



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 10:28 AM EDT

PDB ID : 9OCE / pdb\_00009oce  
EMDB ID : EMD-70312  
Title : 2.48A cryo-EM structure of the Measles Virus L-P-C in complex with ERdRp-0519  
Authors : Liu, B.; Wang, D.; Yang, G.  
Deposited on : 2025-04-24  
Resolution : 2.48 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

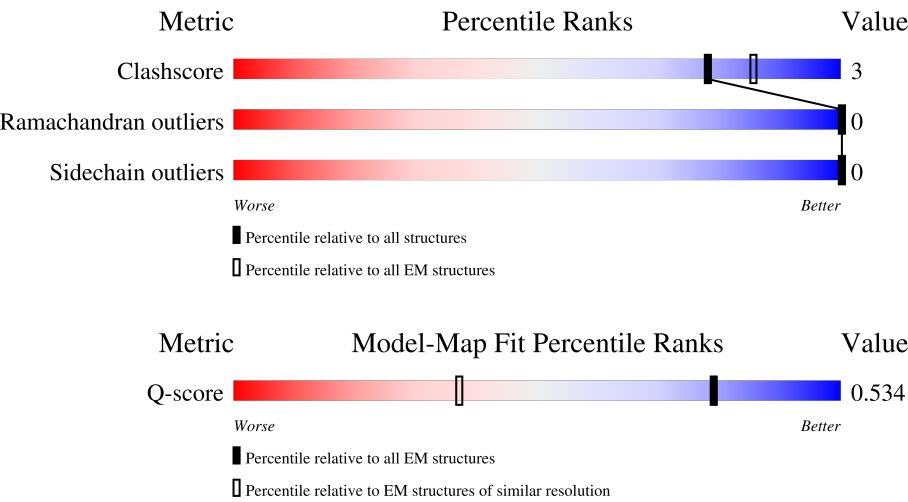
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.48 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	6178 ( 1.98 - 2.98 )

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  $\geq 3$ , 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	
3	F	186	
3	G	186	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20404 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	1997	Total	C	N	O	S	0	0
			15972	10232	2729	2922	89		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	74	Total	C	N	O	S	1	0
			581	370	103	107	1		
2	C	132	Total	C	N	O	S	0	0
			1038	658	185	189	6		
2	D	57	Total	C	N	O	S	0	0
			442	279	77	85	1		
2	E	74	Total	C	N	O	S	1	0
			576	365	97	113	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 a protein called Protein C.

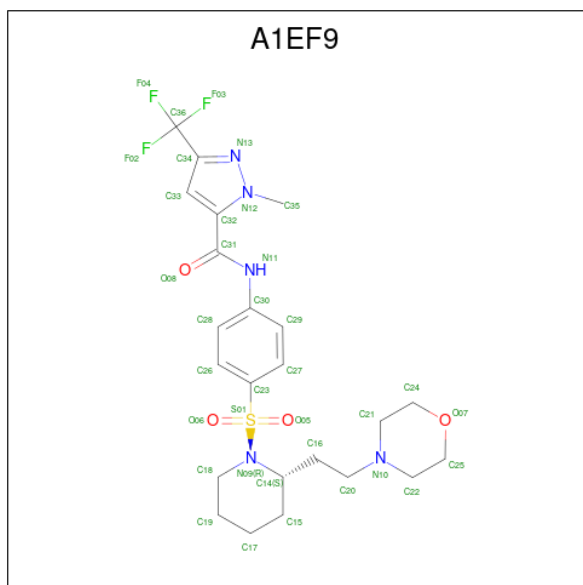
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	115	Total	C	N	O	S	0	0
			900	579	152	160	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	109	Total	C	N	O	S	0	0
			859	554	143	153	9		

- 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: C<sub>23</sub>H<sub>30</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).

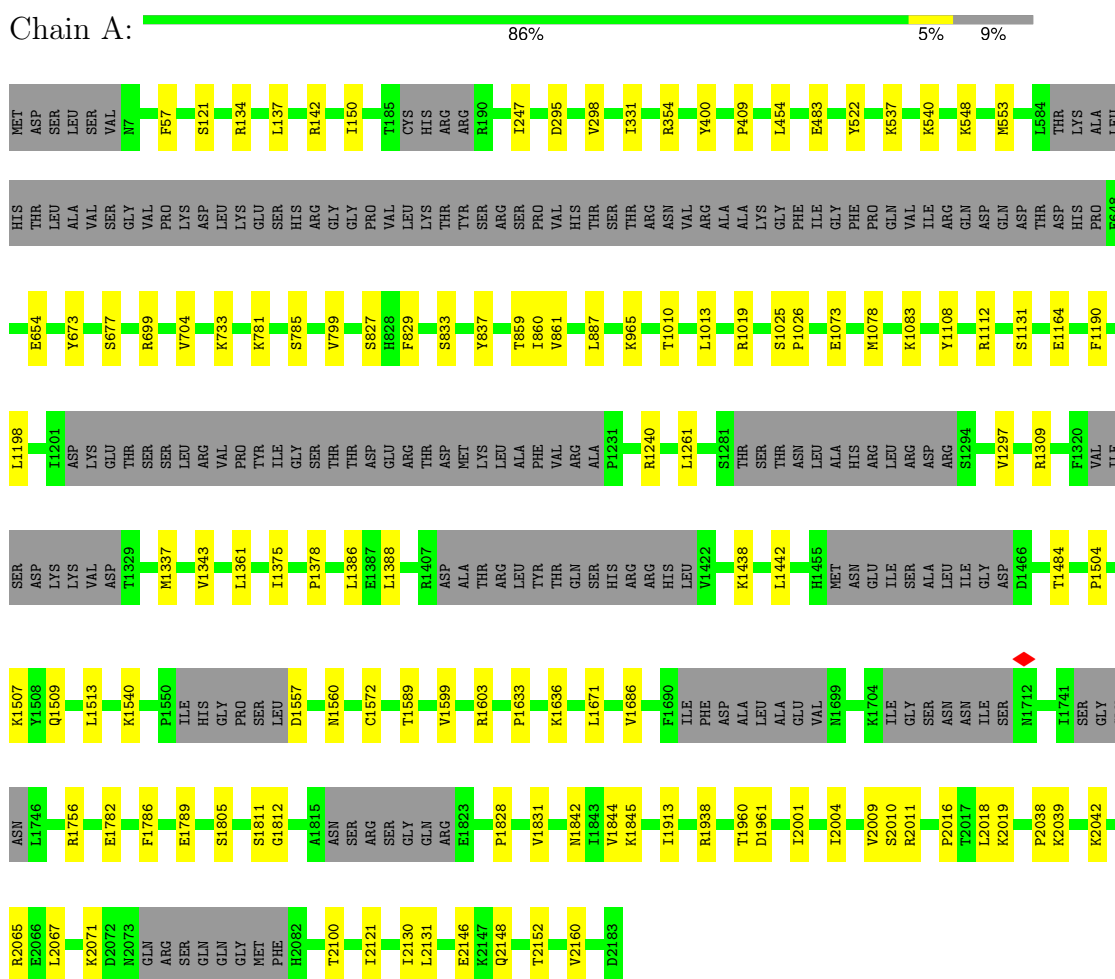


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	F	N	O	S	0
			36	23	3	5	4	1	

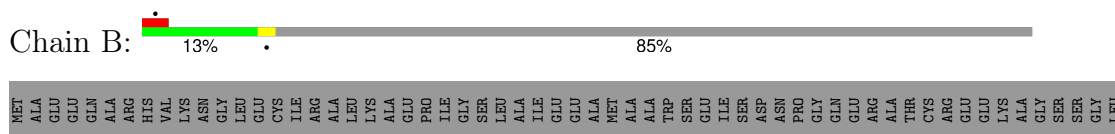
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: RNA-directed RNA polymerase L



