



Full wwPDB EM Validation Report ⓘ

Aug 25, 2025 – 11:09 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

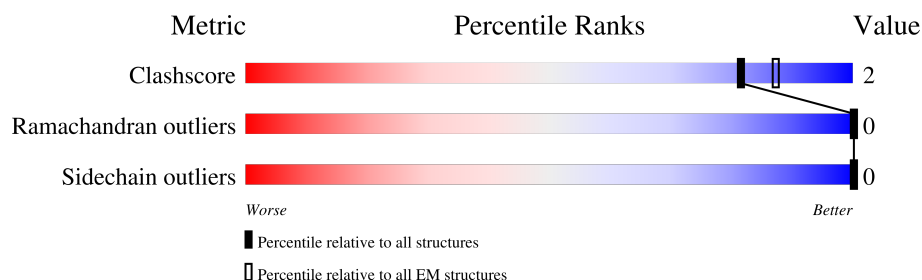
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




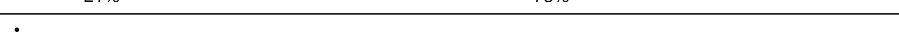

The reported resolution of this entry is 2.73 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2183	
2	B	509	
2	C	509	
2	D	509	
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		

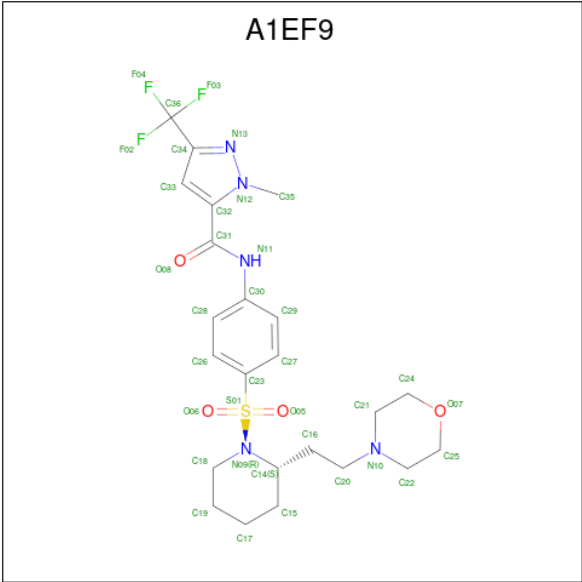
- Molecule 2 is a protein called Phosphoprotein.

