



wwPDB EM Validation Summary Report ⓘ

Jul 4, 2026 – 01:08 PM JST

PDB ID : 9VXX / pdb_00009vxx
EMDB ID : EMD-65444
Title : Cryo-EM Structure of Measles Virus Polymerase in complex with ERDRP-0519
Authors : Xue, L.; Gui, J.; Chang, T.; Pan, H.; Xiong, X.
Deposited on : 2025-07-20
Resolution : 2.73 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

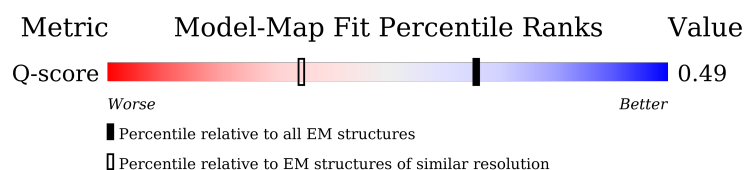
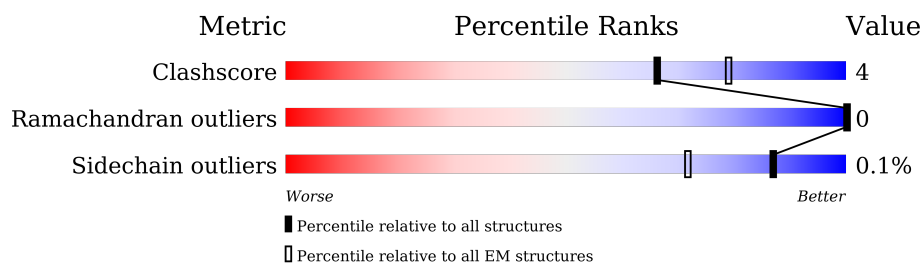
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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.



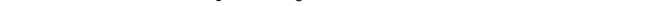
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	2183	
2	B	507	
2	C	507	
2	D	507	

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	E	507	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12608 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1254	Total	C	N	O	S	0	0
			10077	6440	1742	1840	55		

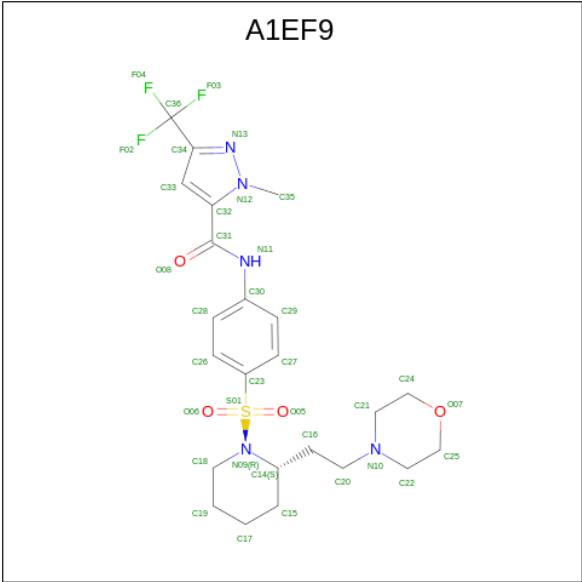
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	148	Total	C	N	O	S	0	0
			1159	736	208	210	5		
2	C	47	Total	C	N	O	S	0	0
			372	233	65	73	1		
2	D	70	Total	C	N	O	S	0	0
			538	337	91	109	1		
2	E	55	Total	C	N	O	S	0	0
			425	269	74	81	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

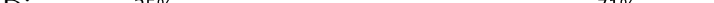
- Molecule 4 is 2-methyl- {N}-[4-[(2 {S})-2-(2-morpholin-4-ylethyl)piperidin-1-yl]sulfonylphenyl]-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EF9) (formula: C₂₃H₃₀F₃N₅O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

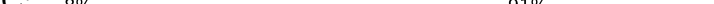
L Y S	ARG	VAL	PRO	LEU	ALA	TYR	VAL	LYS
	GLU	GLY	ARG	PRO	PRO	LYS	ILE	ARG
	LEU	GLY	TYR	ASN	TYR	ASN	GLU	ALA
	ALA	VAL	SER	ASP	VAL	GLU	ILE	ARG
	PHE	SER	PHE	THR	GLU	ILE	SER	LEU
	LYS	ARG	ILE	ILE	VAL	SER	ARG	PRO
	ASP	GLY	SER	GLU	VAL	THR	GLY	ASN
	ASN	ILE	THR	GLU	ARG	CYS	ASP	TRP
	ILE	PRO	LEU	LEU	ARG	GLY	ASP	LYS
	PHE	LYS	VAL	ALA	MET	GLY	PHE	ASN
H I S	GLN	LYS	GLU	LEU	ARG	GLY	GLY	ASN
	ASN	ILE	THR	GLU	VAL	GLY	GLY	ASN
	LEU	THR	ASP	LEU	VAL	GLY	GLY	ASN
	PHE	LYS	LEU	SER	ASN	ILE	ASP	ILE
	MET	LEU	ASN	MET	VAL	GLY	ASP	ILE
	THR	THR	LYS	ASN	VAL	GLY	ASP	ILE
	ALA	PRO	LYS	ASN	VAL	GLY	ASP	ILE
	TYR	ILE	ALA	ALA	VAL	GLY	ASP	ILE
	PRO	GLU	SER	LEU	VAL	LEU	GLY	ASN
	VAL	GLN	ARG	LEU	VAL	PHE	GLY	ASN
L Y S	LEU	VAL	LEU	GLY	PHE	GLY	GLY	ASN
	VAL	ILE	ASN	LYS	ASN	GLY	GLY	ASN
	SER	ILE	SER	ILE	ILE	GLY	GLY	ASN
	THR	ILE	PRO	ILE	VAL	GLY	GLY	ASN
	ALA	ALA	GLN	VAL	VAL	GLY	GLY	ASN
	GLU	LYS	ASN	LEU	VAL	GLY	GLY	ASN
	GLY	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	GLY	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	GLY	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	GLY	GLY	GLY	LEU	VAL	GLY	GLY	ASN
A L A	GLU	VAL	ILE	VAL	VAL	GLY	GLY	ASN
	LEU	ILE	ASN	VAL	VAL	GLY	GLY	ASN
	VAL	ASN	GLN	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
	VAL	GLY	GLY	LEU	VAL	GLY	GLY	ASN
P R O	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
T Y R	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
L E U	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
A R G	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN
	ASN	VAL	ASN	ASN	ASN	ASN	ASN	ASN