#### • Molecule 2: Phosphoprotein



- Molecule 2: Phosphoprotein



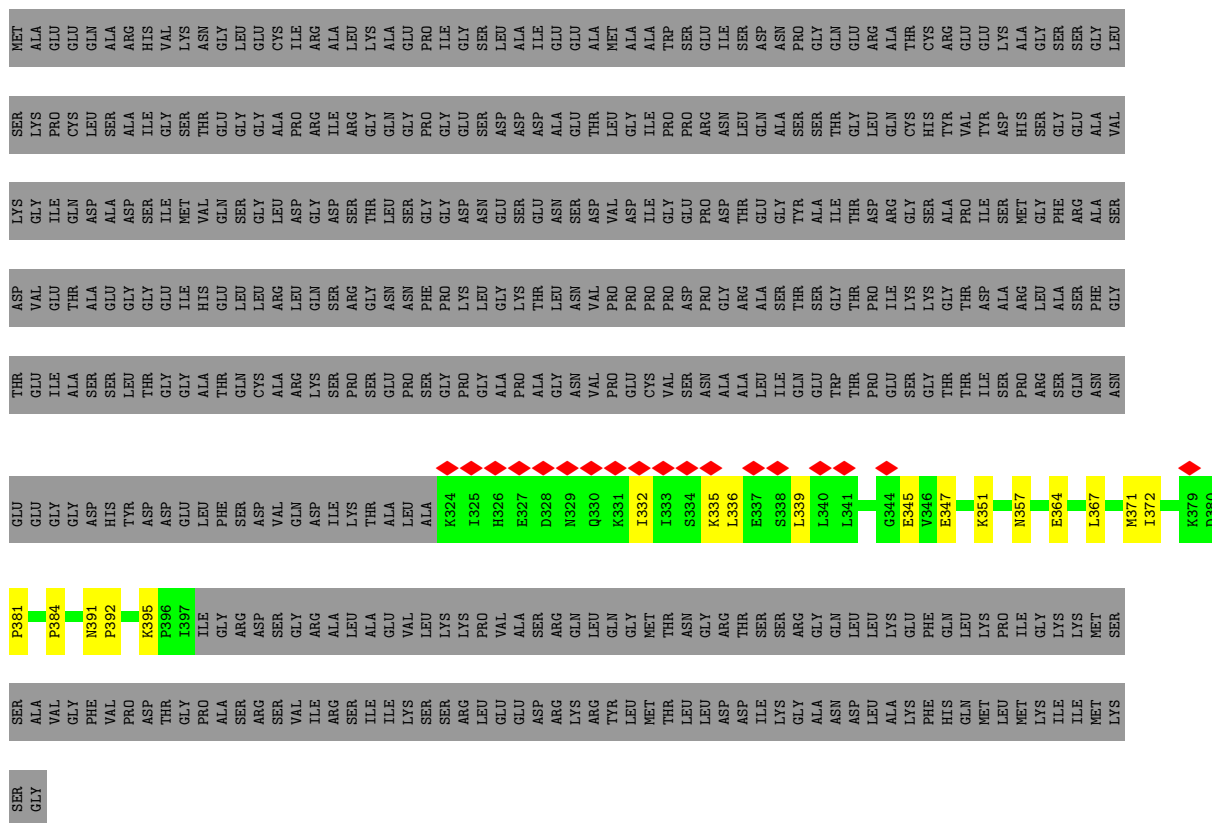
ASP	PRO	THR	ALA	ASP	VAL	GLU	GLU	THR	ASP	LYS	SER	MET
PRO	THR	ALA	ASP	ASP	VAL	GLU	GLU	ILE	GLU	ILE	PRO	ALA
ALA	ALA	ALA	GLY	ASP	THR	GLY	GLY	ALA	THR	GLN	CYS	GLU
ASP	ASP	ASP	ASP	HIS	SER	SER	TYR	SER	GLU	ALA	SER	GLN
VAL	VAL	THR	HIS	TYR	SER	LEU		LEU	GLY	ASP	ALA	ARG
GLU	GLU	THR	ASP	ASP	THR	THR		THR	GLY	SER	ILE	HIS
ILE	ILE	GLY	ASP	ASP	GLY	GLY		GLY	GLU	ILE	GLY	VAL
ASN	ASN	GLY	ASP	ASP	GLY	GLY		GLY	ILE	SER	LYS	VAL
PRO	PRO	ALA	LEU	LEU	ALA	ALA		ALA	HIS	ASN	THR	GLY
ASP	ASP	ASP	PHE	ASP	THR	THR		THR	GLU	GLN	GLU	GLY
LEU	LEU	LEU	ASP	ASP	GLN	GLN		GLN	LEU	SER	GLY	LEU
LYS	LYS	GLY	ASP	ASP	CYS	CYS		CYS	LEU	LEU	GLY	LEU
PRO	PRO	THR	ASP	ASP	ALA	ALA		ALA	ARG	SER	THR	LYS
ILE	ILE	ILE	VAL	VAL	ALA	ALA		ALA	GLY	GLY	GLY	CYS
GLY	GLY	GLY	GLN	GLN	LYS	LYS		LYS	GLN	GLY	ARG	ILE
ARG	ARG	ARG	ILE	ILE	PRO	PRO		PRO	SER	SER	ILE	ALA
ASP	ASP	THR	LYS	THR	ASN	ASN		ASN	GLY	ASP	GLY	LEU
GLY	GLY	ALA	LEU	ALA	GLU	GLY		GLY	THR	GLY	GLY	LYS
ARG	ARG	ALA	LEU	LEU	SER	SER		SER	ASN	ASP	GLN	ALA
ALA	ALA	ALA	ALA	ALA	ALA	ALA		ALA	VAL	VAL	ALA	GLY
LEU	LEU	ALA	K324	K324	PRO	PRO		PRO	LYS	ASN	GLY	LEU
ALA	ALA	ALA	K325	K325	GLY	GLY		GLY	ASN	ASP	GLY	GLY
VAL	VAL	VAL	K326	K326	ALA	ALA		ALA	VAL	ASP	THR	ALA
LEU	LEU	LEU	K327	K327	PRO	PRO		PRO	PHE	SER	GLY	GLY
LYS	LYS	LYS	K328	K328	ASN	ASN		ASN	ASN	SER	GLY	GLY
PRO	PRO	PRO	K329	K329	VAL	VAL		VAL	VAL	ASP	THR	ALA
VAL	VAL	VAL	K330	K330	PRO	PRO		PRO	PRO	VAL	LEU	MET
ALA	ALA	ALA	K331	K331	GLU	GLU		GLU	PRO	ASP	GLY	ALA
SER	SER	SER	K332	K332	CYS	CYS		CYS	PRO	ILE	ILE	ALA
ARG	ARG	ARG	K333	K333	VAL	VAL		VAL	PRO	GLY	PRO	THR
LEU	LEU	LEU	K334	K334	SER	SER		SER	ASP	GLU	PRO	SER
GLN	GLN	GLN	K337	K337	ASN	ASN		ASN	PRO	GLU	ARG	GLY
MET	MET	MET	E337	E337	ALA	ALA		ALA	GLY	ASP	ASN	ILE
GLY	GLY	GLY	E337	E337	ALA	ALA		ALA	ARG	THR	LEU	SER
THR	THR	THR	L340	L340	LEU	LEU		LEU	ALA	GLU	GLN	ARG
ASN	ASN	ASN	L341	L341	ILE	ILE		ILE	SER	GLY	ALA	ASN
GLY	GLY	GLY	L341	L341	GLN	GLN		GLN	THR	TYR	SER	PRO
ARG	ARG	ARG	L343	L343	GLU	GLU		GLU	SER	ALA	GLY	THR
THR	THR	THR	K343	K343	TRP	TRP		TRP	GLY	ILE	THR	GLN
SER	SER	SER	R355	R355	THR	THR		THR	THR	ASP	VAL	ARG
S429	S429	S429	R356	R356	PRO	PRO		PRO	PRO	ASP	GLU	GLU
R430	R430	R430	R356	R356	GLU	GLU		ILE	ILE	ARG	GLN	ARG
K444	K444	K444	L363	L363	SER	SER		LYS	LYS	GLY	CYS	THR
S462	S462	S462	E364	E364	THR	THR		GLY	GLY	ALA	VAL	GLU
M502	M502	M502	L367	L367	ILE	ILE		THR	THR	PRO	THR	GLU
K507	K507	K507	T370	T370	SER	SER		SER	ALA	MET	ASP	LYS
S507	S507	S507	K371	K371	ARG	ARG		ARG	LEU	GLY	HIS	ALA
GLY	GLY	GLY	G376	G376	GLN	GLN		GLN	SER	PHE	ARG	GLY
			LEU	LEU	ASN	ASN		ASN	PHE	ALA	ALA	GLY
			GLY	GLY	ASN	ASN		ASN	GLY	SER	VAL	LEU
			LYS	LYS	LYS	LYS		LYS	ASP	ALA	ALA	GLY
			ASP	ASP	ASP	ASP		ASP	PRO	PRO	PRO	GLY
			ASN	ASN	ASN	ASN		ASN	ASN	ASN	ASN	GLY

- Molecule 2: Phosphoprotein



MET	ALA	GLU	GLU	GLN	ALA	ARG	HIS	ARG	VAL	LYS	ASN	GLY	LEU	GLU	CYS	ILE	ILE	ARG	ALA	ALA	LEU	LYS	GLU	ALA	GLU	PRO	ILE	GLY	GLY	SER	LEU	ALA	ALA	ILE	ILE	GLU	GLU	GLU	GLU	ILE	ILE	SER	ASP	ASN	PRO	GLY	GLN	GLU	GLU	ARG	ALA	ALA	CYS	ARG	GLU	GLU	LYS	GLY	GLY	SER	SER	GLY
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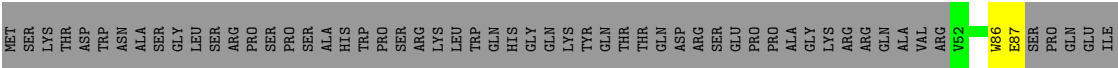
- Molecule 2: Phosphoprotein



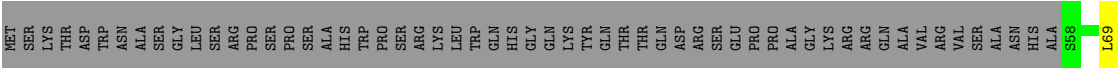
- Molecule 3: Protein C







● Molecule 3: Protein C



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	524675	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	0.729	Depositor
Minimum map value	-0.290	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	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	0.25	0/16320	0.54	3/22101 (0.0%)
2	B	0.27	0/588	0.45	0/784
2	C	0.28	0/1047	0.47	0/1393
2	D	0.29	0/444	0.42	0/592
2	E	0.33	0/585	0.72	2/789 (0.3%)
3	F	0.31	0/914	0.53	0/1236
3	G	0.24	0/873	0.56	2/1180 (0.2%)
All	All	0.26	0/20771	0.54	7/28075 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	833	SER	N-CA-C	6.65	118.53	111.28
2	E	381	PRO	CA-C-N	5.53	132.10	121.54
2	E	381	PRO	C-N-CA	5.53	132.10	121.54
1	A	2038	PRO	CA-C-N	5.34	131.74	121.54
1	A	2038	PRO	C-N-CA	5.34	131.74	121.54
3	G	102	VAL	CA-C-N	5.21	131.35	121.97
3	G	102	VAL	C-N-CA	5.21	131.35	121.97

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	15972	0	16072	72	0
2	B	581	0	643	8	0
2	C	1038	0	1124	17	0
2	D	442	0	479	8	0
2	E	576	0	615	15	0
3	F	900	0	943	9	0
3	G	859	0	902	6	0
4	A	36	0	0	0	0
All	All	20404	0	20778	111	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 3.

