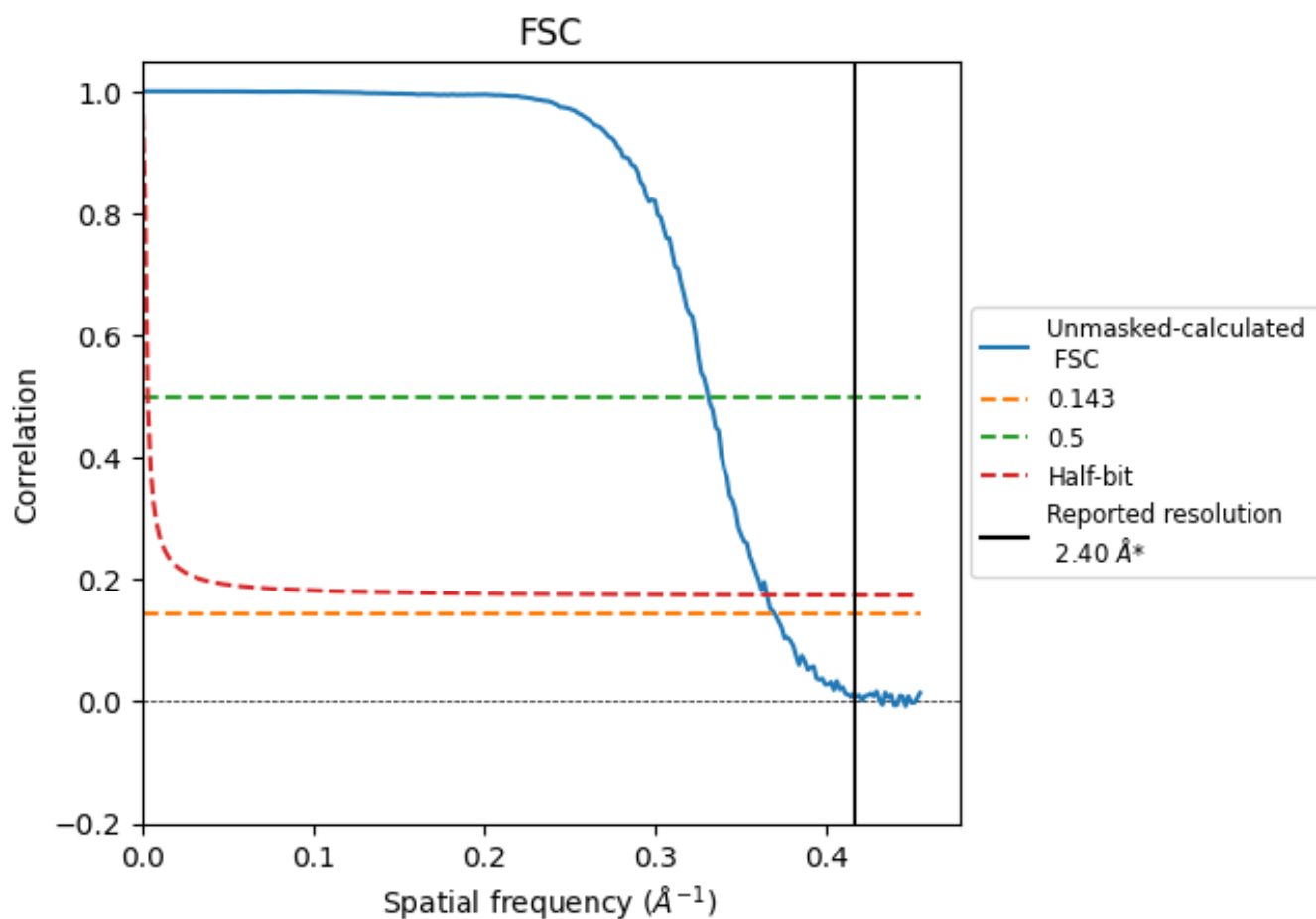


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

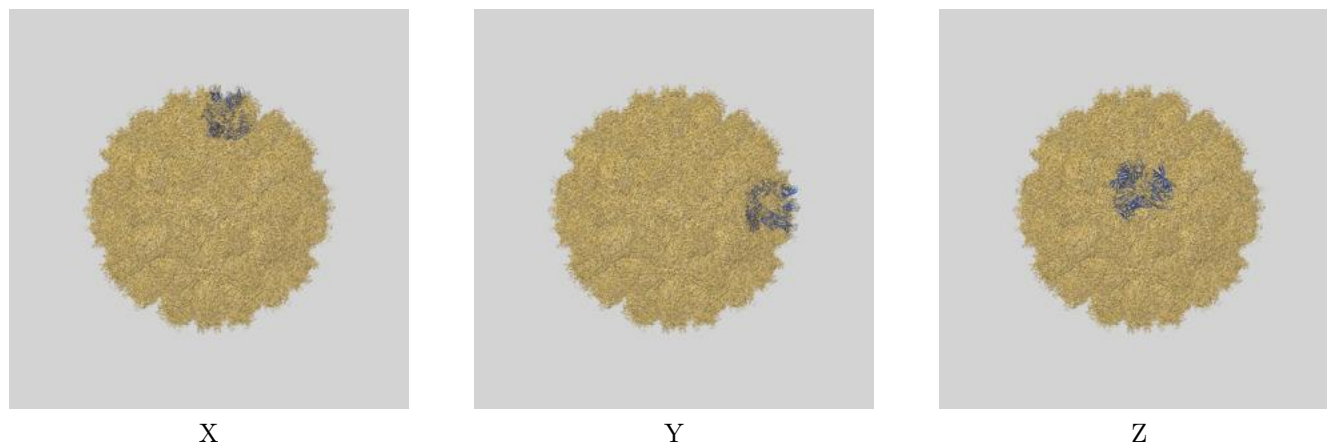
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	3.02	2.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.71 differs from the reported value 2.4 by more than 10 %