- Molecule 2: Phosphoprotein

Chain B:  25% 71%

PRO	ASN	ASP	PRO	THR	ASP	GLU	THR	ASP	LYS	SER	MET
ASN	ASP	GLY	ILE	GLU	VAL	GLY	GLU	VAL	GLY	LYS	ALA
PRO	PRO	GLY	ALA	THR	THR	ALA	ALA	THR	GLN	PRO	LYS
THR	THR	ASP	SER	SER	ALA	ASP	LEU	GLY	ASP	LEU	GLN
ALA	ASP	TYR	LEU	LEU	GLY	ALA	LEU	GLY	ASP	SER	ARG
ASP	TYR	ASP	THR	THR	GLY	THR	THR	GLY	SER	ILE	HIS
VAL	ASP	ASP	GLY	GLY	ILE	ILE	GLY	ILE	GLY	VAL	LYS
LEU	LEU	GLU	ALA	ALA	HIS	VAL	GLN	VAL	ASN	THR	GLY
ASN	ASN	PHE	THR	THR	GLU	GLU	GLU	GLY	GLN	THR	GLY
PRO	PRO	SER	GLN	GLN	LEU	SER	SER	SER	SER	GLY	LEU
ASP	ASP	ASP	CYS	CYS	LEU	LEU	LEU	LEU	GLY	GLY	GLU
L394	K395	VAL	ALA	ALA	LYS	LYS	LYS	LYS	CYS	ALA	GLU
L406	GLN	ARG	ARG	ARG	GLN	GLY	GLY	GLY	ARG	ILE	ALA
L409	LYS	SER	SER	PRO	SER	ILE	SER	ARG	SER	ARG	LYS
L410	THR	THR	SER	SER	GLY	LYS	PRO	GLY	THR	GLY	LEU
K411	ALA	ALA	GLU	GLU	ASN	ALA	GLU	ASN	ALA	GLN	ALA
LYS	LEU	LEU	PRO	PRO	ASN	PHE	SER	PHE	GLY	SER	PRO
PRO	ALA	LYS	GLY	GLY	PRO	LYS	PRO	LYS	ASP	GLY	GLY
VAL	VAL	LYS	PRO	PRO	LYS	ILE	PRO	LYS	ASP	GLY	GLY
ALA	ALA	H326	ALA	ALA	LEU	H326	PRO	LYS	ASP	GLY	GLY
VAL	SER	H326	SER	GLY	GLY	H326	GLY	LEU	ASP	ASP	SER
ARG	ARG	E327	ARG	ALA	ALA	E327	ALA	GLY	ASP	ASP	LEU
GLN	GLN	D328	GLN	PRO	PRO	D328	PRO	LYS	SER	ASP	ALA
LEU	LEU	M329	LEU	ALA	ALA	M329	ALA	THR	GLU	ASP	VAL
GLN	GLN	Q330	GLN	ASN	ASN	Q330	ASN	LEU	ASN	ALA	GLU
GLY	GLY	K331	VAL	VAL	VAL	K331	VAL	VAL	ASP	GLU	GLU
MET	MET	L332	THR	PRO	PRO	L332	PRO	PRO	ASP	LEU	MET
ASN	ASN	L333	GLU	GLU	GLU	L333	GLU	PRO	ASP	GLY	GLY
ARG	ARG	S334	CYS	CYS	CYS	S334	CYS	PRO	ILE	ALA	ALA
GLY	GLY	K335	VAL	VAL	VAL	K335	VAL	PRO	GLY	PRO	TRP
THR	THR	L336	SER	SER	SER	L336	SER	ASN	GLY	SER	SER
SER	SER	GLN	ASN	ASN	ASN	GLN	ASN	PRO	ASP	ARG	GLY
S429	R430	L339	ALA	ALA	ALA	L339	ALA	SER	ASP	ASN	ILE
R430	L433	L340	ALA	ALA	ALA	L340	ALA	ARG	THR	LEU	SER
L433	L434	L341	ILE	ILE	ILE	L341	ILE	ALA	GLY	ALA	ASN
L434	K435	V346	GLN	GLN	GLN	V346	GLN	THR	TYR	ALA	ASN
E436	V450	K350	GLU	GLU	GLU	K350	GLU	SER	GLY	SER	PRO
V450	S462	K351	THR	THR	THR	K351	THR	THR	THR	GLY	GLN
S462	M506	Q352	PRO	PRO	PRO	Q352	PRO	ILE	ASP	LEU	ALA
M506	K507	R355	GLU	GLU	GLU	R355	GLU	LYS	ARG	GLN	ARG
K507	L367	E364	SER	SER	SER	E364	SER	LYS	GLY	THR	THR
L367	T374	L367	THR	THR	THR	L367	THR	ASP	PRO	VAL	GLU
T374	P375	L374	SER	SER	SER	L374	SER	ALA	SER	THR	GLU
P375	GLY	L374	ARG	ARG	ARG	L374	ARG	LEU	HIS	HIS	ALA
GLY	GLY	L374	SER	SER	SER	L374	SER	ALA	PHE	GLY	SER
GLY	GLY	L374	GLN	GLN	GLN	L374	GLN	SER	ARG	GLY	GLY
GLY	GLY	L374	ASN	ASN	ASN	L374	ASN	PHE	ALA	SER	GLY

- Molecule 2: Phosphoprotein

Chain C:  8% 91%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2590005	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.688	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	394.2016, 394.2016, 394.2016	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9476, 0.9476, 0.9476	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: ZN, A1EF9

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	0.17	0/10302	0.34	0/13958
2	B	0.17	0/1168	0.36	0/1556
2	C	0.20	0/373	0.34	0/497
2	D	0.19	0/543	0.42	0/733
2	E	0.21	0/427	0.41	0/570
All	All	0.17	0/12813	0.35	0/17314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	10077	0	10087	74	0
2	B	1159	0	1261	15	0
2	C	372	0	398	6	0
2	D	538	0	560	12	0
2	E	425	0	462	11	0
3	A	1	0	0	0	0
4	A	36	0	0	1	0
All	All	12608	0	12768	100	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 4.

The worst 5 of 100 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:148:LYS:HD2	1:A:247:ILE:HA	1.70	0.74
1:A:1180:CYS:SG	1:A:1364:HIS:HE1	2.13	0.72
1:A:801:ARG:HD2	2:B:450:VAL:HG13	1.78	0.64
1:A:10:LEU:HD11	1:A:1087:ARG:HB3	1.79	0.63
1:A:456:LEU:HD13	1:A:510:PRO:HB2	1.80	0.62

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	1240/2183 (57%)	1209 (98%)	31 (2%)	0	100	100
2	B	142/507 (28%)	139 (98%)	3 (2%)	0	100	100
2	C	45/507 (9%)	45 (100%)	0	0	100	100
2	D	68/507 (13%)	66 (97%)	2 (3%)	0	100	100
2	E	53/507 (10%)	52 (98%)	1 (2%)	0	100	100
All	All	1548/4211 (37%)	1511 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1113/1945 (57%)	1112 (100%)	1 (0%)	88	94
2	B	132/416 (32%)	132 (100%)	0	100	100
2	C	45/416 (11%)	45 (100%)	0	100	100
2	D	64/416 (15%)	64 (100%)	0	100	100
2	E	50/416 (12%)	50 (100%)	0	100	100
All	All	1404/3609 (39%)	1403 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	ASN
1	A	1066	HIS
2	C	329	ASN
1	A	1265	GLN
1	A	1334	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
4	A1EF9	A	2202	-	39,39,39	0.66	0	54,57,57	1.16	4 (7%)

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
4	A1EF9	A	2202	-	-	4/31/50/50	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2202	A1EF9	C23-S01-N09	-5.40	97.74	107.36
4	A	2202	A1EF9	O05-S01-N09	3.36	113.10	106.97
4	A	2202	A1EF9	C34-N13-N12	2.70	106.80	104.36
4	A	2202	A1EF9	C32-C33-C34	2.59	106.23	103.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