All (111) 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)
2:C:356:GLN:HE21	2:E:357:ASN:HB3	1.58	0.68
2:C:355:ARG:HH22	2:E:357:ASN:HD22	1.45	0.65
3:F:151:LEU:HA	3:G:103:ILE:HD11	1.80	0.62
1:A:860:ILE:HG12	1:A:1010:THR:HG22	1.81	0.61
2:B:363:LEU:HD21	2:C:364:GLU:HA	1.83	0.61
2:E:391:ASN:OD1	2:E:395:LYS:NZ	2.35	0.59
1:A:1484:THR:HG1	1:A:1572:CYS:HG	1.51	0.58
1:A:2148:GLN:NE2	1:A:2152:THR:OG1	2.36	0.58
2:B:342:LEU:HD21	2:C:343:LYS:HG3	1.86	0.58
2:B:343:LYS:HG2	2:D:342:LEU:HD21	1.85	0.57
3:F:147:ILE:HD12	3:G:147:ILE:HG12	1.87	0.57
1:A:965:LYS:NZ	1:A:1131:SER:O	2.38	0.56
1:A:522:TYR:HB2	1:A:553:MET:HE1	1.87	0.55
1:A:829:PHE:HA	1:A:837:TYR:O	2.05	0.55
1:A:121:SER:HB3	1:A:150:ILE:HA	1.89	0.55
2:E:347:GLU:HG3	2:E:351:LYS:HE3	1.88	0.54
2:C:367:LEU:HD12	2:E:367:LEU:HD21	1.89	0.54
1:A:1828:PRO:HG2	1:A:1845:LYS:HZ2	1.72	0.54
2:E:372:ILE:HG12	2:E:384:PRO:HB2	1.90	0.53
1:A:704:VAL:HG13	1:A:733:LYS:HA	1.90	0.53
3:F:130:VAL:HG13	3:F:131:ILE:HG12	1.91	0.52
1:A:860:ILE:HG22	1:A:1083:LYS:HE2	1.92	0.51
1:A:2065:ARG:NH1	1:A:2146:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:HG23	2:C:502:MET:HE3	1.91	0.51
1:A:1557:ASP:HB3	1:A:1560:ASN:HB3	1.93	0.50
1:A:1504:PRO:HG3	1:A:1513:LEU:HD12	1.93	0.50
1:A:1261:LEU:HB3	1:A:1388:LEU:HD11	1.94	0.49
1:A:295:ASP:OD1	1:A:827:SER:OG	2.31	0.49
2:B:370:ILE:HD13	2:C:371:MET:HB3	1.93	0.49
1:A:1811:SER:OG	1:A:1812:GLY:N	2.46	0.49
1:A:2067:LEU:HG	1:A:2071:LYS:HE3	1.94	0.49
2:B:363:LEU:HD22	2:C:367:LEU:HD22	1.94	0.49
2:C:332:ILE:HG23	2:E:336[A]:LEU:HD11	1.95	0.49
3:F:86:TRP:O	3:F:87:GLU:C	2.54	0.49
1:A:1019:ARG:NH2	1:A:1073:GLU:OE2	2.46	0.48
1:A:1386:LEU:HG	1:A:1388:LEU:HG	1.95	0.48
2:D:350:LYS:NZ	2:E:345:GLU:OE1	2.41	0.48
2:C:332:ILE:HG23	2:E:336[B]:LEU:HD11	1.95	0.48
2:C:329:ASN:HA	2:C:332:ILE:HD12	1.95	0.48
1:A:137:LEU:HD11	1:A:1343:VAL:HG13	1.96	0.48
1:A:673:TYR:O	1:A:677:SER:HB2	2.14	0.48
1:A:134:ARG:NH2	1:A:1164:GLU:O	2.47	0.47
1:A:1504:PRO:HB3	1:A:1509:GLN:HB3	1.96	0.47
1:A:1831:VAL:HG11	1:A:1845:LYS:HE3	1.97	0.47
1:A:354:ARG:NH2	1:A:537:LYS:O	2.48	0.47
2:D:336:LEU:HD13	2:E:335:LYS:HB2	1.97	0.47
1:A:1442:LEU:HD23	1:A:1671:LEU:HD21	1.95	0.46
1:A:781:LYS:HD2	1:A:799:VAL:HG11	1.97	0.46
2:C:363:LEU:HD11	2:E:364:GLU:HG2	1.96	0.46
2:C:370:ILE:HD11	2:E:371:MET:HE3	1.97	0.46
1:A:2016:PRO:HA	1:A:2019:LYS:HG3	1.98	0.46
1:A:57:PHE:HE2	1:A:483:GLU:HG3	1.81	0.45
1:A:1198:LEU:O	1:A:1309:ARG:NH2	2.49	0.45
3:F:143:THR:O	3:F:147:ILE:HG12	2.17	0.45
1:A:699:ARG:HA	1:A:699:ARG:HD2	1.72	0.45
1:A:1756:ARG:HH22	1:A:2018:LEU:HA	1.81	0.45
1:A:331:ILE:HG21	2:C:462:SER:HB3	1.98	0.45
1:A:454:LEU:HG	2:E:392:PRO:HB2	1.99	0.45
1:A:860:ILE:HG13	1:A:861:VAL:HG23	2.00	0.44
1:A:1913:ILE:HG12	1:A:1960:THR:HG23	1.98	0.44
1:A:2039:LYS:HA	1:A:2042:LYS:HB2	1.98	0.44
2:B:349:ILE:O	2:B:353:ILE:HG13	2.17	0.44
3:G:73:VAL:HG13	3:G:110:VAL:HG13	1.98	0.44
1:A:2001:ILE:HA	1:A:2004:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:LYS:HD2	2:D:379:LYS:HA	1.83	0.44
2:B:338:SER:O	2:C:343:LYS:NZ	2.47	0.44
2:D:336:LEU:HD11	2:E:332:ILE:HG23	1.99	0.44
1:A:1599:VAL:HG12	1:A:1603:ARG:HE	1.81	0.44
3:F:139:MET:HE3	3:F:139:MET:HB3	1.94	0.44
1:A:1078:MET:HE2	1:A:1078:MET:HB3	1.94	0.43
1:A:1782:GLU:HA	1:A:1805:SER:H	1.82	0.43
1:A:1540:LYS:HD3	1:A:1540:LYS:HA	1.87	0.43
1:A:1686:VAL:HB	3:F:112:ARG:NE	2.34	0.43
1:A:1828:PRO:HG2	1:A:1845:LYS:NZ	2.34	0.43
1:A:1938:ARG:HB2	1:A:1961:ASP:HB2	2.01	0.43
1:A:654:GLU:HG3	1:A:785:SER:HB3	2.00	0.42
1:A:1484:THR:OG1	1:A:1572:CYS:SG	2.64	0.42
1:A:1190:PHE:HB2	1:A:1361:LEU:HB3	2.02	0.42
1:A:1375:ILE:HD12	1:A:1378:PRO:HG3	2.00	0.42
1:A:540:LYS:HE3	1:A:540:LYS:HB3	1.83	0.42
1:A:2130:ILE:HG12	1:A:2160:VAL:HG12	2.02	0.42
3:G:119:LEU:HD13	3:G:145:MET:HE1	2.02	0.42
1:A:548:LYS:HB2	1:A:548:LYS:HE3	1.79	0.42
2:D:339:LEU:HD23	2:D:342:LEU:HD12	2.02	0.42
1:A:247:ILE:HG22	1:A:887:LEU:HD13	2.02	0.41
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.94	0.41
1:A:2100:THR:HG23	1:A:2131:LEU:HB2	2.02	0.41
1:A:1786:PHE:HB3	1:A:1789:GLU:HG2	2.02	0.41
2:D:343:LYS:HD2	2:E:339:LEU:HD23	2.01	0.41
3:F:131:ILE:HG23	3:F:131:ILE:HD12	1.79	0.41
1:A:859:THR:OG1	1:A:861:VAL:O	2.31	0.41
1:A:2009:VAL:HB	1:A:2121:ILE:HD13	2.03	0.41
1:A:2010:SER:OG	1:A:2011:ARG:N	2.53	0.41
3:G:69:LEU:HB2	3:G:156:MET:HE2	2.02	0.41
1:A:1297:VAL:HB	1:A:1337:MET:HE2	2.02	0.41
1:A:1108:TYR:CZ	1:A:1112:ARG:HD2	2.55	0.41
1:A:1438:LYS:NZ	1:A:1589:THR:O	2.51	0.41
1:A:1633:PRO:HA	1:A:1636:LYS:HG2	2.03	0.41
1:A:1842:ASN:O	1:A:1844:VAL:N	2.53	0.41
1:A:1845:LYS:HE2	1:A:1845:LYS:HB3	1.73	0.41
1:A:142:ARG:HE	1:A:142:ARG:HB3	1.65	0.40
2:C:444:LYS:HA	2:C:444:LYS:HD2	1.90	0.40
2:D:329:ASN:O	2:D:333:ILE:HG13	2.22	0.40
3:G:131:ILE:HG23	3:G:131:ILE:HD12	1.85	0.40
1:A:1025:SER:HA	1:A:1026:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:ARG:HD2	1:A:1240:ARG:HA	1.92	0.40
1:A:1507:LYS:HE2	1:A:1507:LYS:HB3	1.88	0.40
1:A:1756:ARG:HH12	1:A:2018:LEU:HB3	1.87	0.40
1:A:400:TYR:HB3	1:A:409:PRO:HD3	2.04	0.40
2:B:335[A]:LYS:HE2	2:C:333:ILE:HG23	2.03	0.40
3:F:106:MET:HE3	3:F:106:MET:HB2	1.91	0.40

