



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 03:58 pm GMT

PDB ID : 5NEU
EMDB ID : EMD-3635
Title : Localised Reconstruction of Integrin alpha V beta 6 bound to Foot and Mouth Disease Virus O1 Manisa - Pose B.
Authors : Kotecha, A.; Stuart, D.
Deposited on : 2017-03-11
Resolution : 12.30 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

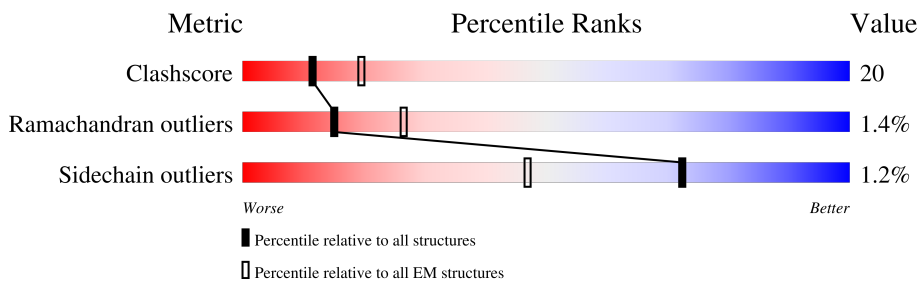
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1	208	
2	2	218	
3	3	220	
4	4	85	
5	A	590	
6	B	470	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13287 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 O1 Manisa VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	208	1611	1015	291	302	3	0	0

- Molecule 2 is a protein called O1 Manisa VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	207	1631	1040	279	305	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	93	TYR	SER	engineered mutation	UNP Q6PMW3

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	220	1687	1081	274	323	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	conflict	UNP A0A1C6ZW60
3	174	VAL	ALA	conflict	UNP A0A1C6ZW60

- Molecule 4 is a protein called O1 Manisa VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	45	345	218	55	70	2	0	0

- Molecule 5 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	590	4572	2900	775	876	21	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P06756
A	?	-	SER	deletion	UNP P06756
A	400	CYS	MET	conflict	UNP P06756
A	?	-	GLN	deletion	UNP P06756
A	?	-	LYS	deletion	UNP P06756

- Molecule 6 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	448	3438	2157	587	663	31	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	249	CYS	ILE	conflict	UNP P18564
B	517	ASN	HIS	conflict	UNP P18564

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	1	1	Total	Mg	0
			1	1	

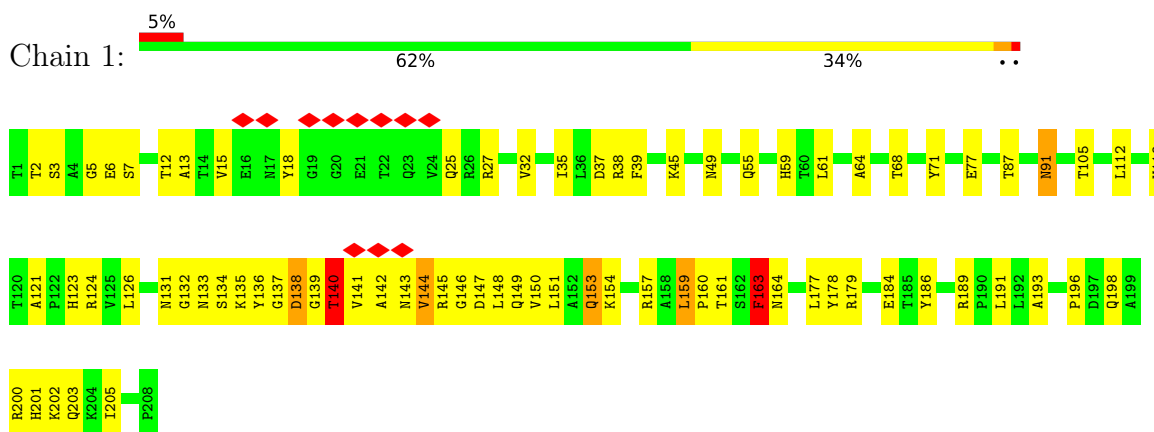
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total	Ca	0
			2	2	

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.

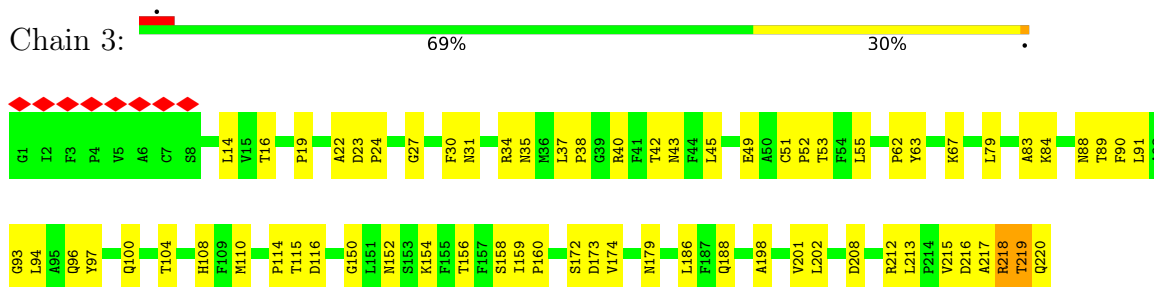
- Molecule 1: O1 Manisa VP1



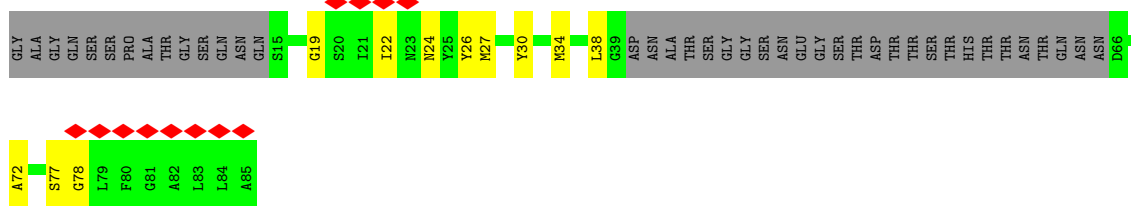
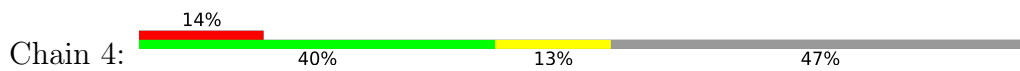
- Molecule 2: O1 Manisa VP2