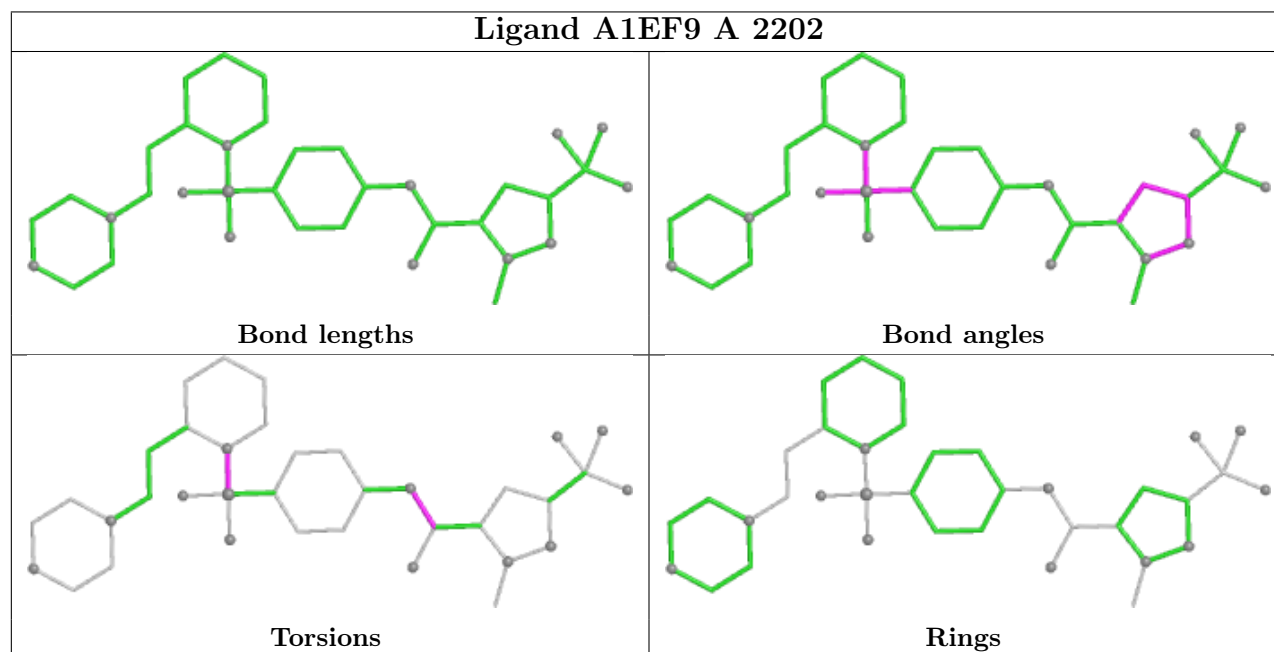
Mol	Chain	Res	Type	Atoms
4	A	2202	A1EF9	O08-C31-N11-C30
4	A	2202	A1EF9	C32-C31-N11-C30
4	A	2202	A1EF9	C14-N09-S01-O06
4	A	2202	A1EF9	C14-N09-S01-O05

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2202	A1EF9	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

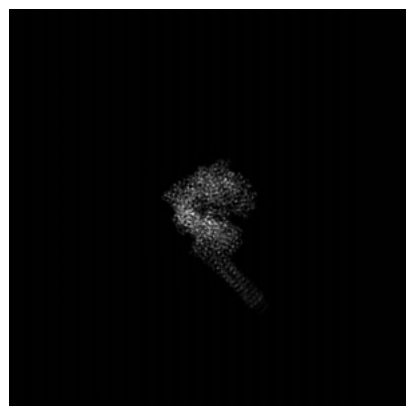
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65444. These allow visual inspection of the internal detail of the map and identification of artifacts.

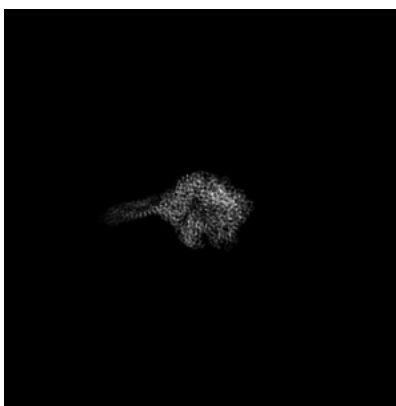
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

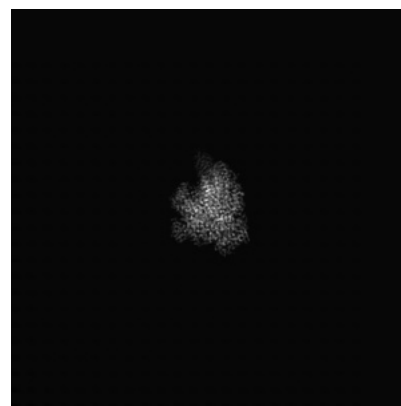
6.1.1 Primary map



X

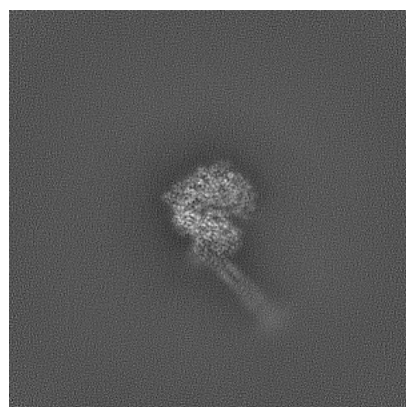


Y

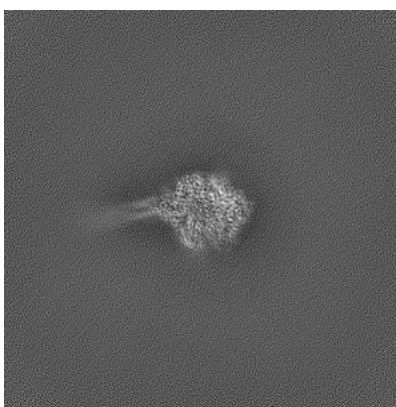


Z

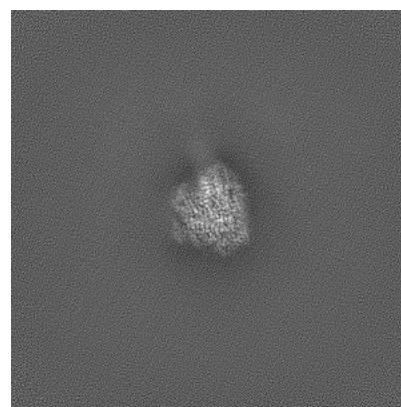
6.1.2 Raw map



X



Y



Z

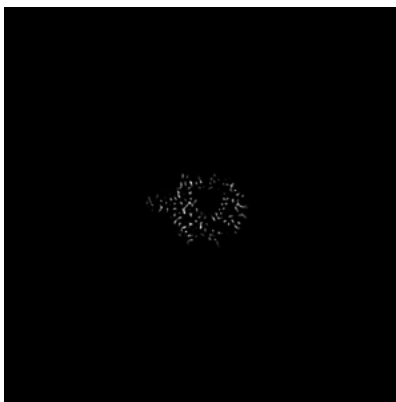
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

