



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 03:35 PM JST

PDB ID : 7FFF
EMDB ID : EMD-31567
Title : Structure of Venezuelan equine encephalitis virus with the receptor LDLRAD3
Authors : Zhang, X.; Xiang, Y.; Ma, J.; Ma, B.; Huang, C.
Deposited on : 2021-07-23
Resolution : 3.00 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.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

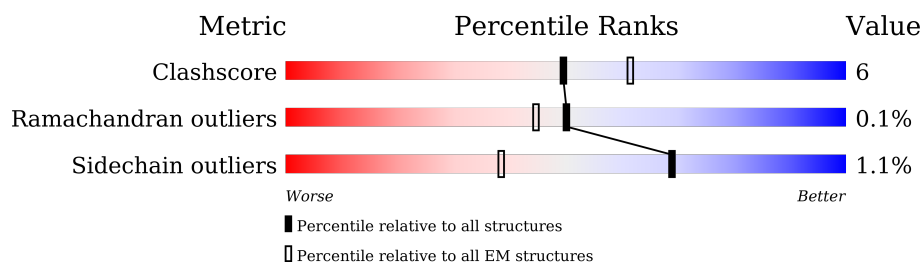
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.




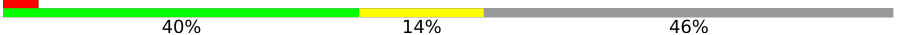
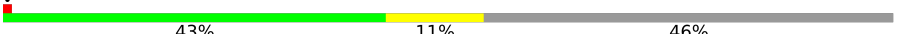
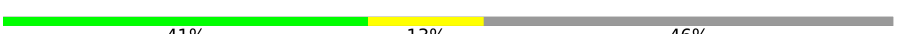




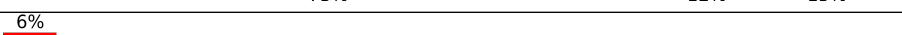
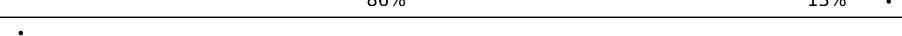
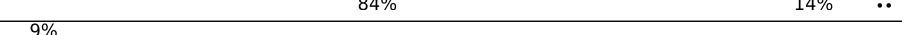

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	275	
1	F	275	
1	K	275	
1	S	275	
2	B	442	
2	C	442	
2	G	442	
2	O	442	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	70	
3	E	70	
3	H	70	
3	M	70	
4	I	59	
4	L	59	
4	P	59	
4	T	59	
5	J	423	
5	N	423	
5	Q	423	
5	R	423	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34356 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	163	Total	C	N	O	S	0	0
			1281	809	228	236	8		
1	S	163	Total	C	N	O	S	0	0
			1281	809	228	236	8		
1	A	163	Total	C	N	O	S	0	0
			1281	809	228	236	8		
1	F	163	Total	C	N	O	S	0	0
			1281	809	228	236	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	64	ASN	LYS	engineered mutation	UNP P05674
S	64	ASN	LYS	engineered mutation	UNP P05674
A	64	ASN	LYS	engineered mutation	UNP P05674
F	64	ASN	LYS	engineered mutation	UNP P05674

- Molecule 2 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
2	B	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
2	C	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
2	O	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		

- Molecule 3 is a protein called Low-density lipoprotein receptor class A domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	38	Total	C	N	O	S	0	0
			287	172	49	59	7		
3	D	38	Total	C	N	O	S	0	0
			287	172	49	59	7		
3	E	38	Total	C	N	O	S	0	0
			287	172	49	59	7		
3	M	38	Total	C	N	O	S	0	0
			287	172	49	59	7		

- Molecule 4 is a protein called assembly protein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	50	Total	C	N	O	S	0	0
			375	237	59	73	6		
4	T	50	Total	C	N	O	S	0	0
			375	237	59	73	6		
4	P	50	Total	C	N	O	S	0	0
			375	237	59	73	6		
4	L	50	Total	C	N	O	S	0	0
			375	237	59	73	6		

- Molecule 5 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	419	Total	C	N	O	S	0	0
			3275	2070	579	601	25		
5	Q	419	Total	C	N	O	S	0	0
			3275	2070	579	601	25		
5	R	419	Total	C	N	O	S	0	0
			3275	2070	579	601	25		
5	N	419	Total	C	N	O	S	0	0
			3275	2070	579	601	25		

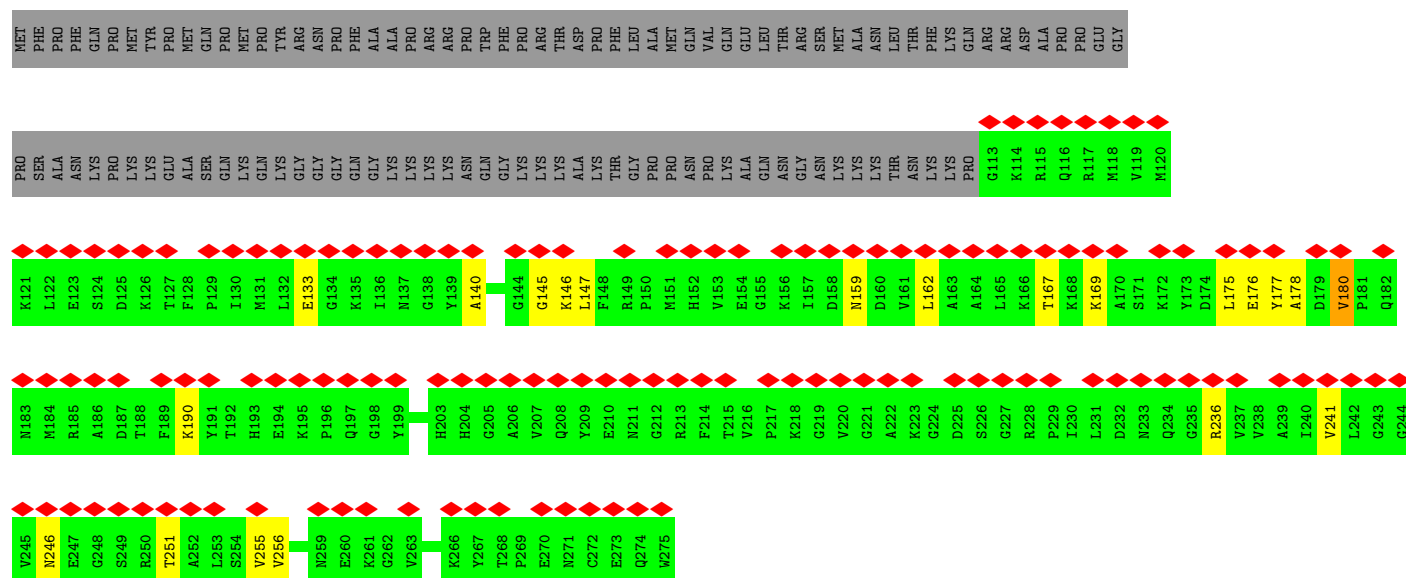
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	H	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