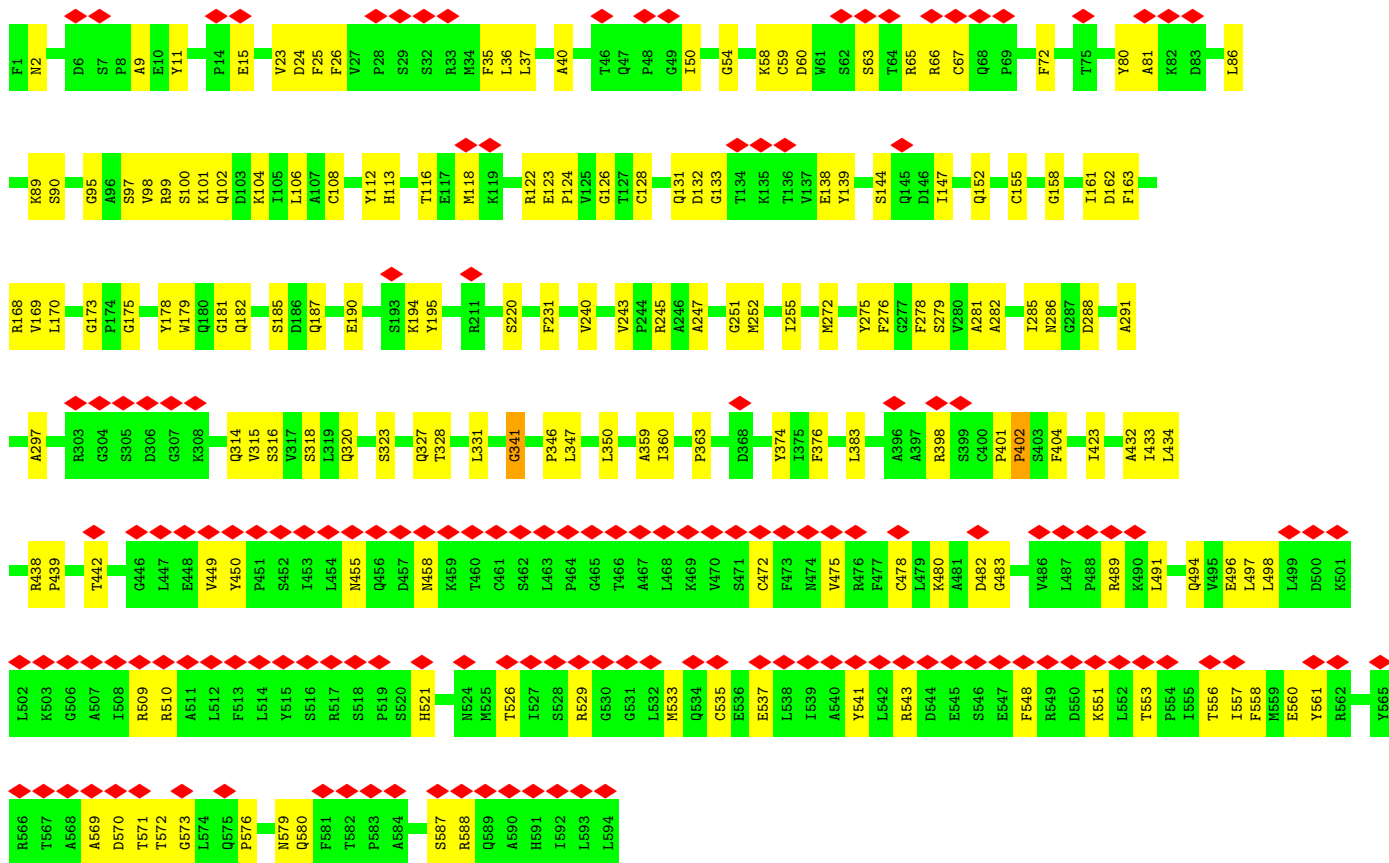
- Molecule 3: Capsid protein



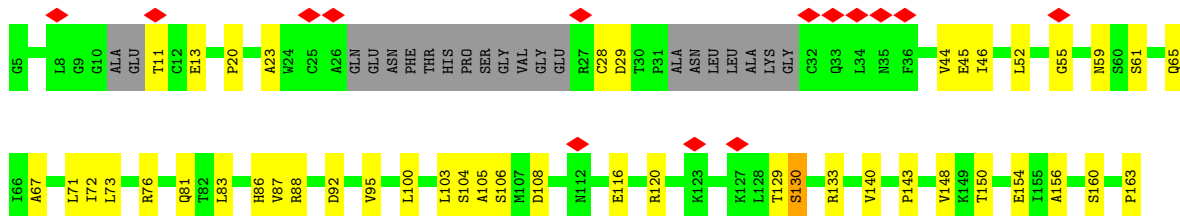
- Molecule 4: O1 Manisa VP4

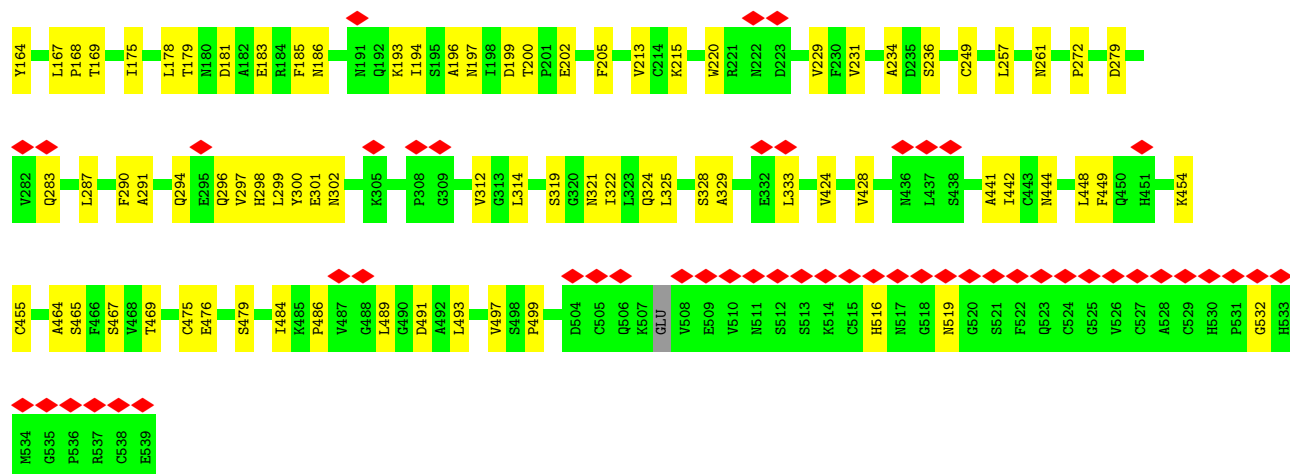


• Molecule 5: Integrin alpha-V



• Molecule 6: Integrin beta-6





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0138	Depositor
Map size (Å)	172.8, 172.8, 172.8	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: MG, 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	1	0.40	0/1647	0.63	2/2250 (0.1%)
2	2	0.45	0/1676	0.63	0/2289
3	3	0.44	0/1737	0.57	1/2373 (0.0%)
4	4	0.37	0/351	0.48	0/470
5	A	0.24	0/4674	0.41	0/6326
6	B	0.23	0/3495	0.40	0/4722
All	All	0.33	0/13580	0.49	3/18430 (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
1	1	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	163	PHE	CA-C-N	-7.68	100.30	117.20
1	1	163	PHE	O-C-N	5.28	131.15	122.70
3	3	186	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	163	PHE	Mainchain

5.2 Too-close contacts [i](#)

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	1	1611	0	1611	259	0
2	2	1631	0	1582	74	0
3	3	1687	0	1610	208	0
4	4	345	0	318	17	0
5	A	4572	0	4425	90	0
6	B	3438	0	3379	108	0
7	1	1	0	0	0	0
8	B	2	0	0	0	0
All	All	13287	0	12925	522	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 20.

The worst 5 of 522 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)
1:1:124:ARG:HH21	3:3:37:LEU:CD1	1.19	1.50
1:1:144:VAL:HB	1:1:145:ARG:CA	1.38	1.50
1:1:153:GLN:HE22	6:B:164:TYR:CB	1.28	1.46
1:1:148:LEU:CD2	6:B:196:ALA:HB1	1.48	1.42
1:1:144:VAL:CB	1:1:145:ARG:HA	1.37	1.42