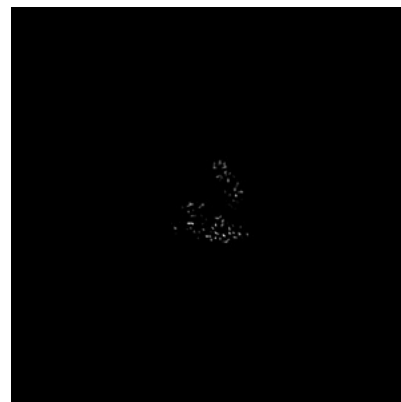
6.2.1 Primary map



X Index: 208

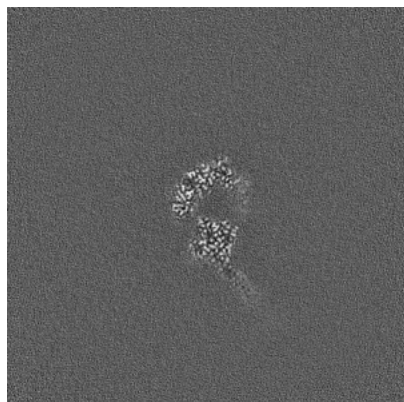


Y Index: 208

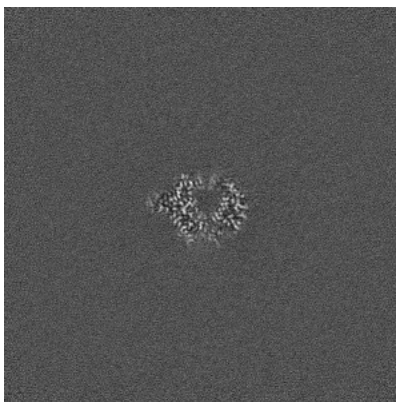


Z Index: 208

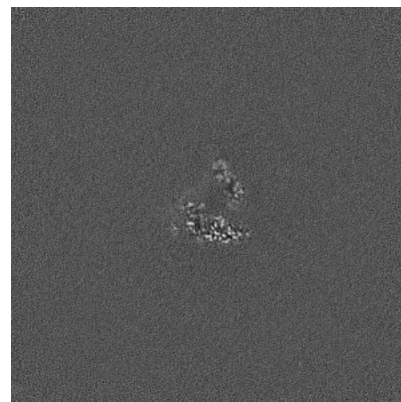
6.2.2 Raw map



X Index: 208



Y Index: 208



Z Index: 208

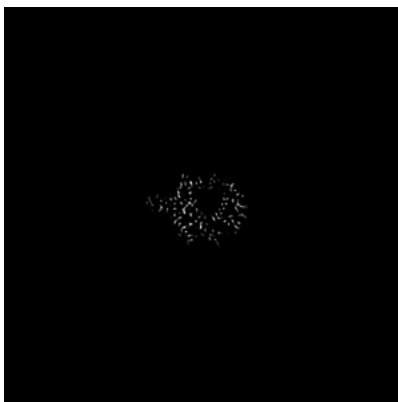
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

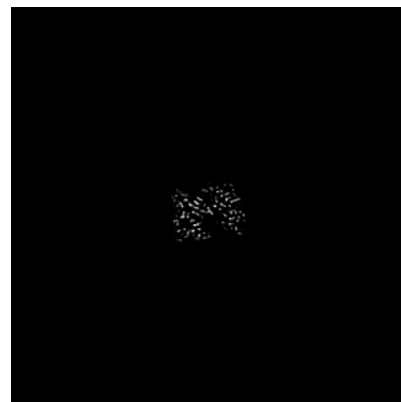
6.3.1 Primary map



X Index: 214

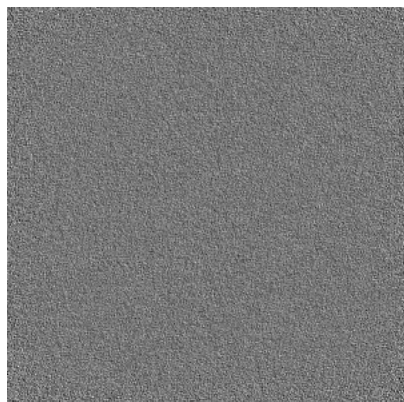


Y Index: 208

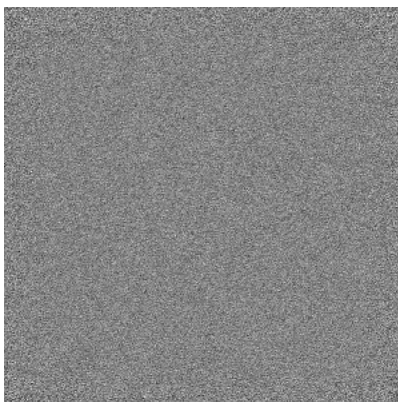


Z Index: 192

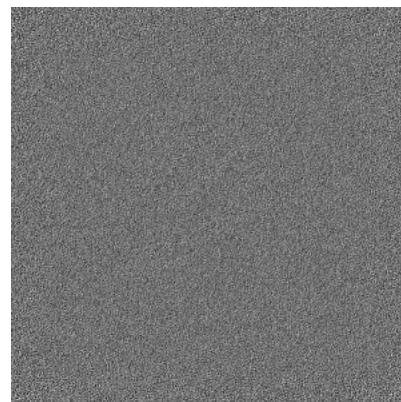
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

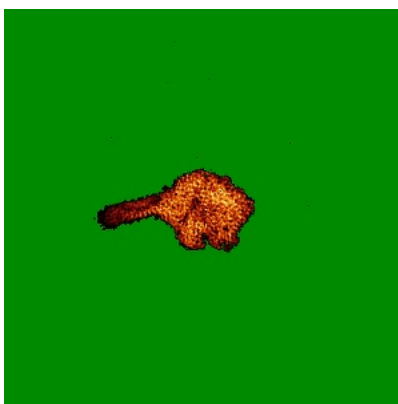
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