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	1969/2183 (90%)	1903 (97%)	66 (3%)	0	100	100
2	B	71/509 (14%)	69 (97%)	2 (3%)	0	100	100
2	C	128/509 (25%)	125 (98%)	3 (2%)	0	100	100
2	D	55/509 (11%)	55 (100%)	0	0	100	100
2	E	73/509 (14%)	66 (90%)	7 (10%)	0	100	100
3	F	111/186 (60%)	110 (99%)	1 (1%)	0	100	100
3	G	105/186 (56%)	103 (98%)	2 (2%)	0	100	100
All	All	2512/4591 (55%)	2431 (97%)	81 (3%)	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	1781/1943 (92%)	1781 (100%)	0	100	100
2	B	68/415 (16%)	68 (100%)	0	100	100
2	C	119/415 (29%)	119 (100%)	0	100	100
2	D	52/415 (12%)	52 (100%)	0	100	100
2	E	69/415 (17%)	69 (100%)	0	100	100
3	F	99/162 (61%)	99 (100%)	0	100	100
3	G	96/162 (59%)	96 (100%)	0	100	100
All	All	2284/3927 (58%)	2284 (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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	HIS
1	A	433	HIS
1	A	473	GLN
1	A	524	HIS
1	A	557	GLN
1	A	719	HIS
1	A	812	HIS
1	A	984	GLN
1	A	1027	ASN
1	A	1105	ASN
1	A	1335	GLN
1	A	1431	GLN
1	A	1535	HIS
1	A	1658	ASN
1	A	1760	ASN
1	A	1810	ASN
1	A	1941	ASN
1	A	2106	HIS
1	A	2148	GLN
2	B	352	GLN
2	C	330	GLN
2	C	366	HIS
2	D	329	ASN
2	D	330	GLN

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Mol	Chain	Res	Type
2	E	329	ASN

### 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	$\# Z  > 2$
4	A1EF9	A	2500	-	38,39,39	2.42	11 (28%)	52,57,57	2.87	16 (30%)

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	2500	-	-	11/28/50/50	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2500	A1EF9	C20-N10	-9.14	1.26	1.47
4	A	2500	A1EF9	S01-N09	6.62	1.73	1.63
4	A	2500	A1EF9	C23-S01	3.77	1.81	1.76
4	A	2500	A1EF9	C18-N09	3.15	1.53	1.48
4	A	2500	A1EF9	C31-N11	2.86	1.44	1.35
4	A	2500	A1EF9	C17-C15	-2.84	1.46	1.53
4	A	2500	A1EF9	C22-N10	-2.80	1.39	1.46
4	A	2500	A1EF9	C21-N10	-2.78	1.39	1.46
4	A	2500	A1EF9	C32-N12	-2.70	1.31	1.36
4	A	2500	A1EF9	O06-S01	2.55	1.46	1.43
4	A	2500	A1EF9	O08-C31	-2.03	1.18	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2500	A1EF9	O06-S01-O05	-13.11	99.13	119.59
4	A	2500	A1EF9	C36-C34-N13	6.42	127.27	119.72
4	A	2500	A1EF9	C34-N13-N12	4.95	108.09	104.37
4	A	2500	A1EF9	O05-S01-C23	4.70	113.94	108.10
4	A	2500	A1EF9	C26-C23-S01	-4.02	115.74	119.73
4	A	2500	A1EF9	O05-S01-N09	3.99	113.94	106.97
4	A	2500	A1EF9	C27-C23-S01	3.85	123.56	119.73
4	A	2500	A1EF9	C22-N10-C21	3.58	116.55	108.84
4	A	2500	A1EF9	O06-S01-N09	3.57	113.22	106.97
4	A	2500	A1EF9	C32-C33-C34	3.36	108.19	103.57
4	A	2500	A1EF9	C33-C34-N13	-3.11	106.86	111.33
4	A	2500	A1EF9	C32-N12-N13	-2.84	109.83	112.76
4	A	2500	A1EF9	O06-S01-C23	2.51	111.22	108.10
4	A	2500	A1EF9	C33-C32-C31	-2.45	120.16	128.22
4	A	2500	A1EF9	C19-C17-C15	2.26	116.06	111.42
4	A	2500	A1EF9	F04-C36-C34	-2.25	108.46	112.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2500	A1EF9	C15-C14-C16-C20
4	A	2500	A1EF9	C18-N09-S01-C23
4	A	2500	A1EF9	C14-N09-S01-O05
4	A	2500	A1EF9	C16-C20-N10-C21
4	A	2500	A1EF9	C16-C20-N10-C22
4	A	2500	A1EF9	C18-N09-S01-O06

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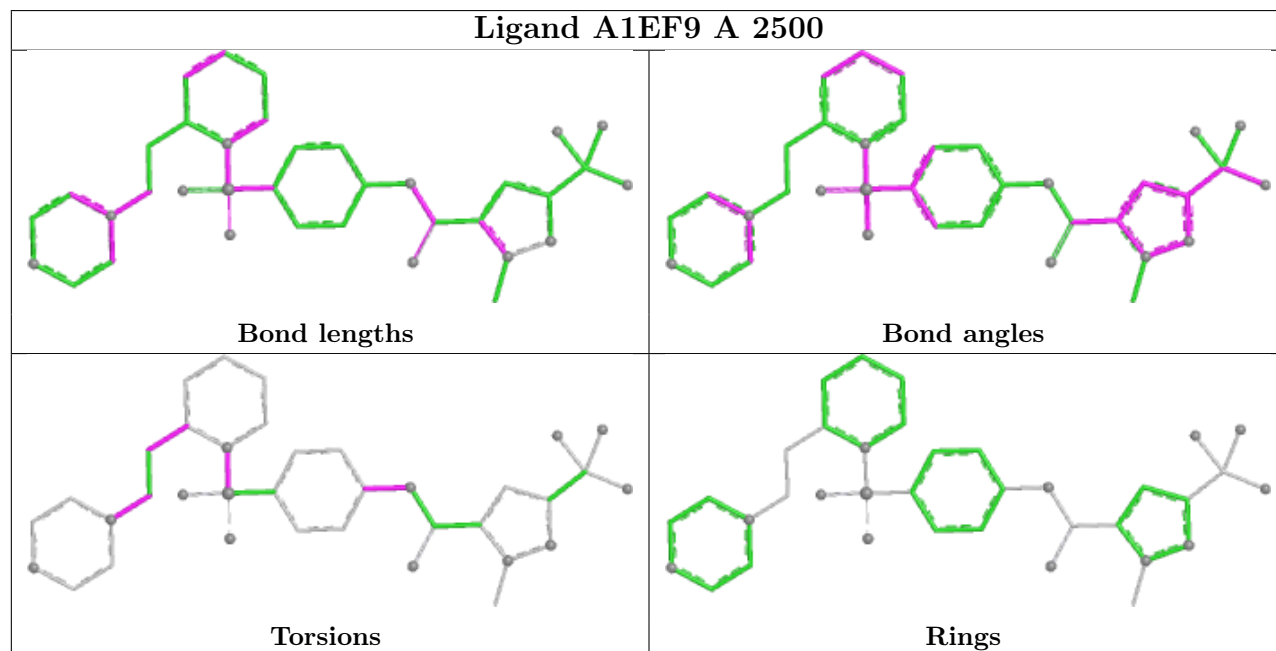
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Mol	Chain	Res	Type	Atoms
4	A	2500	A1EF9	C28-C30-N11-C31
4	A	2500	A1EF9	C29-C30-N11-C31
4	A	2500	A1EF9	C18-N09-S01-O05
4	A	2500	A1EF9	N09-C14-C16-C20
4	A	2500	A1EF9	C14-N09-S01-C23

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

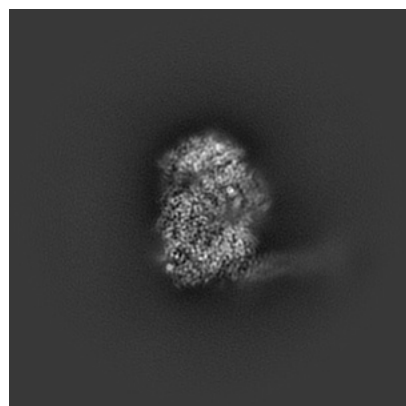
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70312. These allow visual inspection of the internal detail of the map and identification of artifacts.

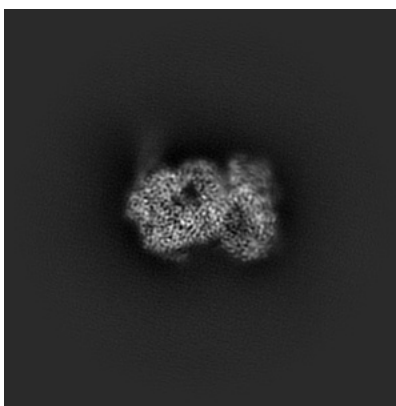
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