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	1	206/208 (99%)	185 (90%)	18 (9%)	3 (2%)	10	46
2	2	205/218 (94%)	188 (92%)	17 (8%)	0	100	100
3	3	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
4	4	41/85 (48%)	39 (95%)	1 (2%)	1 (2%)	6	33
5	A	584/590 (99%)	495 (85%)	75 (13%)	14 (2%)	6	33
6	B	430/470 (92%)	375 (87%)	49 (11%)	6 (1%)	11	46
All	All	1684/1791 (94%)	1490 (88%)	170 (10%)	24 (1%)	15	46

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	144	VAL
1	1	140	THR
5	A	72	PHE
5	A	571	THR
5	A	63	SER

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	1	170/170 (100%)	166 (98%)	4 (2%)	49	69
2	2	179/190 (94%)	173 (97%)	6 (3%)	37	60
3	3	177/177 (100%)	173 (98%)	4 (2%)	50	70
4	4	36/67 (54%)	35 (97%)	1 (3%)	43	65
5	A	484/484 (100%)	483 (100%)	1 (0%)	93	96
6	B	394/410 (96%)	393 (100%)	1 (0%)	92	95
All	All	1440/1498 (96%)	1423 (99%)	17 (1%)	72	83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	185	PHE
2	2	77	ARG
2	2	135	ARG
2	2	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	179	ASN
5	A	145	GLN
6	B	197	ASN
4	4	31	GLN
5	A	187	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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
6	B	4
5	A	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	333:LEU	C	334:ARG	N	13.51
1	A	29:SER	C	32:SER	N	10.55
1	B	93:TYR	C	94:PRO	N	7.04
1	B	91:GLU	C	92:ASP	N	5.99
1	B	336:GLU	C	424:VAL	N	3.99

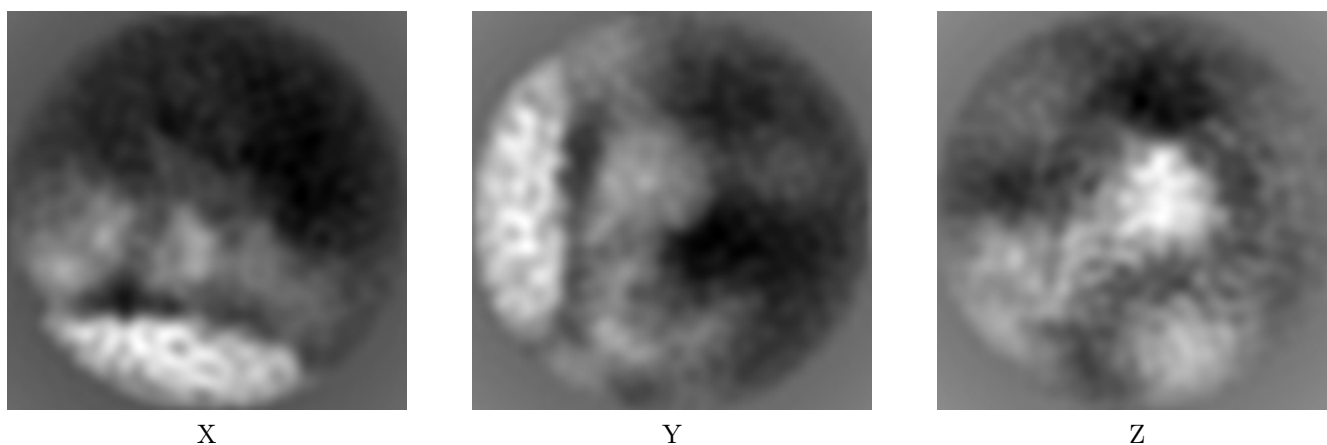
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3635. 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](#)

