



wwPDB EM Validation Summary Report ⓘ

May 17, 2026 – 02:52 PM JST

PDB ID : 9VUL / pdb_00009vul
EMDB ID : EMD-65367
Title : Cryo-EM structure of the human measles virus RNA-dependent RNA polymerase bound to allosteric inhibitor ERDRP-0519
Authors : Du, T.; Wang, J.; Wu, S.; Ru, H.
Deposited on : 2025-07-13
Resolution : 3.13 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

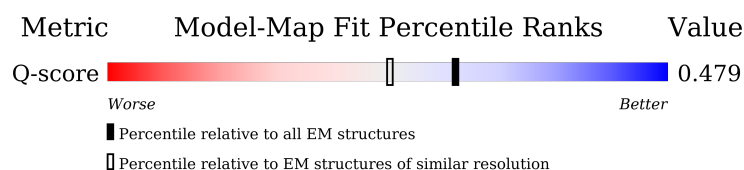
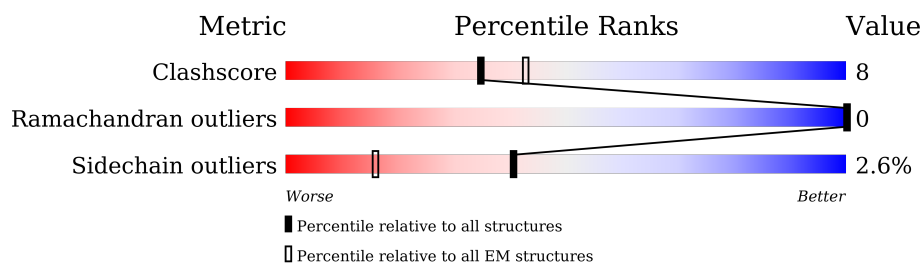
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 (2.63 - 3.63)

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	602	
1	B	602	
1	C	602	
1	D	602	

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Mol	Chain	Length	Quality of chain
2	L	2630	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12206 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 Maltose/maltodextrin-binding periplasmic protein, Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1034	655	187	186	6		
1	B	32	Total	C	N	O	S	0	0
			249	156	44	48	1		
1	C	59	Total	C	N	O	S	0	0
			443	279	75	88	1		
1	D	42	Total	C	N	O	S	0	0
			317	199	56	61	1		

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-94	MET	-	initiating methionine	UNP P0AEX9
A	-93	GLY	-	expression tag	UNP P0AEX9
A	-92	SER	-	expression tag	UNP P0AEX9
A	-91	SER	-	expression tag	UNP P0AEX9
A	-90	HIS	-	expression tag	UNP P0AEX9
A	-89	HIS	-	expression tag	UNP P0AEX9
A	-88	HIS	-	expression tag	UNP P0AEX9
A	-87	HIS	-	expression tag	UNP P0AEX9
A	-86	HIS	-	expression tag	UNP P0AEX9
A	-85	HIS	-	expression tag	UNP P0AEX9
A	-84	GLY	-	expression tag	UNP P0AEX9
A	-83	THR	-	expression tag	UNP P0AEX9
A	-82	LYS	-	expression tag	UNP P0AEX9
A	-81	THR	-	expression tag	UNP P0AEX9
A	284	GLY	-	linker	UNP P0AEX9
A	285	THR	-	linker	UNP P0AEX9
A	286	ASP	-	linker	UNP P0AEX9
A	287	TYR	-	linker	UNP P0AEX9
A	288	ASP	-	linker	UNP P0AEX9
A	289	ILE	-	linker	UNP P0AEX9
A	290	PRO	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	291	THR	-	linker	UNP P0AEX9
A	292	THR	-	linker	UNP P0AEX9
A	293	LEU	-	linker	UNP P0AEX9
A	294	GLU	-	linker	UNP P0AEX9
A	295	VAL	-	linker	UNP P0AEX9
A	296	LEU	-	linker	UNP P0AEX9
A	297	PHE	-	linker	UNP P0AEX9
A	298	GLN	-	linker	UNP P0AEX9
A	299	GLY	-	linker	UNP P0AEX9
A	300	PRO	-	linker	UNP P0AEX9
A	301	LEU	-	linker	UNP P0AEX9
A	302	GLY	-	linker	UNP P0AEX9
A	303	SER	-	linker	UNP P0AEX9
B	-94	MET	-	initiating methionine	UNP P0AEX9
B	-93	GLY	-	expression tag	UNP P0AEX9
B	-92	SER	-	expression tag	UNP P0AEX9
B	-91	SER	-	expression tag	UNP P0AEX9
B	-90	HIS	-	expression tag	UNP P0AEX9
B	-89	HIS	-	expression tag	UNP P0AEX9
B	-88	HIS	-	expression tag	UNP P0AEX9
B	-87	HIS	-	expression tag	UNP P0AEX9
B	-86	HIS	-	expression tag	UNP P0AEX9
B	-85	HIS	-	expression tag	UNP P0AEX9
B	-84	GLY	-	expression tag	UNP P0AEX9
B	-83	THR	-	expression tag	UNP P0AEX9
B	-82	LYS	-	expression tag	UNP P0AEX9
B	-81	THR	-	expression tag	UNP P0AEX9
B	284	GLY	-	linker	UNP P0AEX9
B	285	THR	-	linker	UNP P0AEX9
B	286	ASP	-	linker	UNP P0AEX9
B	287	TYR	-	linker	UNP P0AEX9
B	288	ASP	-	linker	UNP P0AEX9
B	289	ILE	-	linker	UNP P0AEX9
B	290	PRO	-	linker	UNP P0AEX9
B	291	THR	-	linker	UNP P0AEX9
B	292	THR	-	linker	UNP P0AEX9
B	293	LEU	-	linker	UNP P0AEX9
B	294	GLU	-	linker	UNP P0AEX9
B	295	VAL	-	linker	UNP P0AEX9
B	296	LEU	-	linker	UNP P0AEX9
B	297	PHE	-	linker	UNP P0AEX9
B	298	GLN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	GLY	-	linker	UNP P0AEX9
B	300	PRO	-	linker	UNP P0AEX9
B	301	LEU	-	linker	UNP P0AEX9
B	302	GLY	-	linker	UNP P0AEX9
B	303	SER	-	linker	UNP P0AEX9
C	-94	MET	-	initiating methionine	UNP P0AEX9
C	-93	GLY	-	expression tag	UNP P0AEX9
C	-92	SER	-	expression tag	UNP P0AEX9
C	-91	SER	-	expression tag	UNP P0AEX9
C	-90	HIS	-	expression tag	UNP P0AEX9
C	-89	HIS	-	expression tag	UNP P0AEX9
C	-88	HIS	-	expression tag	UNP P0AEX9
C	-87	HIS	-	expression tag	UNP P0AEX9
C	-86	HIS	-	expression tag	UNP P0AEX9
C	-85	HIS	-	expression tag	UNP P0AEX9
C	-84	GLY	-	expression tag	UNP P0AEX9
C	-83	THR	-	expression tag	UNP P0AEX9
C	-82	LYS	-	expression tag	UNP P0AEX9
C	-81	THR	-	expression tag	UNP P0AEX9
C	284	GLY	-	linker	UNP P0AEX9
C	285	THR	-	linker	UNP P0AEX9
C	286	ASP	-	linker	UNP P0AEX9
C	287	TYR	-	linker	UNP P0AEX9
C	288	ASP	-	linker	UNP P0AEX9
C	289	ILE	-	linker	UNP P0AEX9
C	290	PRO	-	linker	UNP P0AEX9
C	291	THR	-	linker	UNP P0AEX9
C	292	THR	-	linker	UNP P0AEX9
C	293	LEU	-	linker	UNP P0AEX9
C	294	GLU	-	linker	UNP P0AEX9
C	295	VAL	-	linker	UNP P0AEX9
C	296	LEU	-	linker	UNP P0AEX9
C	297	PHE	-	linker	UNP P0AEX9
C	298	GLN	-	linker	UNP P0AEX9
C	299	GLY	-	linker	UNP P0AEX9
C	300	PRO	-	linker	UNP P0AEX9
C	301	LEU	-	linker	UNP P0AEX9
C	302	GLY	-	linker	UNP P0AEX9
C	303	SER	-	linker	UNP P0AEX9
D	-94	MET	-	initiating methionine	UNP P0AEX9
D	-93	GLY	-	expression tag	UNP P0AEX9
D	-92	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-91	SER	-	expression tag	UNP P0AEX9
D	-90	HIS	-	expression tag	UNP P0AEX9
D	-89	HIS	-	expression tag	UNP P0AEX9
D	-88	HIS	-	expression tag	UNP P0AEX9
D	-87	HIS	-	expression tag	UNP P0AEX9
D	-86	HIS	-	expression tag	UNP P0AEX9
D	-85	HIS	-	expression tag	UNP P0AEX9
D	-84	GLY	-	expression tag	UNP P0AEX9
D	-83	THR	-	expression tag	UNP P0AEX9
D	-82	LYS	-	expression tag	UNP P0AEX9
D	-81	THR	-	expression tag	UNP P0AEX9
D	284	GLY	-	linker	UNP P0AEX9
D	285	THR	-	linker	UNP P0AEX9
D	286	ASP	-	linker	UNP P0AEX9
D	287	TYR	-	linker	UNP P0AEX9
D	288	ASP	-	linker	UNP P0AEX9
D	289	ILE	-	linker	UNP P0AEX9
D	290	PRO	-	linker	UNP P0AEX9
D	291	THR	-	linker	UNP P0AEX9
D	292	THR	-	linker	UNP P0AEX9
D	293	LEU	-	linker	UNP P0AEX9
D	294	GLU	-	linker	UNP P0AEX9
D	295	VAL	-	linker	UNP P0AEX9
D	296	LEU	-	linker	UNP P0AEX9
D	297	PHE	-	linker	UNP P0AEX9
D	298	GLN	-	linker	UNP P0AEX9
D	299	GLY	-	linker	UNP P0AEX9
D	300	PRO	-	linker	UNP P0AEX9
D	301	LEU	-	linker	UNP P0AEX9
D	302	GLY	-	linker	UNP P0AEX9
D	303	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,RNA-directed RNA polymerase L,Strep II and FLAG tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	1262	Total	C	N	O	S	0	0
			10125	6474	1740	1855	56		

