



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 01:15 AM UTC

PDB ID : 8U3A / pdb_00008u3a
EMDB ID : EMD-41855
Title : TRPV1 in nanodisc bound with PI-Br4 bound in Conformation 1 (monomer)
Authors : Arnold, W.R.; Julius, D.; Cheng, Y.
Deposited on : 2023-09-07
Resolution : 2.30 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

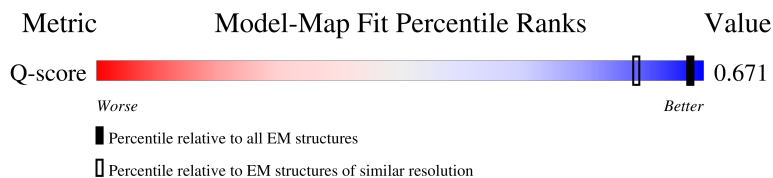
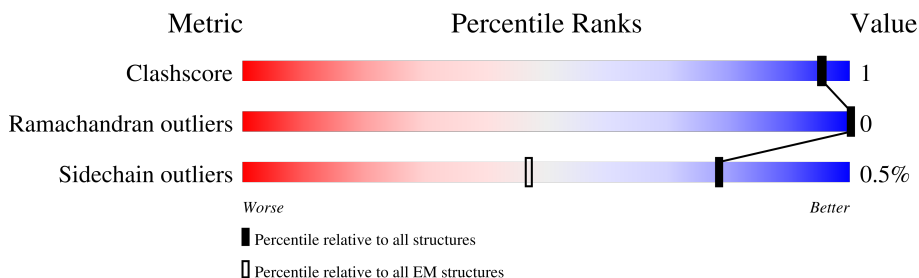
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	635	
1	D	635	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6970 atoms, of which 3539 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	284	Total	C	H	N	O	S	0	0
			4741	1569	2388	362	404	18		
1	D	121	Total	C	H	N	O	S	0	0
			2019	661	1032	147	170	9		

There are 52 discrepancies between the modelled and reference sequences:

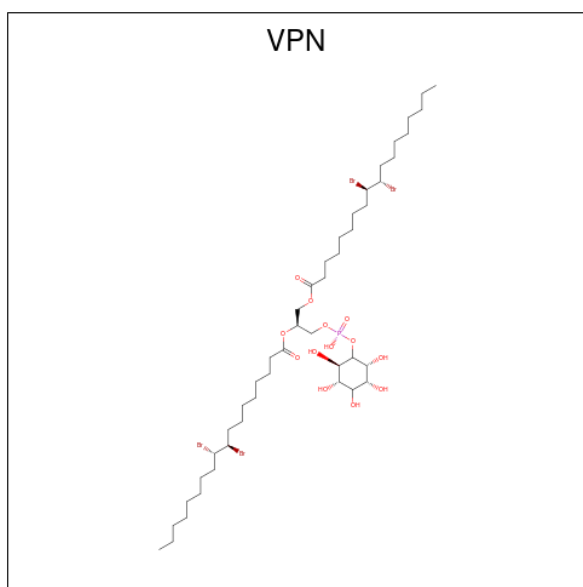
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	-	initiating methionine	UNP O35433
A	108	GLY	-	expression tag	UNP O35433
A	109	SER	-	expression tag	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	LEU	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	MET	deletion	UNP O35433
A	?	-	GLU	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	THR	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	HIS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	ARG	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	ALA	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433

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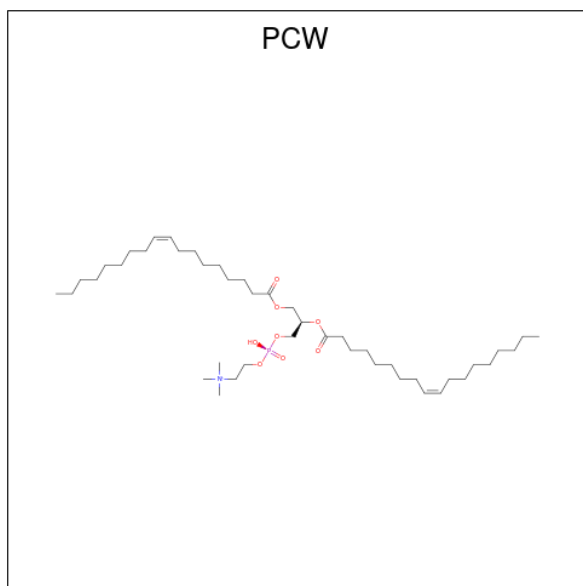
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP O35433
D	107	MET	-	initiating methionine	UNP O35433
D	108	GLY	-	expression tag	UNP O35433
D	109	SER	-	expression tag	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	LEU	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	MET	deletion	UNP O35433
D	?	-	GLU	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	THR	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	HIS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	ARG	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	ALA	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433

- Molecule 2 is (2S)-2-[(9,10-dibromooctadecanoyl)oxy]-3-[[[(S)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9R,10S)-9,10-dibromooctadecanoate (CCD ID: VPN) (formula: C₄₅H₈₃Br₄O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	Br	C	H	O	P	
2	A	1	105	2	32	57	13	1	0

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	68	20	38	1	8	1	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Na	0
			1	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			AltConf
5	A	7	Total	H	O	0
			21	14	7	
5	D	5	Total	H	O	0
			15	10	5	

