



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 10:29 AM EDT

PDB ID : 9OCF / pdb_00009ocf
EMDB ID : EMD-70313
Title : 2.73A cryo-EM structure of the Measles Virus L-P in complex with ERdRp-0519
Authors : Liu, B.; Wang, D.; Yang, G.
Deposited on : 2025-04-24
Resolution : 2.73 Å(reported)

This is a Full wwPDB EM Validation 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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

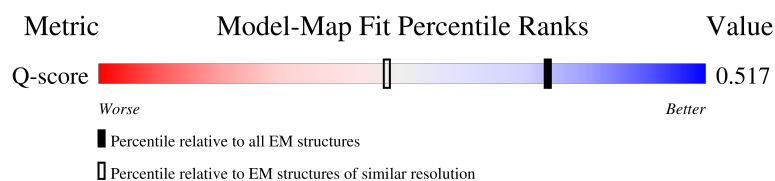
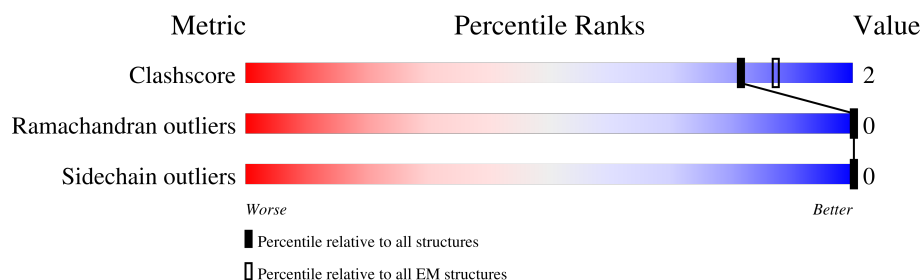
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	509	
2	C	509	
2	D	509	

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Mol	Chain	Length	Quality of chain
2	E	509	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12449 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	1281	Total	C	N	O	S	0	0
			10283	6567	1771	1888	57		

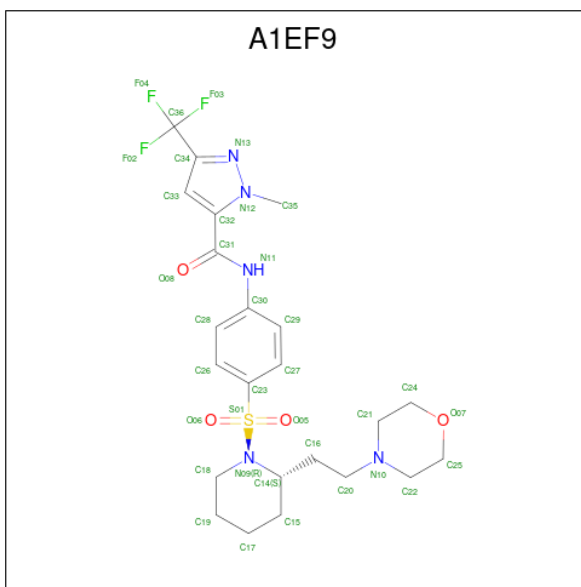
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	60	Total	C	N	O	S	0	0
			457	291	81	84	1		
2	C	114	Total	C	N	O	S	0	0
			896	568	160	162	6		
2	D	43	Total	C	N	O	S	0	0
			324	205	56	62	1		
2	E	60	Total	C	N	O	S	0	0
			453	286	76	90	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	508	SER	-	expression tag	UNP Q83623
B	509	GLY	-	expression tag	UNP Q83623
C	508	SER	-	expression tag	UNP Q83623
C	509	GLY	-	expression tag	UNP Q83623
D	508	SER	-	expression tag	UNP Q83623
D	509	GLY	-	expression tag	UNP Q83623
E	508	SER	-	expression tag	UNP Q83623
E	509	GLY	-	expression tag	UNP Q83623

- Molecule 3 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	
3	A	1	36	23	3	5	4	1	0

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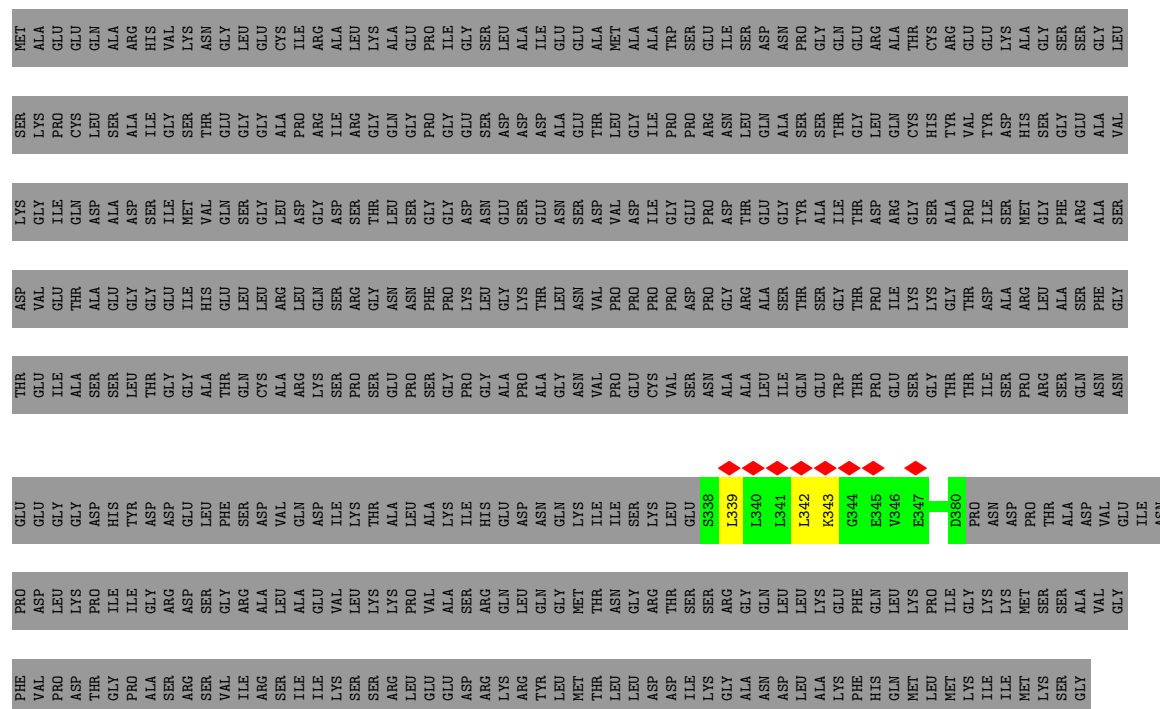
- Molecule 2: Phosphoprotein