There are 34 discrepancies between the modelled and reference sequences:

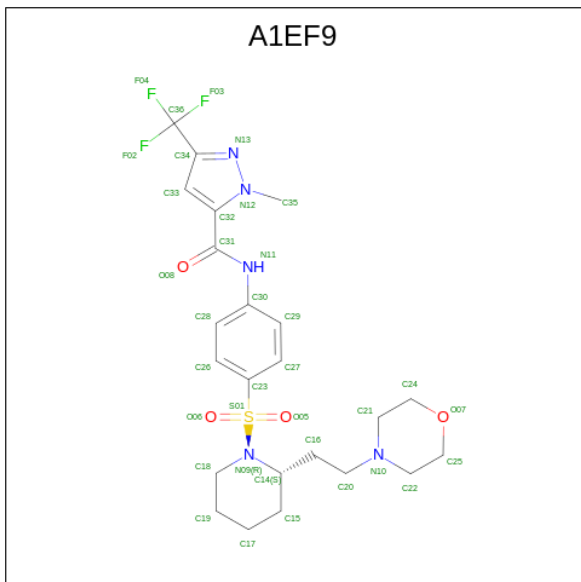
Chain	Residue	Modelled	Actual	Comment	Reference
L	-397	MET	-	initiating methionine	UNP P0AEX9
L	-396	GLY	-	expression tag	UNP P0AEX9
L	-395	SER	-	expression tag	UNP P0AEX9
L	-394	SER	-	expression tag	UNP P0AEX9
L	-393	HIS	-	expression tag	UNP P0AEX9
L	-392	HIS	-	expression tag	UNP P0AEX9
L	-391	HIS	-	expression tag	UNP P0AEX9
L	-390	HIS	-	expression tag	UNP P0AEX9
L	-389	HIS	-	expression tag	UNP P0AEX9
L	-388	HIS	-	expression tag	UNP P0AEX9
L	-387	GLY	-	expression tag	UNP P0AEX9
L	-386	THR	-	expression tag	UNP P0AEX9
L	-385	LYS	-	expression tag	UNP P0AEX9
L	-384	THR	-	expression tag	UNP P0AEX9
L	-19	GLY	-	linker	UNP P0AEX9
L	-18	THR	-	linker	UNP P0AEX9
L	-17	ASP	-	linker	UNP P0AEX9
L	-16	TYR	-	linker	UNP P0AEX9
L	-15	ASP	-	linker	UNP P0AEX9
L	-14	ILE	-	linker	UNP P0AEX9
L	-13	PRO	-	linker	UNP P0AEX9
L	-12	THR	-	linker	UNP P0AEX9
L	-11	THR	-	linker	UNP P0AEX9
L	-10	LEU	-	linker	UNP P0AEX9
L	-9	GLU	-	linker	UNP P0AEX9
L	-8	VAL	-	linker	UNP P0AEX9
L	-7	LEU	-	linker	UNP P0AEX9
L	-6	PHE	-	linker	UNP P0AEX9
L	-5	GLN	-	linker	UNP P0AEX9
L	-4	GLY	-	linker	UNP P0AEX9
L	-3	PRO	-	linker	UNP P0AEX9
L	-2	LEU	-	linker	UNP P0AEX9
L	-1	GLY	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9

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

Mol	Chain	Residues	Atoms	AltConf
3	L	2	Total Zn 2 2	0

- Molecule 4 is 2-methyl- {N}-[4-[(2 {S})-2-(2-morpholin-4-ylethyl)piperidin-1-yl]sul

fonylphenyl]-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EF9) (formula: $C_{23}H_{30}F_3N_5O_4S$) (labeled as "Ligand of Interest" by depositor).