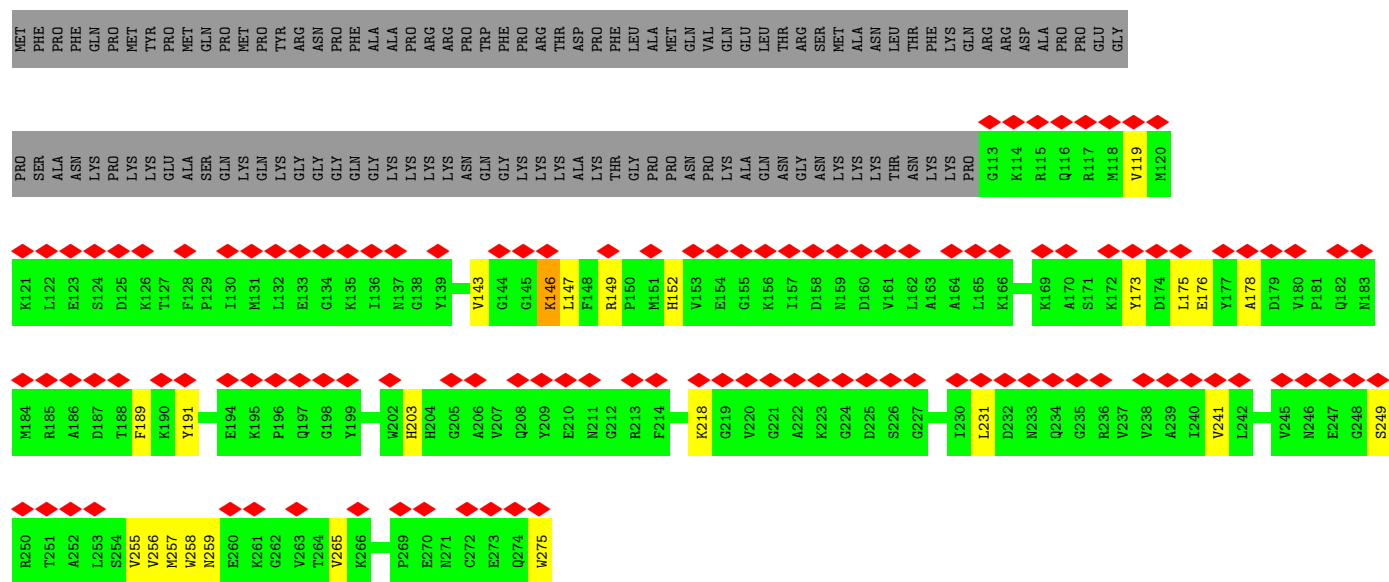
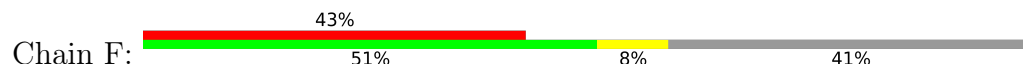
Continued on next page...

Continued from previous page...

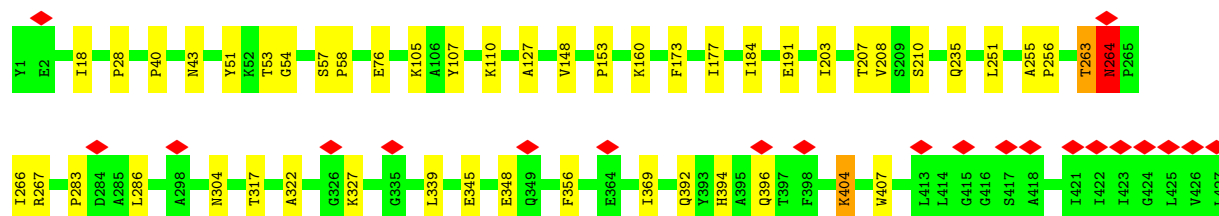
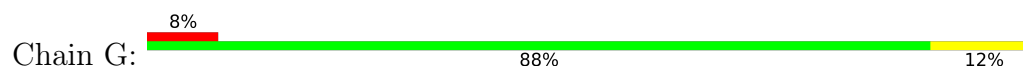
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
6	M	1	1	1	0



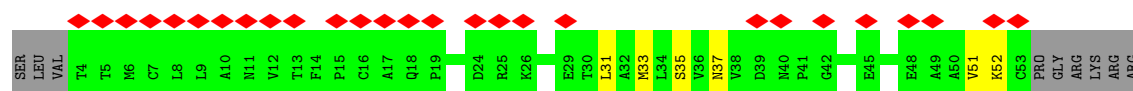
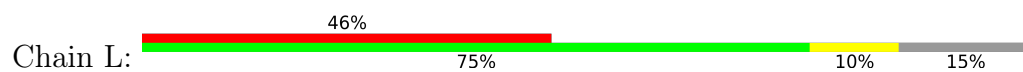
• Molecule 1: Capsid protein



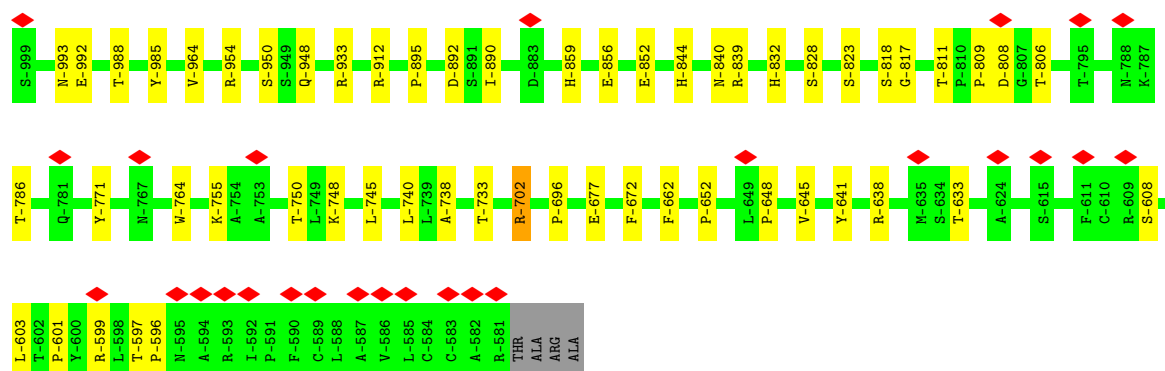
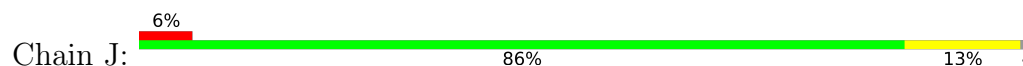
• Molecule 2: Spike glycoprotein E1