SER	ARG	ASN	GLU	THR	GLY	THR	ASP	LYS	SER	MET
SER	ARG	ASP	GLU	GLY	GLU	ILE	VAL	GLY	LYS	ALA
SER	VAL	THR	GLY	THR	GLY	ALA	THR	GLN	PRO	GLU
ILE	ARG	ALA	ASP	SER	HIS	SER	ALA	ASP	LEU	GLN
SER	VAL	ASP	TYR	LEU	TYR	LEU	GLY	ASP	ALA	ARG
ILE	GLU	ILE	ASP	THR	ASP	THR	GLY	ILE	ILE	HIS
LYS	SER	ASN	GLU	GLY	GLU	GLY	ILE	MET	SER	LYS
SER	SER	P3992	LEU	ALA	LEU	ALA	HIS	VAL	THR	ASN
SER	ARG	D3993	PHE	THR	PHE	THR	GLU	GLN	GLU	GLY
LEU	LEU	P4113	ASP	CYS	ASP	CYS	LEU	LEU	GLY	LEU
GLU	GLU	VAL	VAL	ALA	VAL	ALA	ARG	LEU	ALA	CYS
ASP	ASP	ALA	GLN	LYS	ASP	LYS	GLN	GLY	GLY	ARG
ARG	LYS	SER	ILE	SER	ILE	SER	SER	ASP	ILE	ALA
LYS	ARG	ARG	THR	PRO	THR	PRO	ARG	THR	ARG	LEU
TYR	GLN	GLN	THR	GLU	THR	GLU	ASN	GLY	GLY	LYS
LEU	GLN	LEU	LEU	PRO	LEU	PRO	ASN	SER	GLN	ALA
MET	MET	GLY	ALA	SER	ALA	GLY	PHE	GLY	PRO	PRO
THR	THR	THR	LYS	GLY	LYS	GLY	PRO	GLY	GLY	ILE
LEU	LEU	ASN	ILE	PRO	ILE	PRO	LYS	ASP	ASP	GLY
ASP	ASP	ARG	GLU	ALA	GLU	ALA	GLY	GLU	ASP	LEU
ILE	ILE	THR	ASN	PRO	ASP	ALA	THR	GLU	ASP	ALA
LYS	LYS	SER	GLN	GLY	GLN	GLY	LEU	ASN	GLY	GLU
GLY	GLY	SER	LYS	ASN	ILE	ASN	LEU	ASP	ALA	GLU
ALA	ALA	ARG	ILE	VAL	ILE	VAL	VAL	ASP	THR	GLU
ASN	ASN	GLN	ILE	PRO	ILE	PRO	ARG	VAL	GLU	ALA
PHE	PHE	GLU	S338	SER	GLU	ASN	ASP	GLY	PRO	SER
HIS	HIS	PHE	L339	ALA	L339	ALA	GLY	ASP	PRO	GLU
GLN	GLN	GLN	L340	ALA	L340	ALA	ARG	THR	THR	ALA
MET	MET	LEU	L341	LEU	L341	LEU	ALA	GLN	GLN	ASP
LEU	LEU	LYS	L342	ILE	L342	ILE	SER	GLY	ALA	ASN
MET	MET	PRO	K343	GLN	K343	GLN	THR	TYR	SER	PRO
ILE	ILE	GLY	G344	THR	G344	THR	GLY	ILE	ALA	GLY
ILE	ILE	ILE	E347	THR	E347	THR	PRO	ASP	ARG	GLU
MET	MET	LYS	+	GLU	+	GLU	ILE	ARG	LEU	ALA
LYS	SER	SER	N357	SER	N357	GLY	LYS	GLY	CYS	THR
GLY	GLY	ALA	L363	THR	L363	THR	GLY	ALA	ALA	ARG
		VAL	I370	ILE	I370	ILE	ASP	ILE	VAL	GLU
		PHE		SER		SER	ALA	SER	THR	LYS
		GLY		PRO		PRO	ARG	MET	ASP	ALA
		VAL		ARG		ARG	LEU	GLY	GLY	GLY
		ASP	P375	GLN	GLY	GLN	ALA	PHE	ARG	SER
		GLY		SER		SER	THR	GLY	GLU	SER
		PRO		ASN		ASN	PHE	ALA	GLU	GLY
		PRO	L365	GLY	LYS	GLY	GLY	SER	ALA	LEU

- Molecule 2: Phosphoprotein





- Molecule 2: Phosphoprotein

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	358252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.648	Depositor
Minimum map value	-0.332	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	339.968, 339.968, 339.968	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8853333, 0.8853333, 0.8853333	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: 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	0.18	0/10513	0.43	0/14248
2	B	0.12	0/460	0.34	0/615
2	C	0.16	0/903	0.36	0/1200
2	D	0.12	0/325	0.32	0/434
2	E	0.25	0/458	0.72	2/620 (0.3%)
All	All	0.18	0/12659	0.43	2/17117 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	381	PRO	CA-C-N	5.20	131.47	121.54
2	E	381	PRO	C-N-CA	5.20	131.47	121.54

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	10283	0	10280	51	0
2	B	457	0	505	4	0
2	C	896	0	973	6	0
2	D	324	0	354	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	453	0	479	5	0
3	A	36	0	0	0	0
All	All	12449	0	12591	60	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 2.

All (60) 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:829:PHE:HA	1:A:837:TYR:O	1.92	0.70
1:A:965:LYS:NZ	1:A:1131:SER:O	2.35	0.59
2:B:363:LEU:HD21	2:C:364:GLU:HA	1.85	0.57
1:A:1190:PHE:HB2	1:A:1361:LEU:HB3	1.87	0.57
1:A:976:GLU:HG3	1:A:1123:ARG:HE	1.70	0.56
1:A:673:TYR:O	1:A:677:SER:HB2	2.06	0.55
1:A:860:ILE:HG22	1:A:1083:LYS:HE2	1.88	0.54
1:A:121:SER:HB3	1:A:150:ILE:HA	1.90	0.54
1:A:860:ILE:HG12	1:A:1010:THR:HG22	1.90	0.54
1:A:1057:PRO:HG2	1:A:1157:LEU:HD11	1.89	0.53
1:A:1198:LEU:O	1:A:1309:ARG:NH2	2.42	0.53
1:A:522:TYR:HB2	1:A:553:MET:HE1	1.91	0.52
1:A:134:ARG:NH2	1:A:1164:GLU:O	2.43	0.51
2:B:363:LEU:HD22	2:C:367:LEU:HD22	1.93	0.51
1:A:810:ARG:NH1	1:A:813:ASP:OD2	2.44	0.50
1:A:704:VAL:HG13	1:A:733:LYS:HA	1.94	0.50
1:A:860:ILE:HG13	1:A:861:VAL:HG23	1.94	0.49
1:A:1019:ARG:NH2	1:A:1073:GLU:OE2	2.46	0.49
1:A:1239:VAL:HG13	1:A:1278:THR:HG22	1.94	0.48
1:A:251:TYR:O	1:A:254:LEU:HB3	2.14	0.47
1:A:781:LYS:HD2	1:A:799:VAL:HG11	1.96	0.47
1:A:1261:LEU:HB3	1:A:1388:LEU:HD11	1.97	0.47
1:A:530:LEU:HD11	1:A:547:ALA:HB1	1.96	0.47
2:B:343:LYS:HG2	2:D:342:LEU:HD21	1.97	0.46
1:A:126:GLN:HG2	1:A:129:ARG:HH21	1.79	0.46
1:A:354:ARG:NH2	1:A:537:LYS:O	2.49	0.46
1:A:701:GLU:HG2	1:A:736:MET:HG2	1.98	0.46
1:A:128:LEU:HD13	1:A:886:TYR:HB3	1.98	0.45
1:A:266:ASP:HA	1:A:269:PHE:HD2	1.80	0.45
1:A:416:HIS:HA	2:E:358:ILE:HG23	1.98	0.45
1:A:331:ILE:HG21	2:C:462:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:HA	1:A:699:ARG:HD2	1.80	0.45
2:B:370:ILE:HD13	2:C:371:MET:HB3	1.97	0.45
1:A:1386:LEU:HG	1:A:1388:LEU:HG	1.98	0.45
1:A:206:SER:OG	1:A:207:ARG:N	2.51	0.44
1:A:657:SER:HA	1:A:779:VAL:O	2.17	0.44
1:A:747:TRP:O	1:A:751:THR:OG1	2.28	0.44
1:A:286:LEU:HD11	1:A:312:ILE:HD11	1.99	0.44
1:A:847:LEU:HD23	1:A:850:ILE:HD12	1.98	0.44
1:A:57:PHE:HE2	1:A:483:GLU:HG3	1.83	0.44
2:C:367:LEU:HD12	2:E:367:LEU:HD21	1.99	0.43
1:A:540:LYS:HE3	1:A:540:LYS:HB3	1.85	0.43
2:D:343:LYS:NZ	2:E:338:SER:O	2.44	0.43
2:E:347:GLU:HG3	2:E:351:LYS:HE3	1.99	0.43
1:A:247:ILE:HG22	1:A:887:LEU:HD13	1.99	0.43
1:A:30:GLU:HB3	1:A:49:ILE:HG21	2.01	0.43
1:A:682:ARG:HA	1:A:682:ARG:HD3	1.88	0.42
2:C:363:LEU:HD11	2:E:364:GLU:HG2	2.01	0.42
1:A:568:ILE:HD11	1:A:686:ILE:HG21	2.00	0.42
1:A:771:GLN:HG2	1:A:832:TYR:HA	2.01	0.42
1:A:295:ASP:OD1	1:A:827:SER:OG	2.38	0.42
1:A:664:LEU:HD11	1:A:775:GLN:HB2	2.01	0.41
1:A:954:GLY:HA3	1:A:1159:VAL:HG21	2.03	0.41
1:A:447:LYS:HE3	1:A:447:LYS:HB2	1.88	0.41
1:A:1081:THR:HA	1:A:1085:LEU:HD12	2.02	0.41
2:D:339:LEU:HD23	2:D:342:LEU:HD12	2.02	0.41
1:A:42:ASP:OD1	1:A:42:ASP:N	2.54	0.41
1:A:548:LYS:HE3	1:A:548:LYS:HB2	1.83	0.41
1:A:1078:MET:HE2	1:A:1078:MET:HB3	1.98	0.41
1:A:1108:TYR:CZ	1:A:1112:ARG:HD2	2.56	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	1269/2183 (58%)	1237 (98%)	32 (2%)	0	100	100
2	B	56/509 (11%)	54 (96%)	2 (4%)	0	100	100
2	C	110/509 (22%)	109 (99%)	1 (1%)	0	100	100
2	D	41/509 (8%)	41 (100%)	0	0	100	100
2	E	58/509 (11%)	51 (88%)	7 (12%)	0	100	100
All	All	1534/4219 (36%)	1492 (97%)	42 (3%)	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	1139/1943 (59%)	1139 (100%)	0	100	100
2	B	53/415 (13%)	53 (100%)	0	100	100
2	C	103/415 (25%)	103 (100%)	0	100	100
2	D	38/415 (9%)	38 (100%)	0	100	100
2	E	54/415 (13%)	54 (100%)	0	100	100
All	All	1387/3603 (38%)	1387 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	433	HIS
1	A	473	GLN
1	A	524	HIS
1	A	557	GLN
1	A	562	ASN
1	A	711	HIS
1	A	719	HIS