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

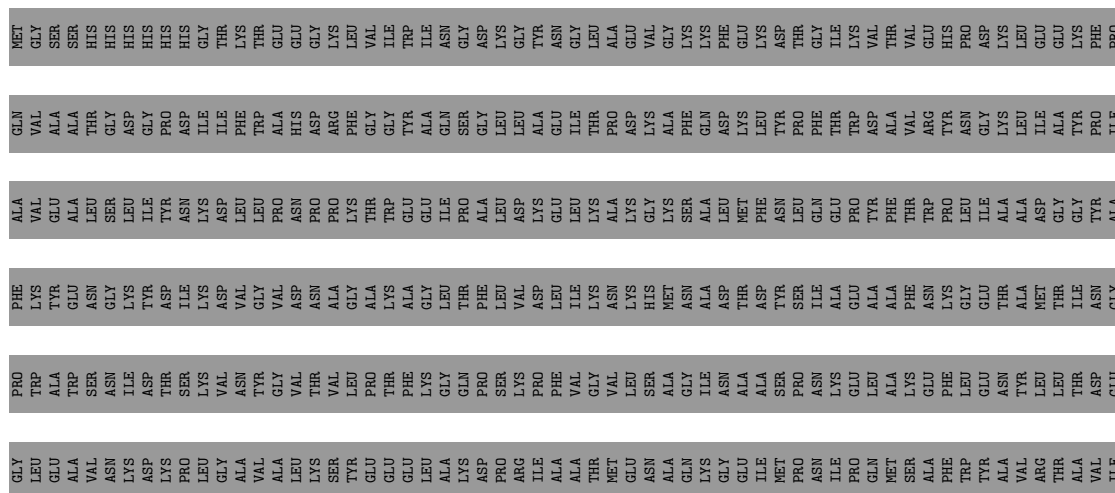
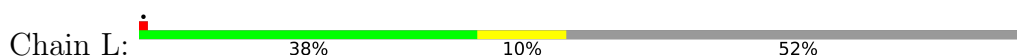
[illegible]

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Phosphoprotein

Chain C: 8% 90%

SER	LYS	HIS	ASN	GLY	PRO	PHE	ALA	GLN	MET
	LYS	GLU	ALA	LEU	TRP	LYS	VAL	VAL	GLY
	PRO	ASP	ALA	GLU	TRP	TRP	GLU	ALA	GLY
	VAL	ASN	GLY	VAL	SER	ASN	LEU	THR	GLY
	ALA	GLN	GLY	ASN	ASN	GLY	SER	GLY	GLY
	SER	LYS	GLN	ASP	ILE	LYS	LEU	ASP	GLY
	ARG	ILE	THR	LYS	ASP	TRP	ILE	GLY	HIS
	GLN	LYS	VAL	ASP	THR	ASP	TRP	PRO	HIS
	LEU	SER	ASN	GLY	SER	ILE	LYS	ASP	HIS
	GLY	GLU	ALA	LEU	VAL	VAL	ASP	ASP	GLY
ASN	THR	LEU	THR	LEU	THR	VAL	THR	ARG	LYS
	THR	GLU	GLY	TYR	LEU	GLY	THR	PHE	LEU
	ARG	GLY	THR	SER	VAL	ALA	PRO	ARG	GLY
	ARG	G344	ASP	GLU	PRO	ALA	THR	GLY	VAL
	GLY	E345	ASP	GLU	THR	LYS	TRP	GLY	ILE
	ASN	V346	TYR	GLU	PHE	ALA	GLU	TYR	TRP
	ASP	E347	ASP	LEU	LYS	GLY	GLU	ALA	ILE
	LEU	S348	ILE	ALA	GLY	LEU	PRO	ASN	ASN
	ALA	I349	PRO	LYS	GLN	THR	ILE	GLU	GLY
	LYS	K350	THR	ASP	PRO	PHE	ALA	GLY	ASP
HIS	PHE	K351	THR	PRO	SER	LEU	LEU	LEU	LYS
	GLN		LEU	ARG	LYS	VAL	LYS	ASP	GLY
	PRO	Q356	GLU	ILE	PRO	ASP	LYS	ALA	TYR
	LYS		VAL	ALA	PHE	LEU	GLU	GLU	ASN
	ILE	L367	LEU	ALA	GLY	ILE	VAL	LEU	GLY
	GLY		GLN	THR	MET	GLY	MET	PRO	GLY
	LYS	I370	GLY	ILE	VAL	LYS	LYS	ALA	GLY
	LYS	M371	PRO	ASN	SER	HIS	LYS	ASP	VAL
	MET	G378	LEU	GLY	ALA	MET	GLY	ALA	GLY
	SER	K379	SER	GLN	GLY	ASN	SER	PHE	LYS
VAL	ALA	D380	GLY	GLY	ASN	ASP	ALA	GLN	LYS
	VAL	P381	ASP	ILE	ALA	THR	MET	LYS	PHE
	GLY	N382	TYR	GLU	ALA	ASP	PHE	LEU	GLY
	PHE		TYR	MET	ALA	TRP	ASP	LEU	ASP
	VAL	V388	ASP	PRO	PRO	SER	LEU	TYR	THR
	ASP		GLU	ILE	LYS	ALA	GLU	TRP	ILE
	THR	N391	LEU	PRO	GLU	ALA	PRO	THR	VAL
	GLY	L394	PHE	GLN	LEU	ALA	TYR	ASP	LYS
	PRO		SER	MET	ALA	PHE	THR	VAL	VAL
	ALA	I397	VAL	ALA	GLU	ASN	TRP	ARG	GLU
SER	ARG	I398	GLN	PHE	PHE	LYS	PRO	TYR	HIS
	SER	G399	ASP	TRP	LEU	GLY	LEU	ASN	PRO
	VAL	ARG	ILE	TYR	GLN	GLU	ILE	GLY	ASP
	ILE	ASP	LYS	ALA	ASN	THR	ALA	LYS	LYS
	ARG	SER	THR	VAL	LEU	ALA	VAL	LEU	GLY
	SER	GLY	ALA	ARG	LEU	MET	ASP	ILE	GLU
	ILE	ARG	LEU	THR	LEU	THR	GLY	ALA	GLY
	LYS	ALA	ALA	ALA	THR	ILE	GLY	TYR	LYS
	LYS	LEU	LYS	VAL	ASP	ASN	ASN	PRO	PHE
	SER	GLU	ILE	GLU	GLU	GLY	ALA	ILE	PRO

- Chain D: 5% 93%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177478	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 ($e^-/\text{\AA}^2$)	52.52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.280	Depositor
Minimum map value	-0.866	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	306.36002, 306.36002, 306.36002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8510001, 0.8510001, 0.8510001	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, ZN

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	0.13	0/1043	0.36	0/1388
1	B	0.10	0/249	0.21	0/331
1	C	0.15	0/448	0.34	0/606
1	D	0.12	0/319	0.31	0/427
2	L	0.16	0/10352	0.37	1/14034 (0.0%)
All	All	0.16	0/12411	0.36	1/16786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	864	THR	N-CA-C	6.77	118.66	111.28

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	1034	0	1123	15	0
1	B	249	0	270	7	0
1	C	443	0	466	12	0
1	D	317	0	340	6	0
2	L	10125	0	10132	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2	0	0	0	0
4	L	36	0	0	0	0
All	All	12206	0	12331	195	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 8.