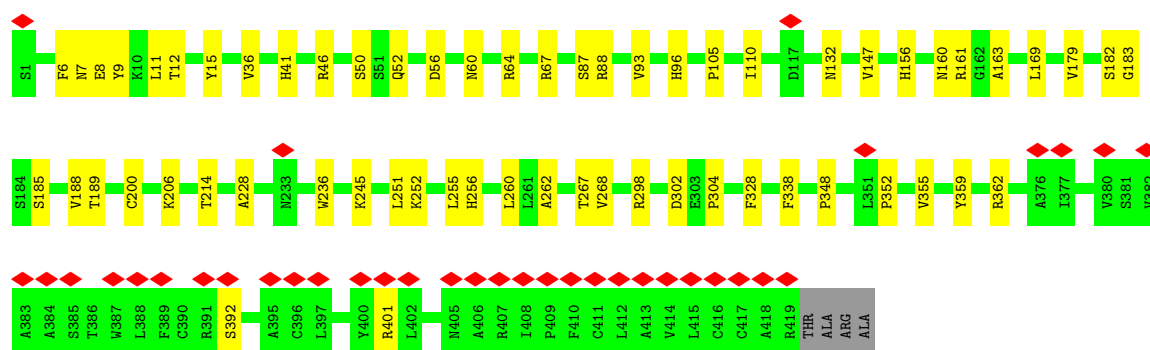
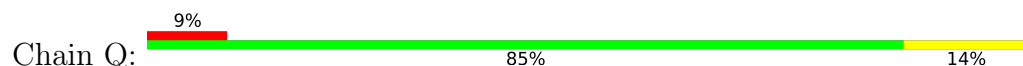
- Molecule 3: Low-density lipoprotein receptor class A domain-containing protein 3



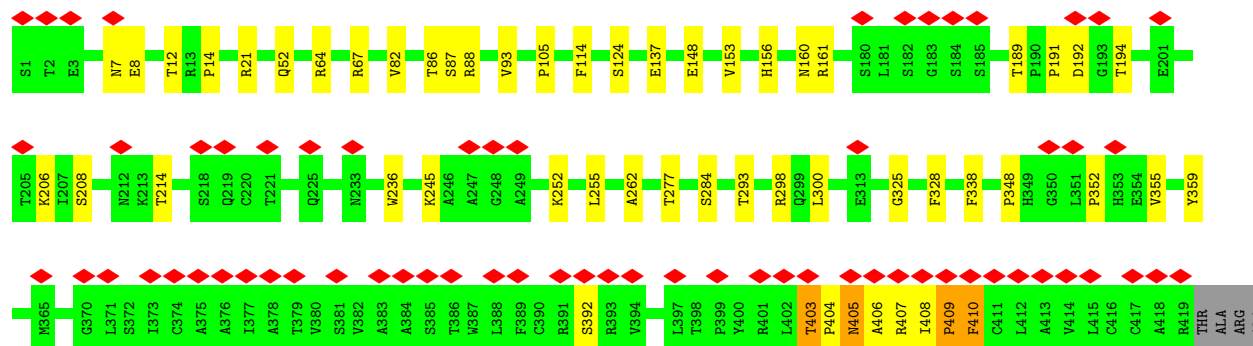
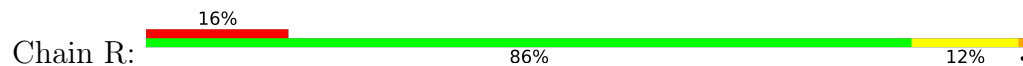
• Molecule 5: Spike glycoprotein E2



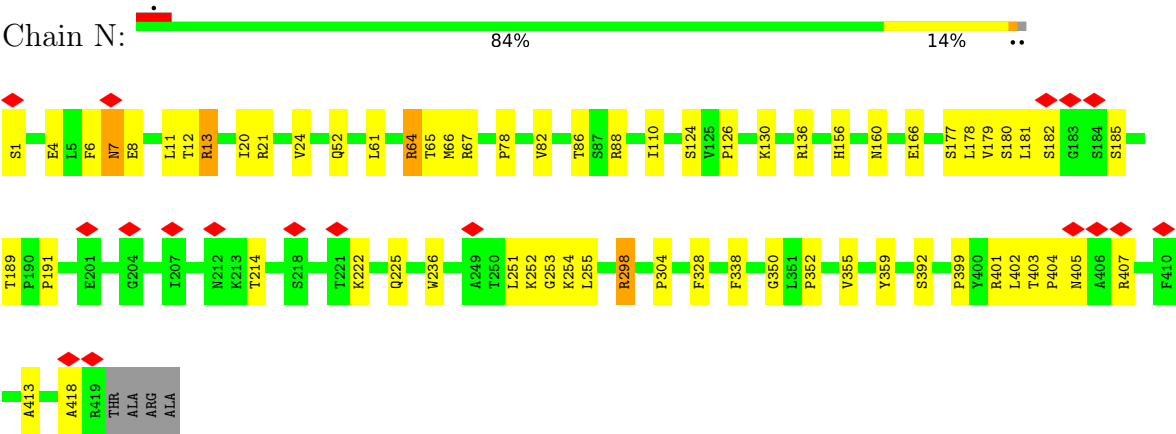
• Molecule 5: Spike glycoprotein E2



• Molecule 5: Spike glycoprotein E2



● Molecule 5: Spike glycoprotein E2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	726076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.32	0/1309	0.51	0/1762
1	F	0.32	0/1309	0.50	0/1762
1	K	0.25	0/1309	0.46	0/1762
1	S	0.25	0/1309	0.47	0/1762
2	B	0.38	0/3461	0.58	0/4731
2	C	0.42	0/3461	0.59	0/4731
2	G	0.41	1/3461 (0.0%)	0.58	0/4731
2	O	0.39	0/3461	0.58	0/4731
3	D	0.36	0/293	0.60	0/394
3	E	0.35	0/293	0.55	0/394
3	H	0.31	0/293	0.59	0/394
3	M	0.35	0/293	0.56	0/394
4	I	0.28	0/382	0.64	1/523 (0.2%)
4	L	0.27	0/382	0.55	0/523
4	P	0.28	0/382	0.60	1/523 (0.2%)
4	T	0.28	0/382	0.62	1/523 (0.2%)
5	J	0.42	0/3366	0.58	0/4578
5	N	0.44	0/3366	0.61	1/4578 (0.0%)
5	Q	0.40	0/3366	0.57	0/4578
5	R	0.42	0/3366	0.65	2/4578 (0.0%)
All	All	0.39	1/35244 (0.0%)	0.58	6/47952 (0.0%)