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Mol	Chain	Res	Type
1	A	771	GLN
1	A	812	HIS
1	A	1027	ASN
1	A	1105	ASN
1	A	1335	GLN
2	B	352	GLN
2	C	356	GLN
2	E	356	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	A1EF9	A	2500	-	38,39,39	2.43	11 (28%)	52,57,57	2.61	15 (28%)

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	A1EF9	A	2500	-	-	12/28/50/50	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2500	A1EF9	C20-N10	-9.00	1.26	1.47
3	A	2500	A1EF9	S01-N09	6.34	1.72	1.63
3	A	2500	A1EF9	C23-S01	4.15	1.82	1.76
3	A	2500	A1EF9	C31-N11	3.16	1.44	1.35
3	A	2500	A1EF9	C18-N09	3.06	1.53	1.48
3	A	2500	A1EF9	O06-S01	3.02	1.46	1.43
3	A	2500	A1EF9	C17-C15	-2.78	1.46	1.53
3	A	2500	A1EF9	C22-N10	-2.69	1.39	1.46
3	A	2500	A1EF9	C21-N10	-2.68	1.39	1.46
3	A	2500	A1EF9	O05-S01	2.61	1.46	1.43
3	A	2500	A1EF9	C32-N12	-2.45	1.32	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2500	A1EF9	O06-S01-O05	-12.09	100.73	119.59
3	A	2500	A1EF9	C36-C34-N13	6.76	127.67	119.72
3	A	2500	A1EF9	C34-N13-N12	4.65	107.86	104.37
3	A	2500	A1EF9	C32-C33-C34	3.39	108.23	103.57
3	A	2500	A1EF9	O06-S01-N09	3.38	112.88	106.97
3	A	2500	A1EF9	O05-S01-N09	3.33	112.80	106.97
3	A	2500	A1EF9	C22-N10-C21	3.30	115.96	108.84
3	A	2500	A1EF9	O05-S01-C23	3.26	112.15	108.10
3	A	2500	A1EF9	C33-C34-N13	-2.98	107.04	111.33
3	A	2500	A1EF9	C32-N12-N13	-2.82	109.84	112.76
3	A	2500	A1EF9	C33-C34-C36	-2.47	125.29	127.93
3	A	2500	A1EF9	O06-S01-C23	2.41	111.09	108.10
3	A	2500	A1EF9	C33-C32-C31	-2.36	120.48	128.22
3	A	2500	A1EF9	C35-N12-C32	-2.24	127.13	129.47
3	A	2500	A1EF9	C19-C17-C15	2.18	115.89	111.42

There are no chirality outliers.

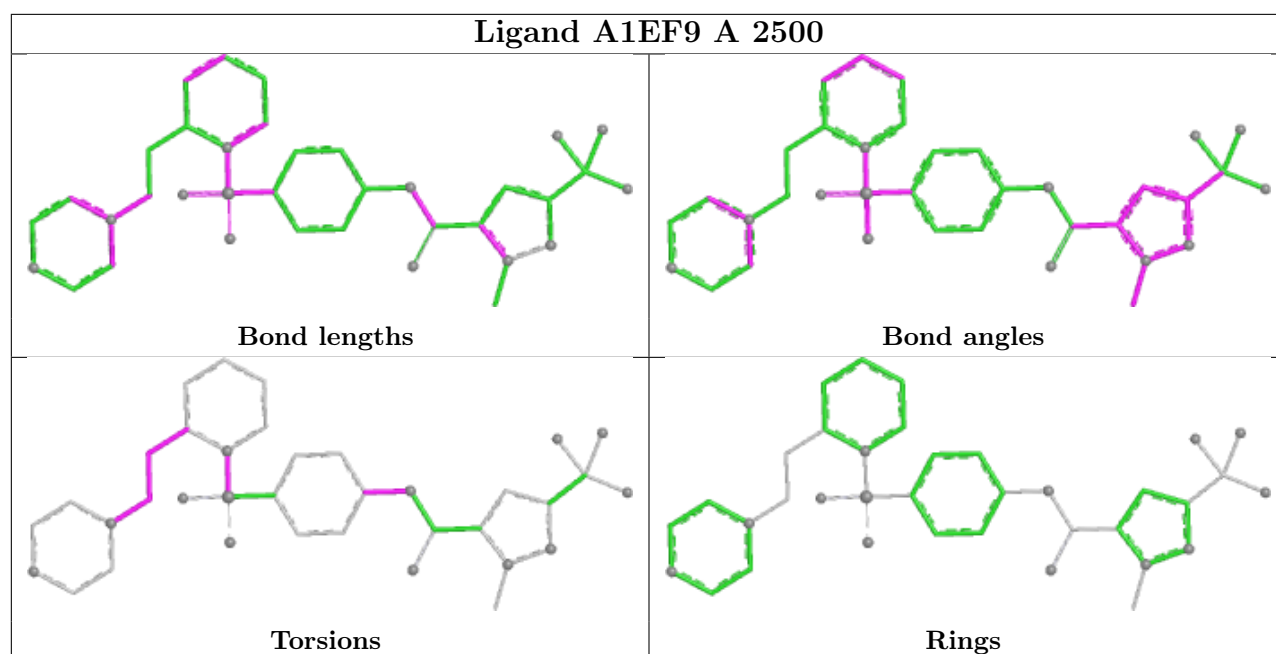
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2500	A1EF9	C15-C14-C16-C20
3	A	2500	A1EF9	N09-C14-C16-C20
3	A	2500	A1EF9	C18-N09-S01-C23
3	A	2500	A1EF9	C16-C20-N10-C21
3	A	2500	A1EF9	C16-C20-N10-C22
3	A	2500	A1EF9	C14-N09-S01-O05
3	A	2500	A1EF9	C18-N09-S01-O06
3	A	2500	A1EF9	C28-C30-N11-C31
3	A	2500	A1EF9	C29-C30-N11-C31
3	A	2500	A1EF9	C18-N09-S01-O05
3	A	2500	A1EF9	C14-N09-S01-C23
3	A	2500	A1EF9	C14-C16-C20-N10

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.

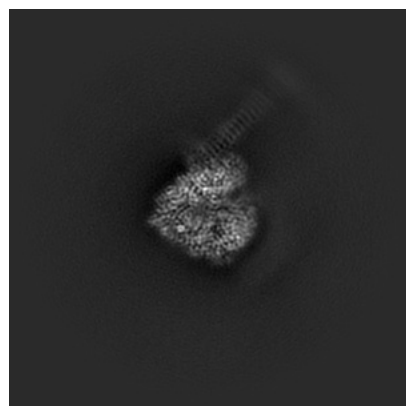
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70313. These allow visual inspection of the internal detail of the map and identification of artifacts.