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

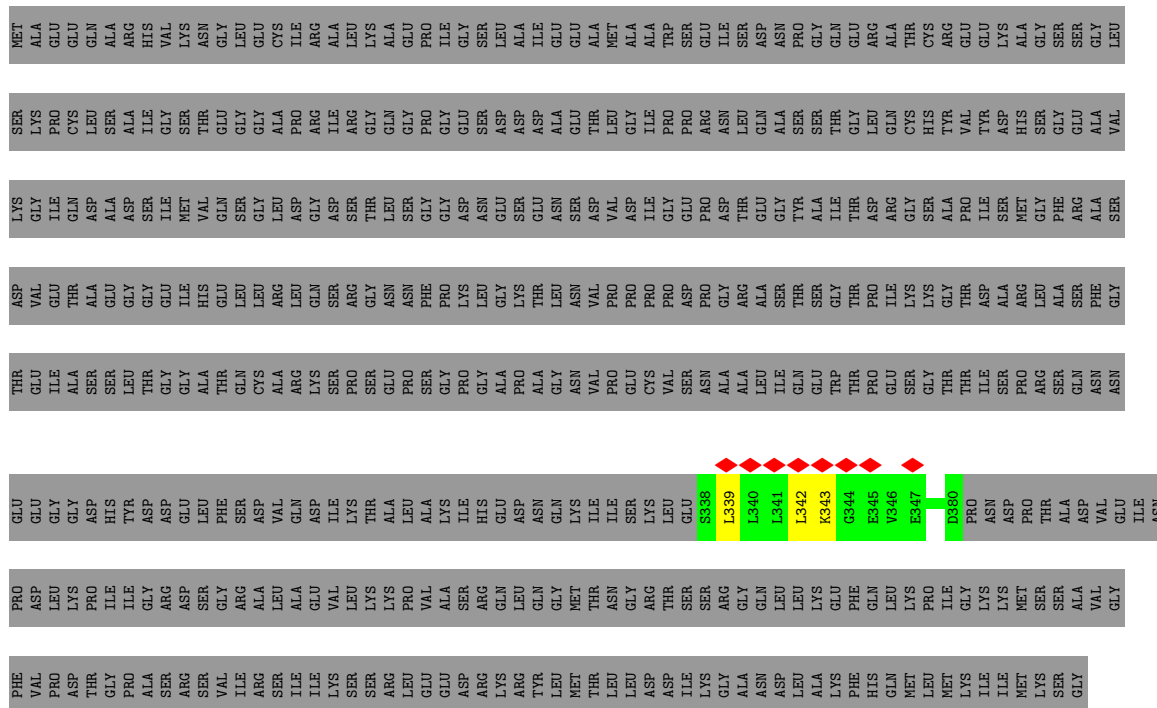


SER	ARG	ASN	GLU	THR	ASP	LYS	SER	ALA	MET
ARG	PRO	ASP	GLU	ILE	ASP	VAL	GLY	LYS	ALA
VAL	SER	PRO	GLY	ILE	THR	GLU	ILE	PRO	ALA
ILE	VAL	ALA	GLY	SER	ALA	THR	GLN	CYS	GLN
ARG	ILE	ASP	HIS	SER	GLU	SER	ALA	ASP	ALA
SER	VAL	VAL	THR	LEU	GLY	GLY	ASP	ALA	ARG
ILE	ILE	GLU	ASP	THR	GLU	THR	ILE	ILE	HIS
LYS	ASN	ASN	GLU	GLY	ILE	GLU	GLY	MET	LYS
SER	<div>◆</div>	P392	LEU	ALA	HIS	VAL	VAL	ASN	THR
SER	<div>◆</div>	D393	PHE	THR	GLU	GLU	GLN	GLY	GLY
ARG	<div>◆</div>	T394	SER	GLN	LEU	LEU	SER	GLY	LEU
LEU	GLU	P413	ASP	CYS	LEU	GLY	GLY	GLY	LEU
GLU	VAL	VAL	VAL	ALA	ARG	ALA	LEU	ALA	CYS
ASP	ALA	ALA	GLN	LYS	GLN	GLY	ASP	GLY	ILE
ARG	SER	SER	ILE	SER	SER	SER	SER	ILE	ALA
LYS	ARG	LYS	LYS	PRO	ARG	ARG	ASP	ARG	LEU
ARG	GLN	GLN	THR	SER	GLY	THR	THR	GLY	LYS
TYR	LEU	TYR	ALA	GLU	ASN	GLU	SER	GLN	ALA
LEU	GLN	GLN	LEU	PRO	ASN	ASN	SER	GLY	GLU
MET	GLY	GLY	ALA	SER	PHE	PHE	GLY	GLY	PRO
THR	MET	THR	LYS	GLY	PRO	PRO	ASP	GLY	ILE
LEU	THR	THR	ILE	PRO	LYS	LYS	ASP	GLY	GLY
LEU	ASN	ASN	HIS	GLY	LEU	HIS	ILE	ASN	LEU
ASP	GLY	GLY	GLU	ALA	GLY	GLY	ASN	ASP	LEU
ILE	ILE	THR	ASN	ALA	THR	THR	GLY	ASP	ALA
LYS	SER	SER	GLN	GLY	LEU	LEU	ASN	ALA	GLU
GLY	ALA	ARG	ILE	VAL	VAL	VAL	ASP	GLU	GLU
ALA	ASN	ILE	ILE	PRO	GLY	PRO	VAL	THR	ALA
ASP	GLN	GLN	ILE	GLU	ARG	PRO	ASP	GLY	MET
LEU	LEU	LEU	LYS	CYS	PRO	PRO	ILE	ILE	ALA
ALA	LEU	LEU	LEU	VAL	VAL	PRO	GLY	PRO	TRP
LYS	LYS	LYS	GLU	SER	ASP	ASP	GLY	ASP	SER
PHE	GLU	<div>◆</div>	S338	ASN	PRO	PRO	GLU	PRO	GLU
HIS	PHE	<div>◆</div>	L339	ALA	GLY	GLY	ASP	ASN	ILE
GLN	GLN	<div>◆</div>	L340	ALA	ARG	ARG	THR	LEU	SER
MET	LEU	<div>◆</div>	L341	LEU	ALA	ALA	GLY	GLN	ASP
LEU	LEU	<div>◆</div>	L342	ILE	SER	SER	GLY	ALA	ASN
MET	PRO	<div>◆</div>	L343	GLN	THR	THR	TYR	SER	PRO
ILE	ILE	<div>◆</div>	K343	GLU	GLY	GLY	ILE	SER	GLY
ILE	LYS	<div>◆</div>	G344	TRP	THR	THR	THR	GLY	GLU
MET	LYS	<div>◆</div>	E347	PRO	PRO	PRO	ASP	LEU	ALA
LYS	MET	<div>◆</div>	<div>+</div>	SER	ILE	ILE	ARG	GLN	ALA
SER	SER	<div>◆</div>	N357	GLU	LYS	LYS	GLY	CYS	THR
ALA	ALA	<div>◆</div>	L363	THR	GLY	GLY	ALA	THR	ARG
VAL	VAL	<div>◆</div>	<div>+</div>	ILE	THR	THR	ALA	VAL	GLU
GLY	GLY	<div>◆</div>	I370	ILE	ASP	ASP	ILE	TYR	GLU
PHE	PHE	<div>◆</div>	<div>+</div>	SER	ALA	ALA	SER	ASP	LYS
VAL	VAL	<div>◆</div>	<div>+</div>	PRO	ARG	ARG	MET	HIS	ALA
PRO	PRO	<div>◆</div>	P375	ARG	LEU	LEU	GLY	ALA	GLY
ASP	ASP	<div>◆</div>	<div>+</div>	SER	ALA	ALA	PHE	SER	SER
GLY	GLY	<div>◆</div>	GLY	GLN	SER	SER	ARG	GLY	GLY
PRO	PRO	<div>◆</div>	L385	ASN	THR	THR	GLY	GLU	ALA
PRO	PRO	<div>◆</div>	<div>+</div>	ASN	GLY	GLY	SER	ALA	ALA

- Molecule 2: Phosphoprotein



- 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

5.1 Standard geometry

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

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.

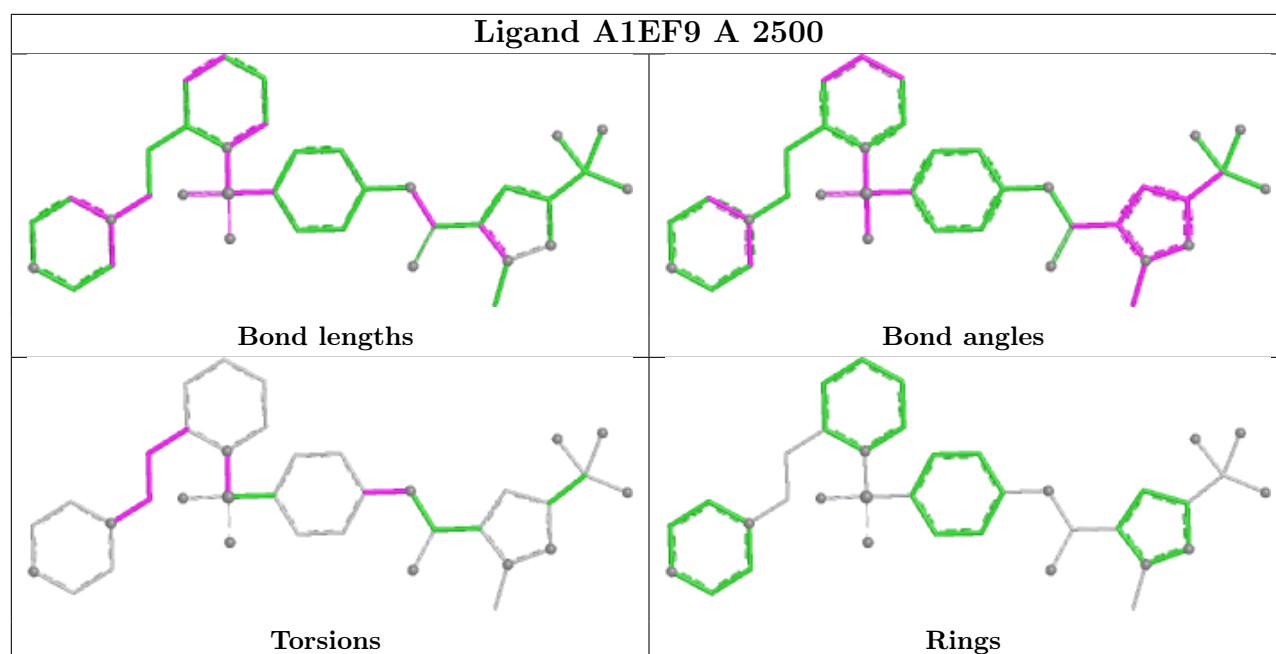
All (12) torsion outliers are listed below:

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.

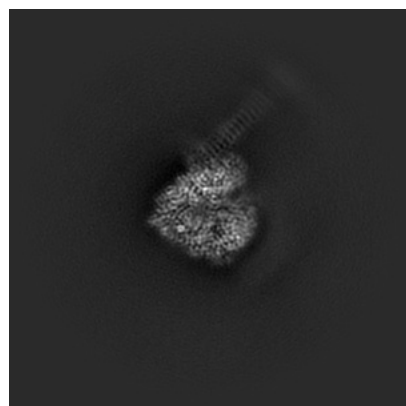
6 Map visualisation [i](#)

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.