LYS	VAL	ASN	THR	GLY	PRO	GLY
LEU	VAL	THR	THR	ASN	ASN	VAL
LEU	LEU	VAL	VAL	ARG	ARG	LEU
GLN	TYR	GLY	ASP	HIS	ALA	ALA
GLY	PHE	TYR	THR	ASP	MET	TYR
PHE	GLN	PHE	THR	LEU	LEU	LEU
THR	ARG	ARG	ARG	LEU	GLN	GLN
PRO	LYS	VAL	THR	VAL	VAL	ARG
ASP	GLY	THR	THR	GLY	GLY	GLY
GLY	TYR	GLY	GLY	PRO	PRO	ILE
LYS	VAL	GLY	ILE	LEU	HIS	HIS
ASP	ALA	ILE	ILE	ASN	ASN	GLY
ASP	SER	LEU	LEU	ARG	PRO	GLY
TYR	MET	SER	SER	LEU	GLY	GLY
ARG	VAL	VAL	VAL	LEU	CYS	CYS
TRP	PHE	SER	SER	GLN	ARG	ARG
CYS	SER	GLY	GLY	ASP	ASP	HIS
PHE	LEU	GLY	GLY	LYS	LYS	LEU
ARG	ALA	VAL	VAL	TRP	TRP	SER
VAL	MET	ARG	MET	TYR	ARG	LYS
GLY	GLY	GLY	GLY	PHE	PHE	PHE
VAL	THR	THR	THR	PHE	VAL	THR
ASN	ASN	ARG	ARG	VAL	LYS	GLY
THR	TRP	MET	GLY	GLY	ARG	TRP
THR	LEU	LEU	ILE	ILE	ALA	ALA
TRP	TYR	TYR	GLN	PHE	PHE	TYR
ASN	THR	THR	TYR	TYR	TYR	GLY
THR	ARG	THR	PHE	PHE	PRO	PRO
ASN	GLY	GLN	GLN	ASN	ASN	VAL
VAL	VAL	PHE	ARG	PHE	HIS	VAL
GLY	0560	ARG	ARG	VAL	SER	SER
ILE	F580	PRO	PRO	TYR	LEU	TYR
ASN	F580	SER	SER	CYS	ASP	ASP
GLU	L669	LYS	LYS	TYR	LEU	LEU
ASP	L669	SER	SER	ILE	CYS	CYS
PRO	L703	LEU	LEU	ILE	ILE	ILE
GLY	L703	PHE	PHE	VAL	PHE	ASP
ILE	THR	ILE	VAL	THR	THR	THR
ASN	LEU	ASP	ASP	ASP	ASP	CYS
GLU	THR	THR	THR	ALA	ALA	GLY
PRO	LYS	GLY	GLY	ALA	LYS	LYS
GLY	SER	SER	ILE	TYR	ASN	ASN
	PHE	PHE	LEU	ARG	SER	VAL
	LYS	LYS	PHE	PRO	LEU	GLY
	CYS	CYS	VAL	VAL	GLY	VAL
	MET	MET	GLN	GLY	GLY	ILE
	ARG	ARG	SER	LEU	LEU	ALA
	LYS	LYS	SER	PRO	PRO	ALA
	ALA	ALA	PHE	TYR	TYR	TYR
	PHE	PHE	MET	TYR	SER	SER
	ARG	ARG	LEU	LYS	SER	SER
	SER	SER	VAL	LYS	GLY	THR
	GLY	GLY	SER	LEU	LEU	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	715030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	267.904, 267.904, 267.904	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.644, 0.644, 0.644	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: NA, PCW, VPN

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	0.48	0/2410	0.80	2/3254 (0.1%)
1	D	0.47	0/1005	0.80	1/1355 (0.1%)
All	All	0.48	0/3415	0.80	3/4609 (0.1%)

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	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	387	ILE	N-CA-C	-6.09	105.75	111.48
1	A	404	SER	CB-CA-C	-5.39	99.01	110.76
1	D	580	PHE	CA-C-O	-5.04	115.53	120.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	491	ARG	Sidechain
1	A	500	ARG	Sidechain

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	2353	2388	2384	7	0
1	D	987	1032	1031	0	0
2	A	48	57	0	0	0
3	A	30	38	34	0	0
4	A	1	0	0	0	0
5	A	7	14	0	0	0
5	D	5	10	0	0	0
All	All	3431	3539	3449	7	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 1.

The worst 5 of 7 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:A:399:ILE:HG23	1:A:412:MET:HE3	1.89	0.54
1:A:386:CYS:HA	1:A:390:CYS:HB2	1.97	0.47
1:A:482:VAL:HG13	1:A:527:VAL:HG21	1.99	0.44
1:A:535:LYS:HE2	1:A:538:VAL:HG21	2.01	0.42
1:A:430:VAL:HG11	1:A:705:ILE:HA	2.03	0.41

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	276/635 (44%)	262 (95%)	14 (5%)	0	100	100
1	D	119/635 (19%)	110 (92%)	9 (8%)	0	100	100
All	All	395/1270 (31%)	372 (94%)	23 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	260/562 (46%)	259 (100%)	1 (0%)	84	92
1	D	108/562 (19%)	107 (99%)	1 (1%)	70	84
All	All	368/1124 (33%)	366 (100%)	2 (0%)	78	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	TYR
1	D	669	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCW	A	802	-	29,29,53	1.46	6 (20%)	35,37,61	1.20	3 (8%)
2	VPN	A	801	-	48,48,63	1.23	5 (10%)	57,62,79	1.25	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	802	-	-	11/33/33/57	-
2	VPN	A	801	-	-	25/46/70/88	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	VPN	O22-C20	3.16	1.42	1.33
2	A	801	VPN	O50-C24	-3.16	1.39	1.46
2	A	801	VPN	O50-C51	2.73	1.42	1.34
3	A	802	PCW	O2-C31	2.64	1.41	1.34
3	A	802	PCW	O3-C11	2.58	1.40	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	VPN	O50-C51-C53	4.23	120.64	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	PCW	O2-C31-C32	3.19	118.38	111.48
3	A	802	PCW	O3-C11-C12	2.71	120.08	111.83
3	A	802	PCW	O1P-P-O2P	-2.66	100.06	112.44
2	A	801	VPN	O22-C20-C19	2.61	119.81	111.83

There are no chirality outliers.

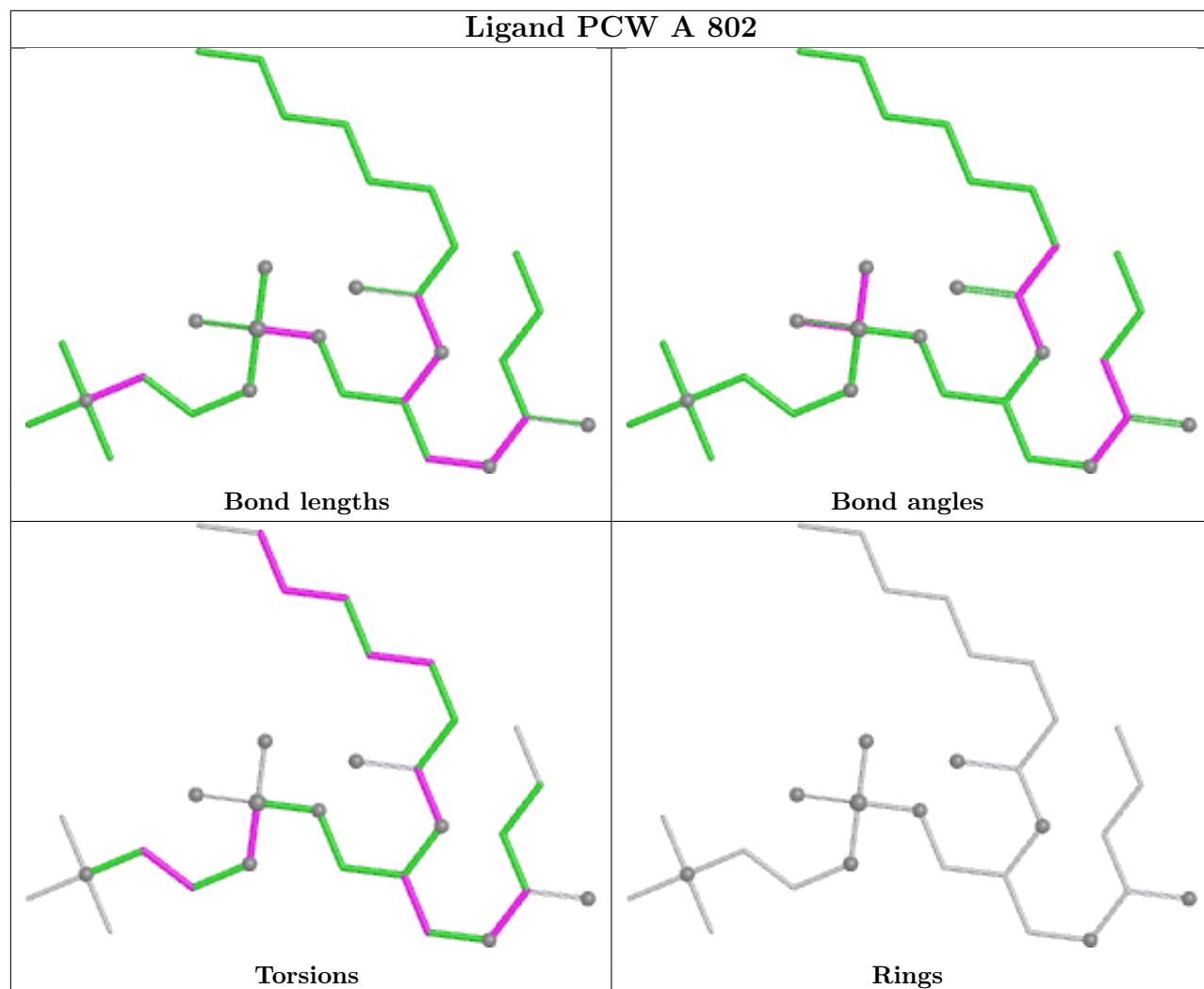
5 of 36 torsion outliers are listed below:

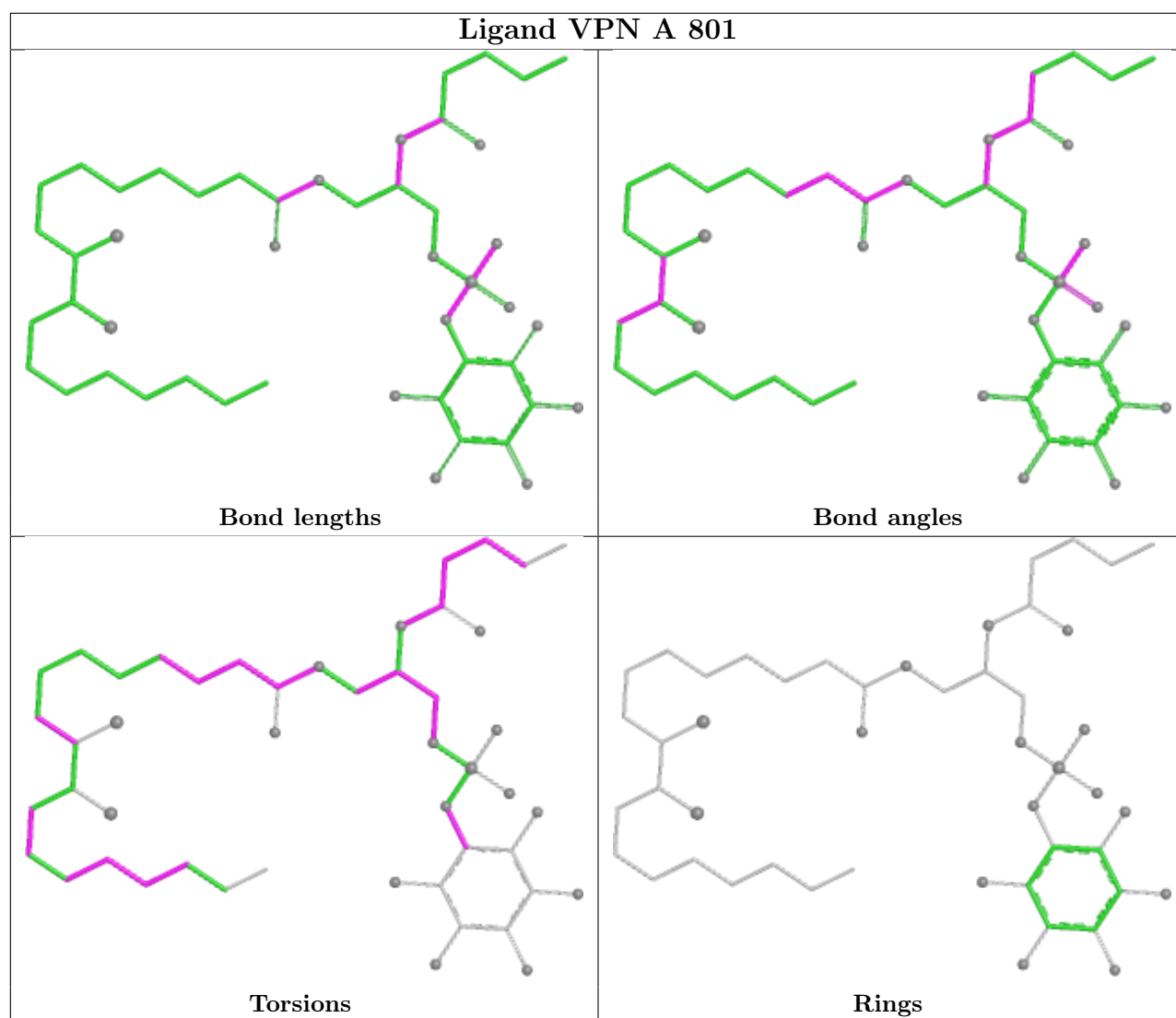
Mol	Chain	Res	Type	Atoms
2	A	801	VPN	BR12-C11-C13-C14
2	A	801	VPN	C53-C51-O50-C24
2	A	801	VPN	C06-C07-C08-C09
3	A	802	PCW	O4P-C4-C5-N
2	A	801	VPN	O21-C20-O22-C23

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

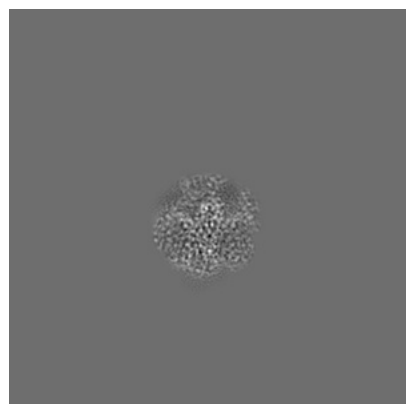
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41855. 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](#)