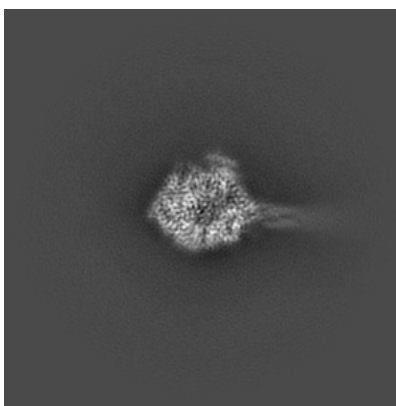
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

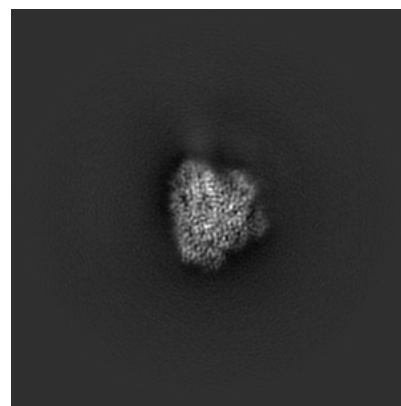
6.1.1 Primary map



X

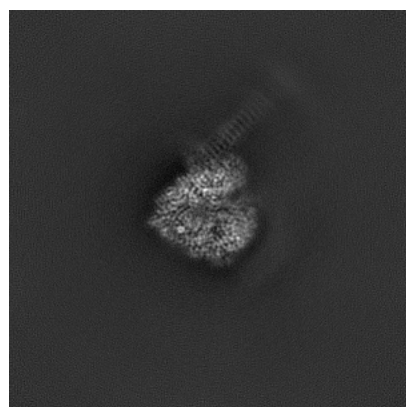


Y

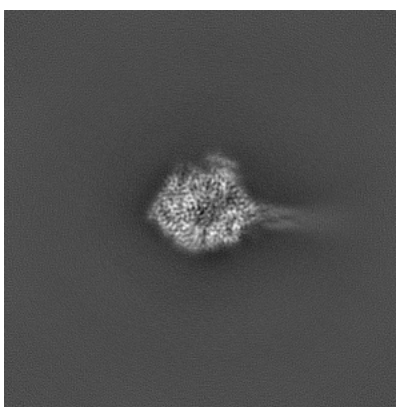


Z

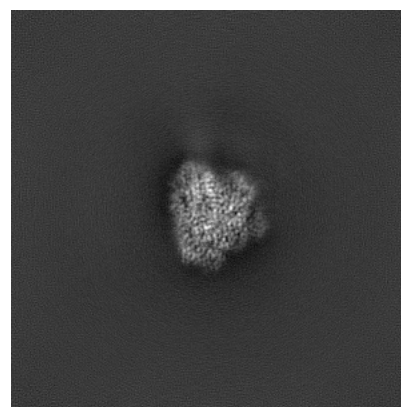
6.1.2 Raw map



X



Y

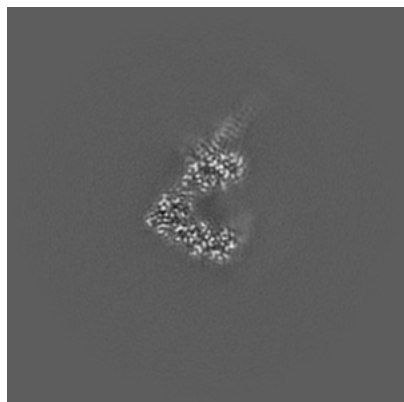


Z

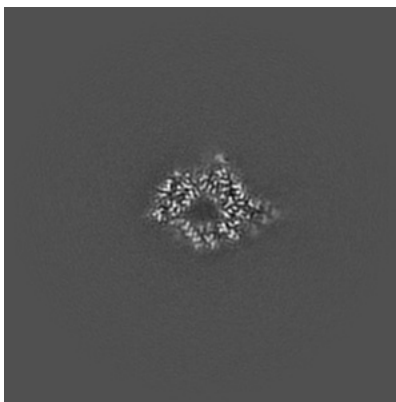
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

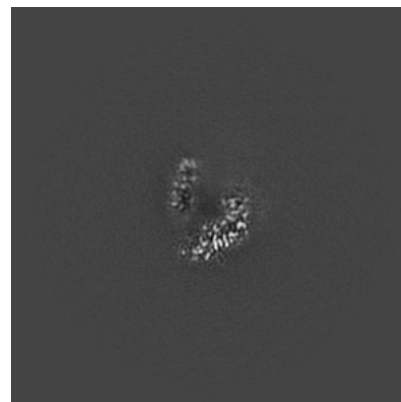
6.2.1 Primary map



X Index: 192

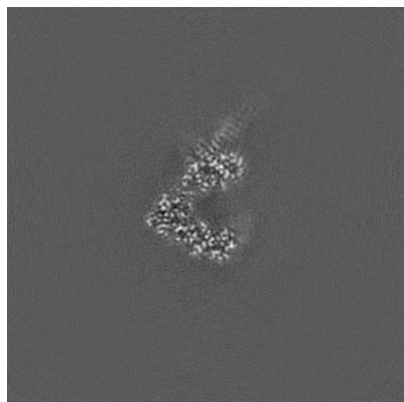


Y Index: 192

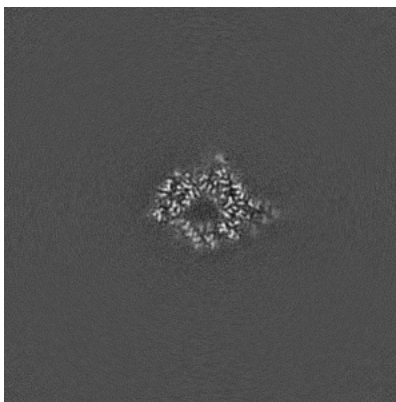


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

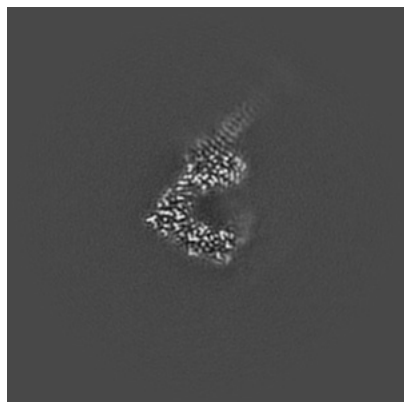


Z Index: 192

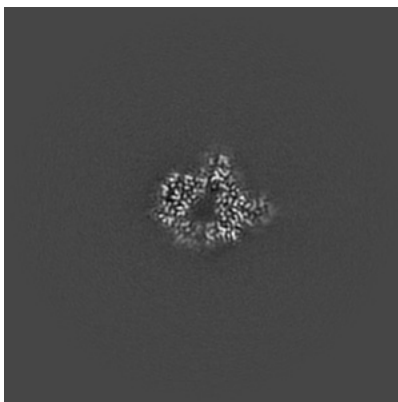
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