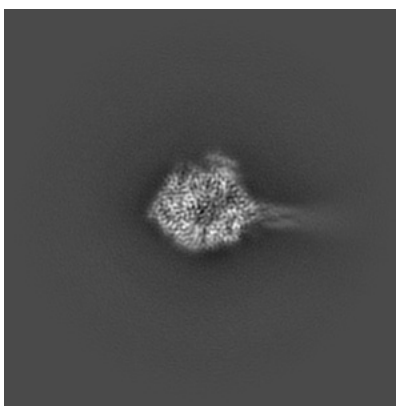
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

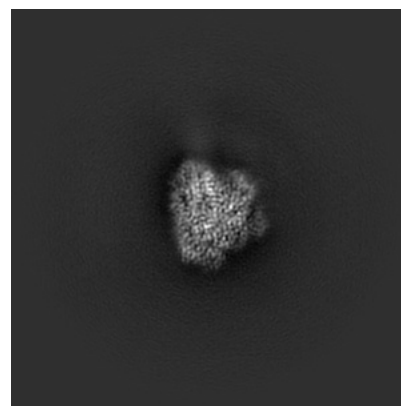
6.1.1 Primary map



X

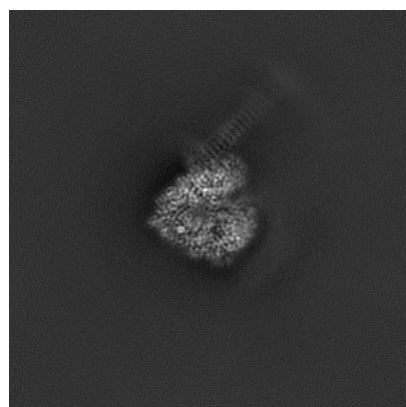


Y

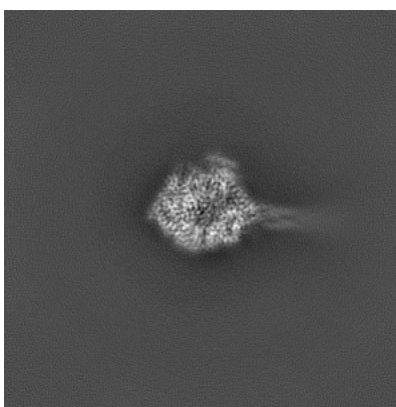


Z

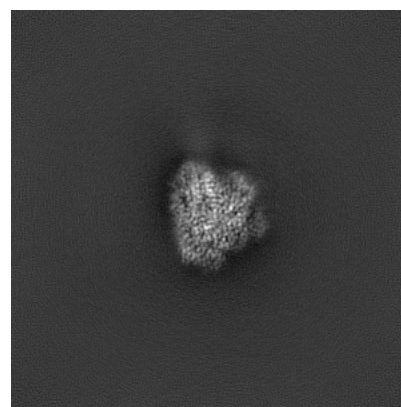
6.1.2 Raw map



X



Y

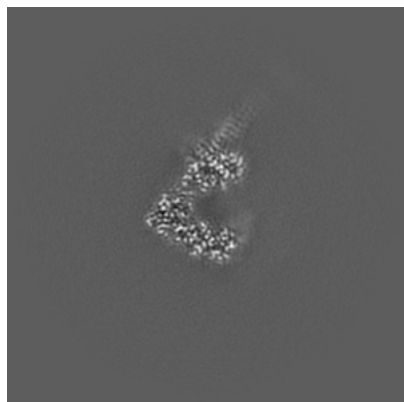


Z

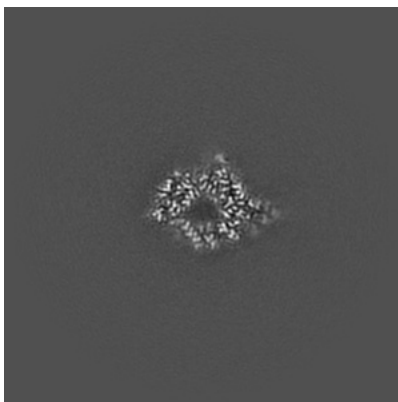
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

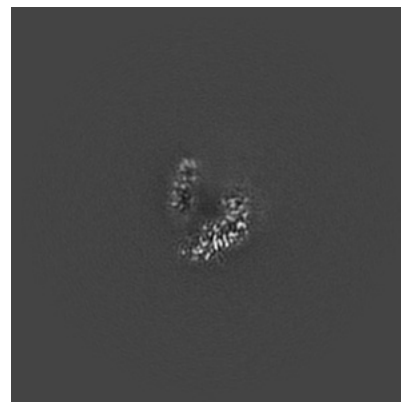
6.2.1 Primary map



X Index: 192

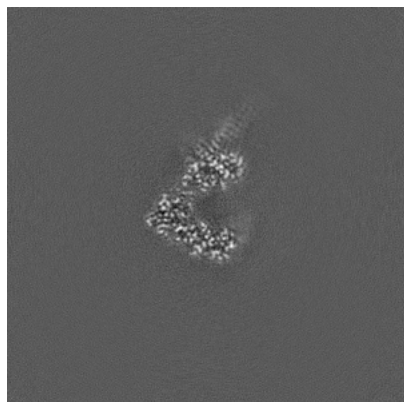


Y Index: 192

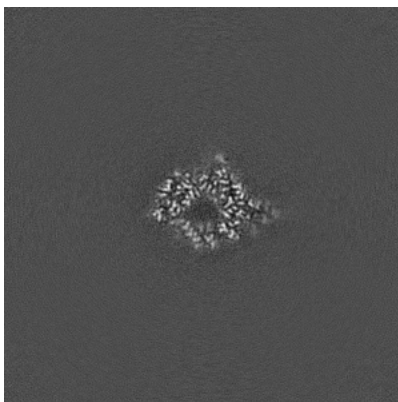


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

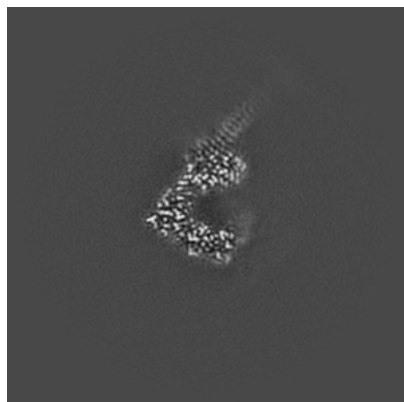


Z Index: 192

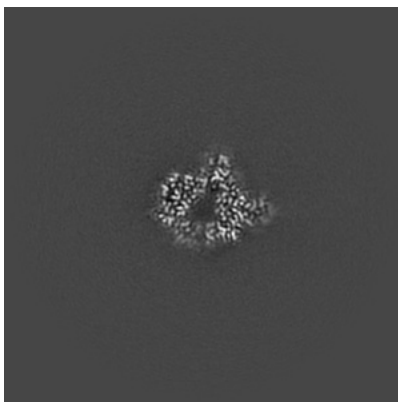
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