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
2	B	0	1
2	C	0	2
2	G	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	3
5	N	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	148	VAL	CB-CG2	-5.04	1.42	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	409	PRO	N-CA-C	14.53	149.88	112.10
5	R	410	PHE	N-CA-CB	11.92	132.06	110.60
5	N	11	LEU	CA-CB-CG	6.94	131.27	115.30
4	T	47	LEU	CA-CB-CG	6.15	129.45	115.30
4	P	47	LEU	CA-CB-CG	5.66	128.32	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	264	ASN	Peptide
2	C	264	ASN	Peptide
2	G	263	THR	Peptide
2	G	264	ASN	Peptide
2	G	369	ILE	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	A	1281	0	1275	15	0
1	F	1281	0	1275	20	0
1	K	1281	0	1275	28	0
1	S	1281	0	1275	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3370	0	3272	28	0
2	C	3370	0	3274	29	0
2	G	3370	0	3274	35	0
2	O	3370	0	3274	40	0
3	D	287	0	246	8	0
3	E	287	0	248	8	0
3	H	287	0	248	13	0
3	M	287	0	248	7	0
4	I	375	0	371	7	0
4	L	375	0	371	6	0
4	P	375	0	371	4	0
4	T	375	0	371	7	0
5	J	3275	0	3212	50	0
5	N	3275	0	3212	51	0
5	Q	3275	0	3212	47	0
5	R	3275	0	3212	38	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	H	1	0	0	0	0
6	M	1	0	0	0	0
All	All	34356	0	33516	373	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 6.

The worst 5 of 373 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)
3:E:37:CYS:CB	3:E:55:CYS:SG	2.14	1.33
3:H:37:CYS:SG	3:H:55:CYS:SG	1.25	1.25
3:H:37:CYS:CB	3:H:55:CYS:SG	2.29	1.21
3:M:37:CYS:SG	3:M:55:CYS:SG	1.09	1.09
1:S:258:TRP:CD1	5:J:-597:THR:HG22	1.89	1.07

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	A	161/275 (58%)	153 (95%)	8 (5%)	0	100	100
1	F	161/275 (58%)	157 (98%)	4 (2%)	0	100	100
1	K	161/275 (58%)	154 (96%)	7 (4%)	0	100	100
1	S	161/275 (58%)	155 (96%)	6 (4%)	0	100	100
2	B	440/442 (100%)	413 (94%)	26 (6%)	1 (0%)	44	77
2	C	440/442 (100%)	416 (94%)	23 (5%)	1 (0%)	44	77
2	G	440/442 (100%)	408 (93%)	31 (7%)	1 (0%)	44	77
2	O	440/442 (100%)	416 (94%)	24 (6%)	0	100	100
3	D	36/70 (51%)	34 (94%)	2 (6%)	0	100	100
3	E	36/70 (51%)	35 (97%)	1 (3%)	0	100	100
3	H	36/70 (51%)	33 (92%)	3 (8%)	0	100	100
3	M	36/70 (51%)	34 (94%)	2 (6%)	0	100	100
4	I	48/59 (81%)	45 (94%)	3 (6%)	0	100	100
4	L	48/59 (81%)	44 (92%)	4 (8%)	0	100	100
4	P	48/59 (81%)	44 (92%)	4 (8%)	0	100	100
4	T	48/59 (81%)	44 (92%)	4 (8%)	0	100	100
5	J	417/423 (99%)	380 (91%)	37 (9%)	0	100	100
5	N	417/423 (99%)	380 (91%)	36 (9%)	1 (0%)	44	77
5	Q	417/423 (99%)	381 (91%)	36 (9%)	0	100	100
5	R	417/423 (99%)	383 (92%)	32 (8%)	2 (0%)	25	61
All	All	4408/5076 (87%)	4109 (93%)	293 (7%)	6 (0%)	50	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	404	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	410	PHE
2	B	404	LYS
2	C	404	LYS
5	R	409	PRO

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	135/230 (59%)	134 (99%)	1 (1%)	81	91
1	F	135/230 (59%)	133 (98%)	2 (2%)	60	83
1	K	135/230 (59%)	134 (99%)	1 (1%)	81	91
1	S	135/230 (59%)	134 (99%)	1 (1%)	81	91
2	B	368/368 (100%)	365 (99%)	3 (1%)	79	90
2	C	368/368 (100%)	366 (100%)	2 (0%)	86	94
2	G	368/368 (100%)	365 (99%)	3 (1%)	79	90
2	O	368/368 (100%)	365 (99%)	3 (1%)	79	90
3	D	33/60 (55%)	31 (94%)	2 (6%)	15	46
3	E	33/60 (55%)	32 (97%)	1 (3%)	36	69
3	H	33/60 (55%)	32 (97%)	1 (3%)	36	69
3	M	33/60 (55%)	31 (94%)	2 (6%)	15	46
4	I	43/51 (84%)	43 (100%)	0	100	100
4	L	43/51 (84%)	43 (100%)	0	100	100
4	P	43/51 (84%)	43 (100%)	0	100	100
4	T	43/51 (84%)	43 (100%)	0	100	100
5	J	362/364 (100%)	359 (99%)	3 (1%)	79	90
5	N	362/364 (100%)	355 (98%)	7 (2%)	52	79
5	Q	362/364 (100%)	360 (99%)	2 (1%)	84	93
5	R	362/364 (100%)	355 (98%)	7 (2%)	52	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3764/4292 (88%)	3723 (99%)	41 (1%)	69 87

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	408	ILE
5	N	160	ASN
3	M	27	ASN
5	N	64	ARG
5	N	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	360	ASN
5	R	121	HIS
2	O	442	ASN
2	O	355	HIS
2	C	392	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

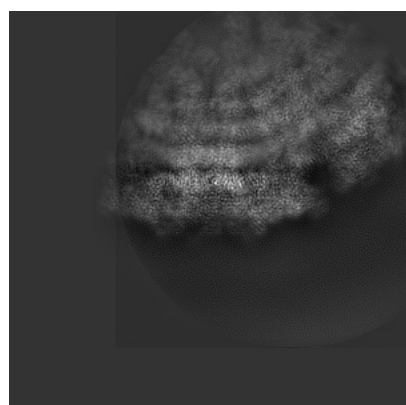
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31567. These allow visual inspection of the internal detail of the map and identification of artifacts.