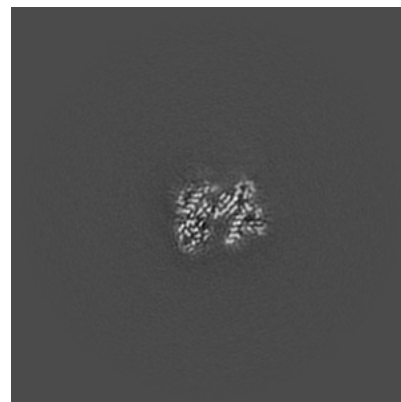
6.3.1 Primary map



X Index: 190

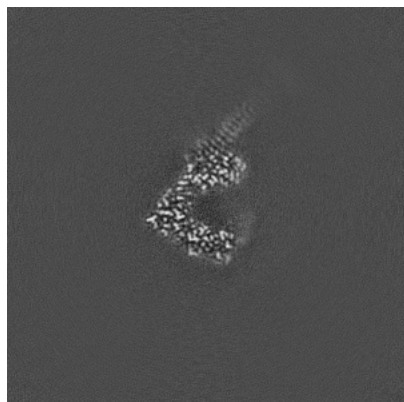


Y Index: 187

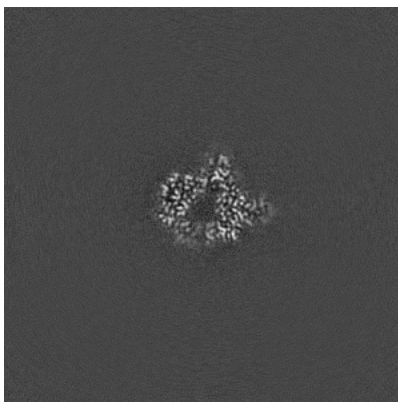


Z Index: 211

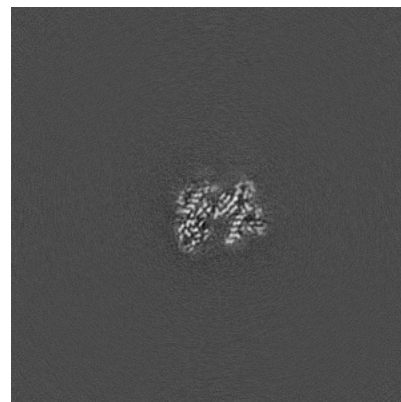
6.3.2 Raw map



X Index: 190



Y Index: 187

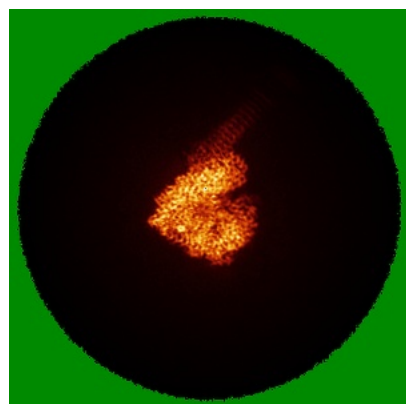


Z Index: 211

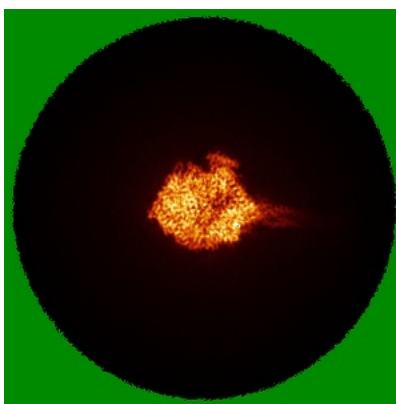
The images above show the largest variance slices of the map in three orthogonal directions.

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

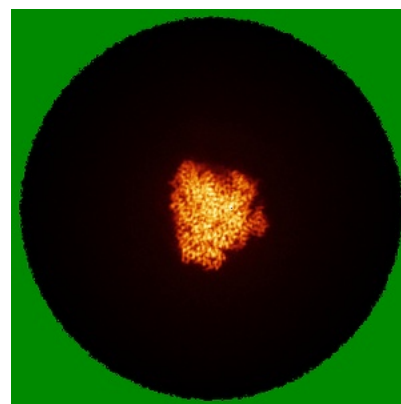
6.4.1 Primary map



X

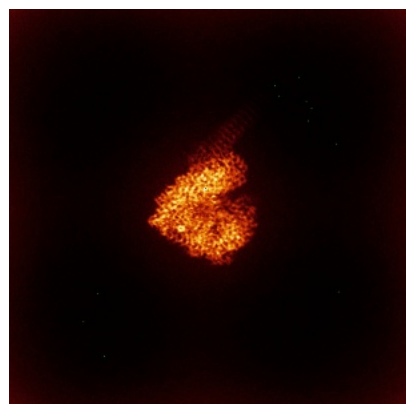


Y

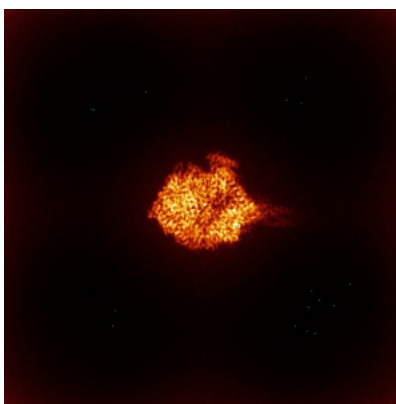


Z

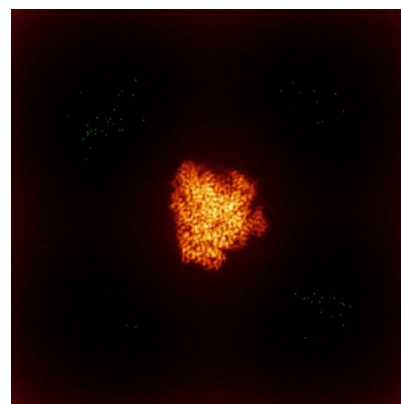
6.4.2 Raw map



X



Y

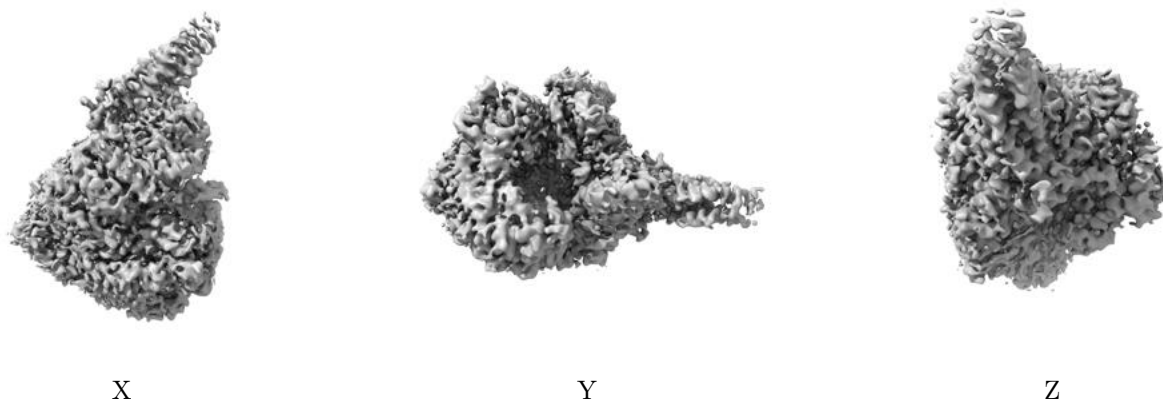


Z

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.

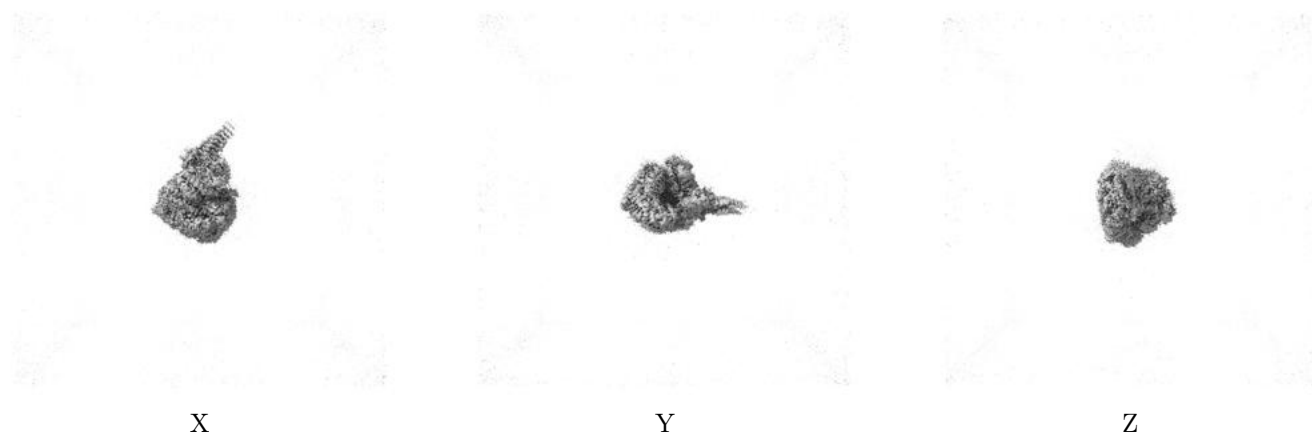
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