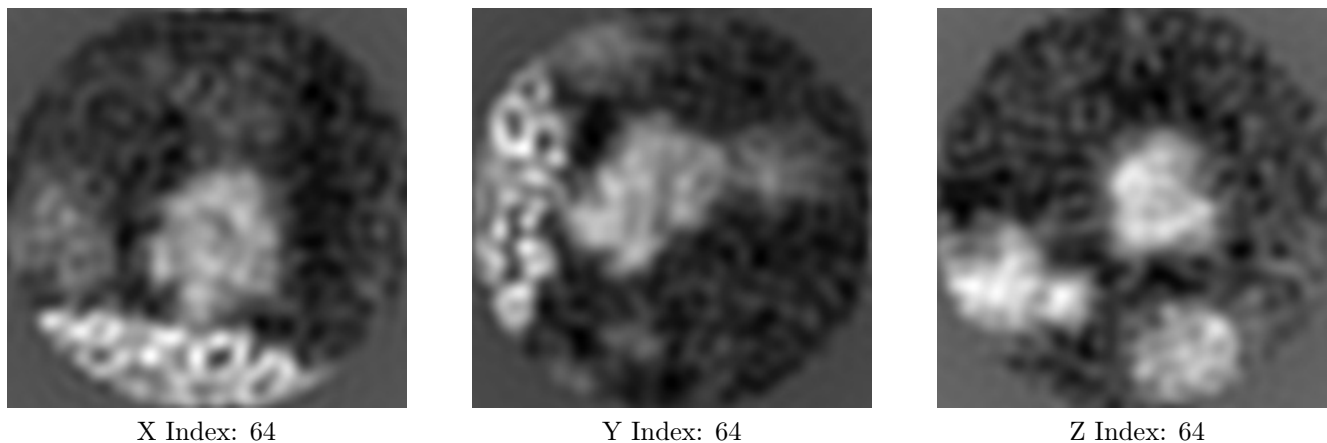
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



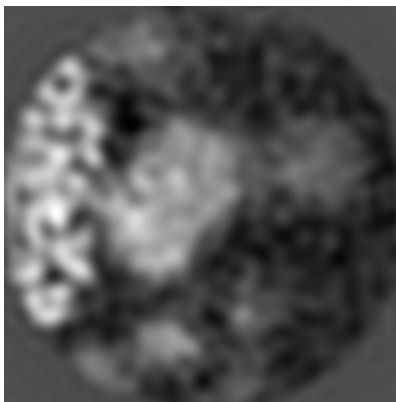
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

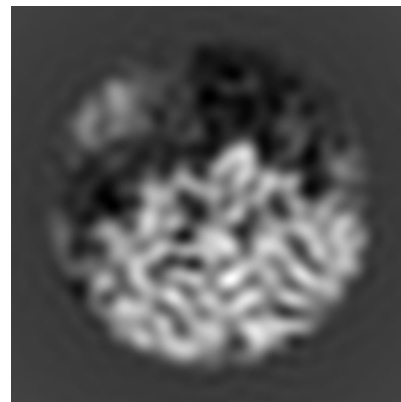
6.3.1 Primary map



X Index: 72



Y Index: 60

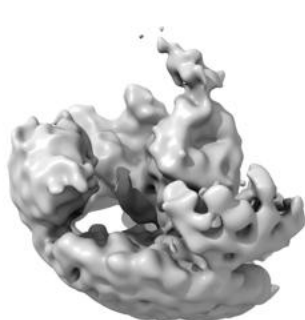


Z Index: 23

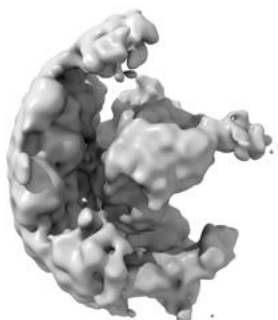
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

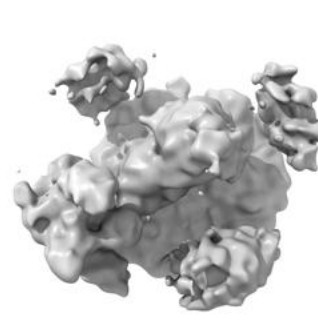
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