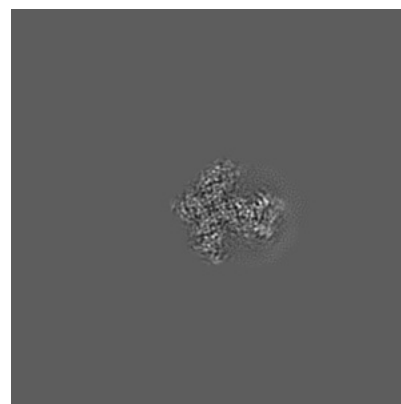
6.1.1 Primary map



X

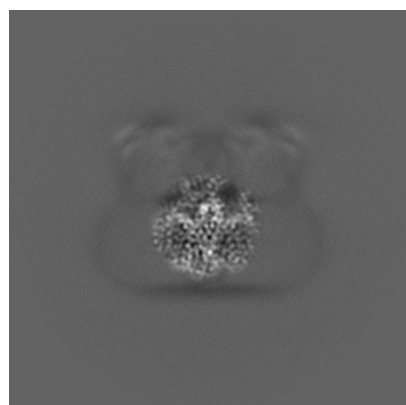


Y

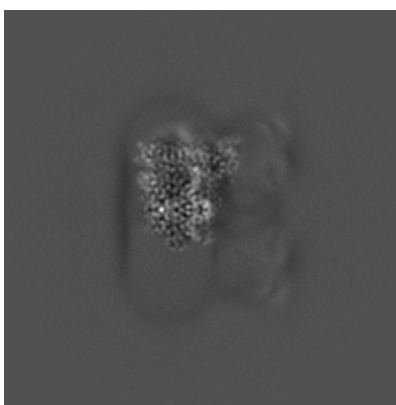


Z

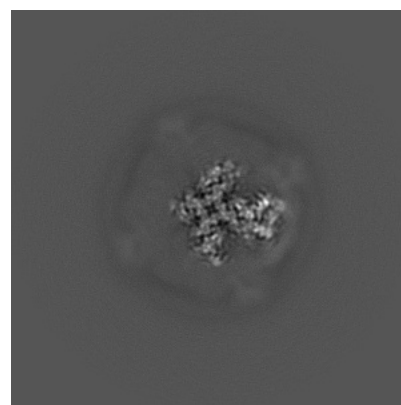
6.1.2 Raw map



X



Y

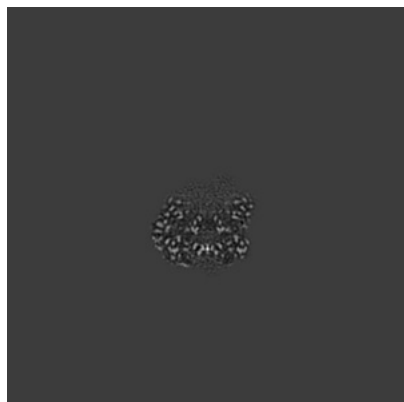


Z

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

6.2 Central slices [i](#)

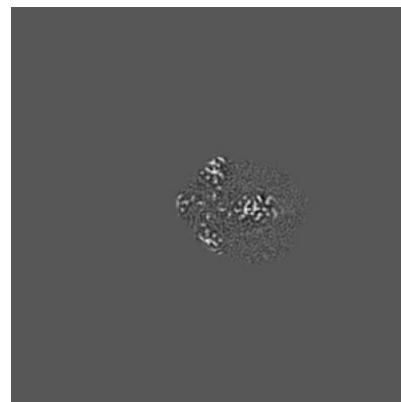
6.2.1 Primary map



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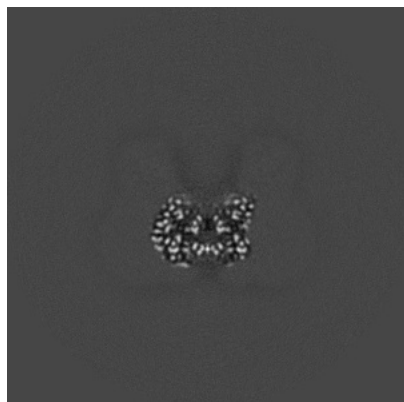