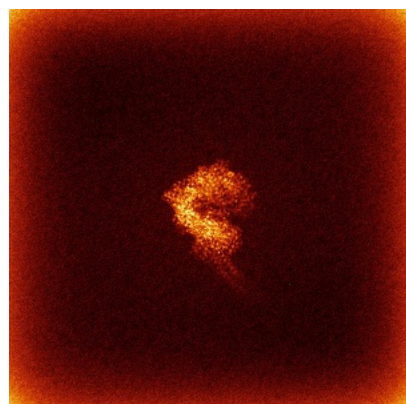


Y

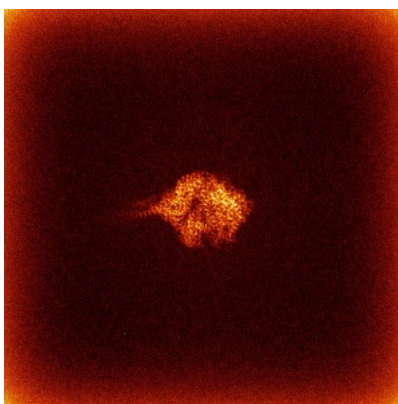


Z

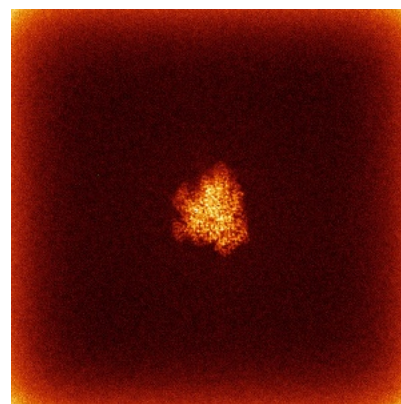
6.4.2 Raw map



X



Y

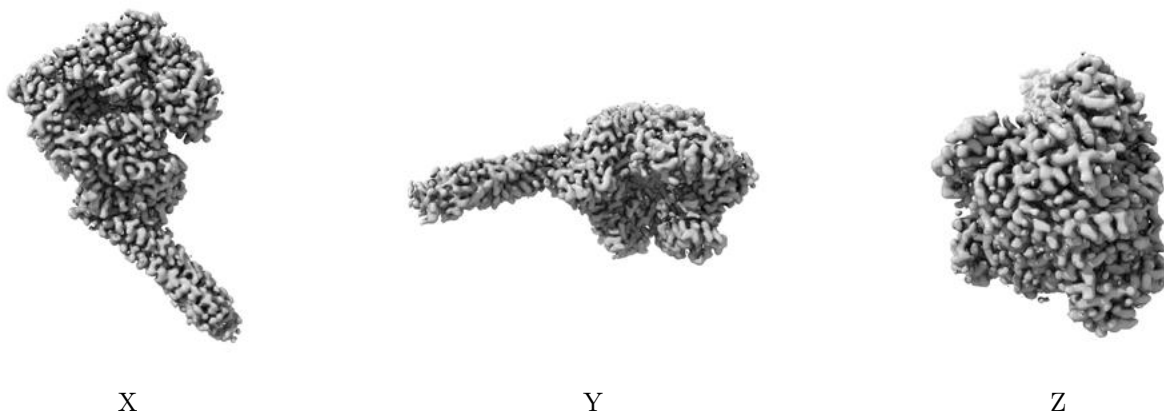


Z

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.

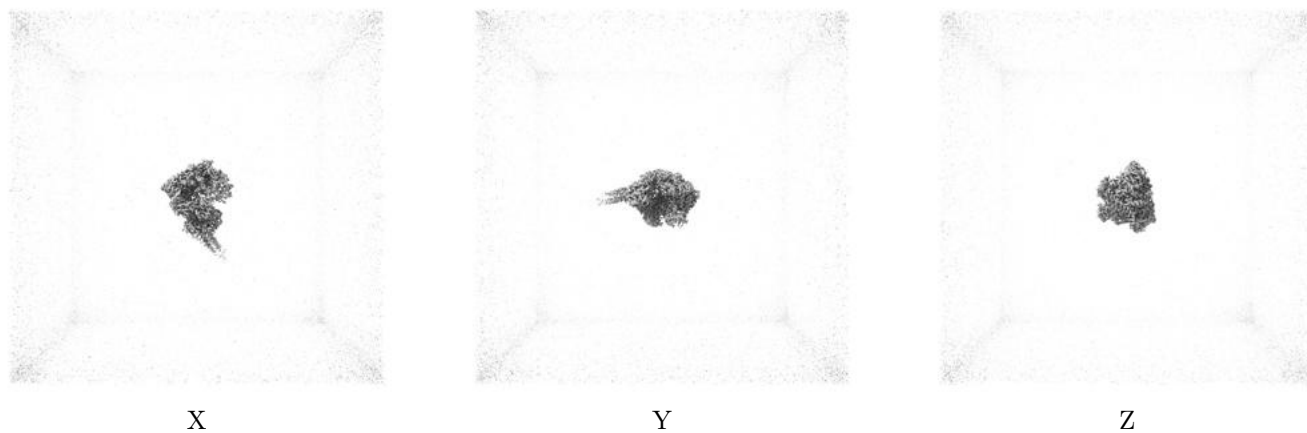
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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



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.

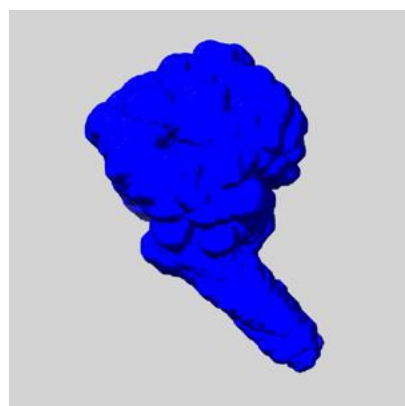
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

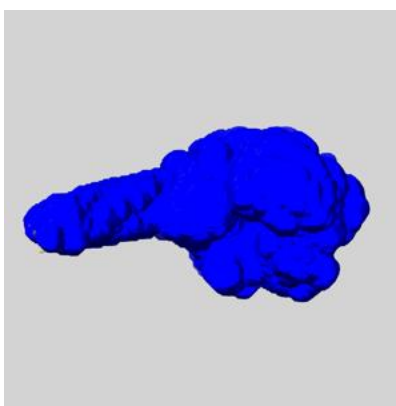
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

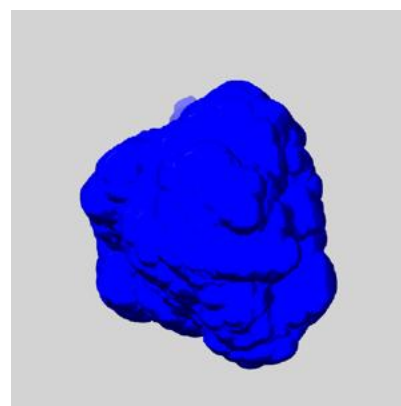
6.6.1 emd_65444_msk_1.map [i](#)