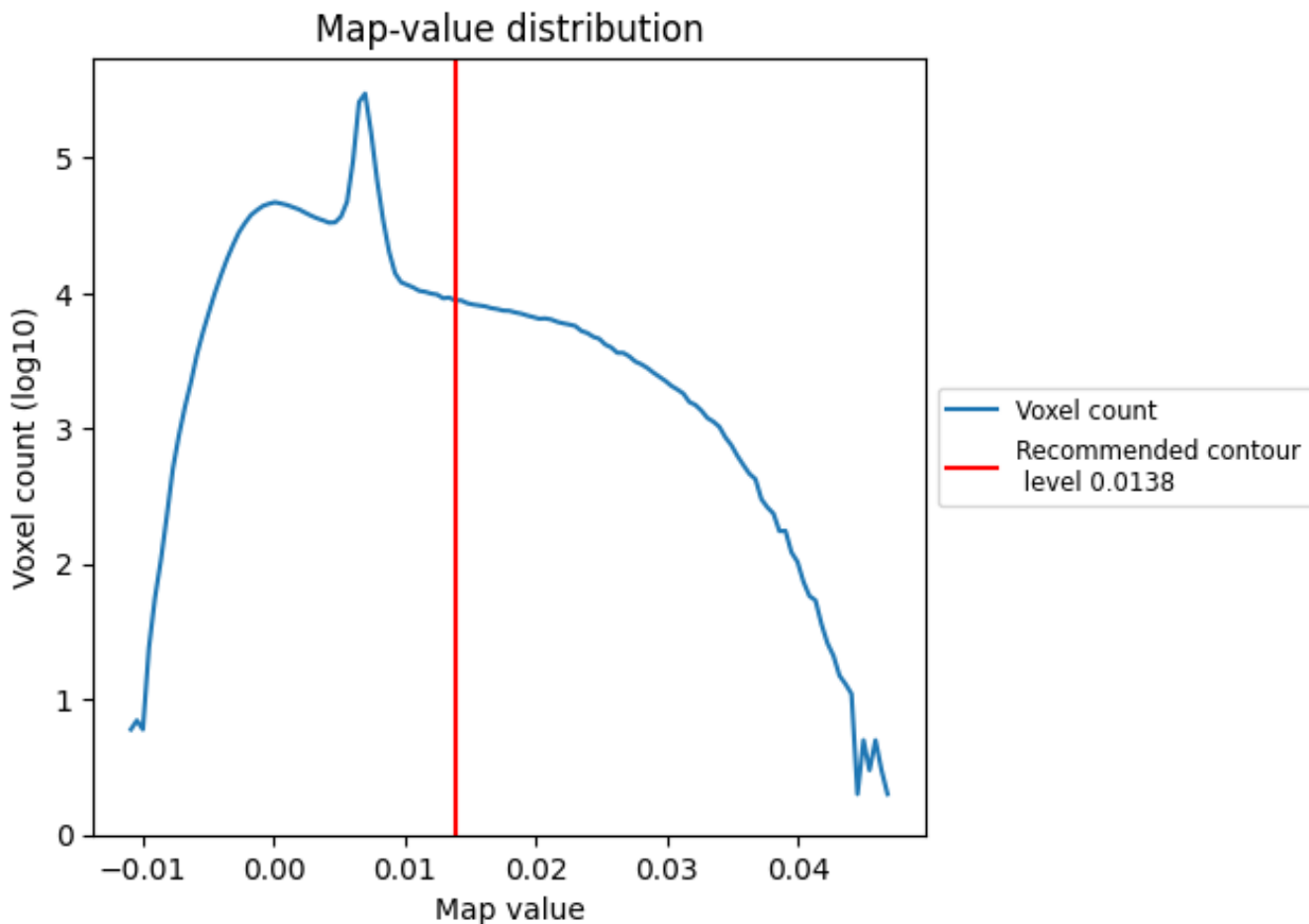
6.5 Mask visualisation

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

7 Map analysis [i](#)

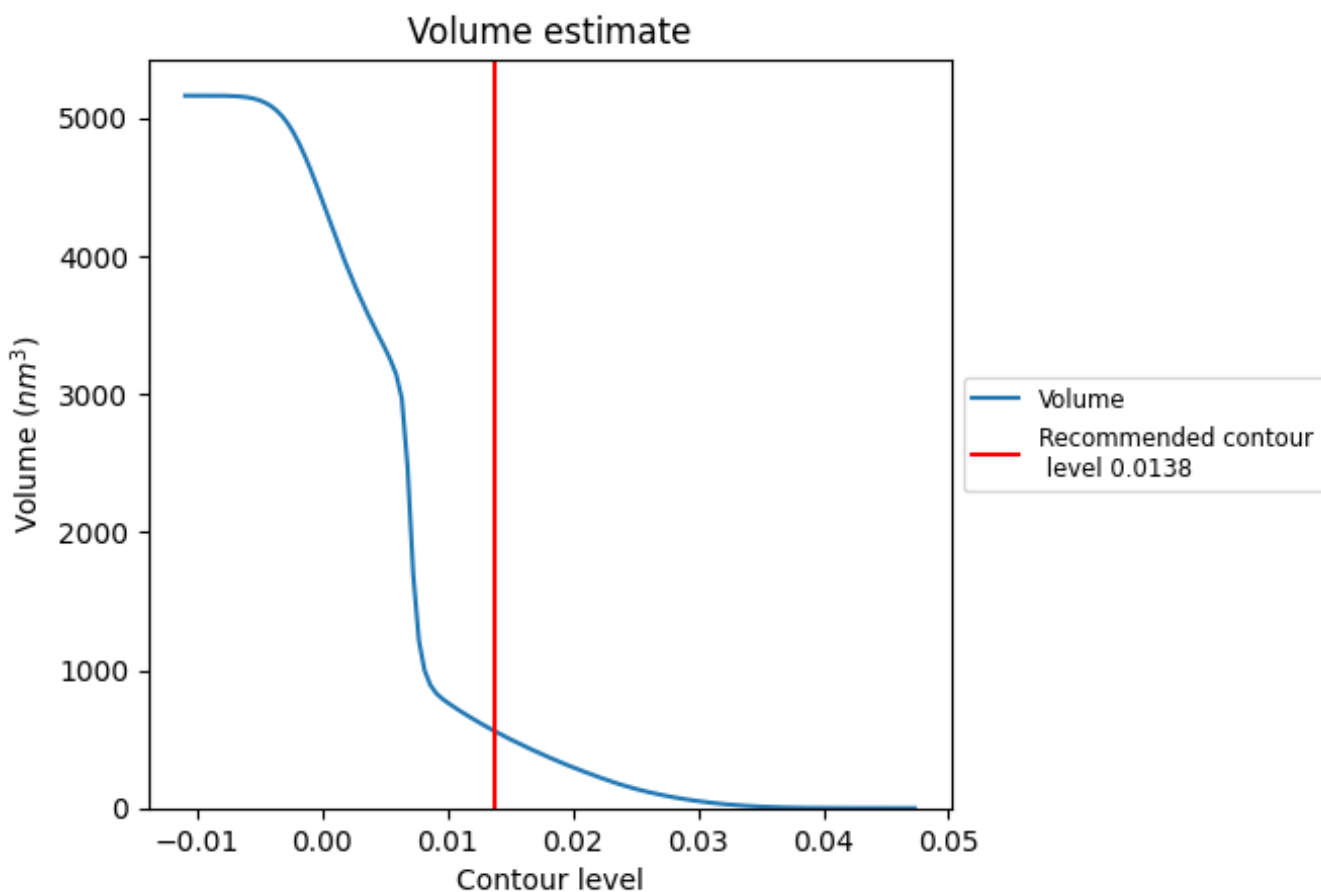
This section contains the results of statistical analysis of the map.

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.