The worst 5 of 195 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:L:1180:CYS:SG	2:L:1364:HIS:HE1	1.92	0.91
2:L:284:GLU:HG3	2:L:285:PRO:HD3	1.59	0.81
2:L:1052:ARG:HD2	2:L:1380:ILE:HG22	1.64	0.80
2:L:464:LEU:HD12	2:L:1078:MET:HE3	1.66	0.76
2:L:1057:PRO:HG2	2:L:1157:LEU:HD11	1.71	0.72

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	127/602 (21%)	123 (97%)	4 (3%)	0	100	100
1	B	30/602 (5%)	30 (100%)	0	0	100	100
1	C	57/602 (10%)	57 (100%)	0	0	100	100
1	D	40/602 (7%)	39 (98%)	1 (2%)	0	100	100
2	L	1250/2630 (48%)	1212 (97%)	38 (3%)	0	100	100
All	All	1504/5038 (30%)	1461 (97%)	43 (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	117/499 (23%)	115 (98%)	2 (2%)	53	70
1	B	30/499 (6%)	30 (100%)	0	100	100
1	C	52/499 (10%)	52 (100%)	0	100	100
1	D	37/499 (7%)	35 (95%)	2 (5%)	20	46
2	L	1121/2301 (49%)	1090 (97%)	31 (3%)	38	62
All	All	1357/4297 (32%)	1322 (97%)	35 (3%)	41	64

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	904	LEU
2	L	928	ILE
2	L	1246	SER
2	L	293	LEU
2	L	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	812	HIS
2	L	909	ASN
2	L	1358	ASN
2	L	1186	ASN
2	L	1268	ASN

5.3.3 RNA

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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	A1EF9	L	4003	-	39,39,39	2.79	15 (38%)	54,57,57	2.74	15 (27%)

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	L	4003	-	-	4/31/50/50	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	4003	A1EF9	C20-N10	-7.36	1.30	1.47
4	L	4003	A1EF9	S01-N09	6.67	1.73	1.63
4	L	4003	A1EF9	C31-N11	6.10	1.48	1.35
4	L	4003	A1EF9	C23-S01	5.82	1.84	1.76
4	L	4003	A1EF9	C30-N11	3.56	1.48	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4003	A1EF9	O06-S01-O05	-10.83	101.98	119.52
4	L	4003	A1EF9	C36-C34-N13	6.23	127.14	119.23
4	L	4003	A1EF9	C15-C14-N09	5.62	119.24	109.50
4	L	4003	A1EF9	C19-C18-N09	5.18	117.90	110.31
4	L	4003	A1EF9	O05-S01-C23	4.50	113.74	108.05

There are no chirality outliers.

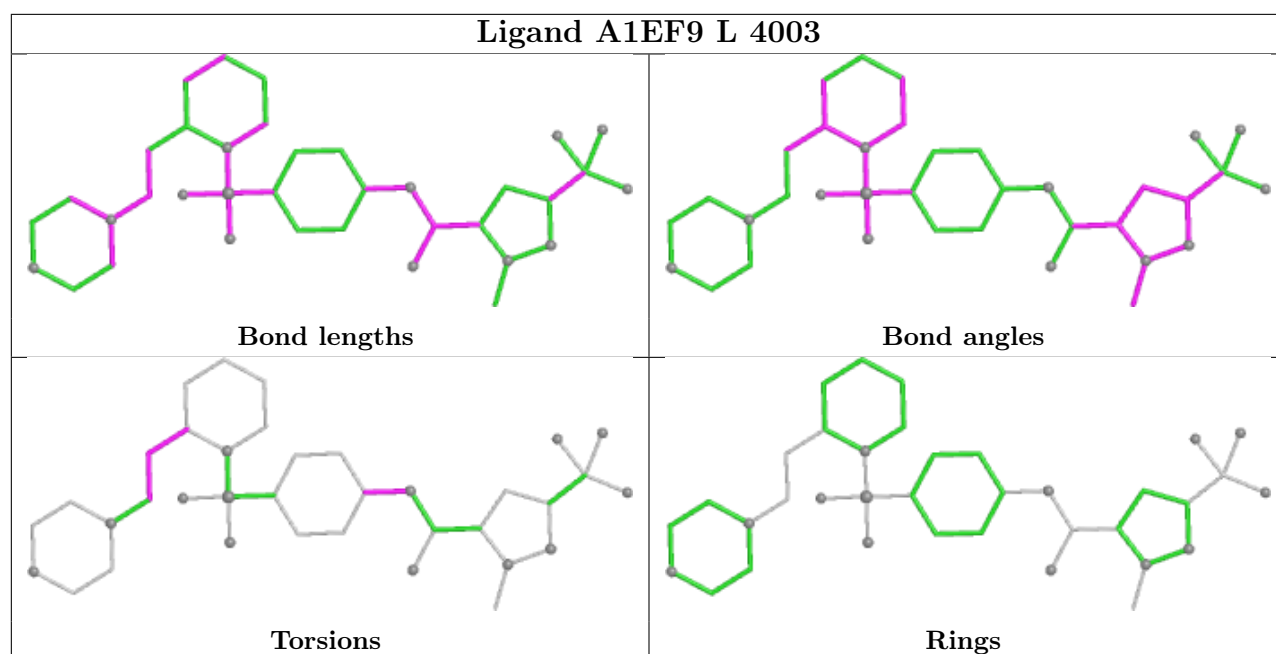
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	4003	A1EF9	C14-C16-C20-N10
4	L	4003	A1EF9	C28-C30-N11-C31
4	L	4003	A1EF9	C29-C30-N11-C31
4	L	4003	A1EF9	C15-C14-C16-C20

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.