Y Index: 208

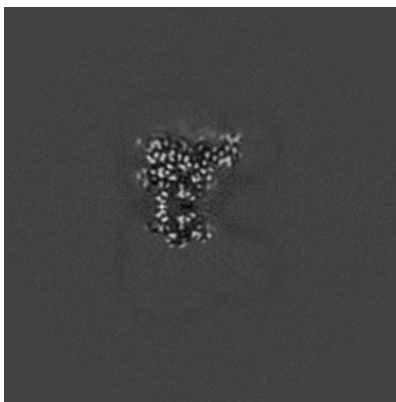


Z Index: 208

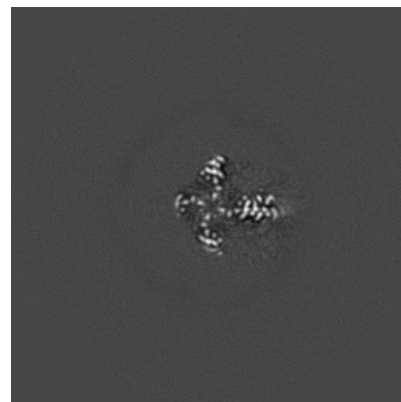
6.2.2 Raw map



X Index: 208



Y Index: 208

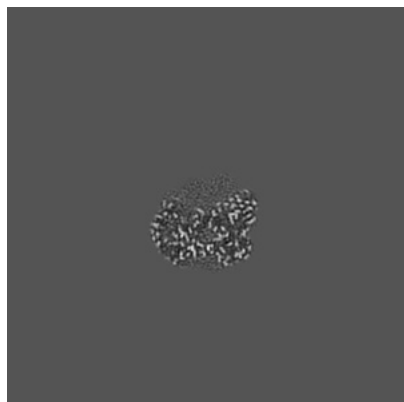


Z Index: 208

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

6.3 Largest variance slices [i](#)

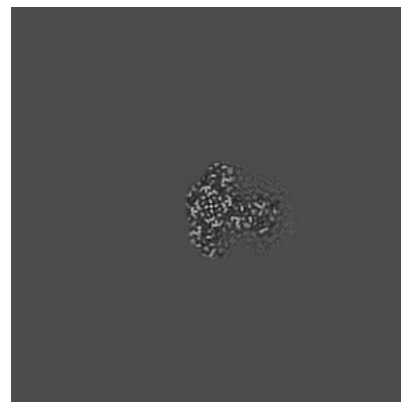
6.3.1 Primary map



X Index: 213

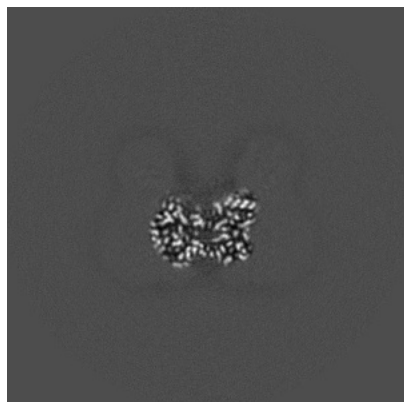


Y Index: 205

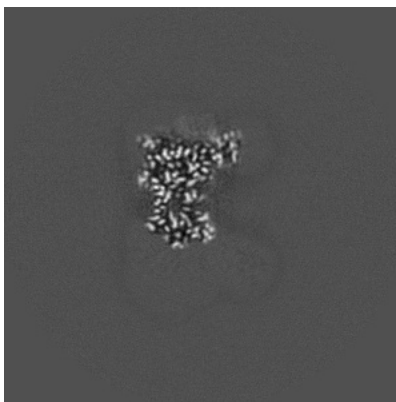


Z Index: 165

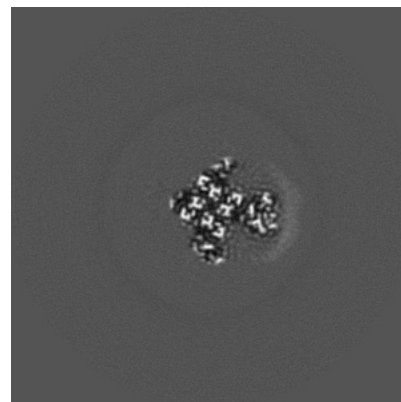
6.3.2 Raw map



X Index: 211



Y Index: 212

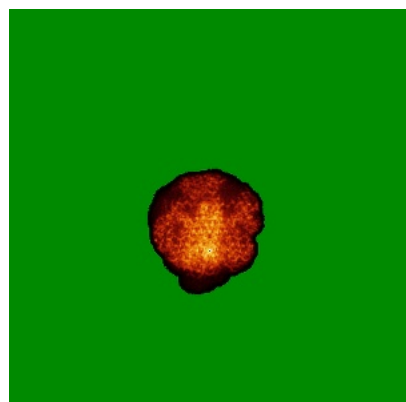


Z Index: 184

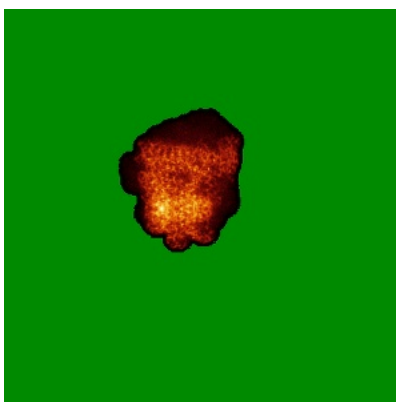
The images above show the largest variance slices of the map in three orthogonal directions.

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

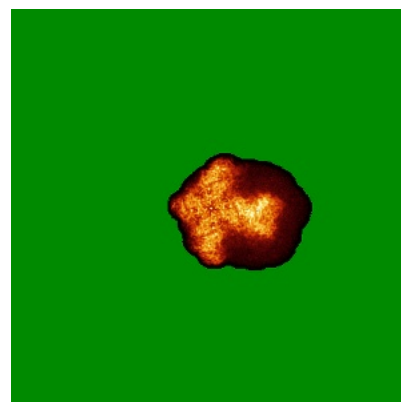
6.4.1 Primary map



X

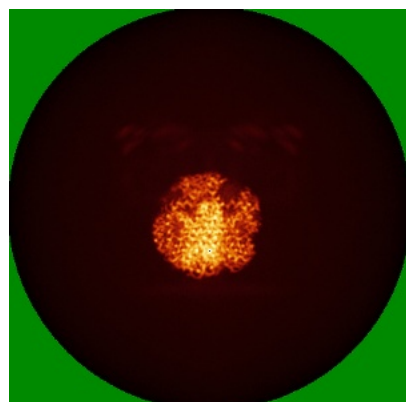


Y

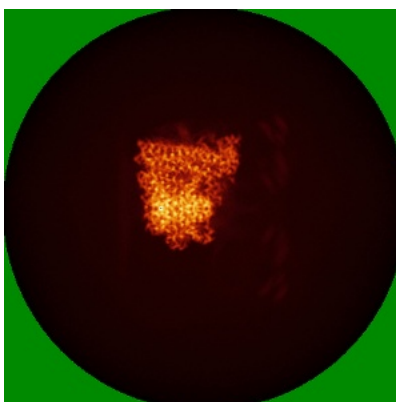


Z

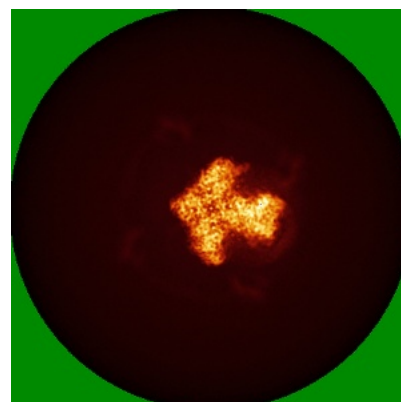
6.4.2 Raw map



X



Y



Z

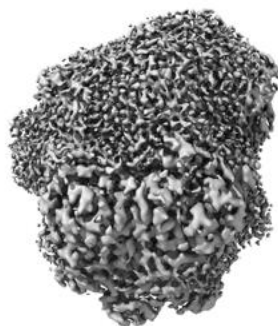
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

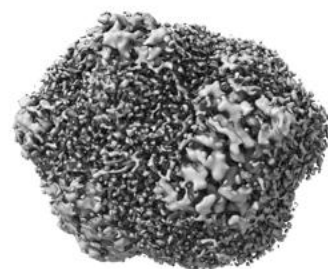
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

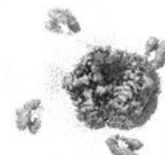
6.5.2 Raw map



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.

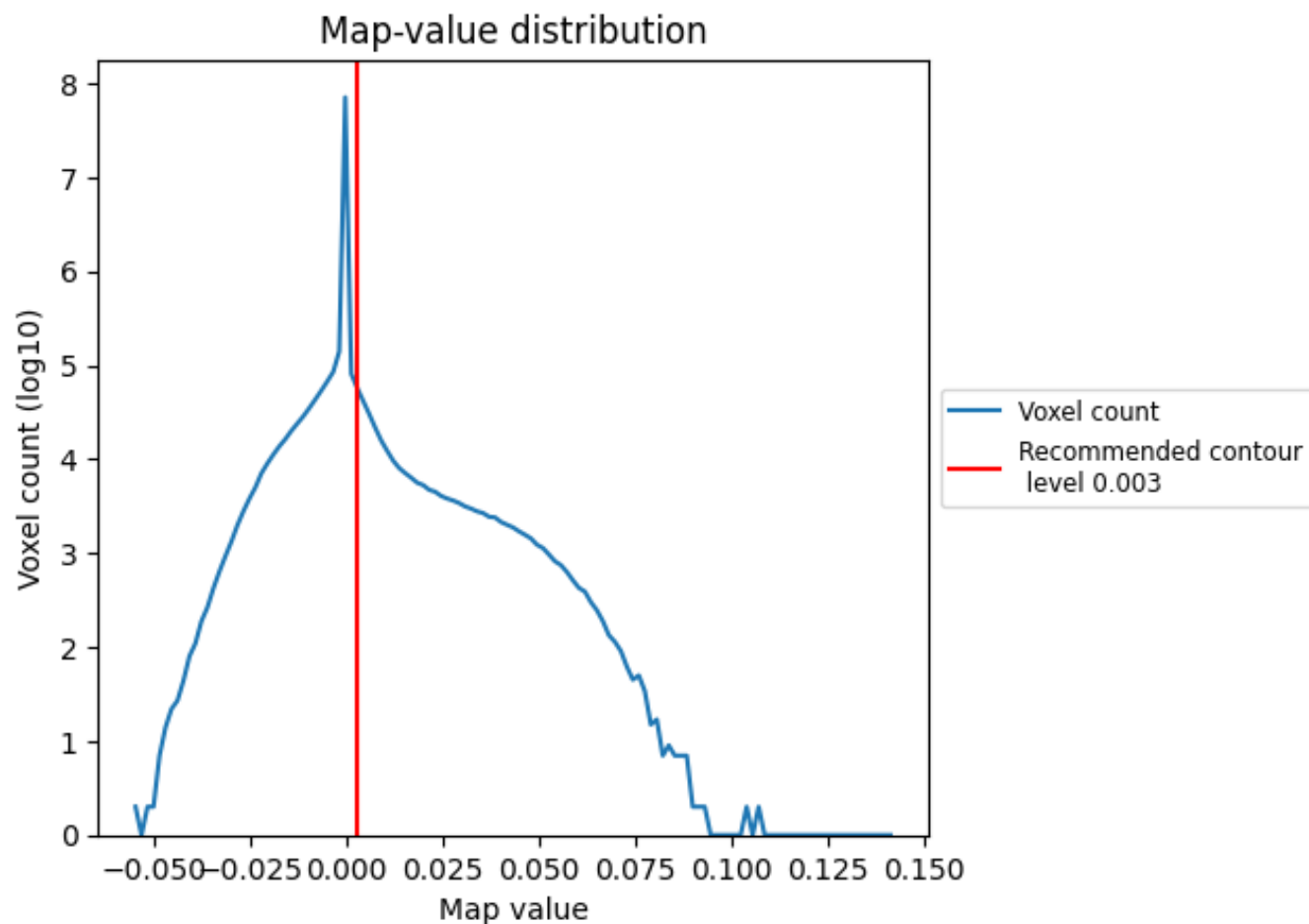
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