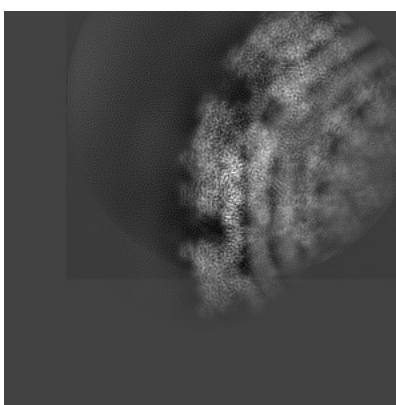
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

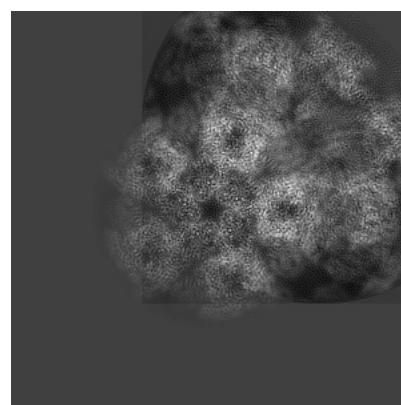
6.1.1 Primary map



X



Y

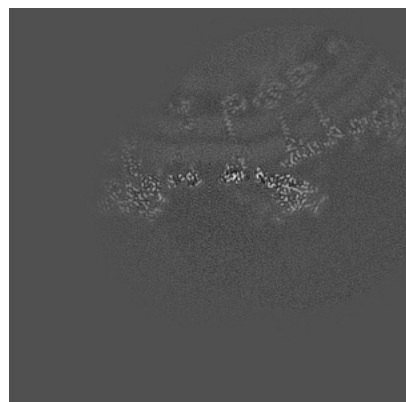


Z

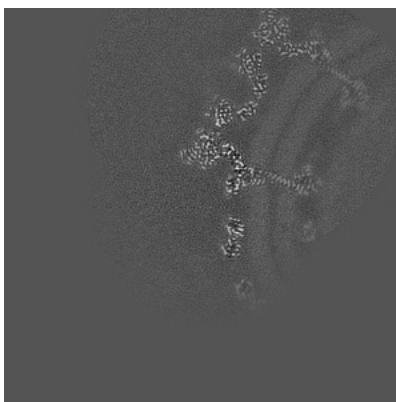
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

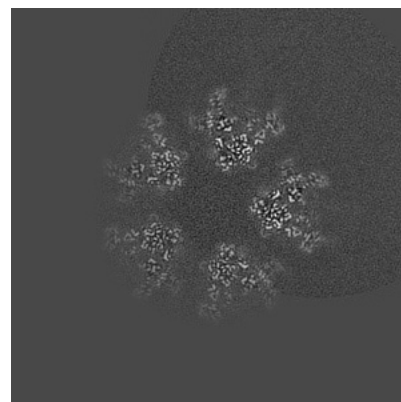
6.2.1 Primary map



X Index: 180



Y Index: 180

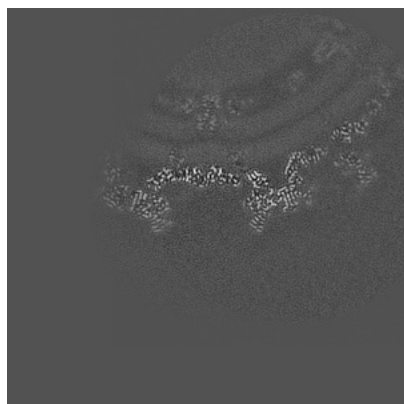


Z Index: 180

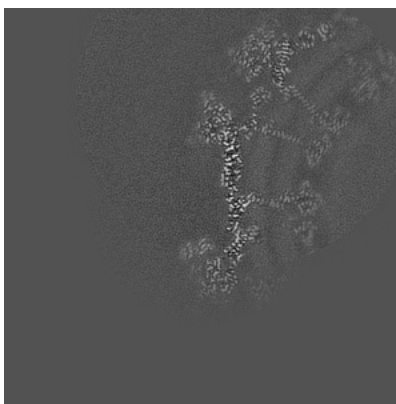
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

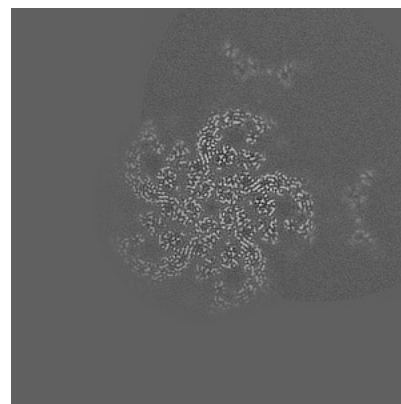
6.3.1 Primary map



X Index: 196



Y Index: 201

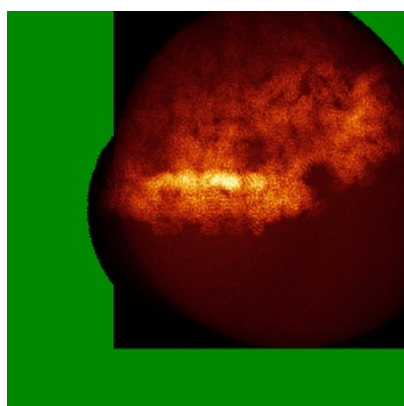


Z Index: 204

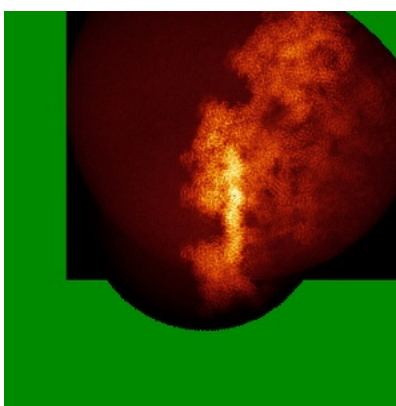
The images above show the largest variance slices of the map in three orthogonal directions.

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

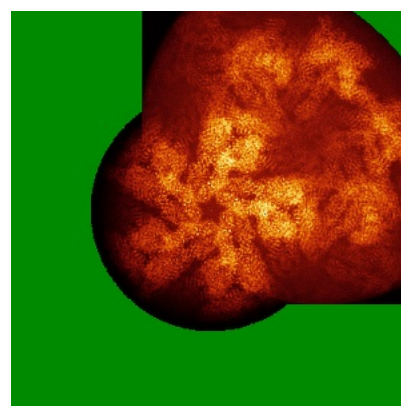
6.4.1 Primary map



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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