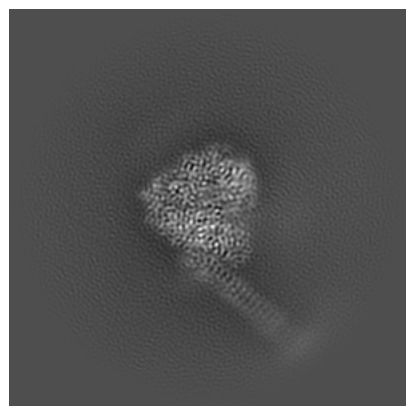
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65367. These allow visual inspection of the internal detail of the map and identification of artifacts.

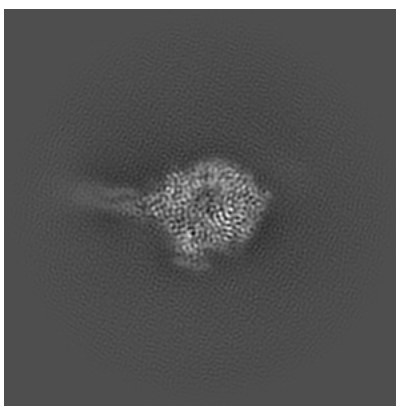
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

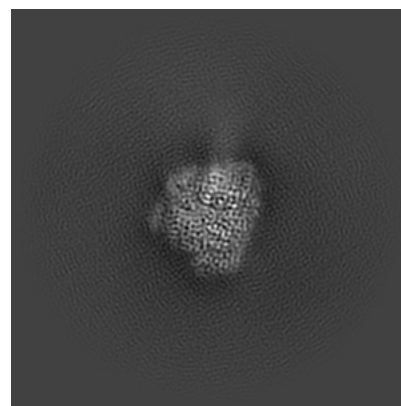
6.1.1 Primary map



X

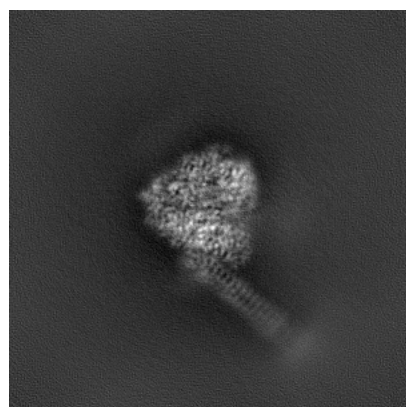


Y

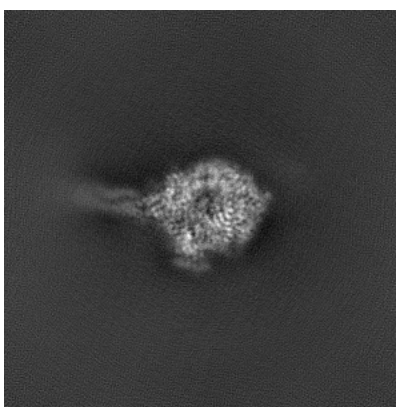


Z

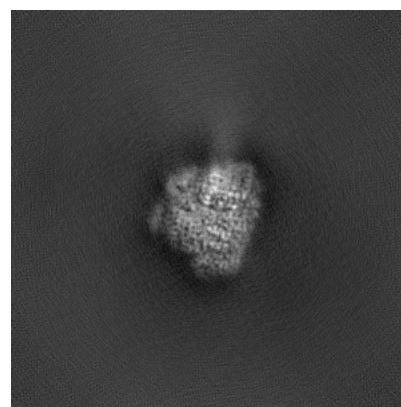
6.1.2 Raw map



X



Y

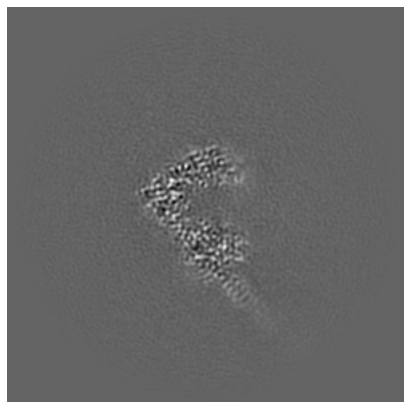


Z

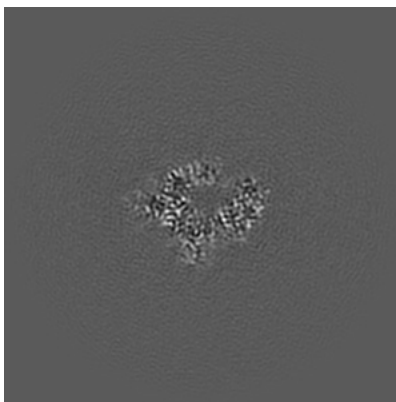
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