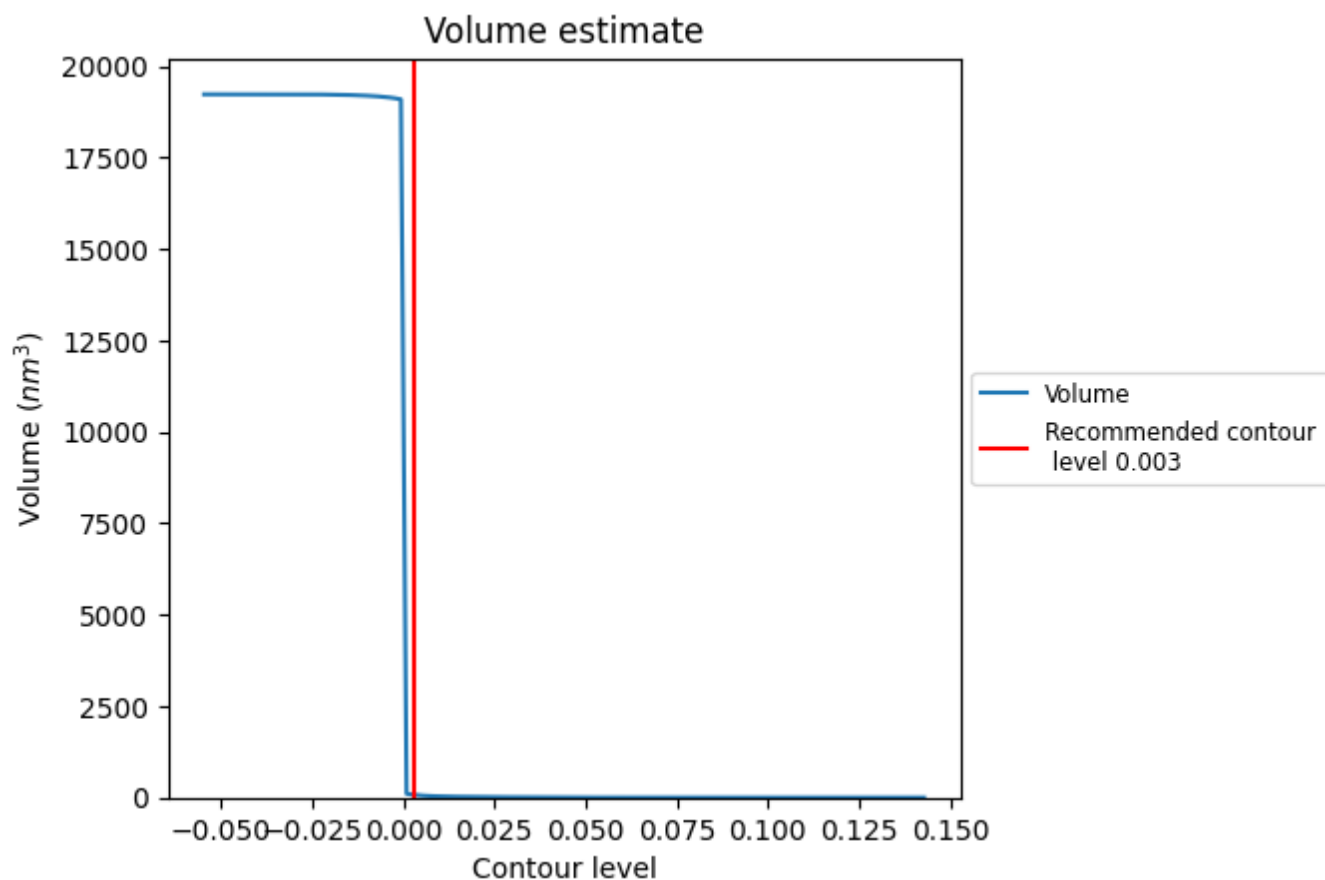
This section contains the results of statistical analysis of the map.

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.