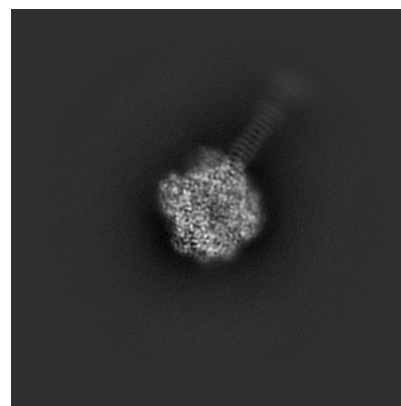
#### 6.1.1 Primary map



X

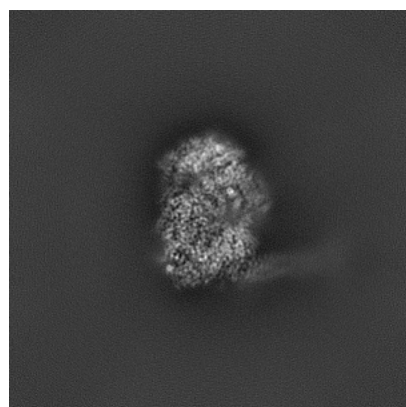


Y

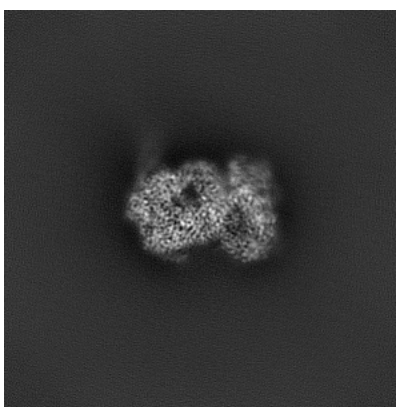


Z

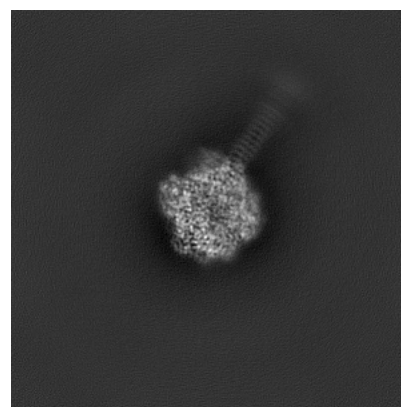
#### 6.1.2 Raw map



X



Y

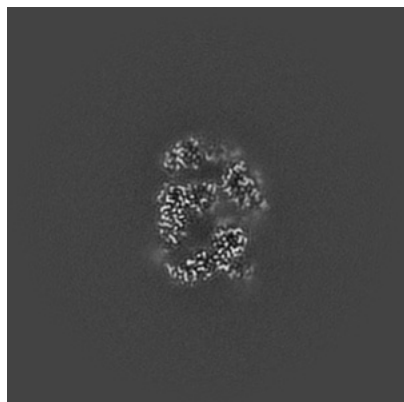


Z

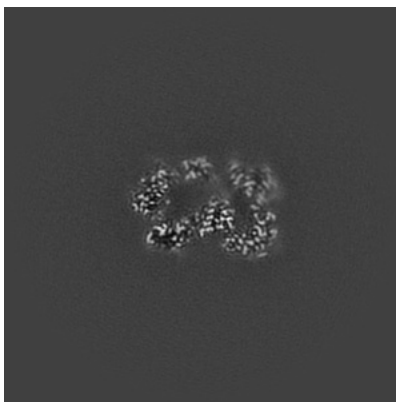
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

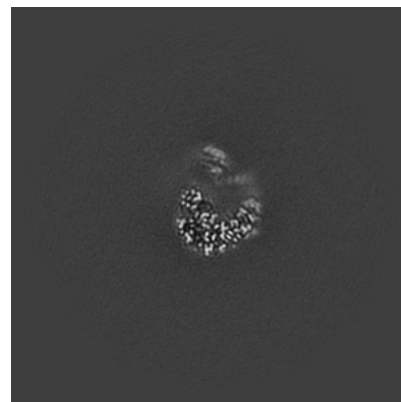
### 6.2.1 Primary map



X Index: 192

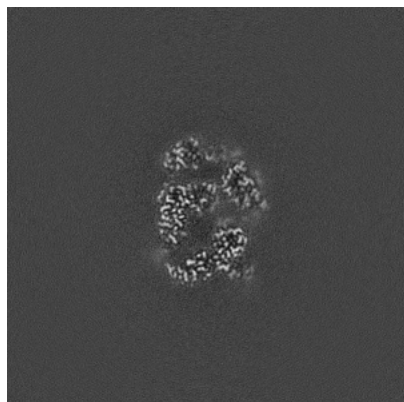


Y Index: 192

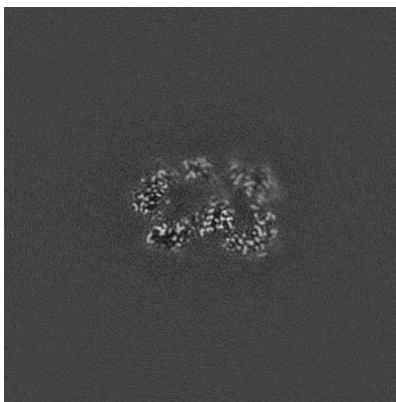


Z Index: 192

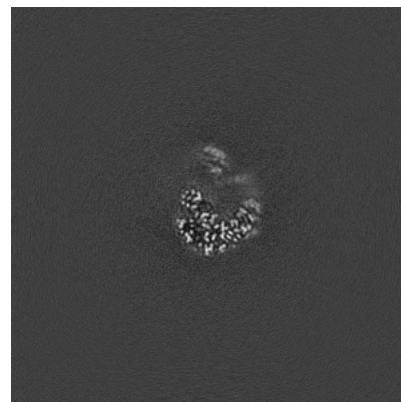
### 6.2.2 Raw map



X Index: 192



Y Index: 192

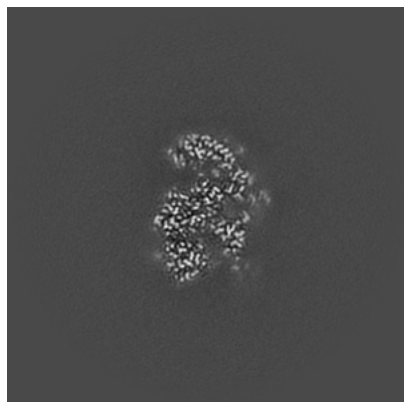


Z Index: 192

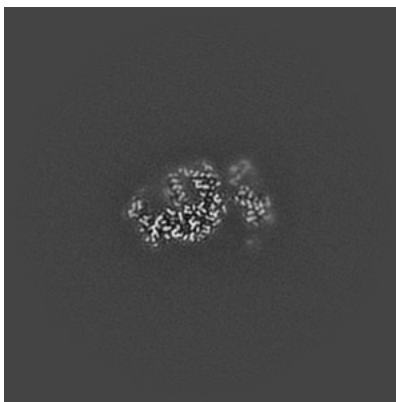
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