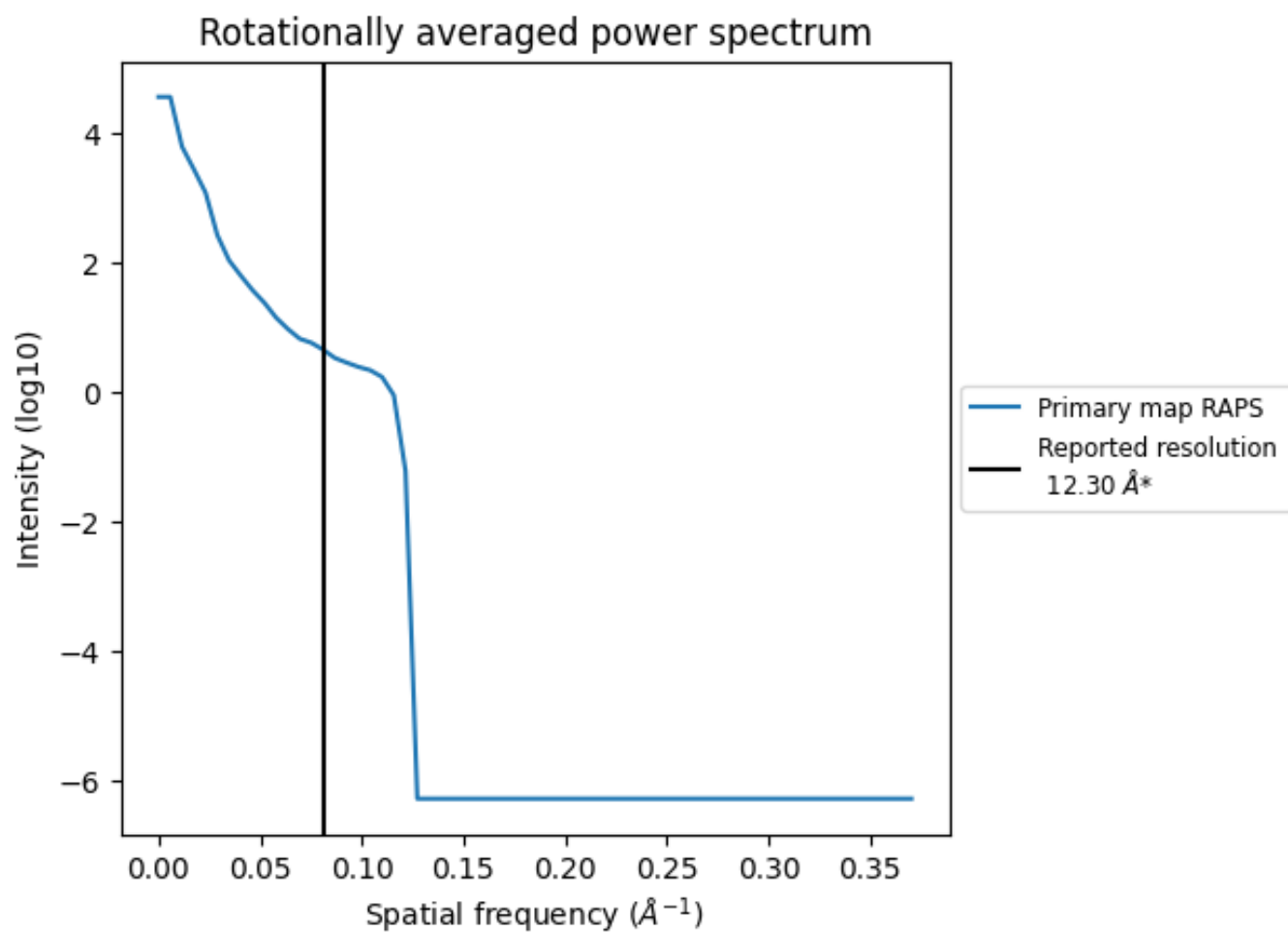
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm^3 ; this corresponds to an approximate mass of 503 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 [i](#)