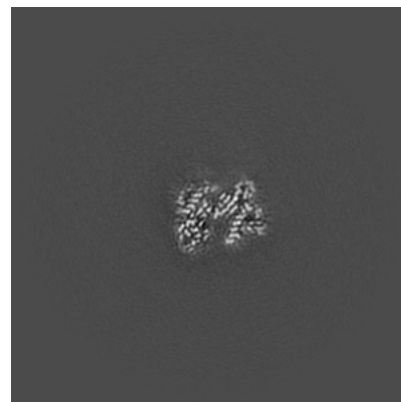
6.3.1 Primary map



X Index: 190

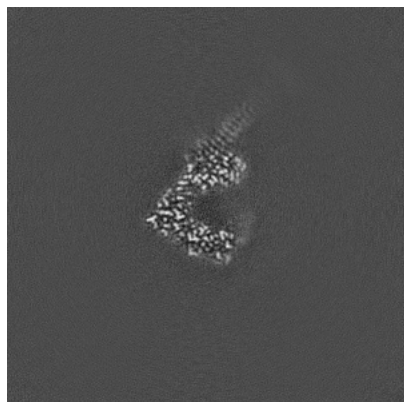


Y Index: 187

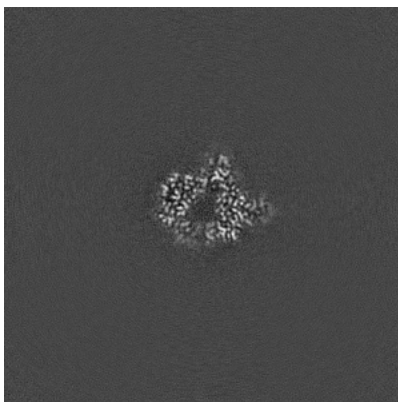


Z Index: 211

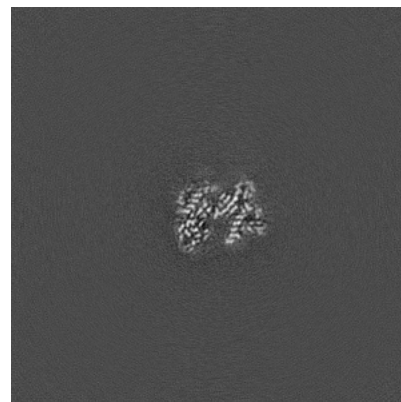
6.3.2 Raw map



X Index: 190



Y Index: 187

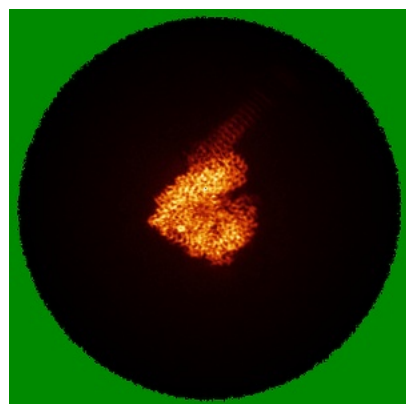


Z Index: 211

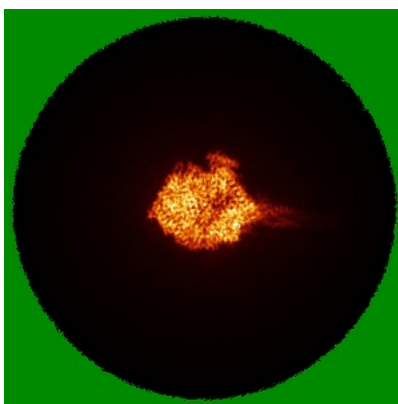
The images above show the largest variance slices of the map in three orthogonal directions.

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

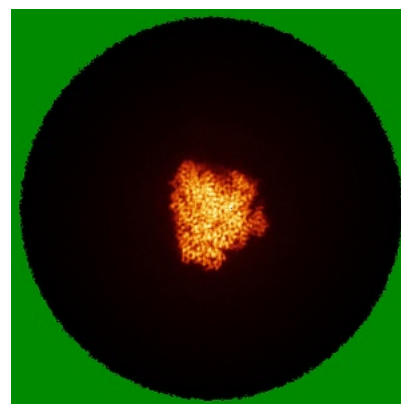
6.4.1 Primary map



X

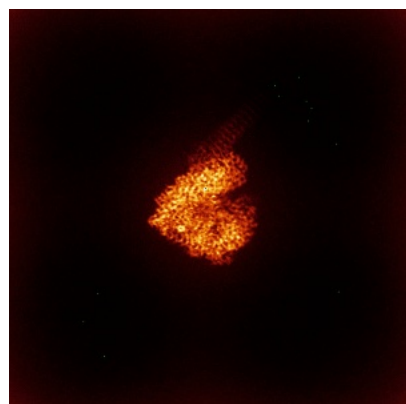


Y

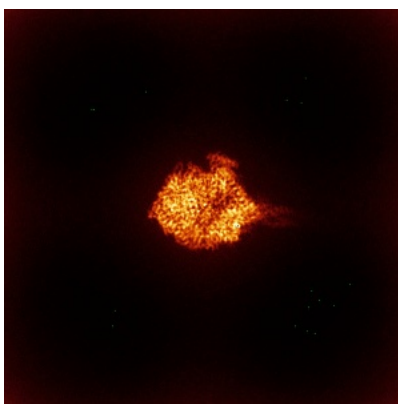


Z

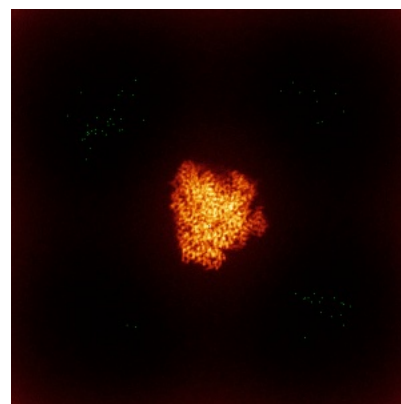
6.4.2 Raw map



X



Y

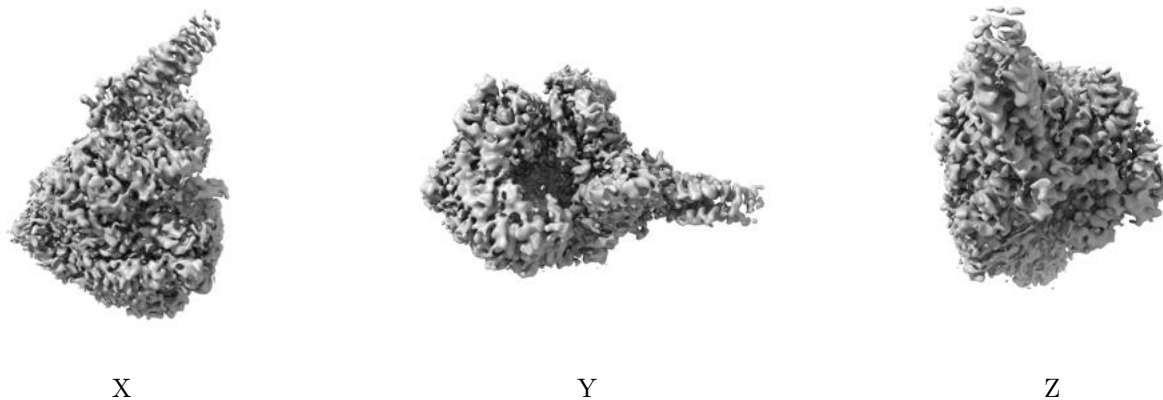


Z

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.