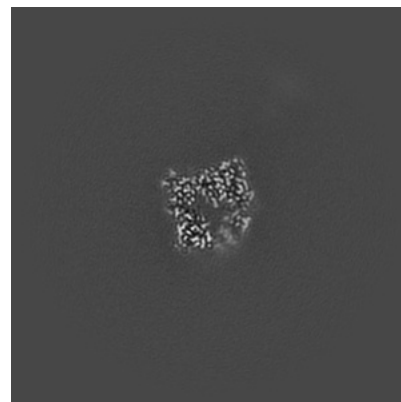
### 6.3.1 Primary map



X Index: 182

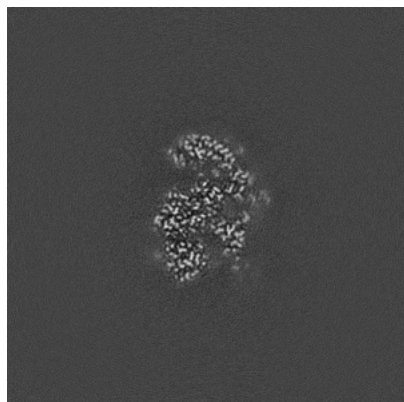


Y Index: 166

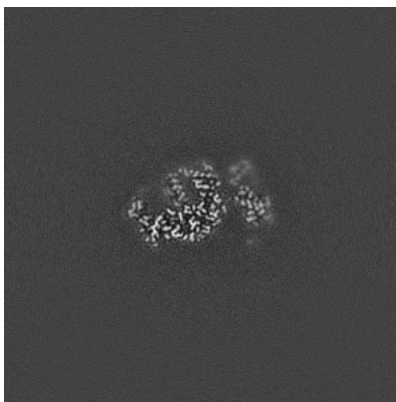


Z Index: 157

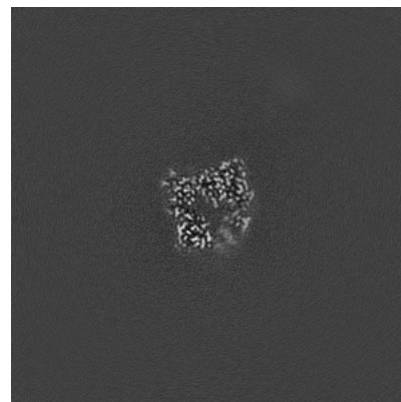
### 6.3.2 Raw map



X Index: 182



Y Index: 166



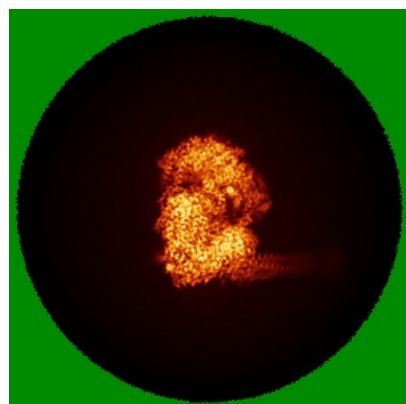
Z Index: 157

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

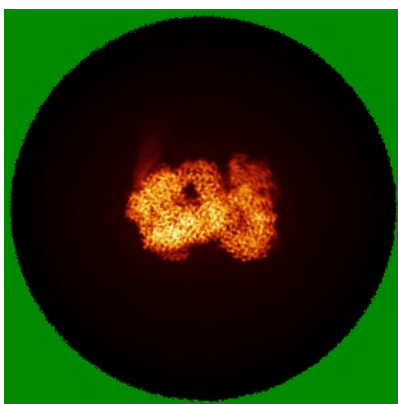


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

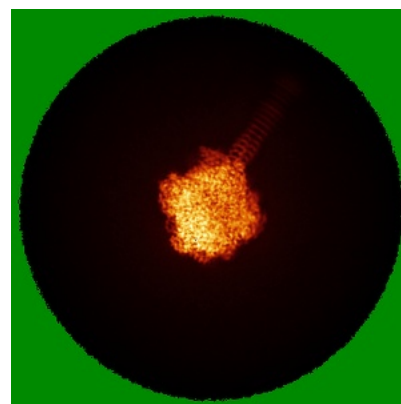
### 6.4.1 Primary map



X

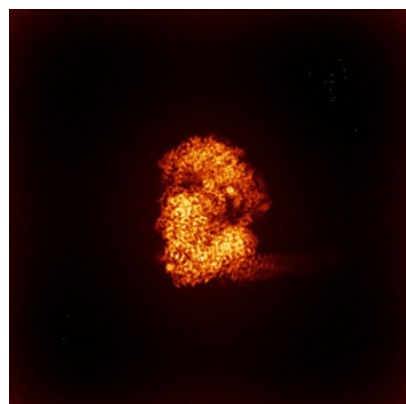


Y

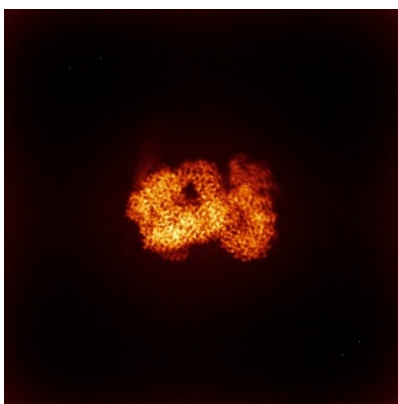


Z

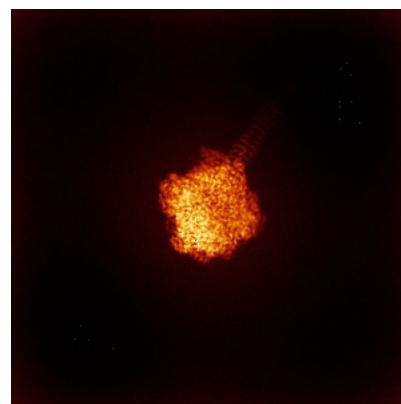
### 6.4.2 Raw map



X



Y



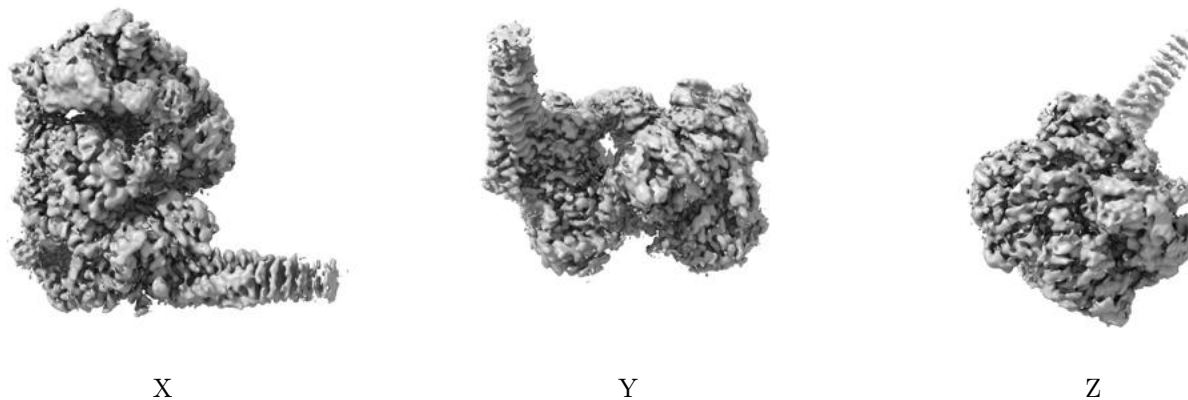
Z

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.



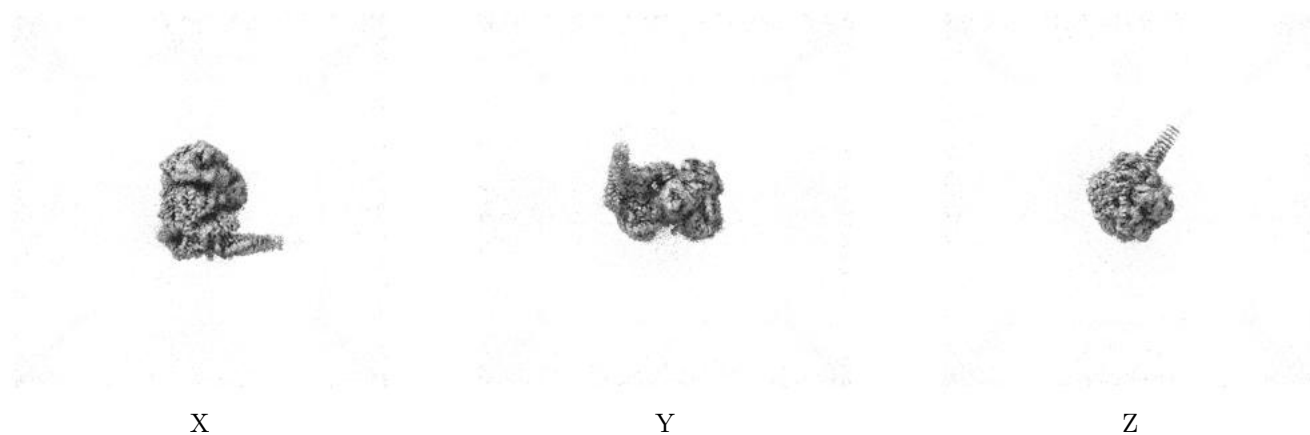
## 6.5 Orthogonal surface views [i](#)

### 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.

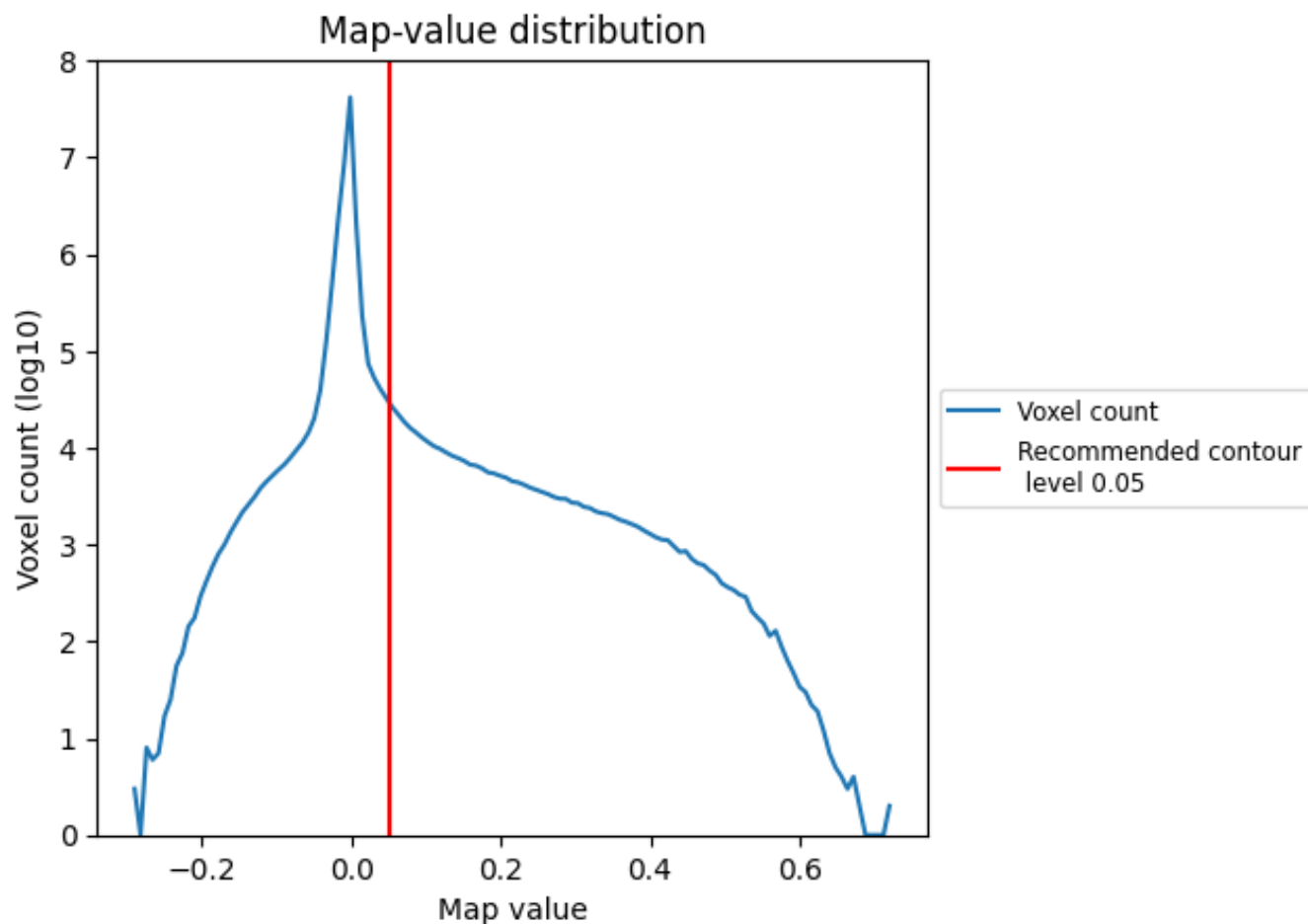
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