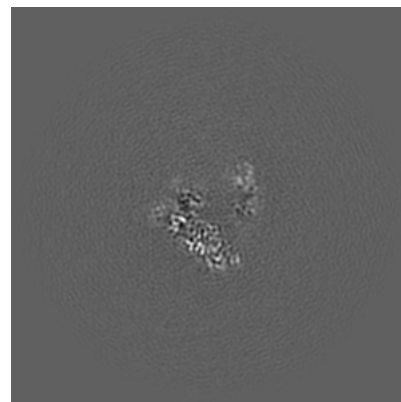
6.2.1 Primary map



X Index: 180

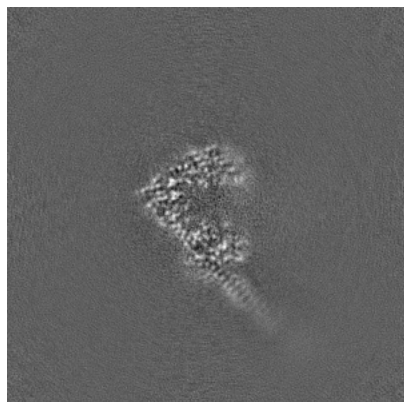


Y Index: 180

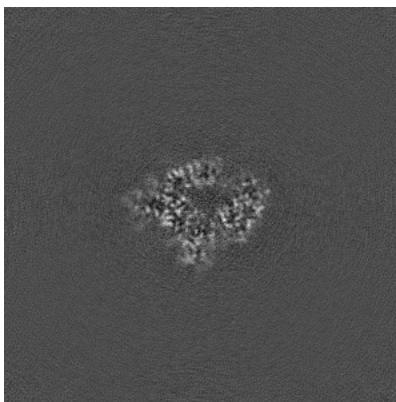


Z Index: 180

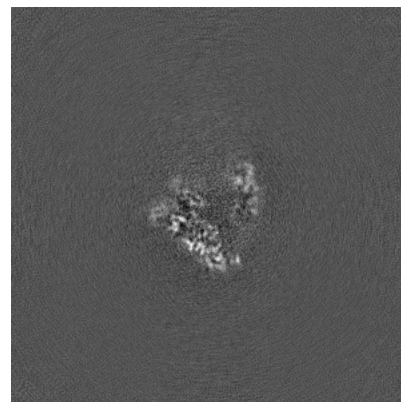
6.2.2 Raw map



X Index: 180



Y Index: 180

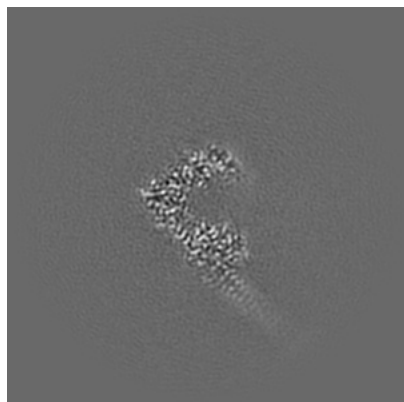


Z Index: 180

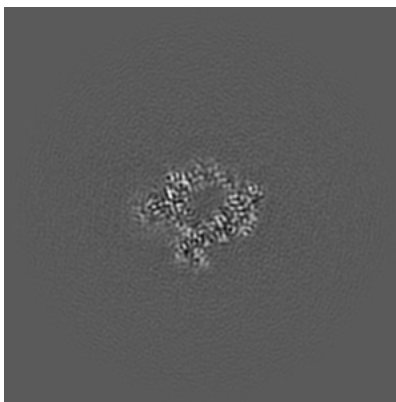
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

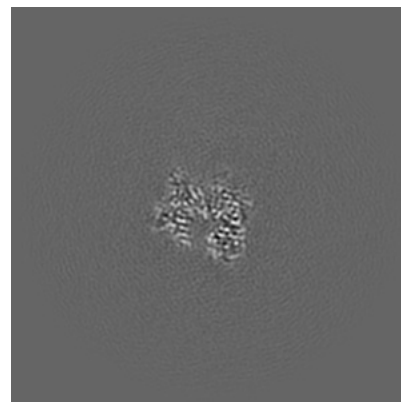
6.3.1 Primary map



X Index: 182

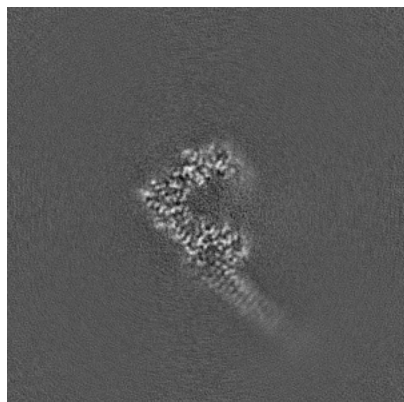


Y Index: 172

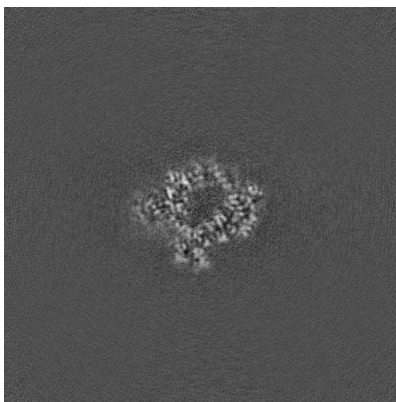


Z Index: 163

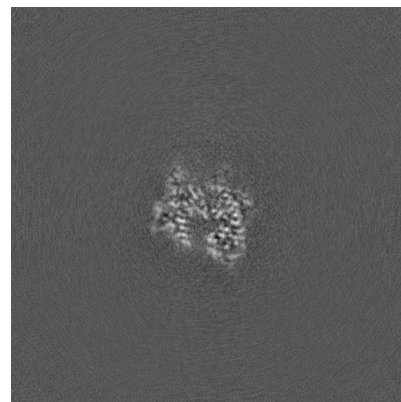
6.3.2 Raw map



X Index: 183



Y Index: 172

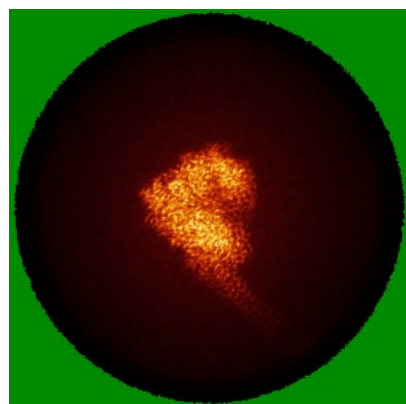


Z Index: 163

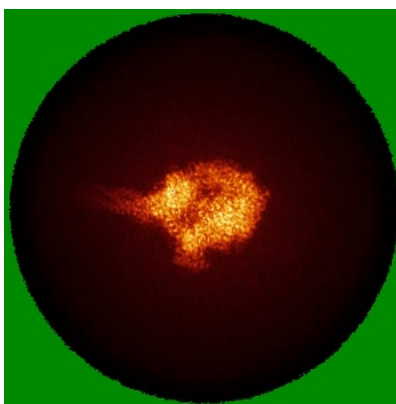
The images above show the largest variance slices of the map in three orthogonal directions.