X



Y

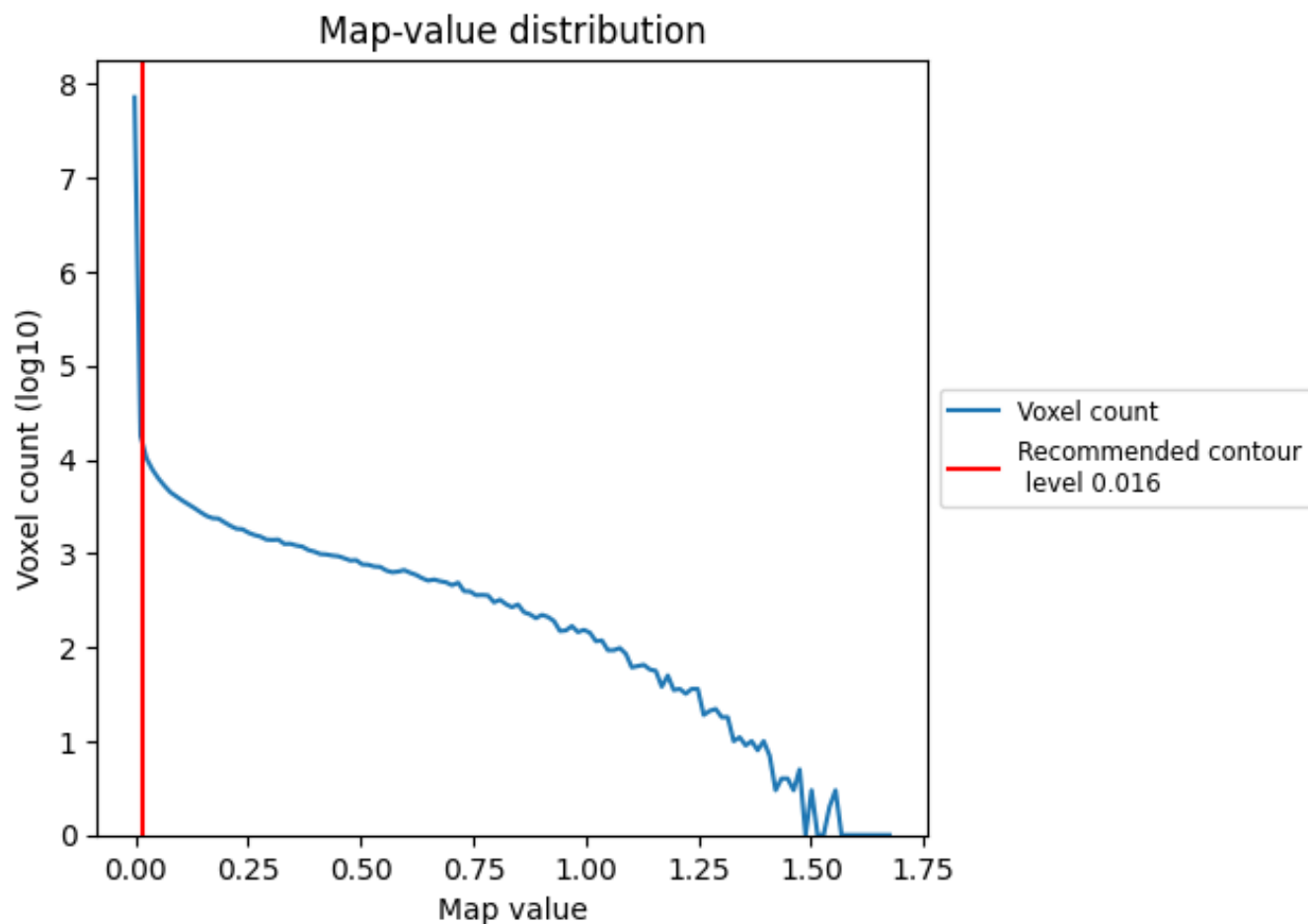


Z

7 Map analysis [i](#)

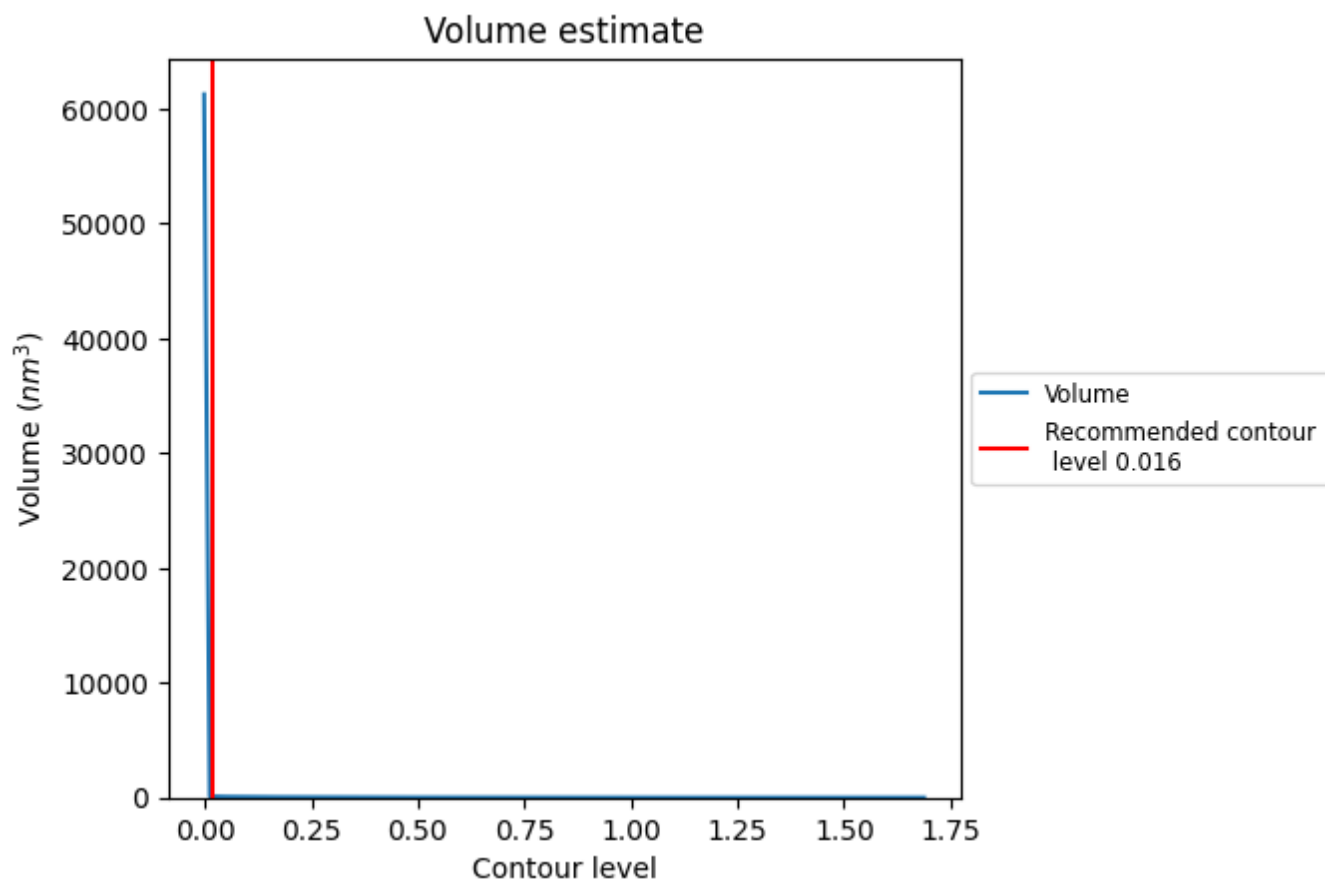
This section contains the results of statistical analysis of the map.

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.

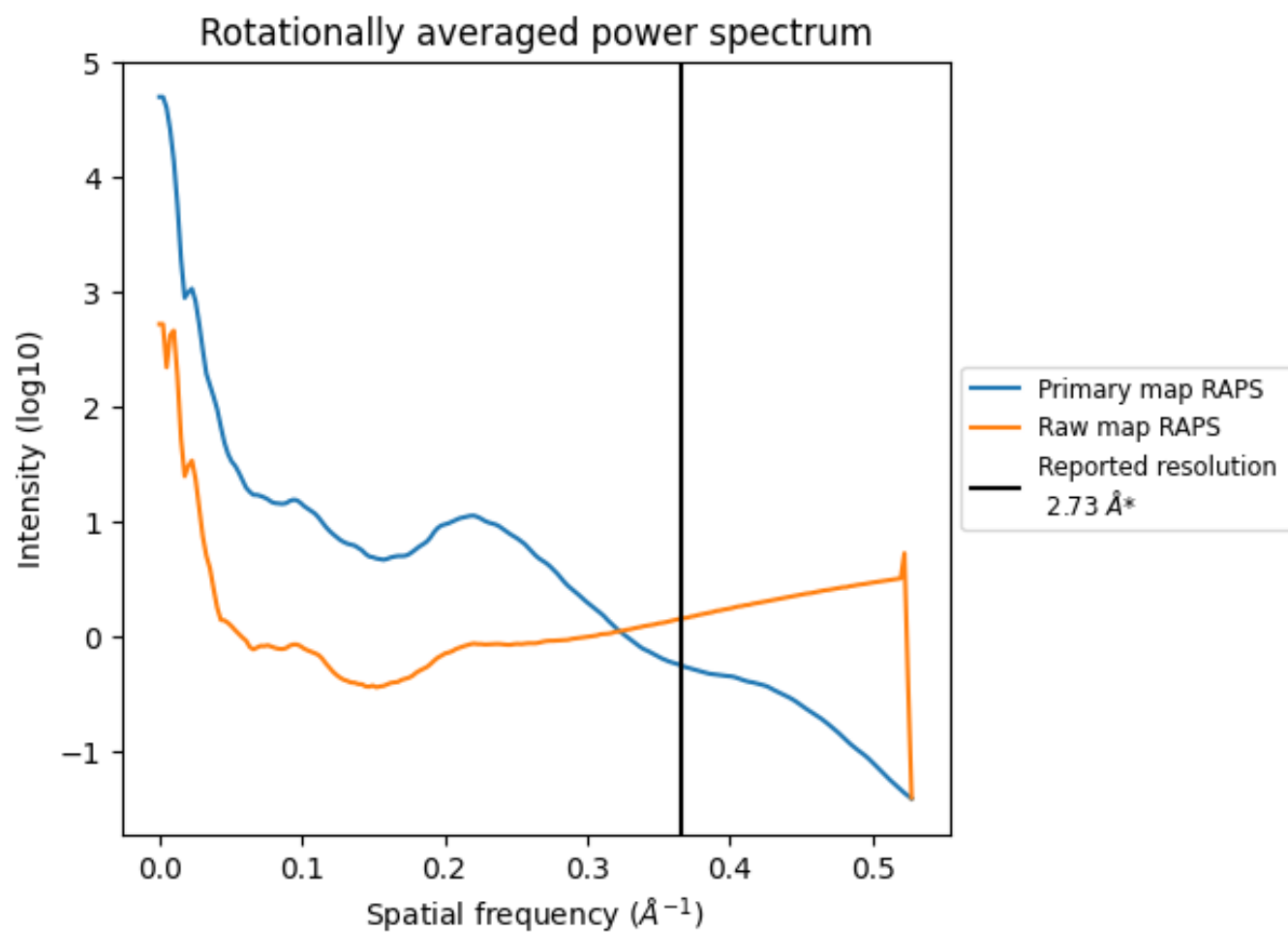
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