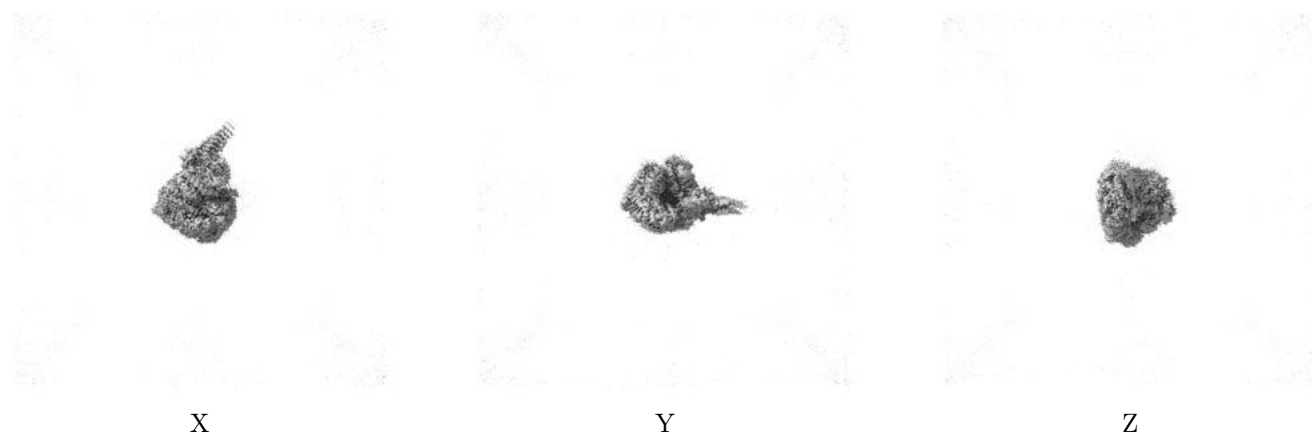
6.5 Orthogonal surface views [i](#)

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.

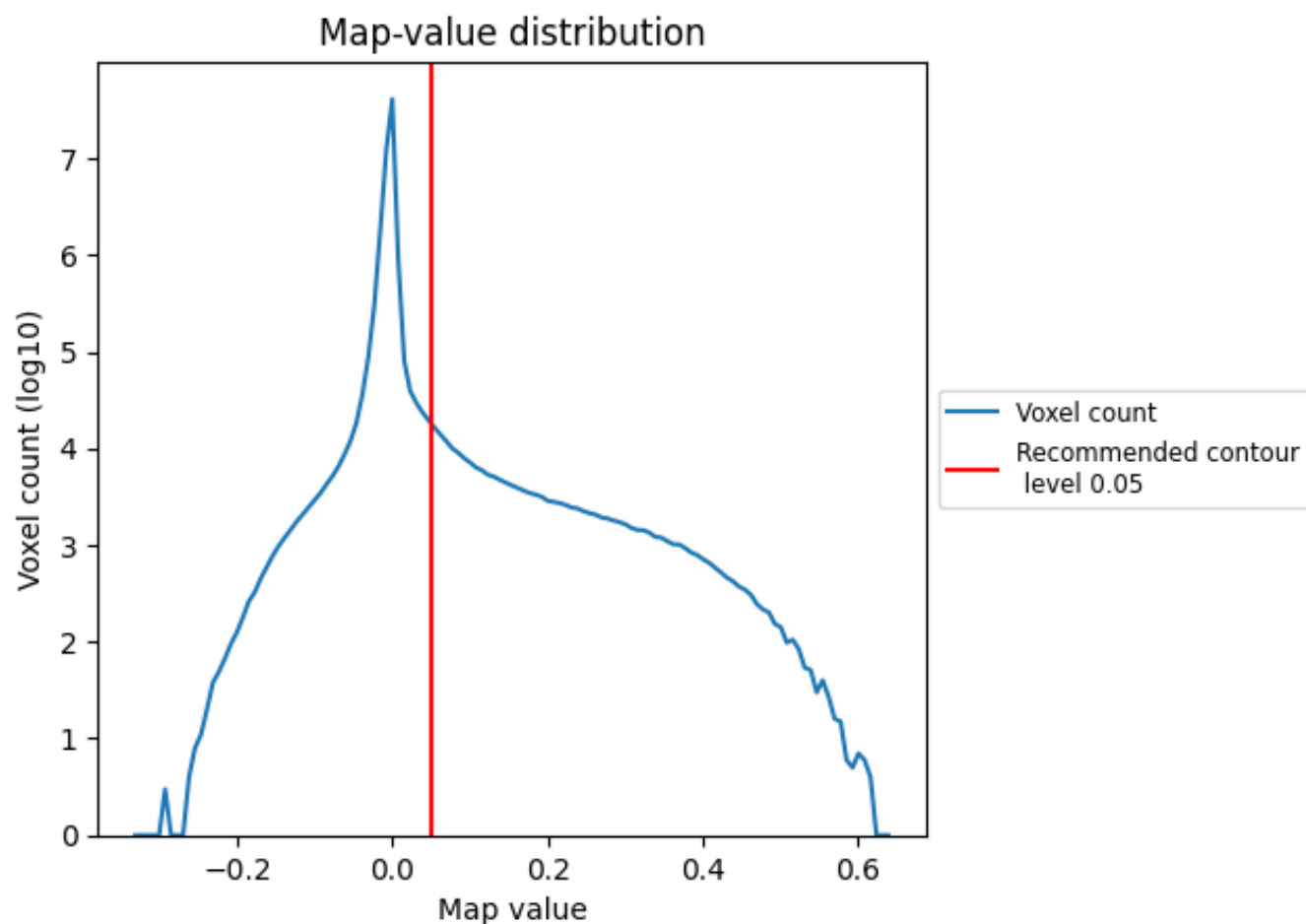
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