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

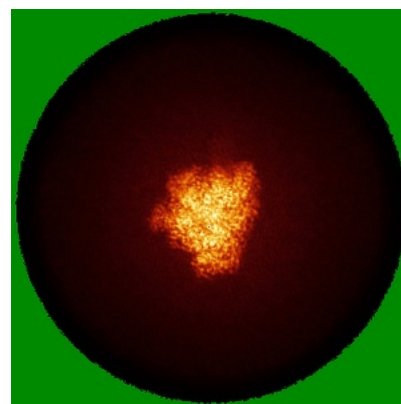
6.4.1 Primary map



X

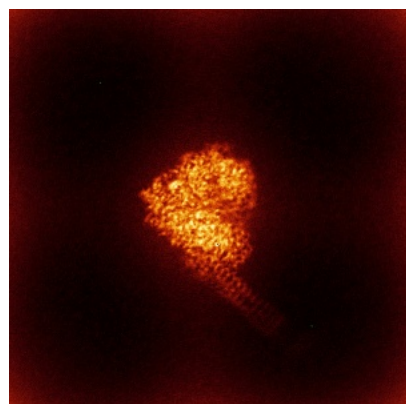


Y

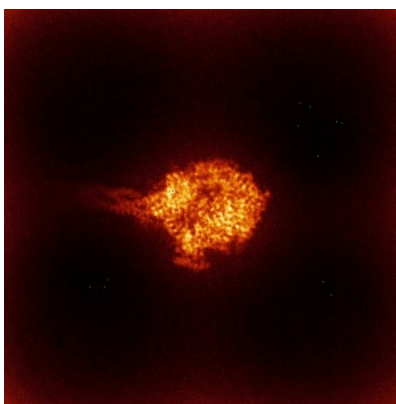


Z

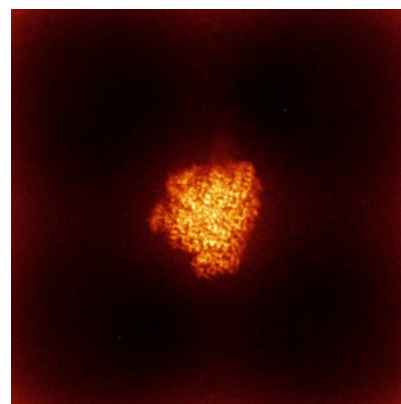
6.4.2 Raw map



X



Y

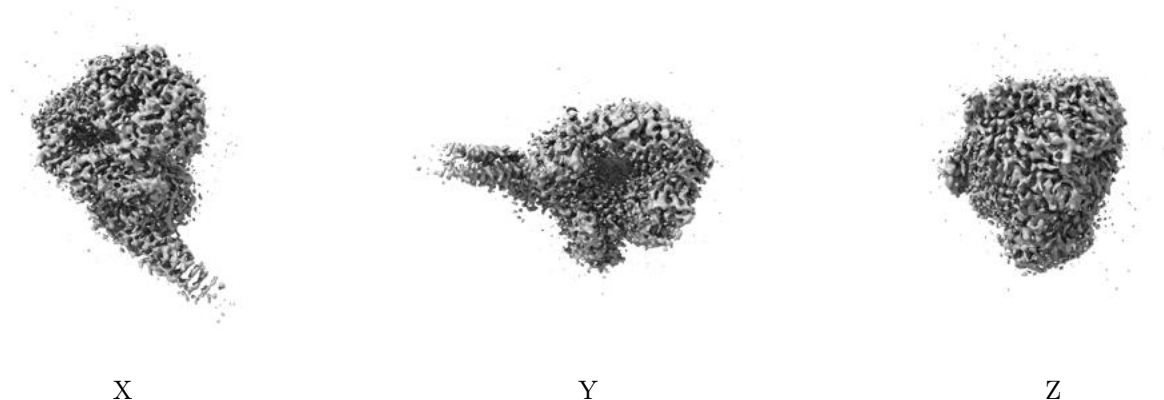


Z

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.

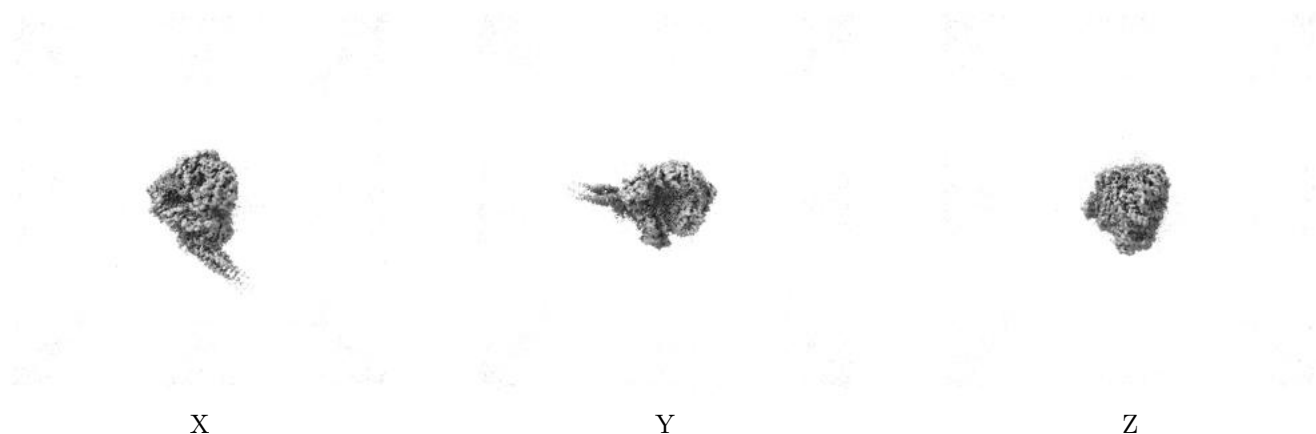
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

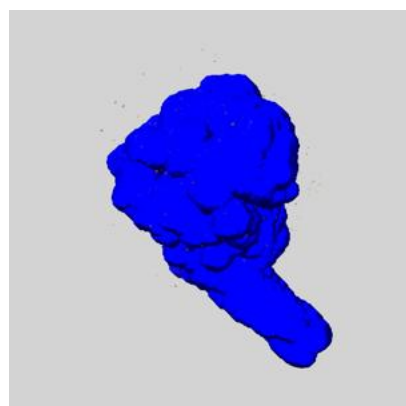
6.6 Mask visualisation [i](#)

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

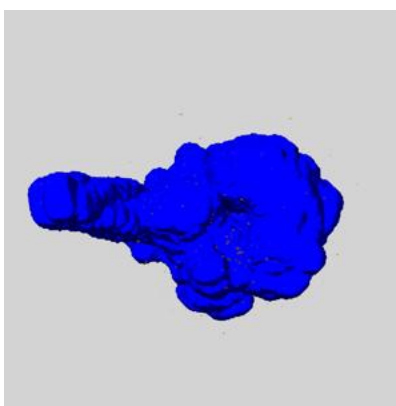
A mask typically either:

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

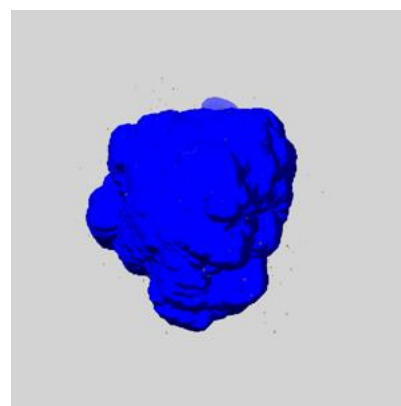
6.6.1 emd_65367_msk_1.map [i](#)