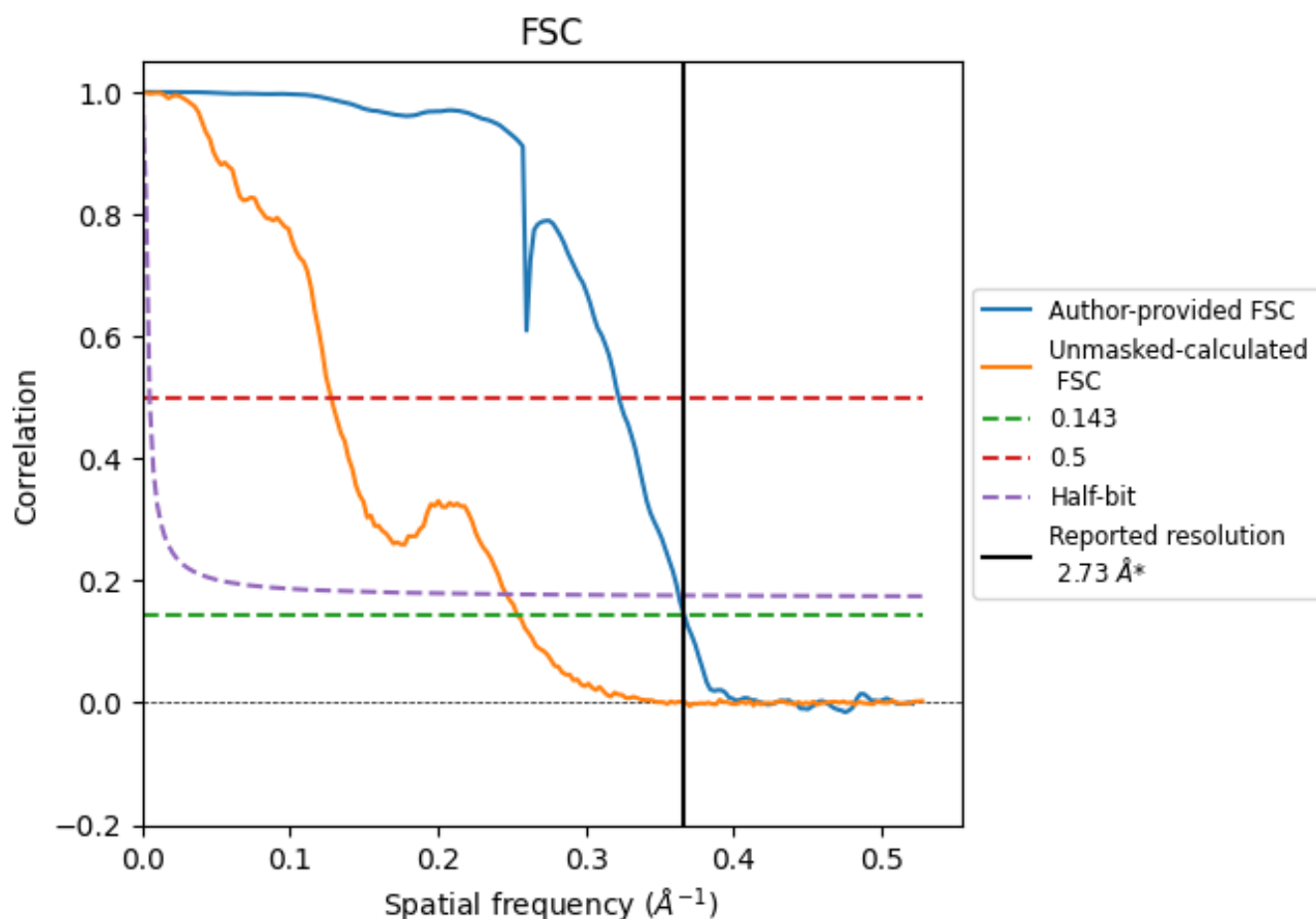


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

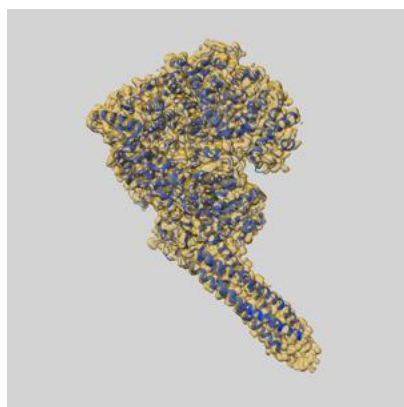
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.10	2.75
Unmasked-calculated*	3.94	7.82	4.06

*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 3.94 differs from the reported value 2.73 by more than 10 %

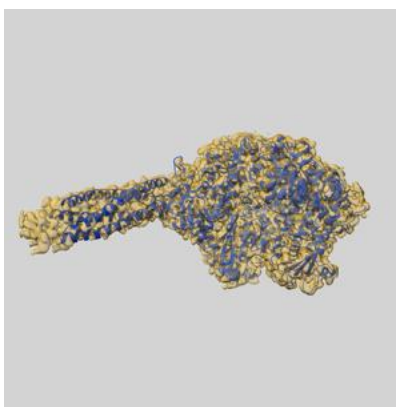
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65444 and PDB model 9VXX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

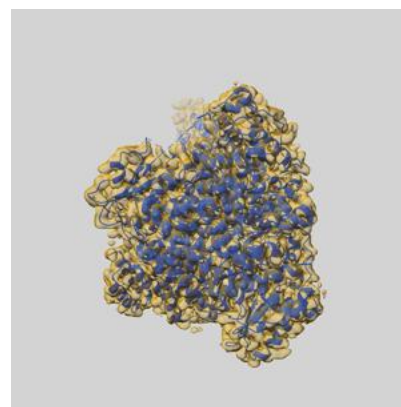
9.1 Map-model overlay [i](#)