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

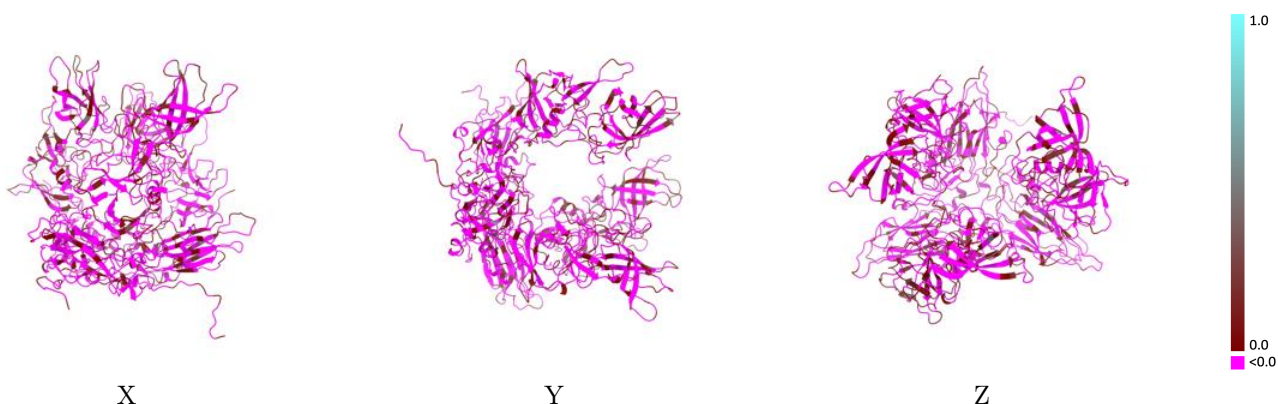
This section contains information regarding the fit between EMDB map EMD-47837 and PDB model 9EAN. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



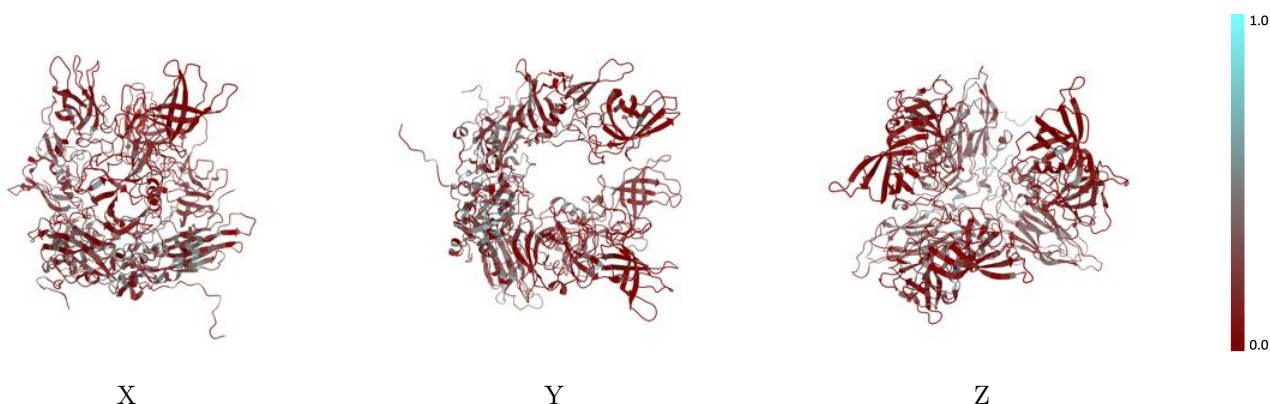
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