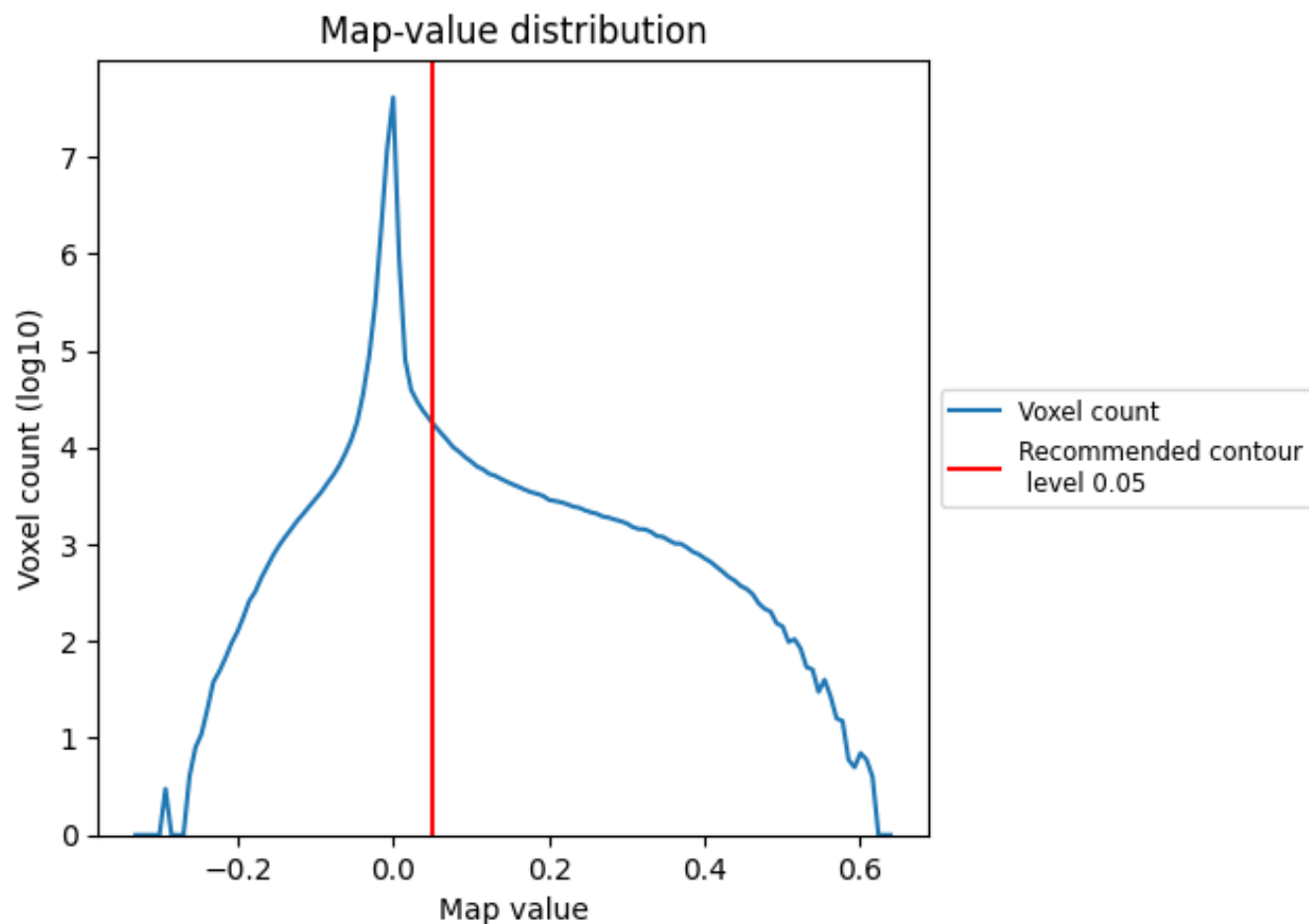
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

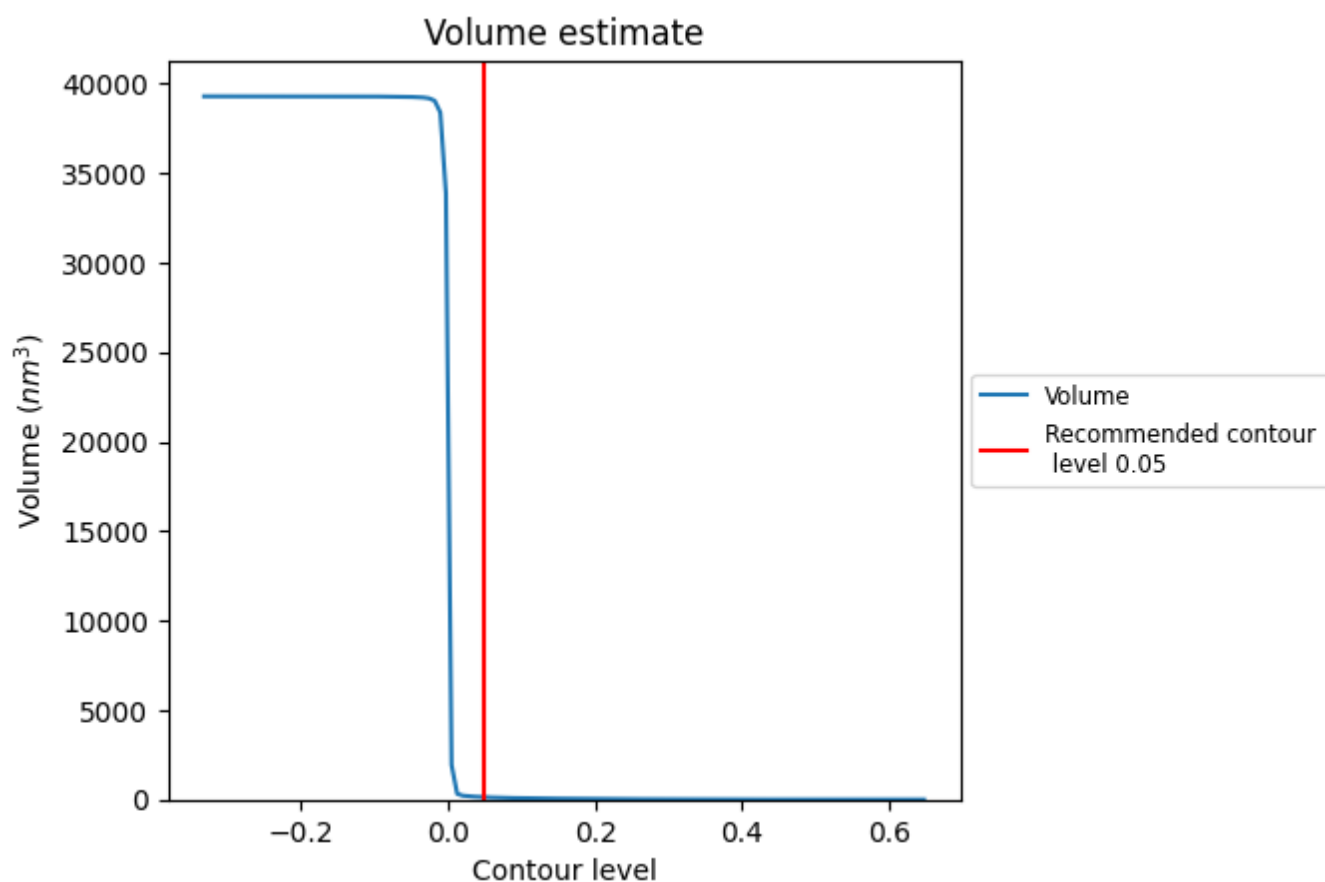
This section contains the results of statistical analysis of the map.

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.