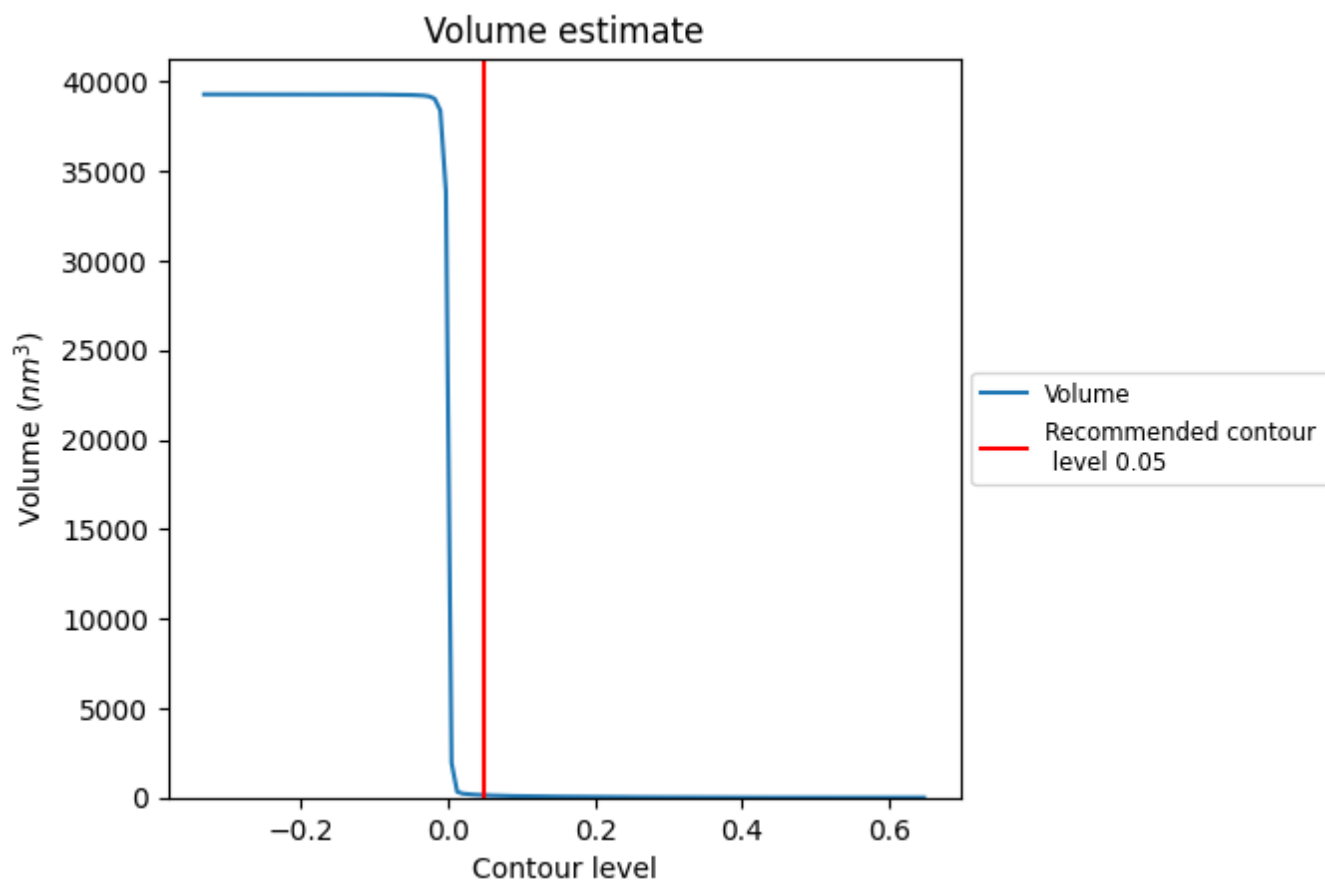
This section contains the results of statistical analysis of the map.

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.

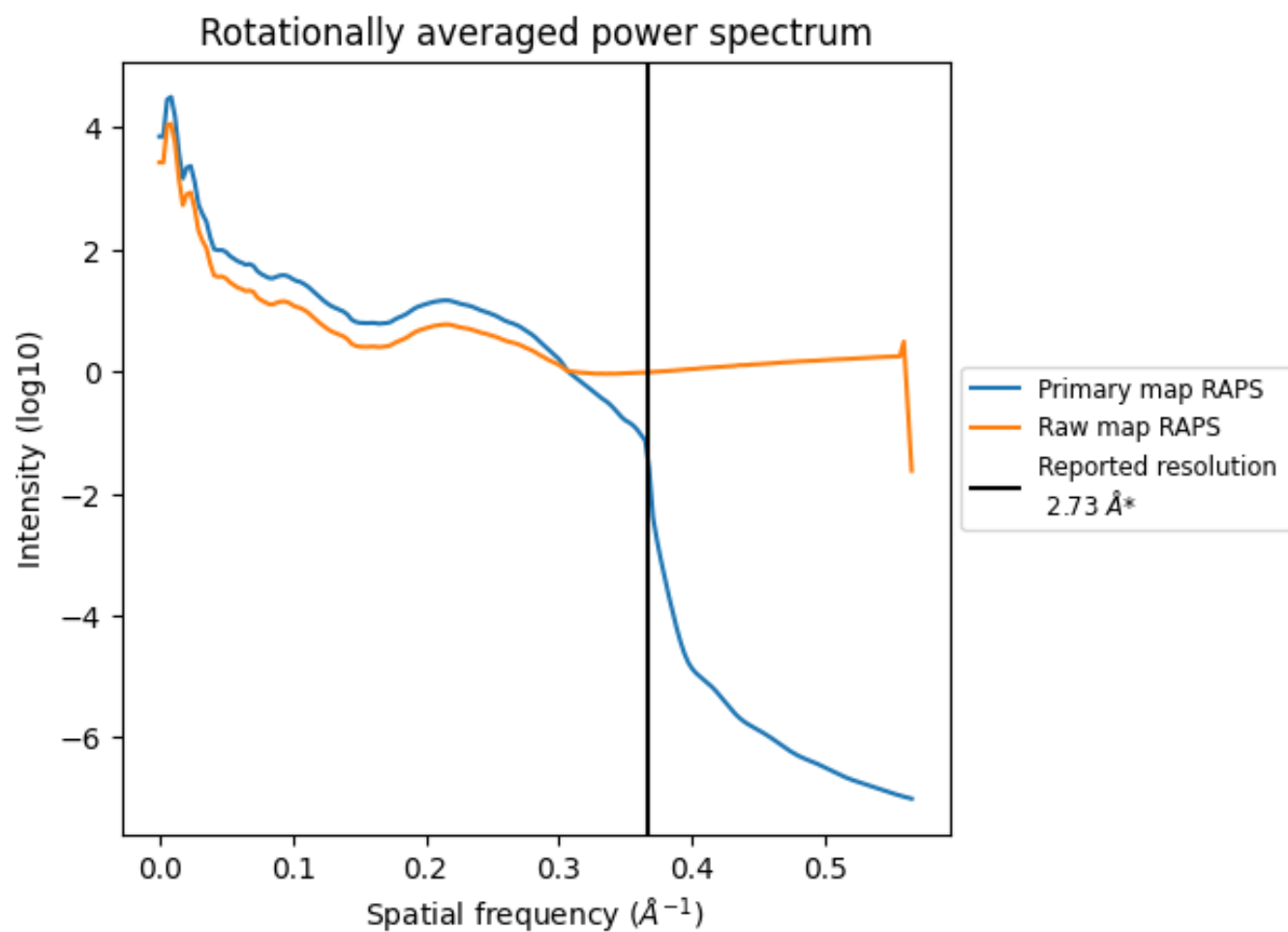
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; 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 ⓘ