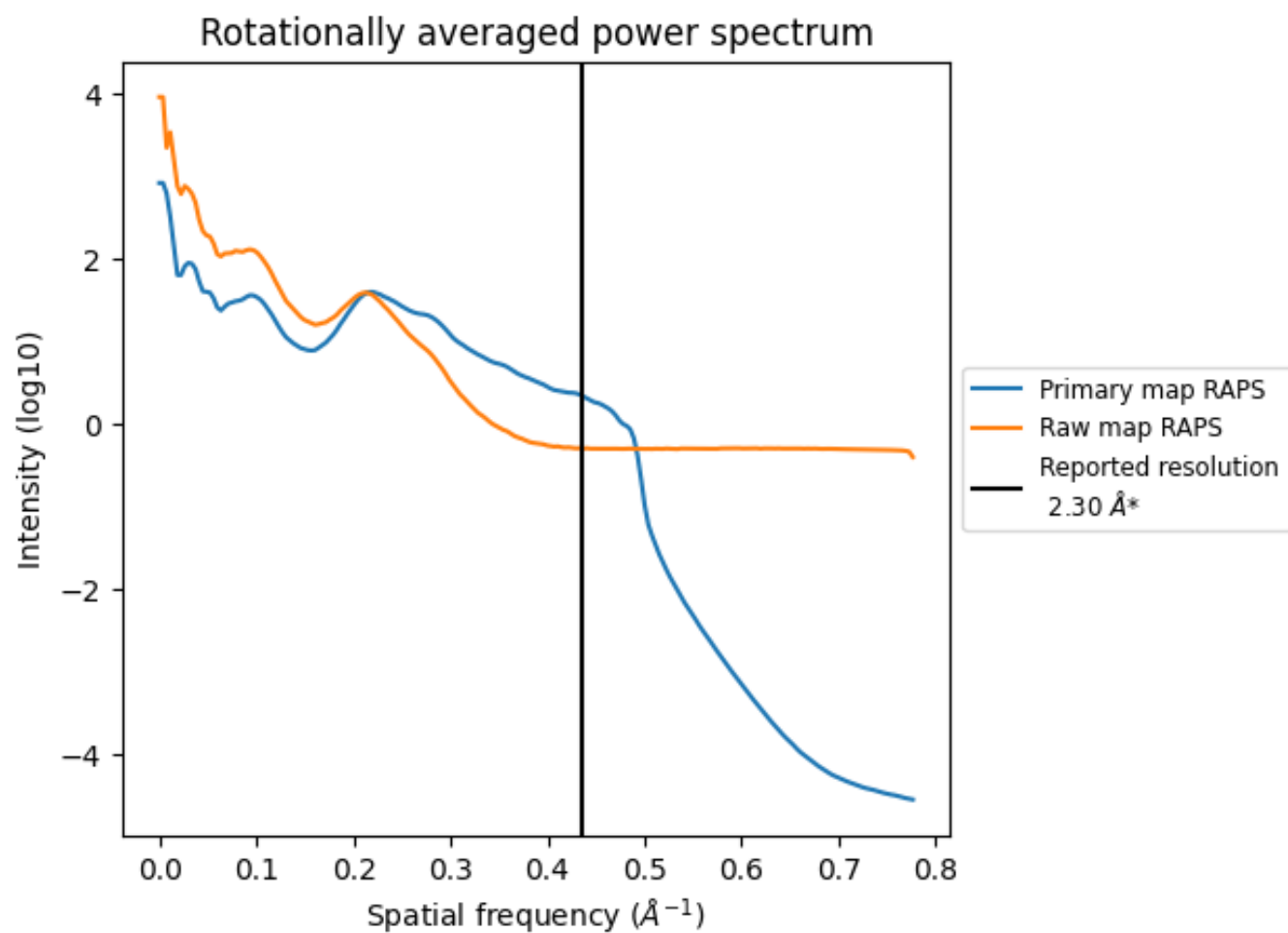
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm^3 ; this corresponds to an approximate mass of 68 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 ⓘ