X



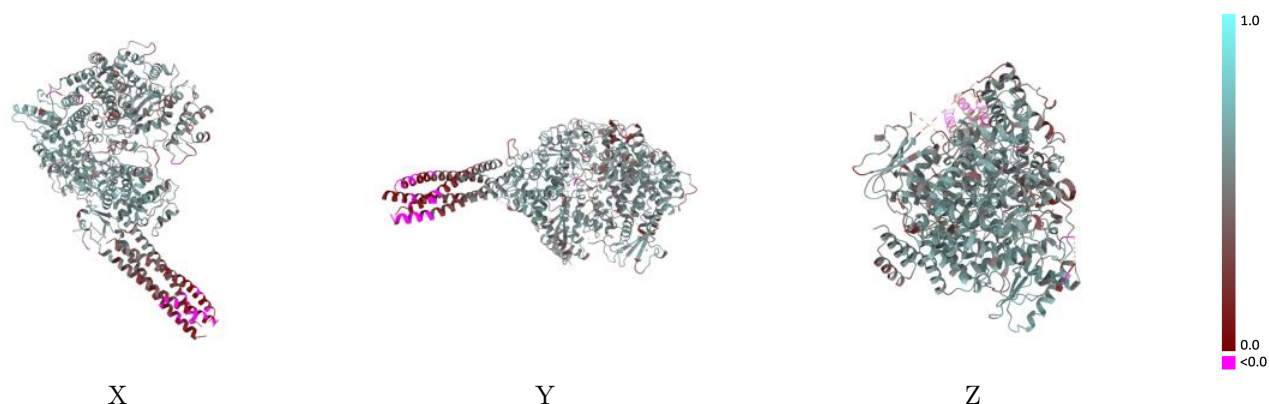
Y



Z

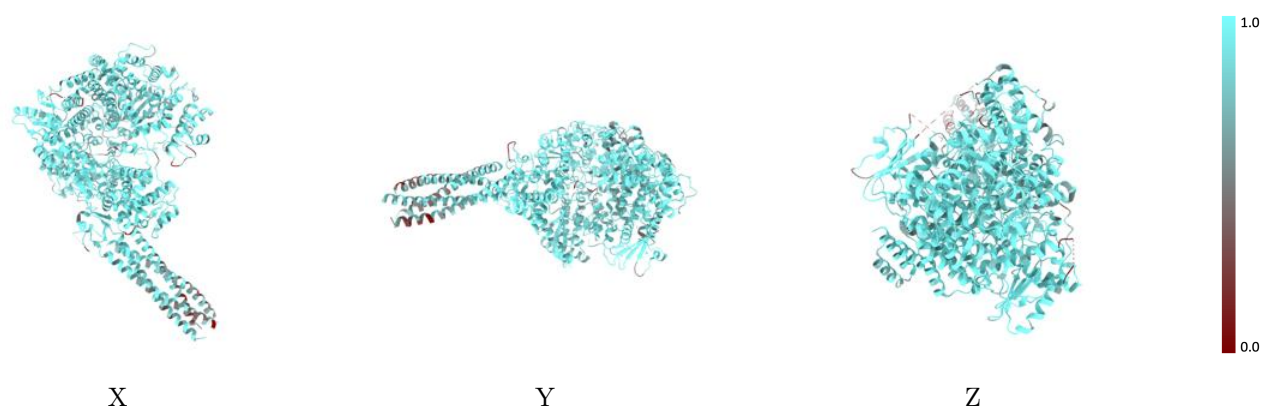
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



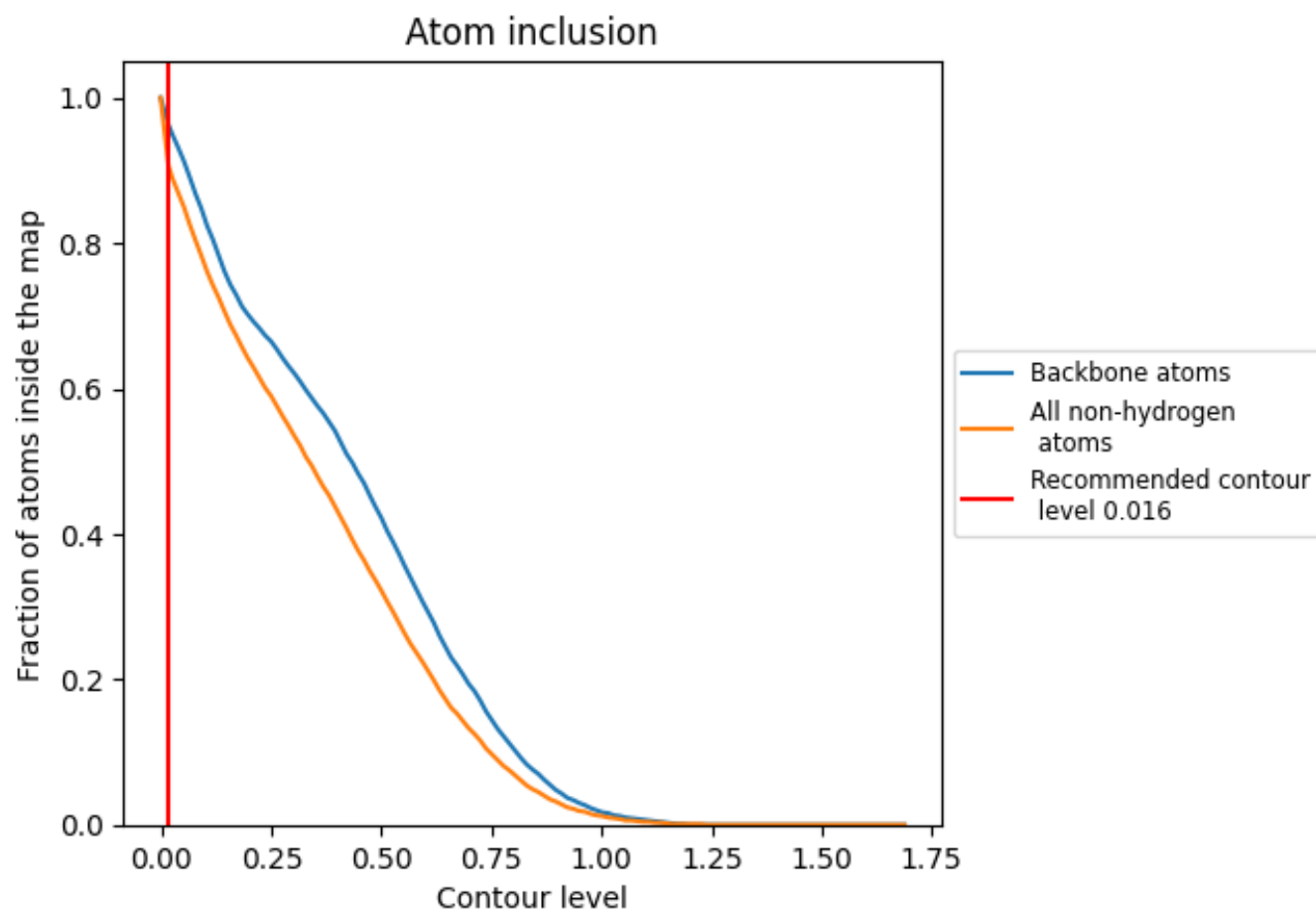
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.4900
A	0.9340	0.5280
B	0.8430	0.3980
C	0.7490	0.2390
D	0.7280	0.3030
E	0.8350	0.2990