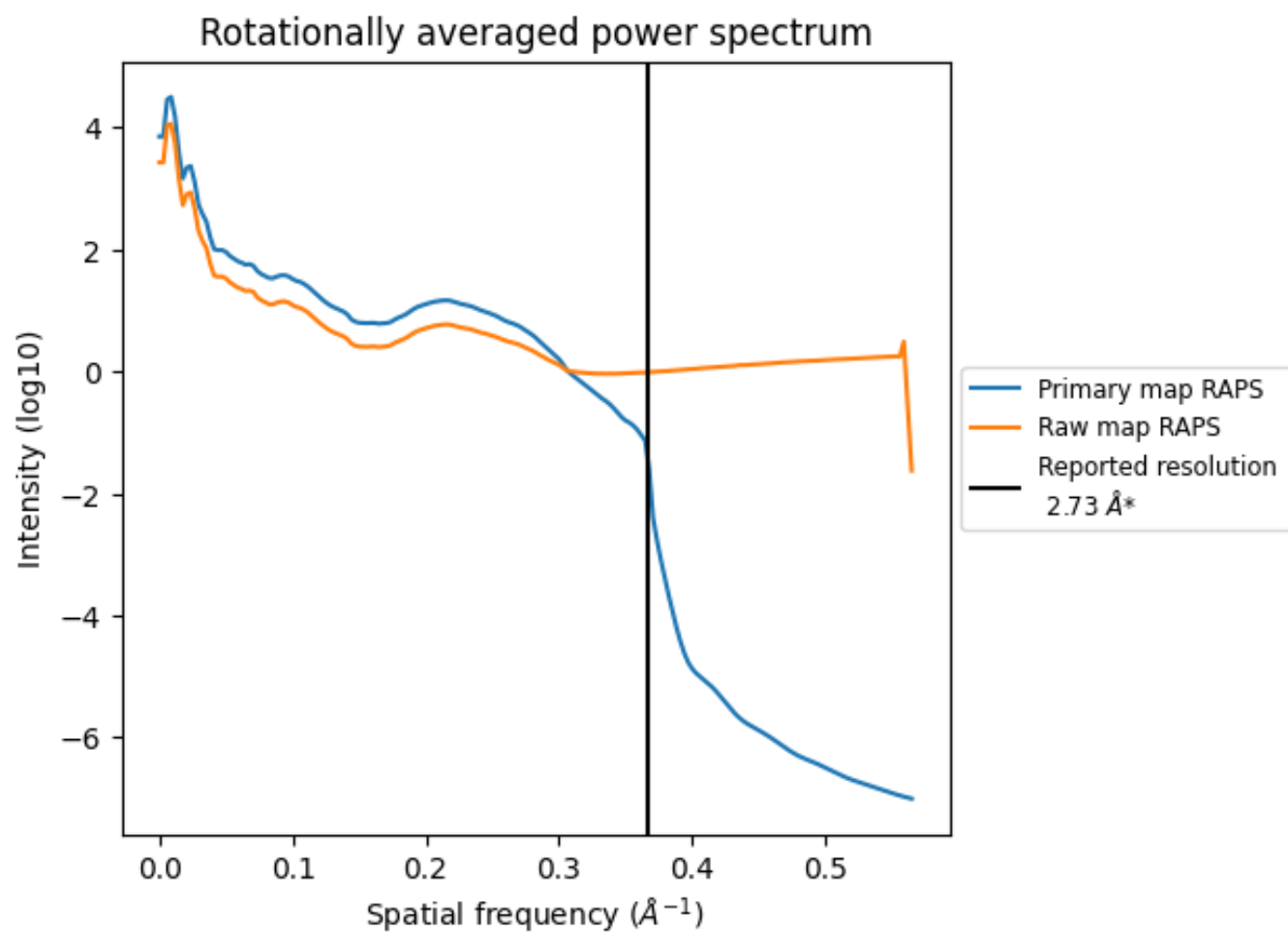
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm^3 ; this corresponds to an approximate mass of 119 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 ⓘ

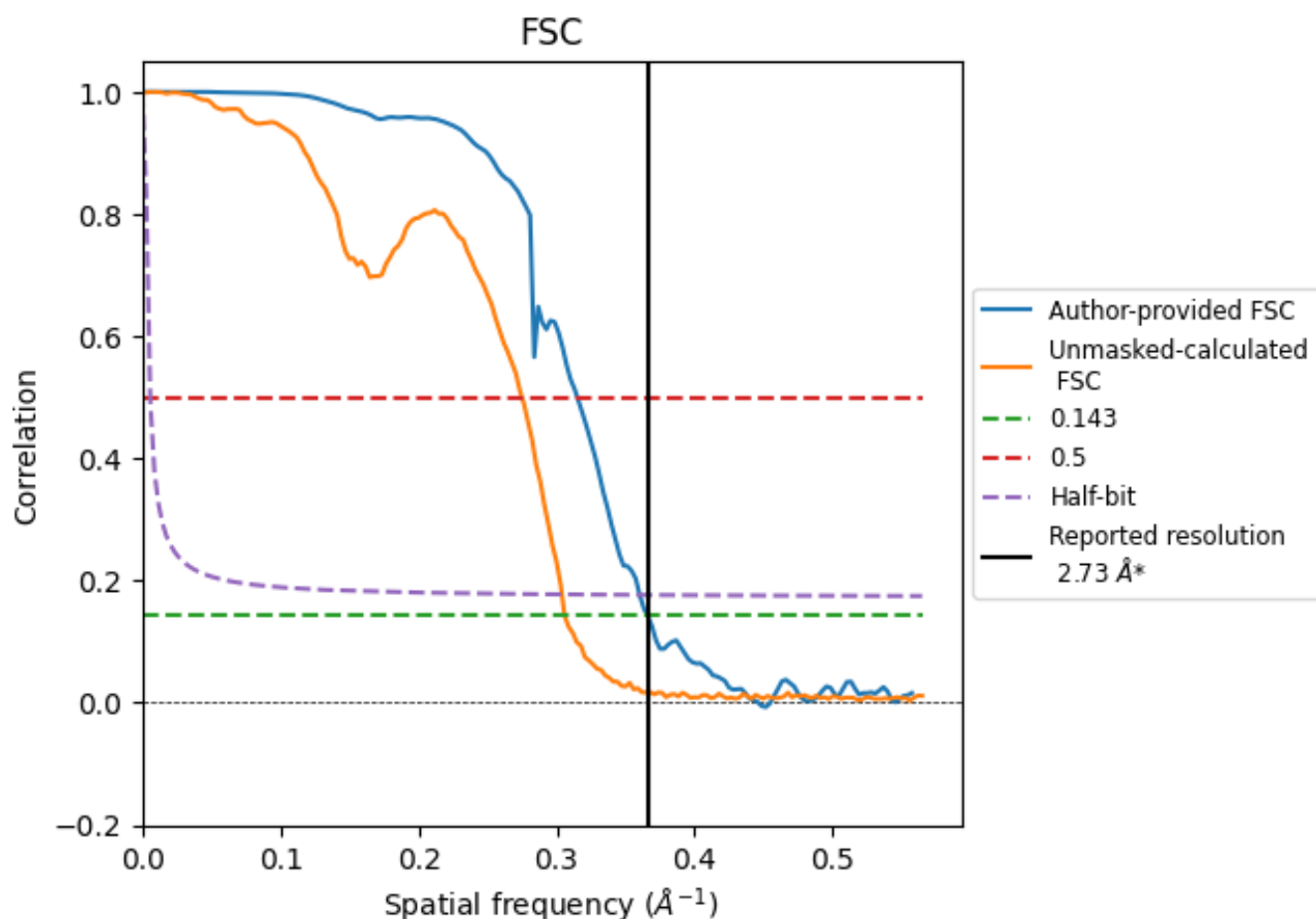


*Reported resolution corresponds to spatial frequency of 0.366 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

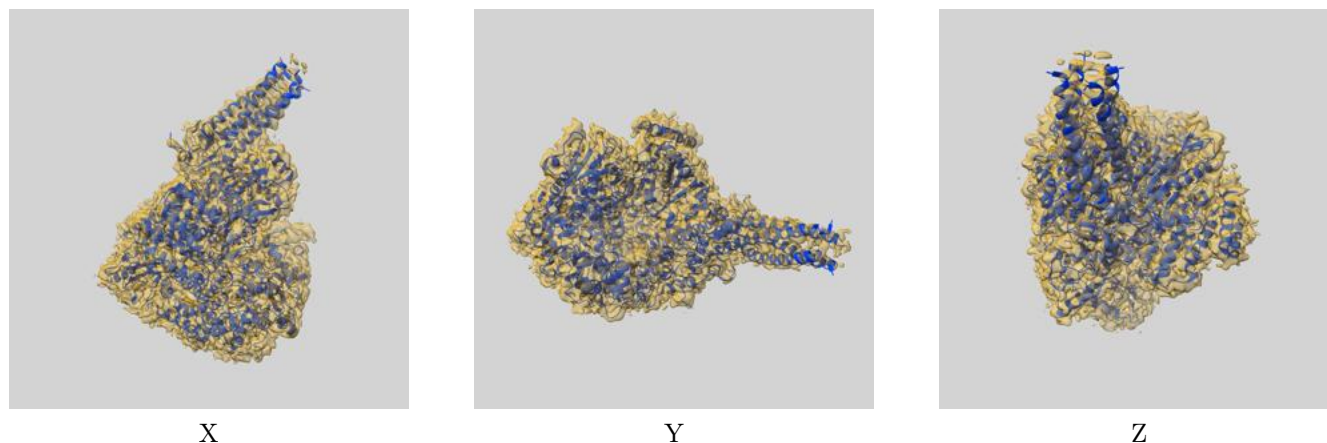
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.17	2.78
Unmasked-calculated*	3.27	3.64	3.29