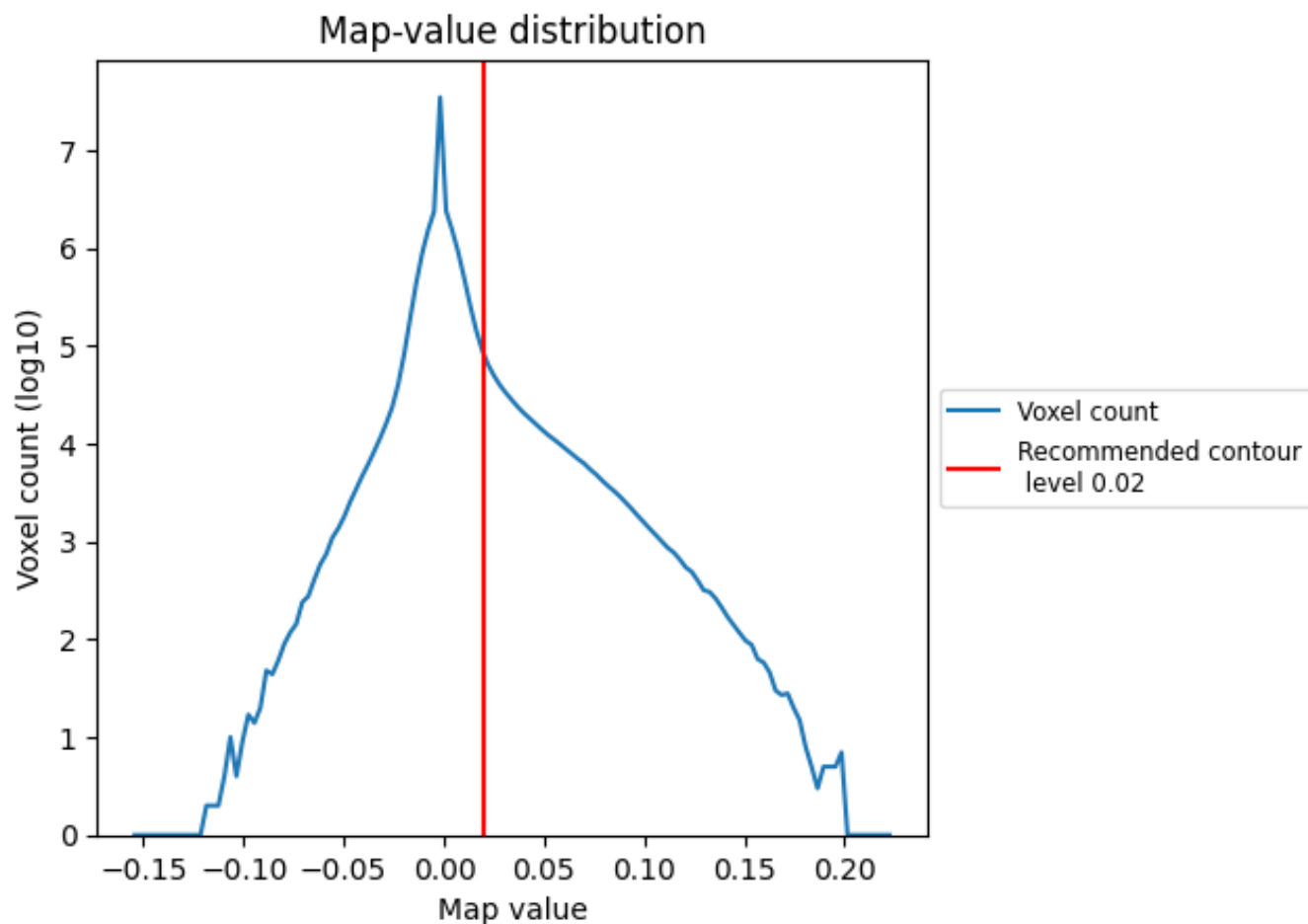
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

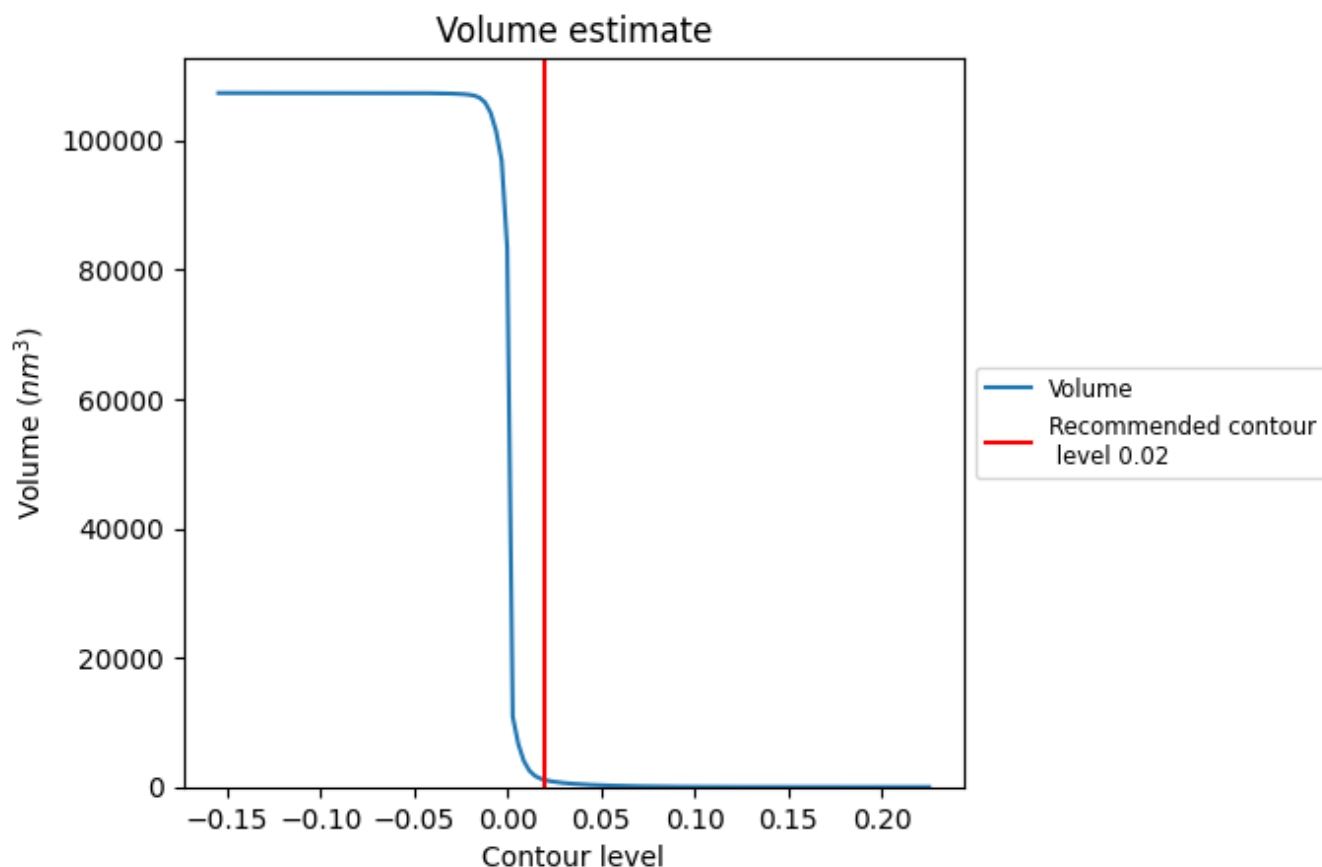
This section contains the results of statistical analysis of the map.

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.