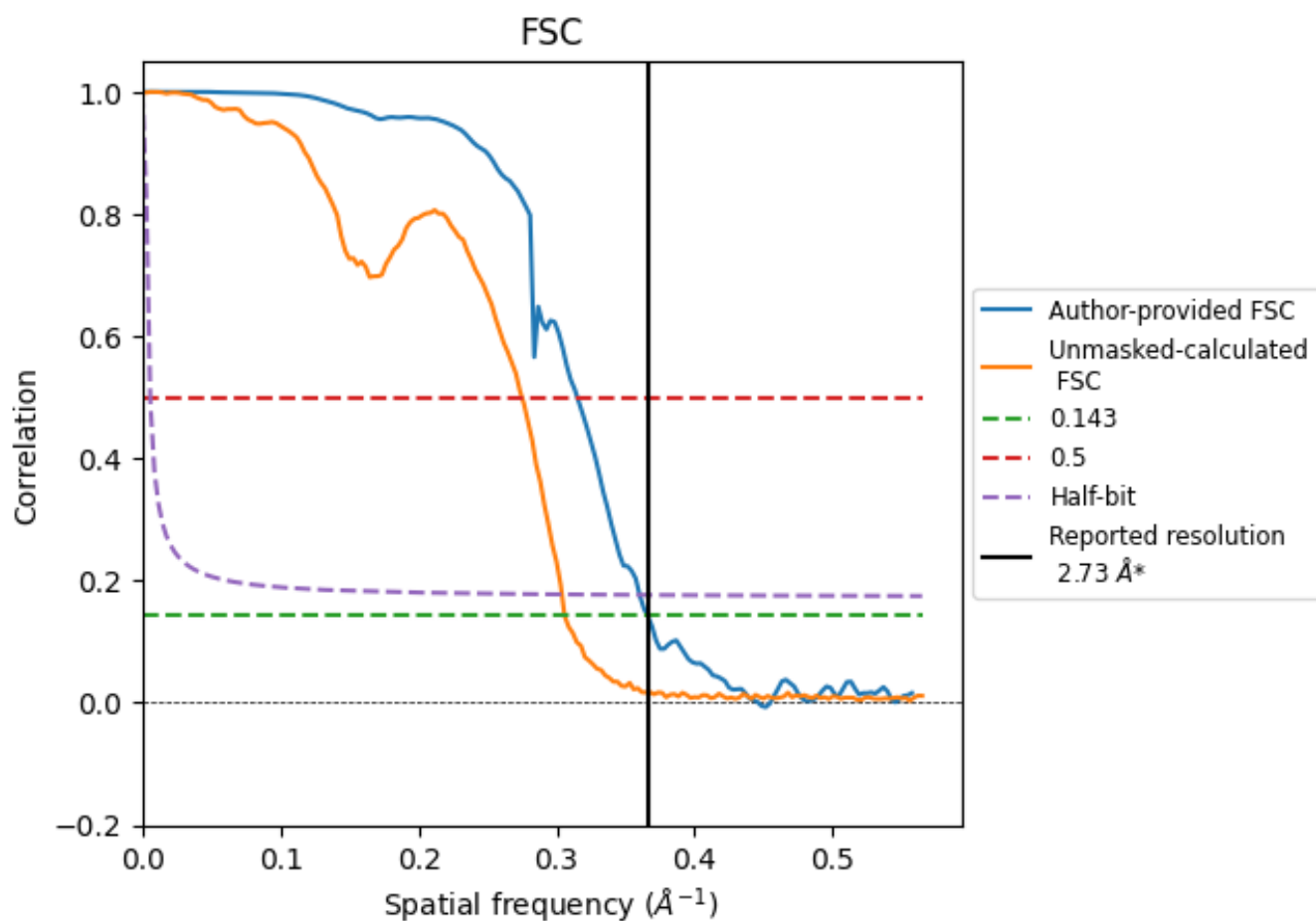


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

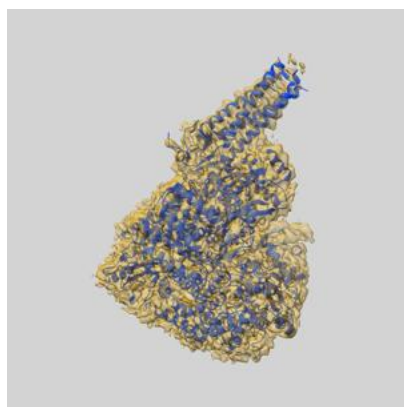
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.17	2.78
Unmasked-calculated*	3.27	3.64	3.29

*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 %

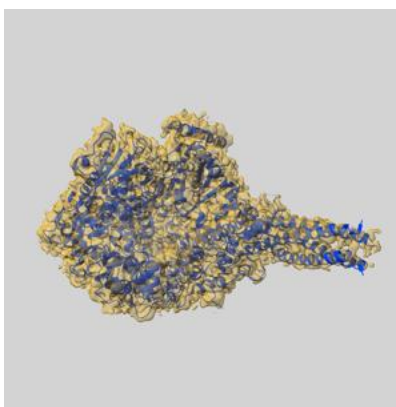
9 Map-model fit [i](#)

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 5](#).