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

9 Map-model fit [i](#)

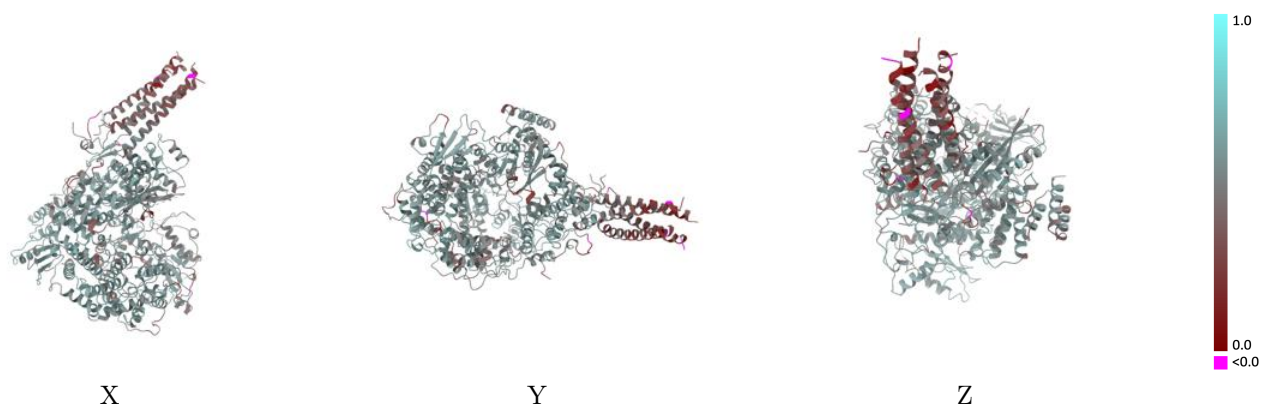
This section contains information regarding the fit between EMDB map EMD-70313 and PDB model 9OCF. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



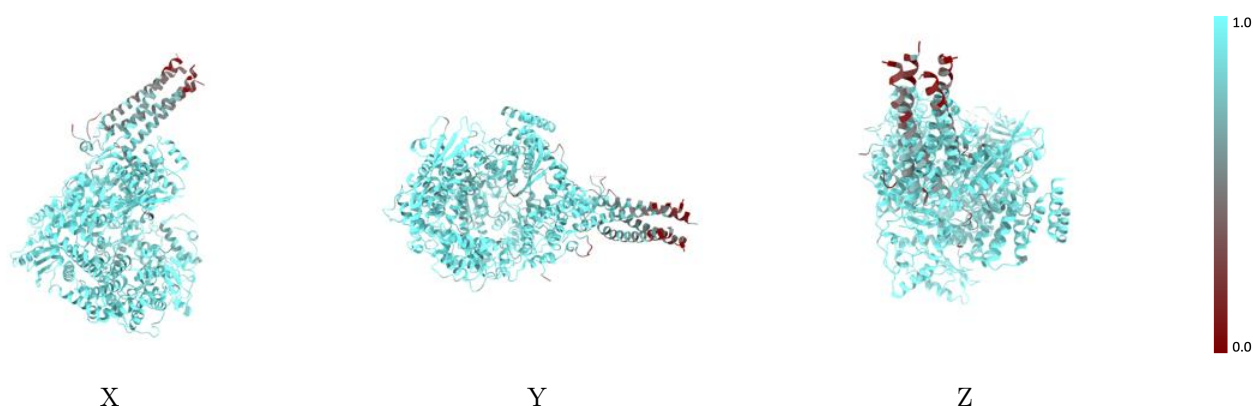
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



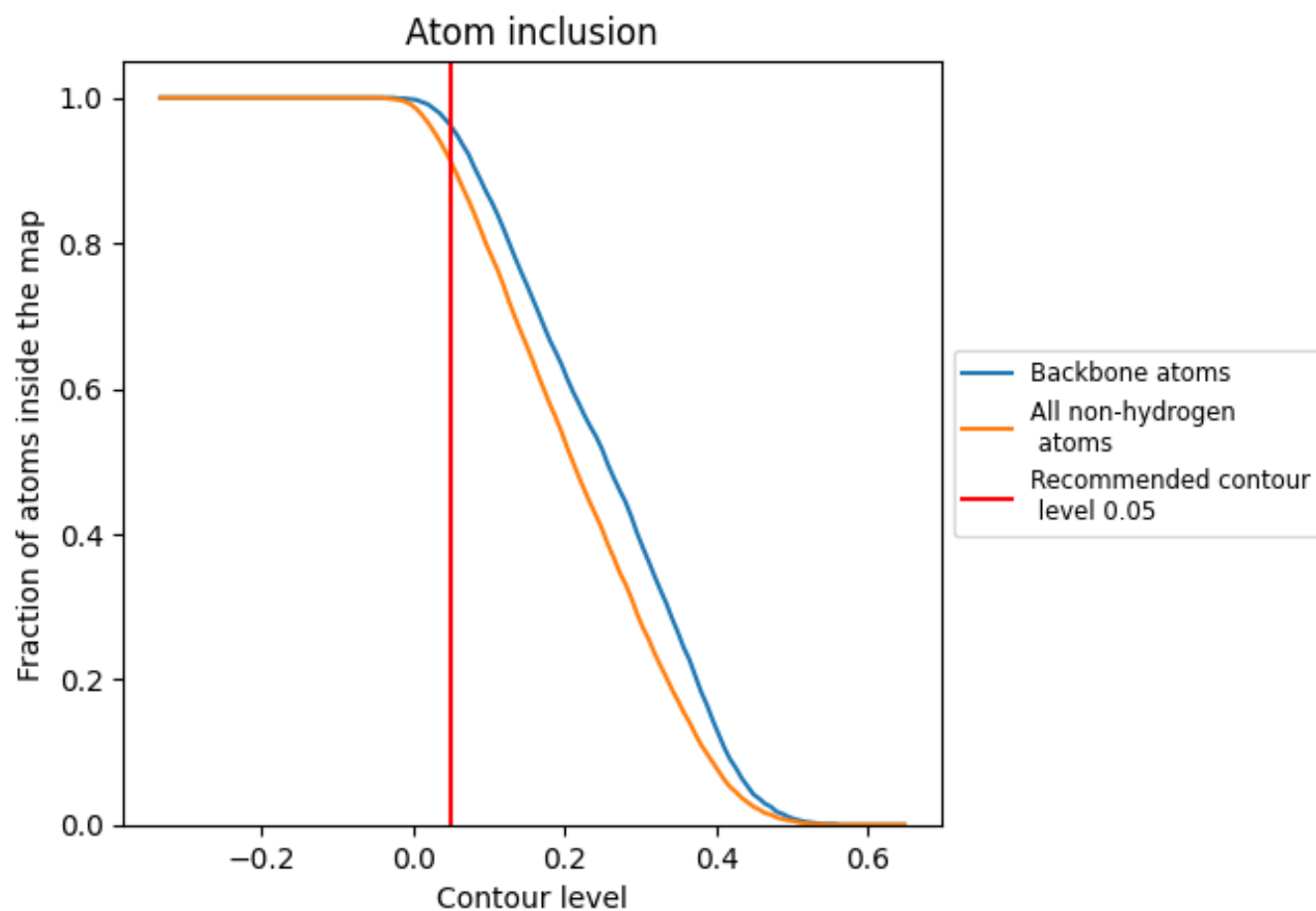
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9130	<div></div> 0.5170
A	<div></div> 0.9590	<div></div> 0.5430
B	<div></div> 0.6230	<div></div> 0.3830
C	<div></div> 0.7500	<div></div> 0.4090
D	<div></div> 0.6650	<div></div> 0.3830
E	<div></div> 0.6760	<div></div> 0.3600