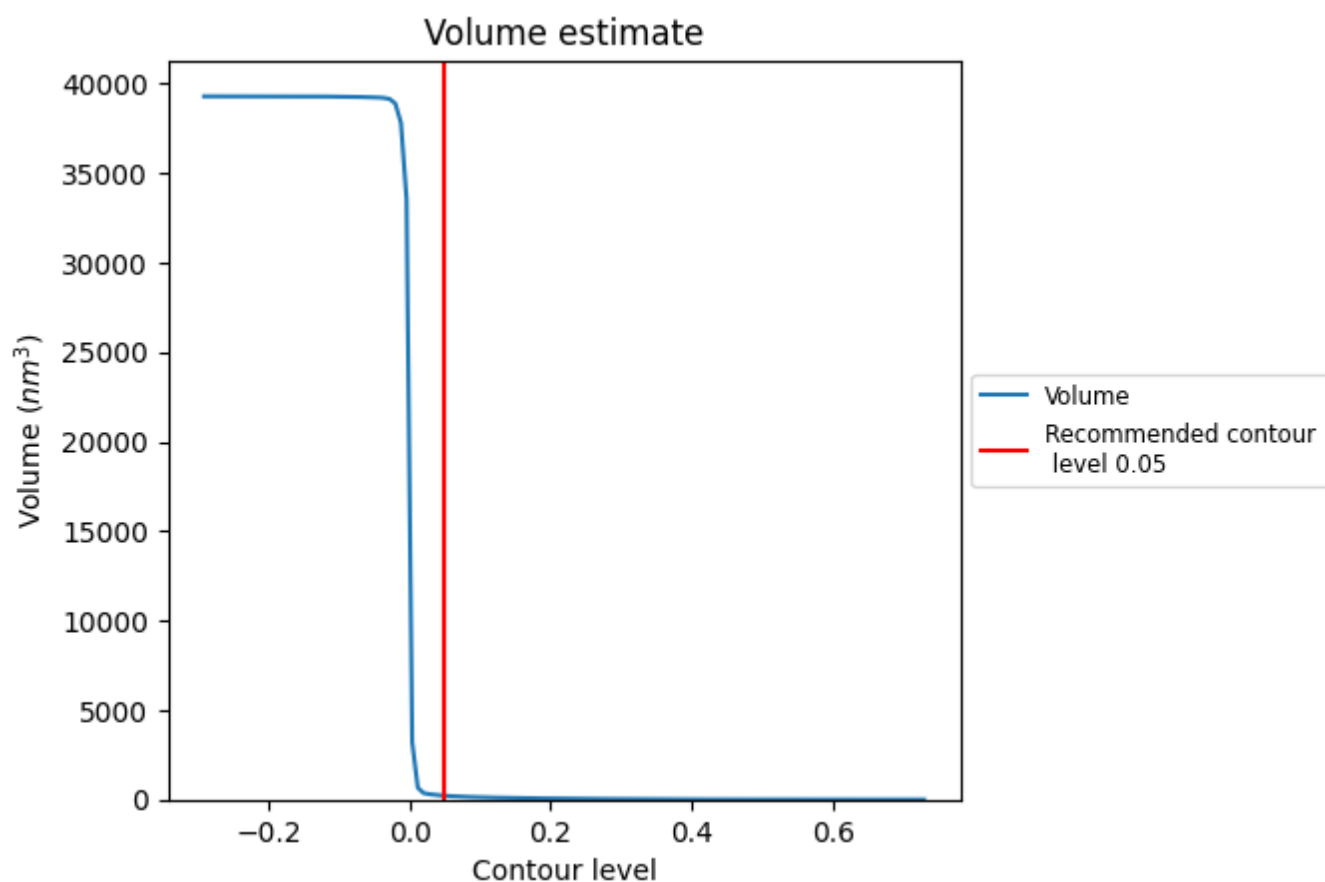
This section contains the results of statistical analysis of the map.

### 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.

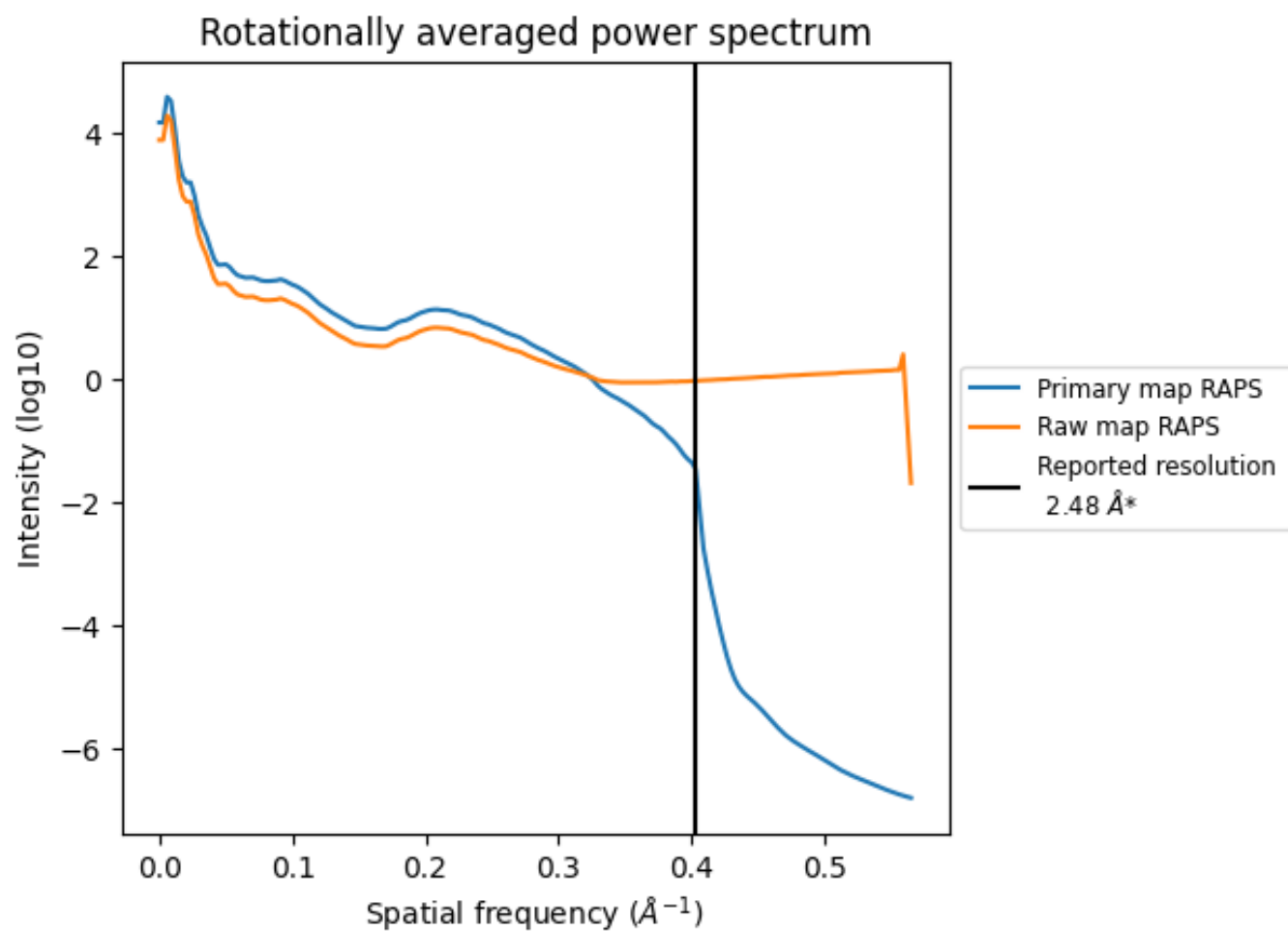
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm<sup>3</sup>; this corresponds to an approximate mass of 194 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

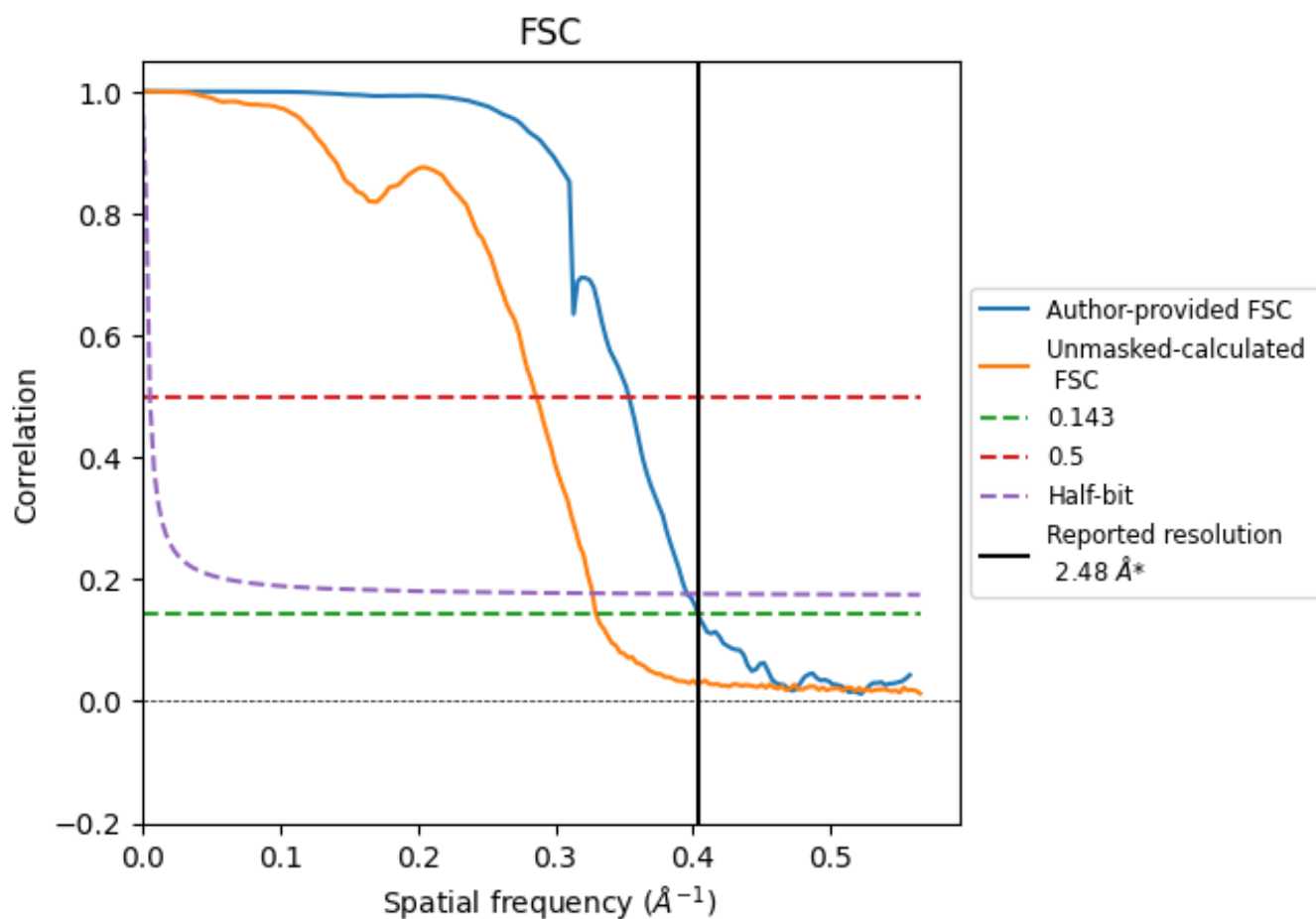


\*Reported resolution corresponds to spatial frequency of  $0.403 \text{ \AA}^{-1}$