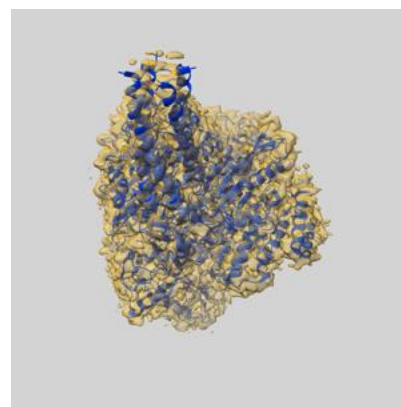
9.1 Map-model overlay [i](#)



X



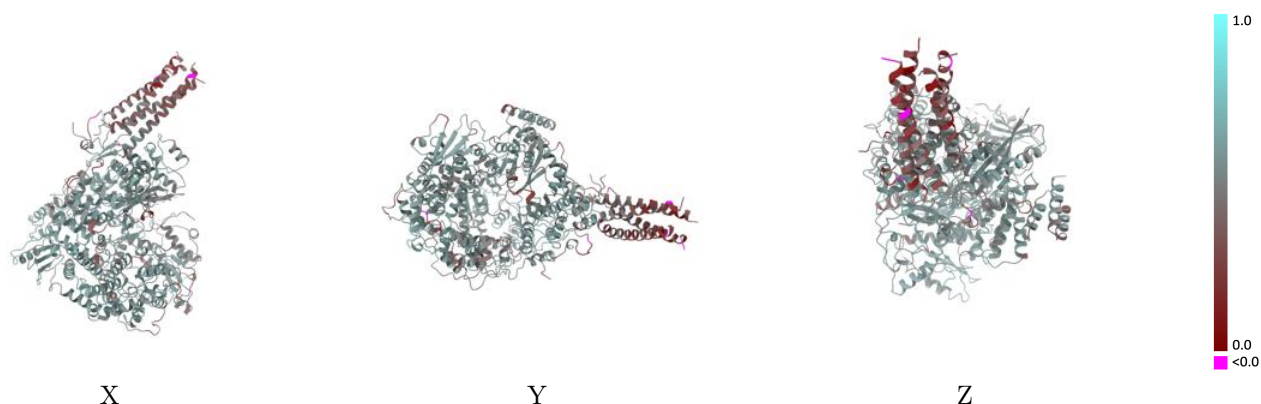
Y



Z

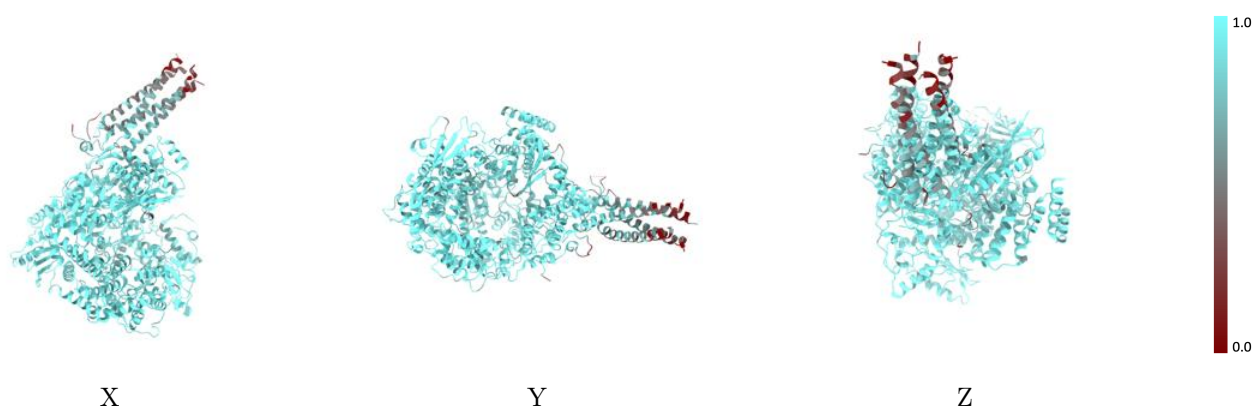
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



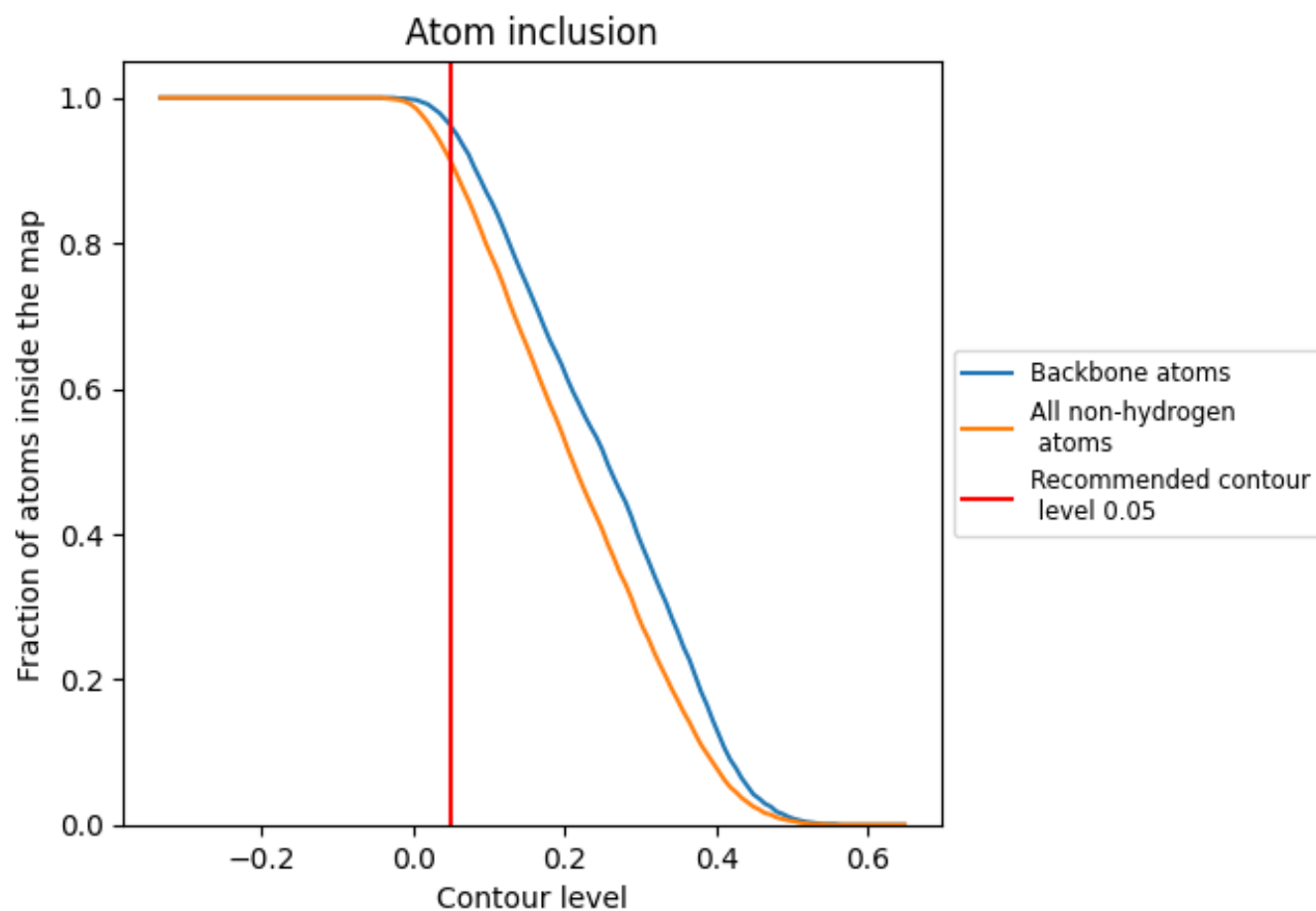
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