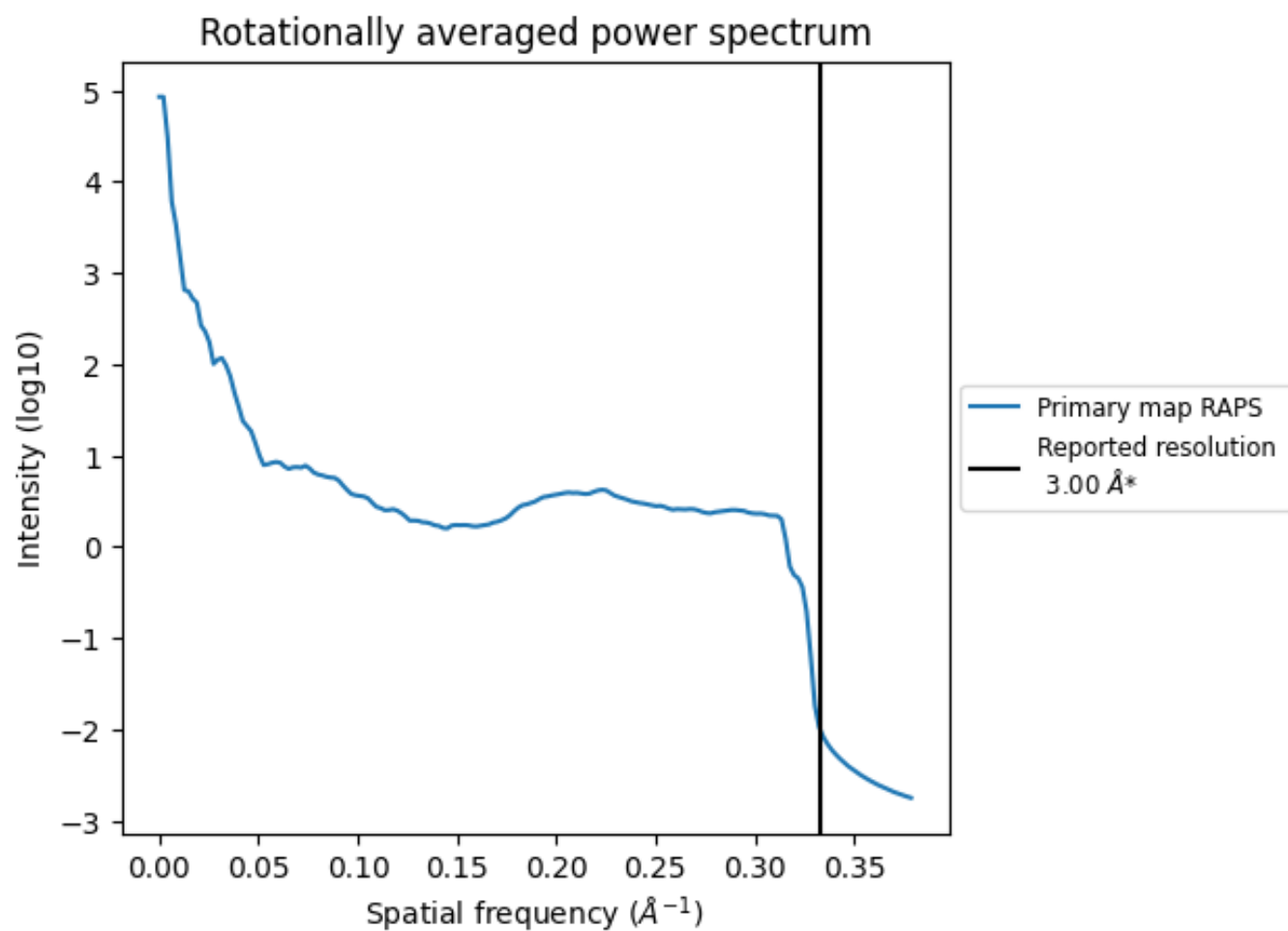
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1090 nm^3 ; this corresponds to an approximate mass of 985 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 0.333 Å⁻¹

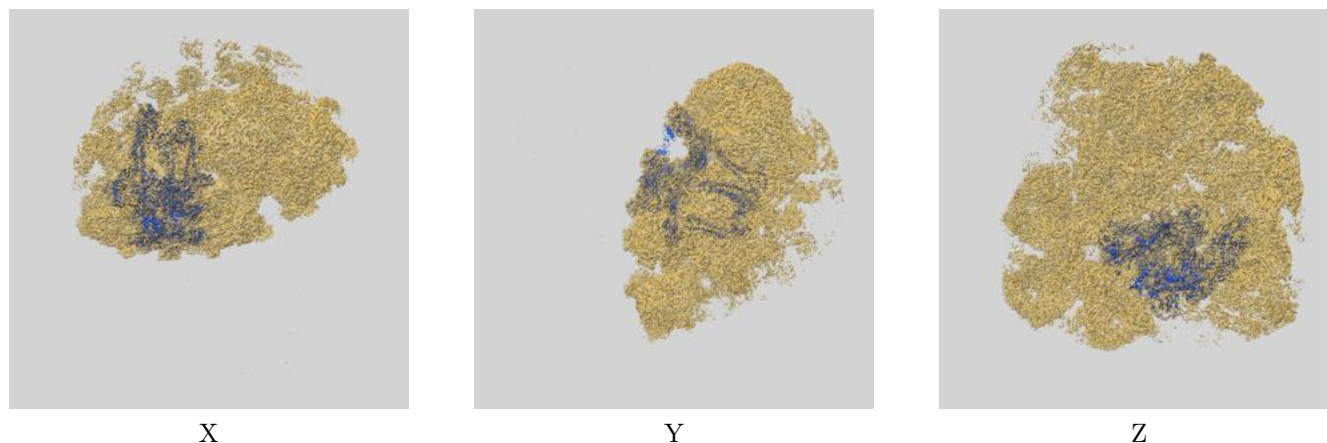
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

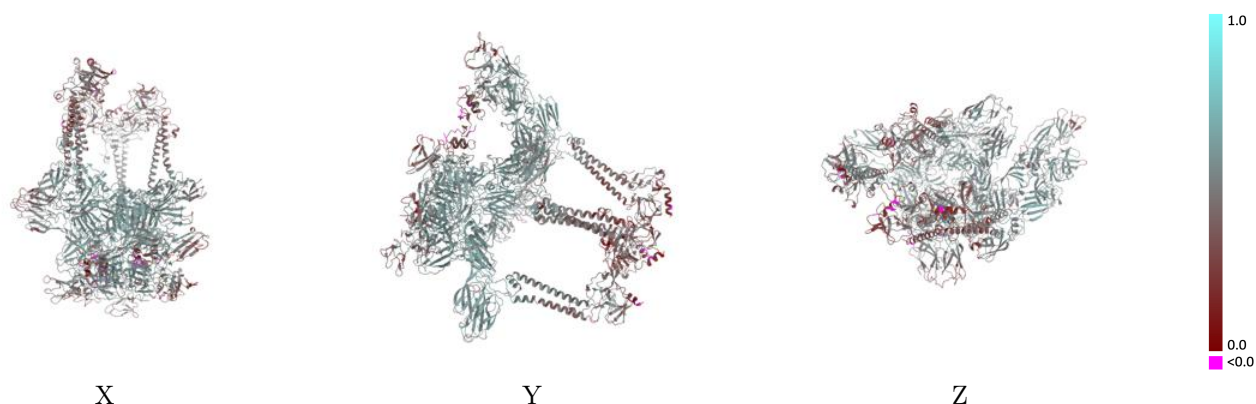
This section contains information regarding the fit between EMDB map EMD-31567 and PDB model 7FFF. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