## 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 0.403  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

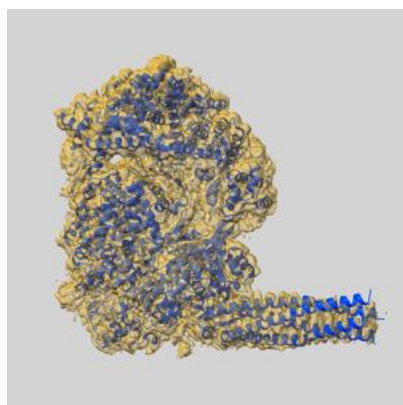
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.83	2.53
Unmasked-calculated*	3.03	3.50	3.06

\*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 3.03 differs from the reported value 2.48 by more than 10 %

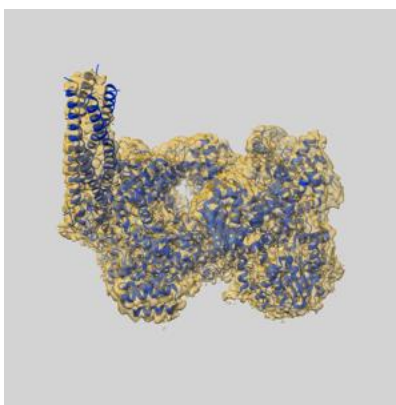
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70312 and PDB model 9OCE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

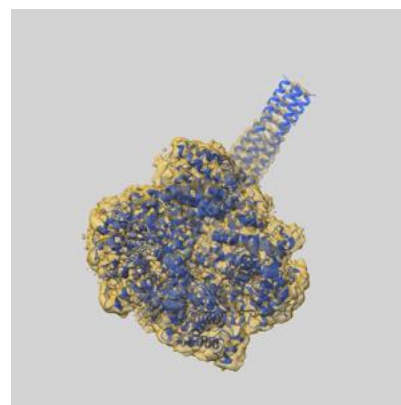
### 9.1 Map-model overlay [i](#)



X



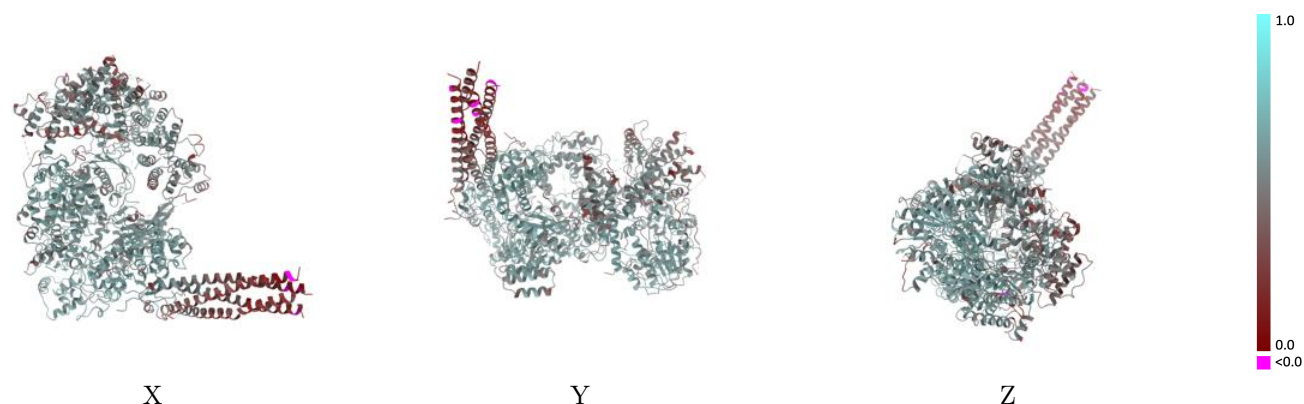
Y



Z

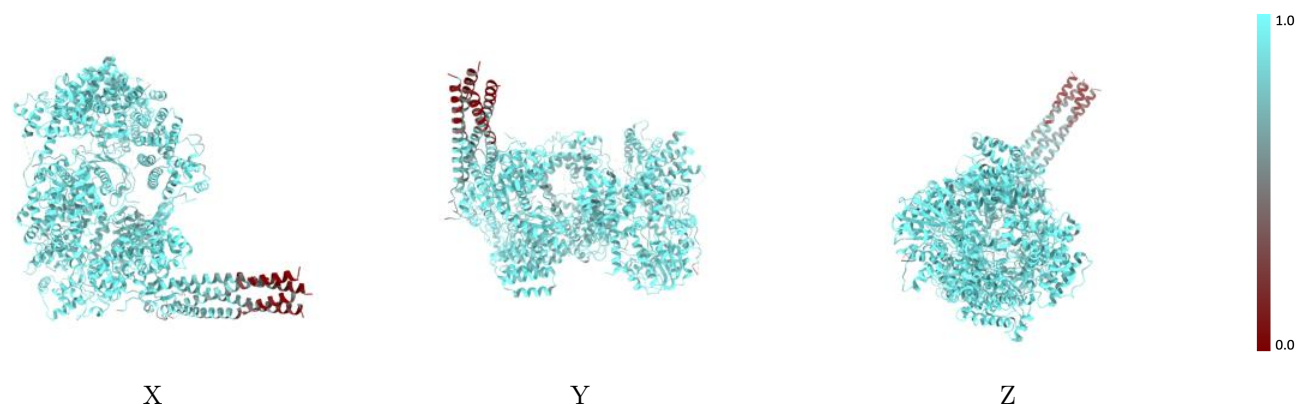
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

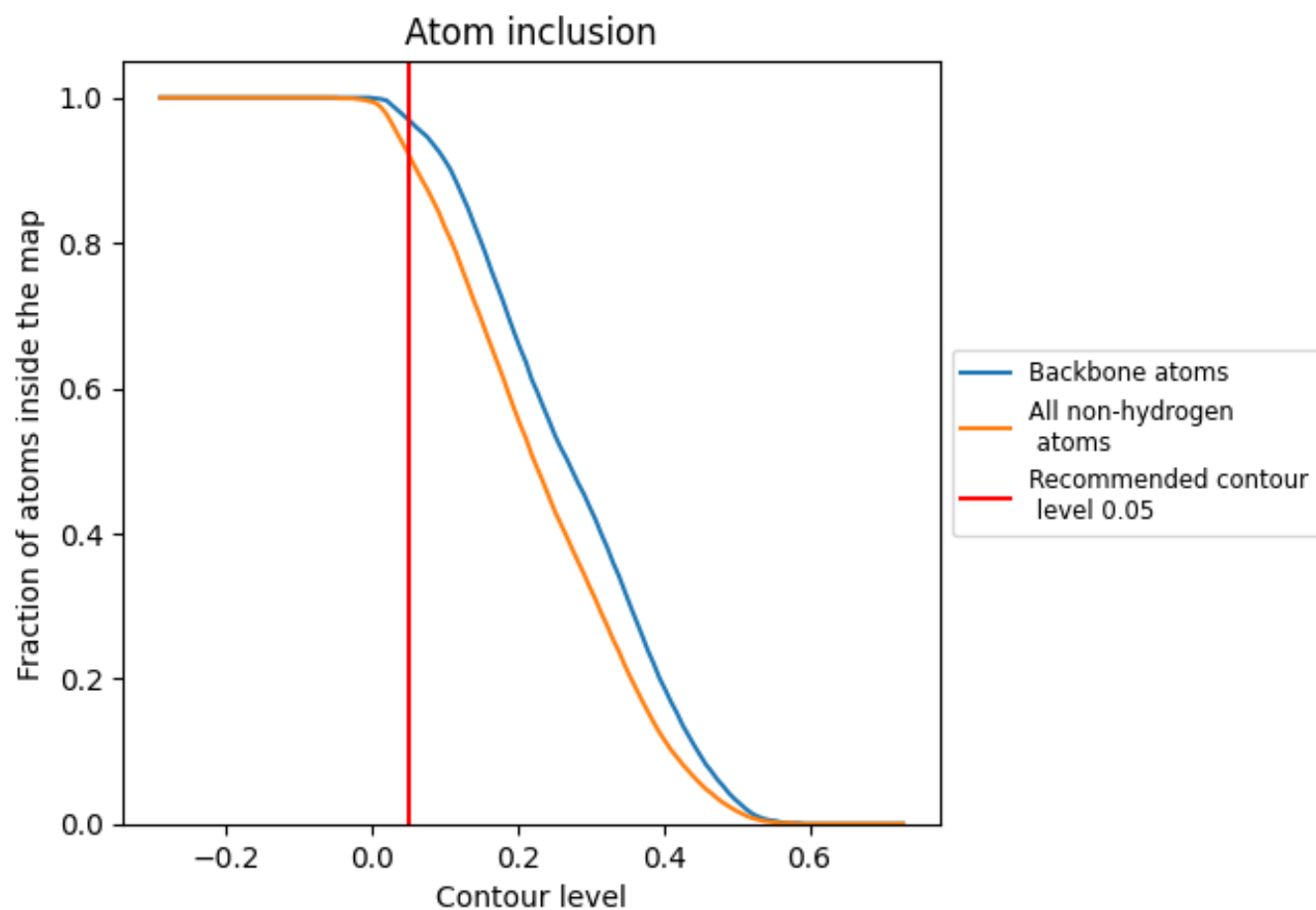
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 97% of all backbone atoms, 92% 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></div>0.9230</div>	<div><div></div>0.5340</div>
A	<div><div></div>0.9610</div>	<div><div></div>0.5630</div>
B	<div><div></div>0.6640</div>	<div><div></div>0.3830</div>
C	<div><div></div>0.7460</div>	<div><div></div>0.4150</div>
D	<div><div></div>0.6520</div>	<div><div></div>0.3470</div>
E	<div><div></div>0.6330</div>	<div><div></div>0.3400</div>
F	<div><div></div>0.9480</div>	<div><div></div>0.5370</div>
G	<div><div></div>0.9080</div>	<div><div></div>0.4650</div>

1.0

0.0

<0.0