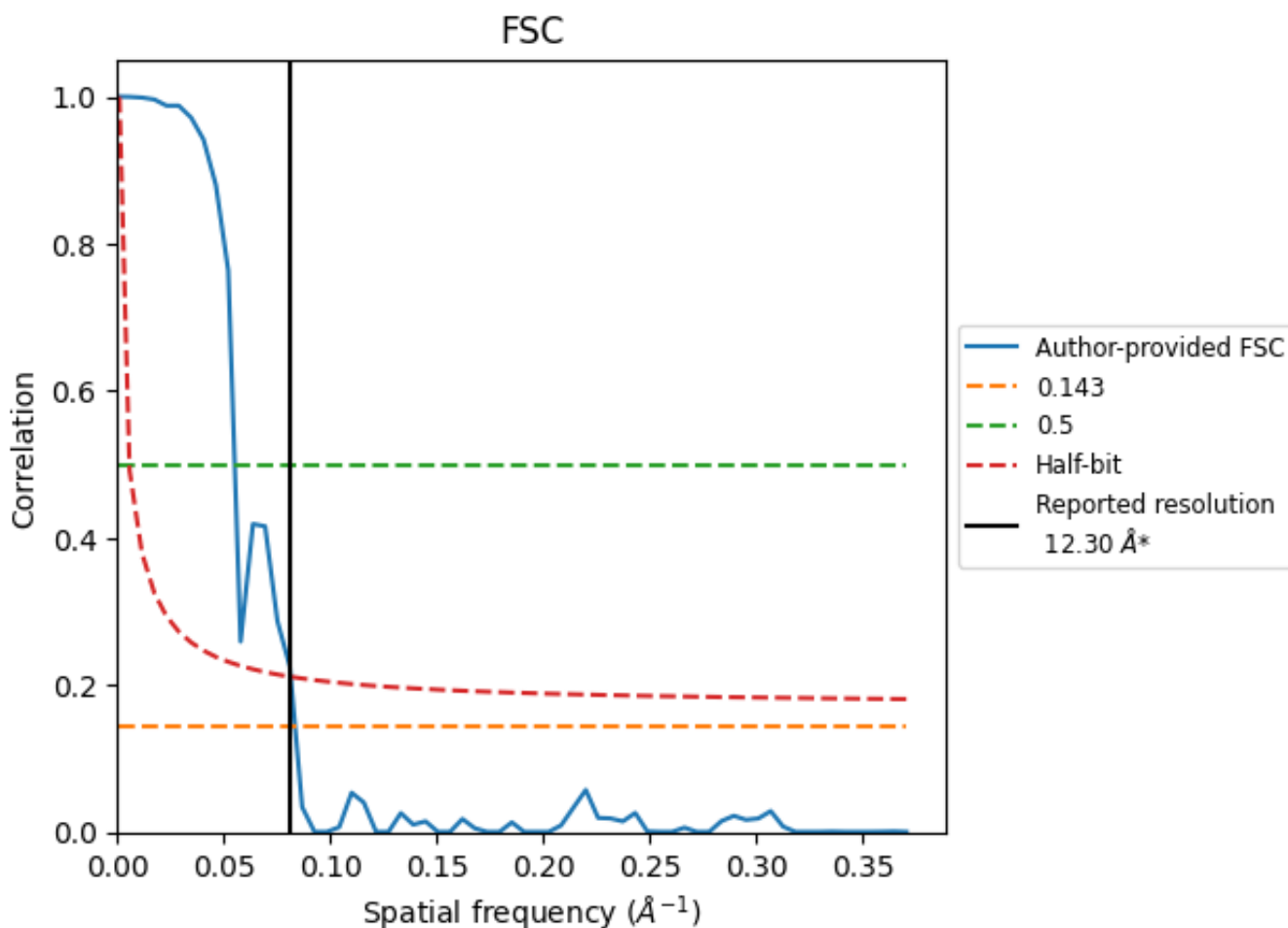


*Reported resolution corresponds to spatial frequency of 0.081 Å⁻¹

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 0.081 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.30	-	-
Author-provided FSC curve	11.98	18.15	12.29
Unmasked-calculated*	-	-	-

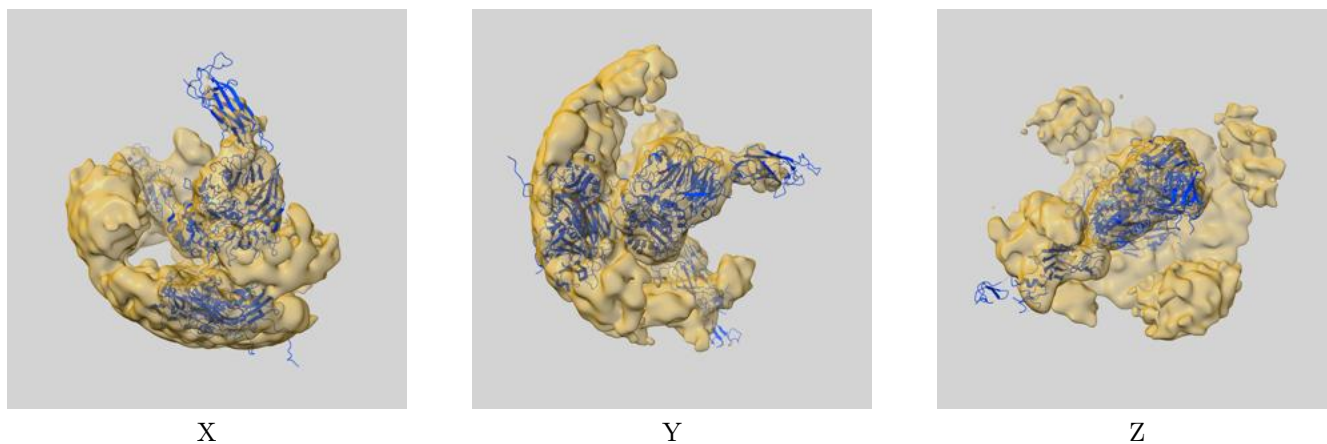
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

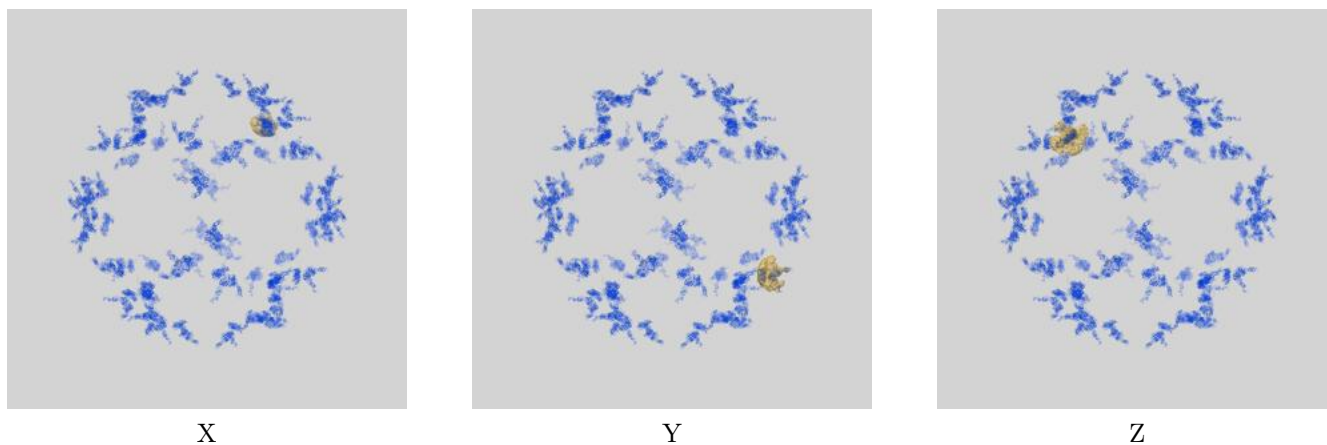
This section contains information regarding the fit between EMDB map EMD-3635 and PDB model 5NEU. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