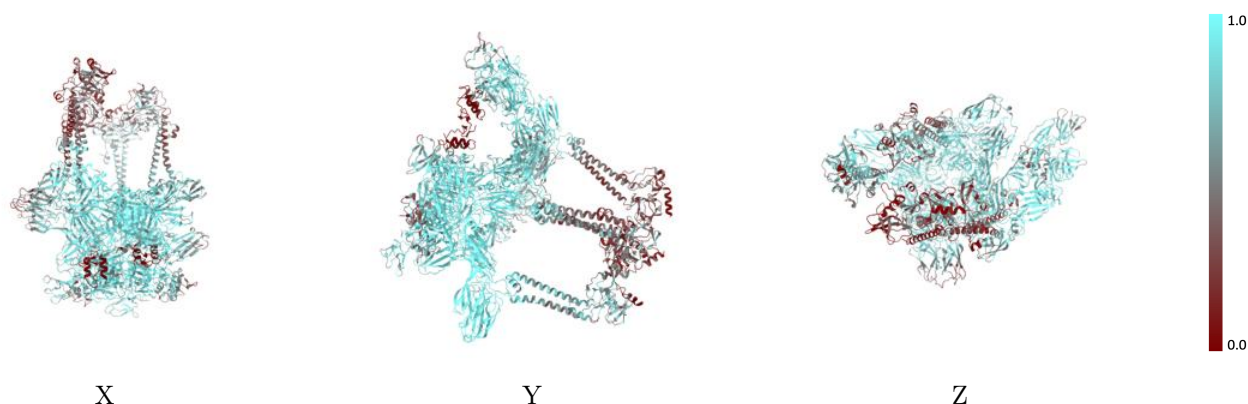
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



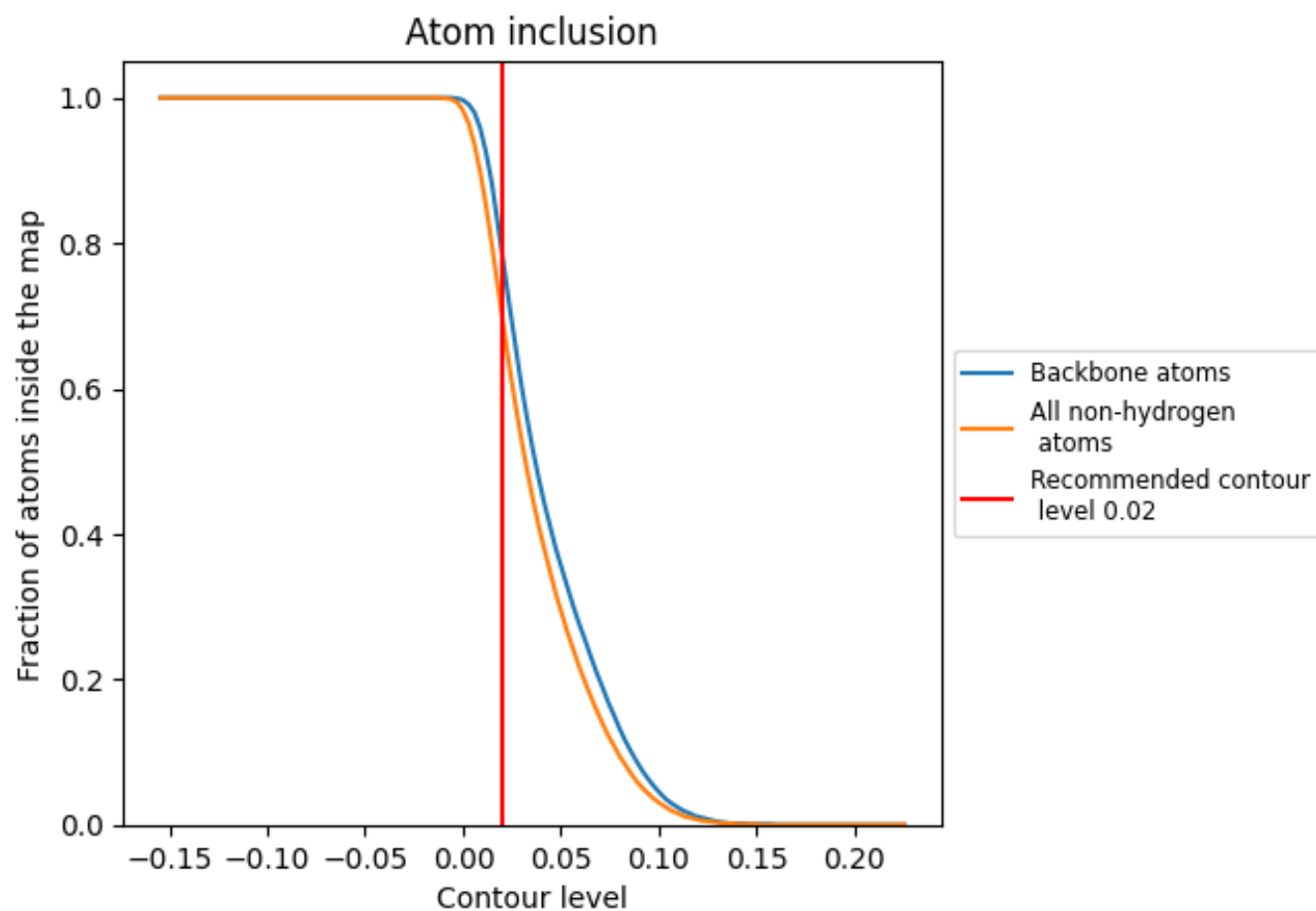
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.4800
A	 0.2340	 0.3160
B	 0.7120	 0.4810
C	 0.7410	 0.5120
D	 0.8630	 0.4990
E	 0.7510	 0.4850
F	 0.2710	 0.3540
G	 0.7710	 0.5190
H	 0.8420	 0.4890
I	 0.0350	 0.2190
J	 0.8070	 0.5160
K	 0.5310	 0.4100
L	 0.3910	 0.3810
M	 0.8810	 0.5060
N	 0.8430	 0.5230
O	 0.8860	 0.5430
P	 0.0510	 0.2720
Q	 0.8160	 0.5120
R	 0.7250	 0.4980
S	 0.4220	 0.3520
T	 0.2750	 0.3020