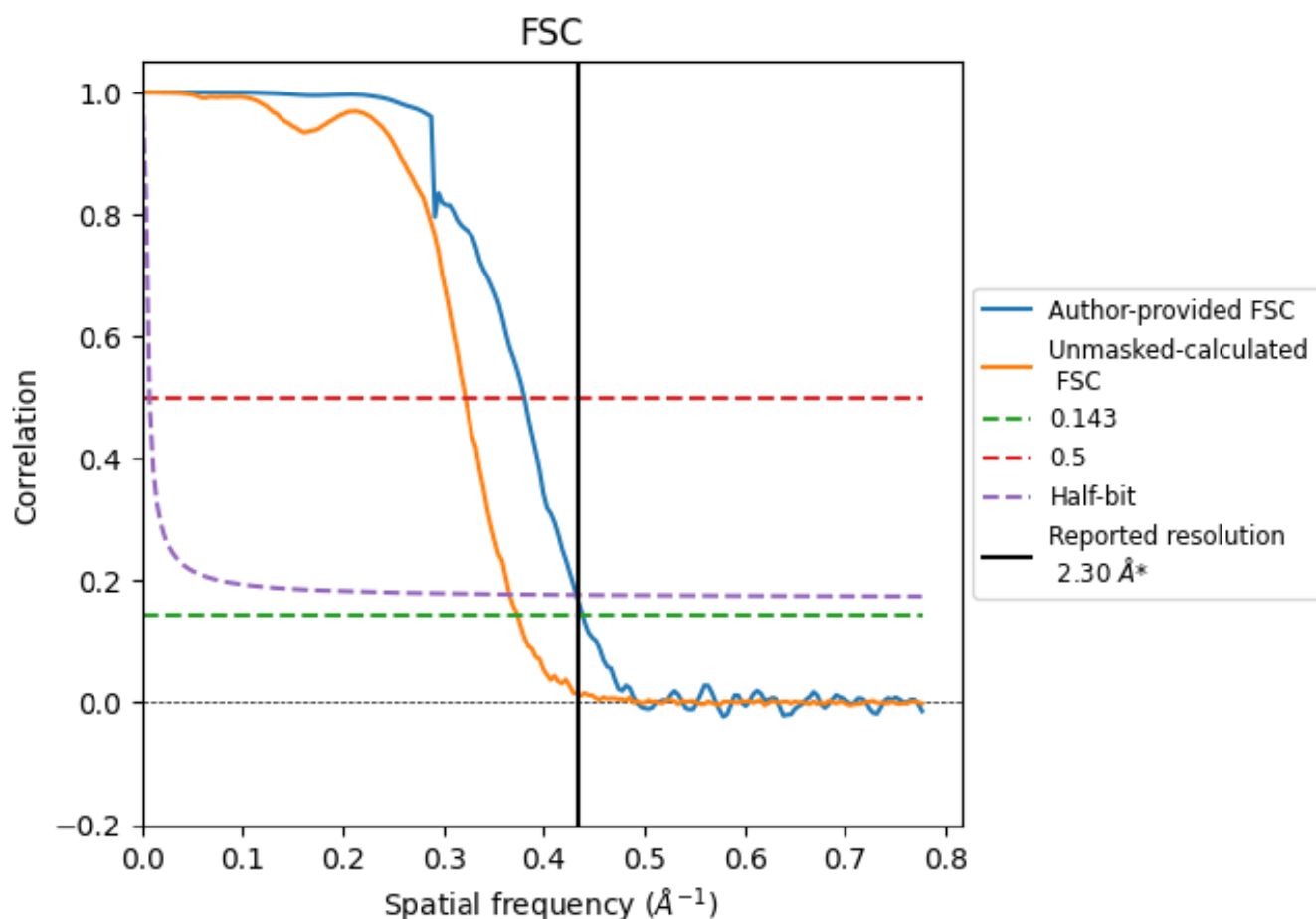


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

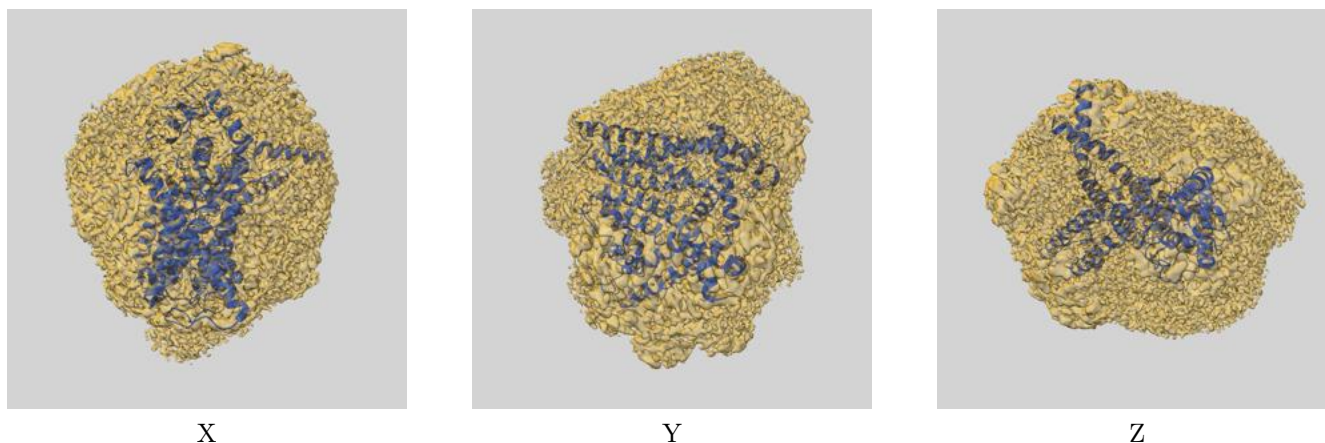
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.28	2.63	2.31
Unmasked-calculated*	2.68	3.11	2.74

*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 2.68 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41855 and PDB model 8U3A. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



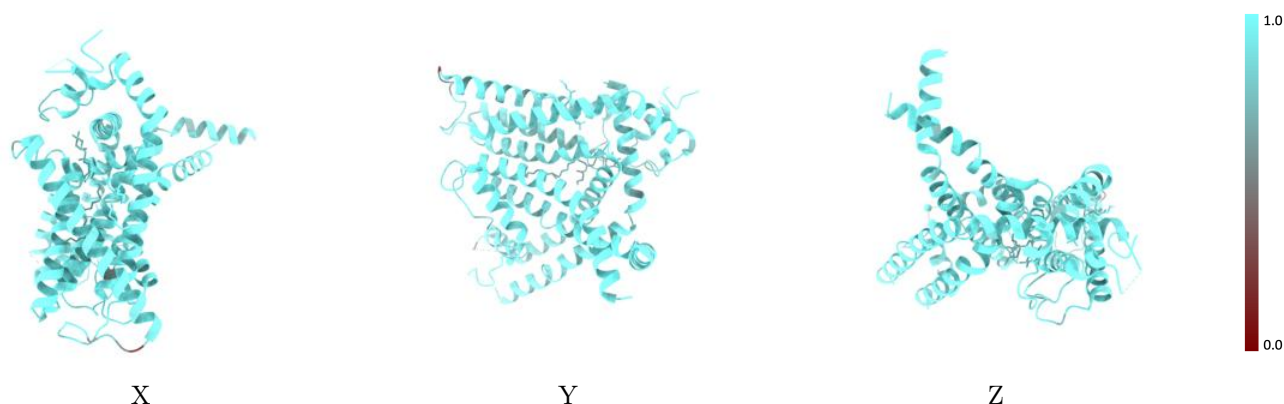
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



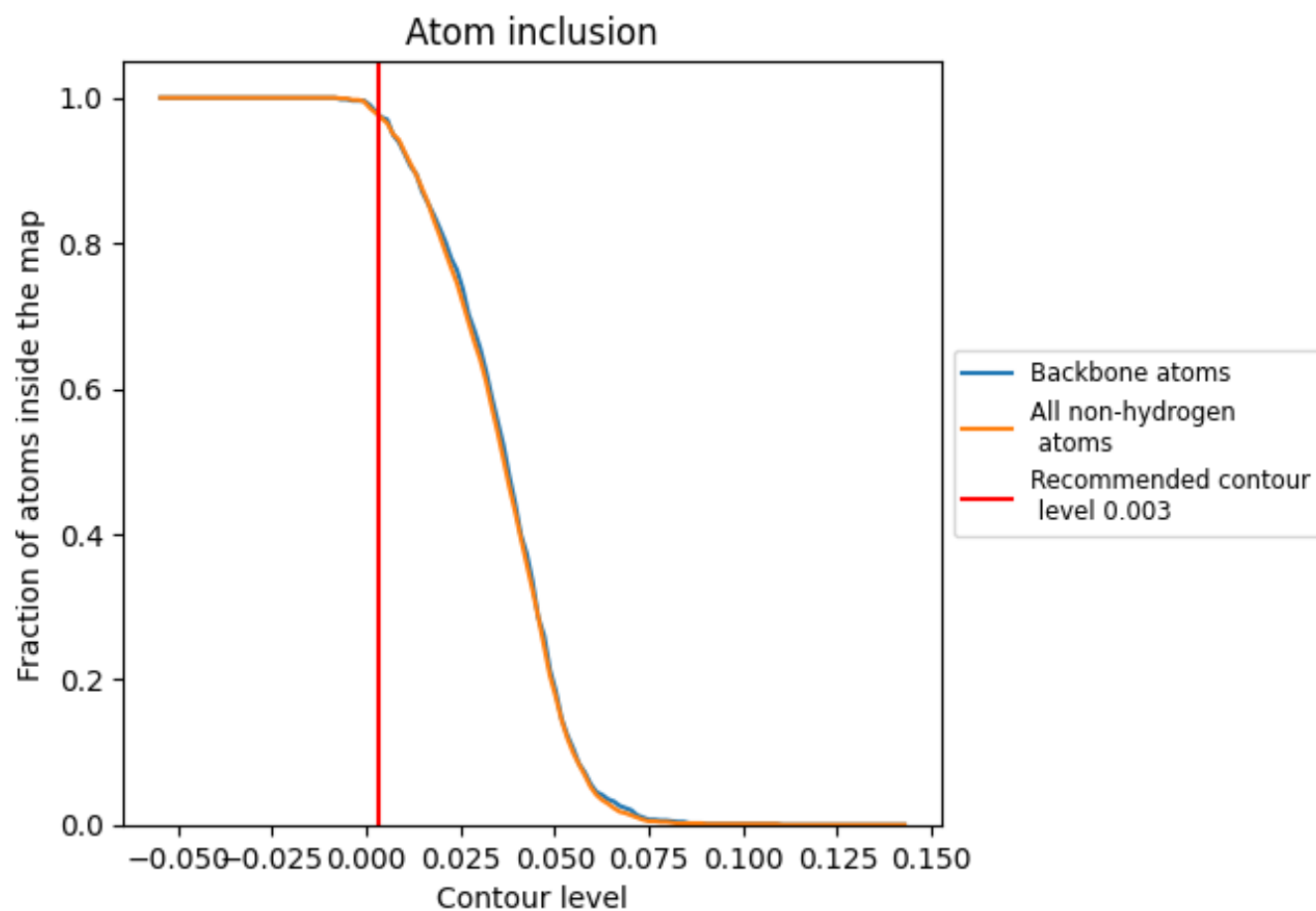
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9770	0.6710
A	0.9630	0.6600
D	0.9830	0.6990