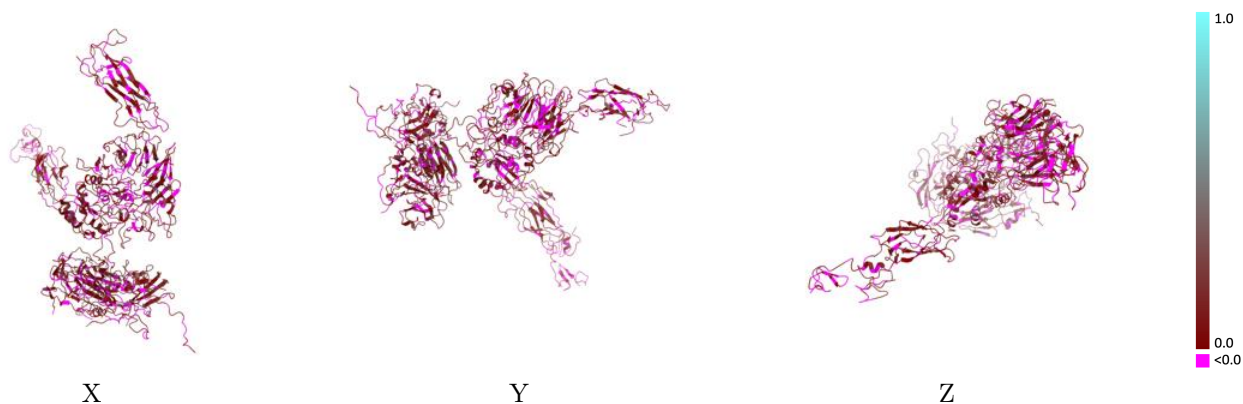


9.1.2 Map-model assembly overlay [i](#)



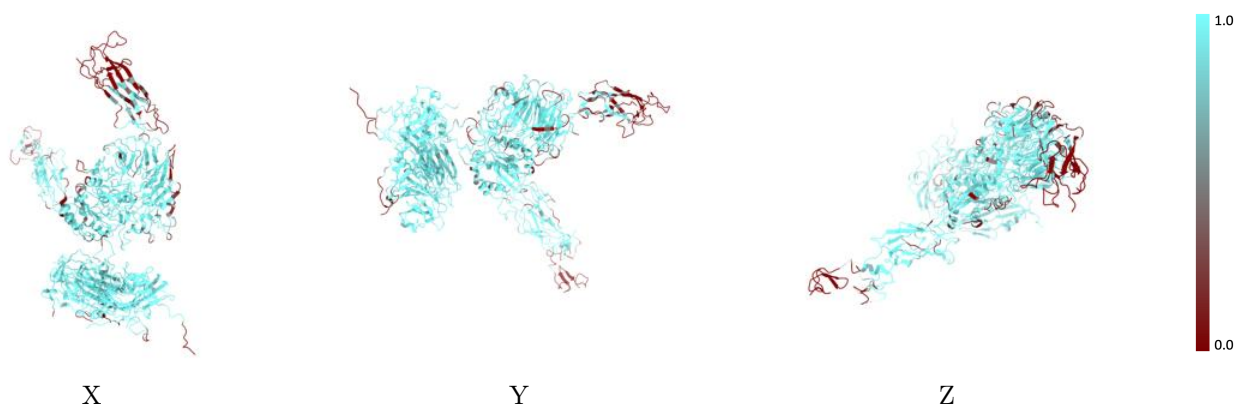
The images above show the 3D surface view of the map at the recommended contour level 0.0138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



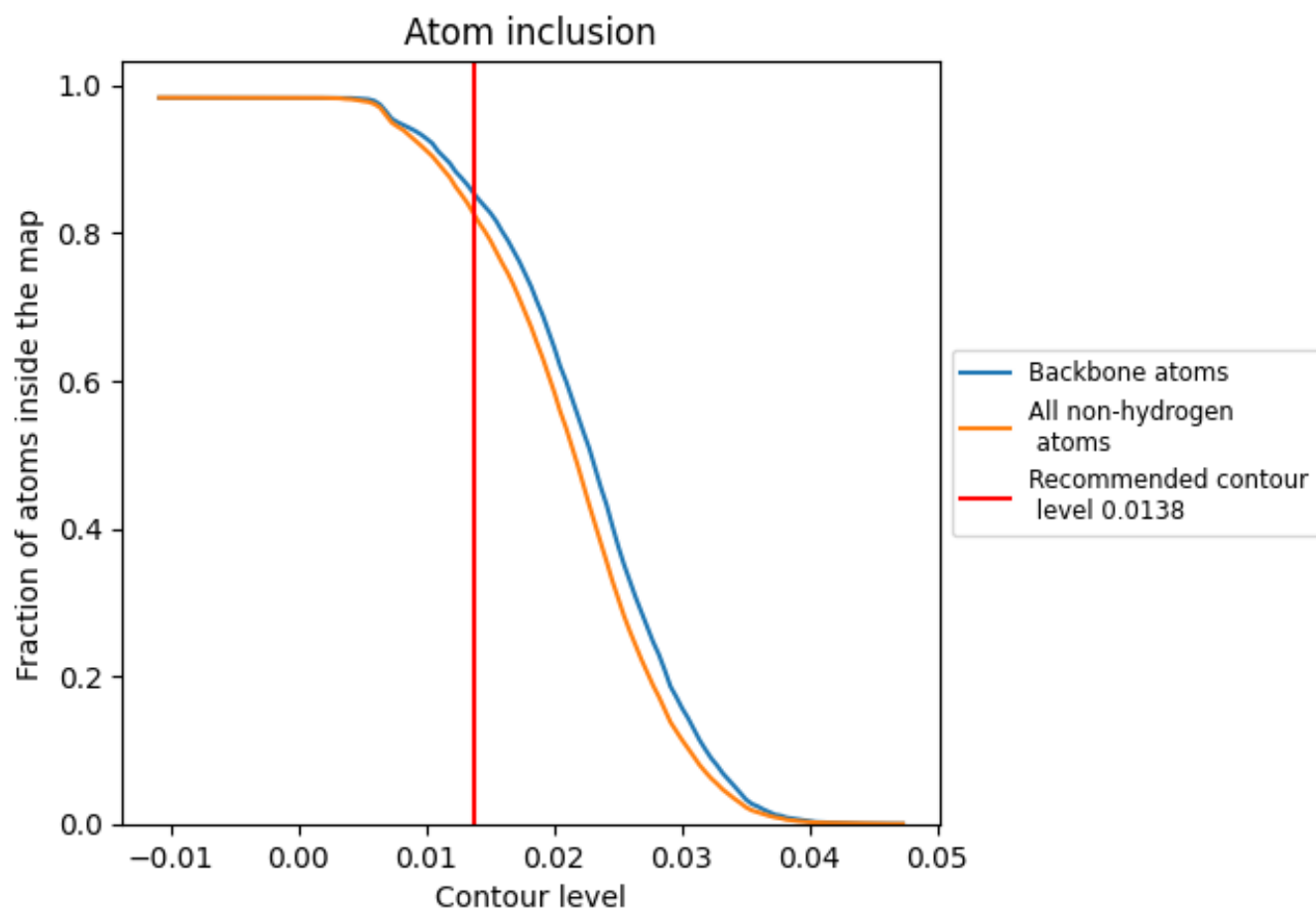
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0138).















9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.0138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8230	 0.0790
1	 0.9175	 0.0960
2	 0.9631	 0.0920
3	 0.9392	 0.0960
4	 0.7155	 0.0740
A	 0.7113	 0.0680
B	 0.8143	 0.0720