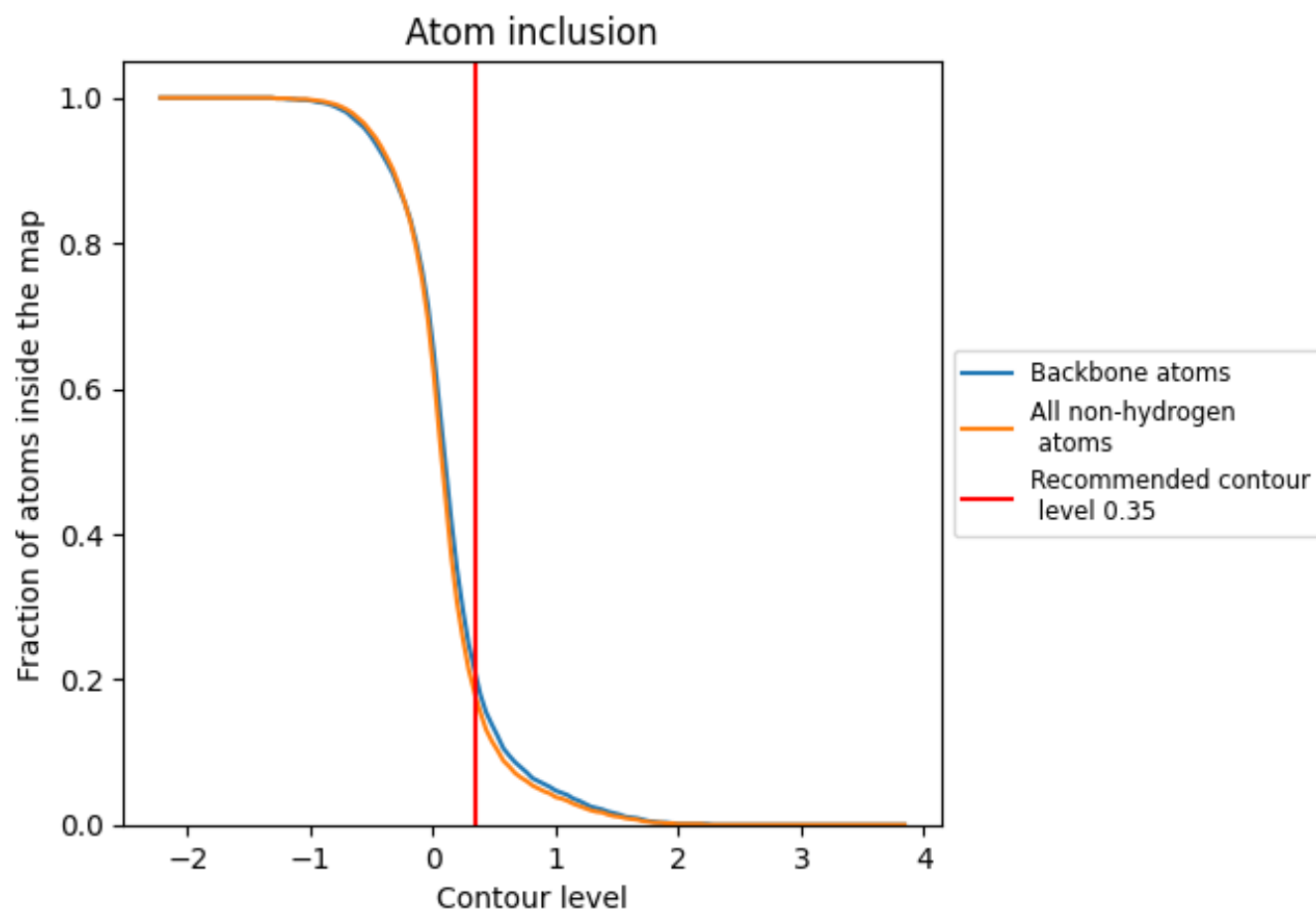
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 21% of all backbone atoms, 18% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.1750	<div></div> -0.0780
A	<div></div> 0.1660	<div></div> -0.0910
B	<div></div> 0.1690	<div></div> -0.0820
C	<div></div> 0.1920	<div></div> -0.0590