X



Y

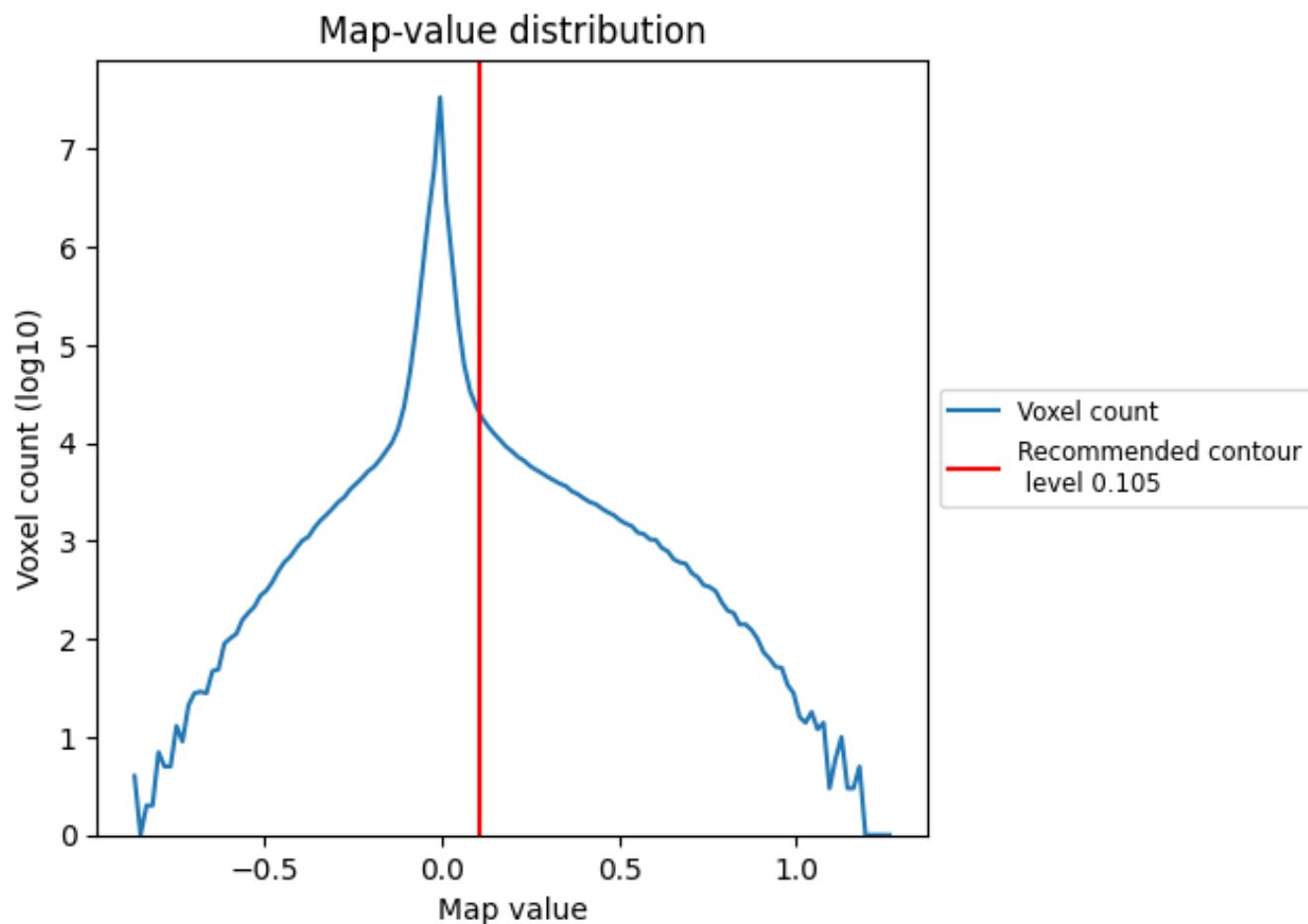


Z

7 Map analysis [i](#)

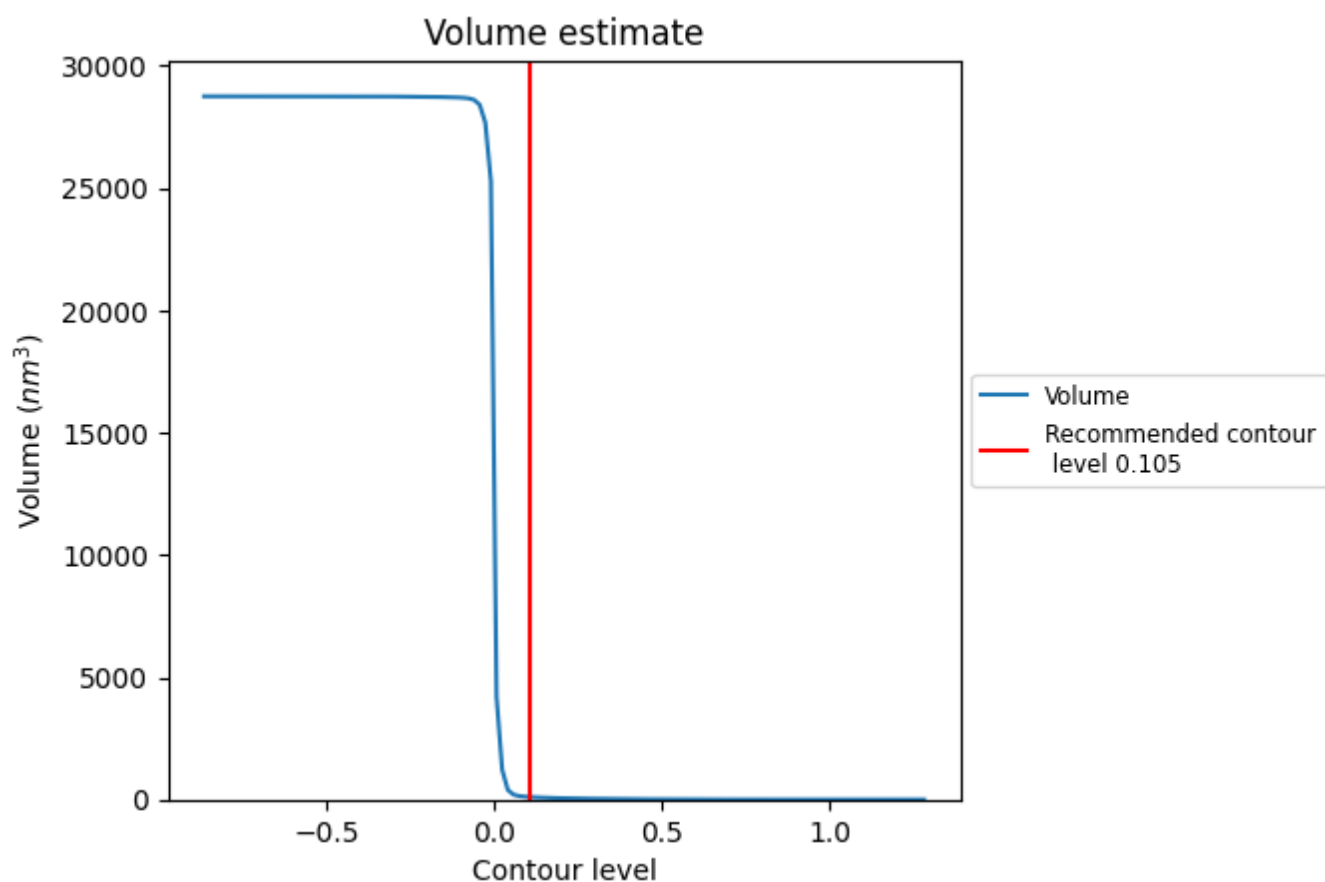
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

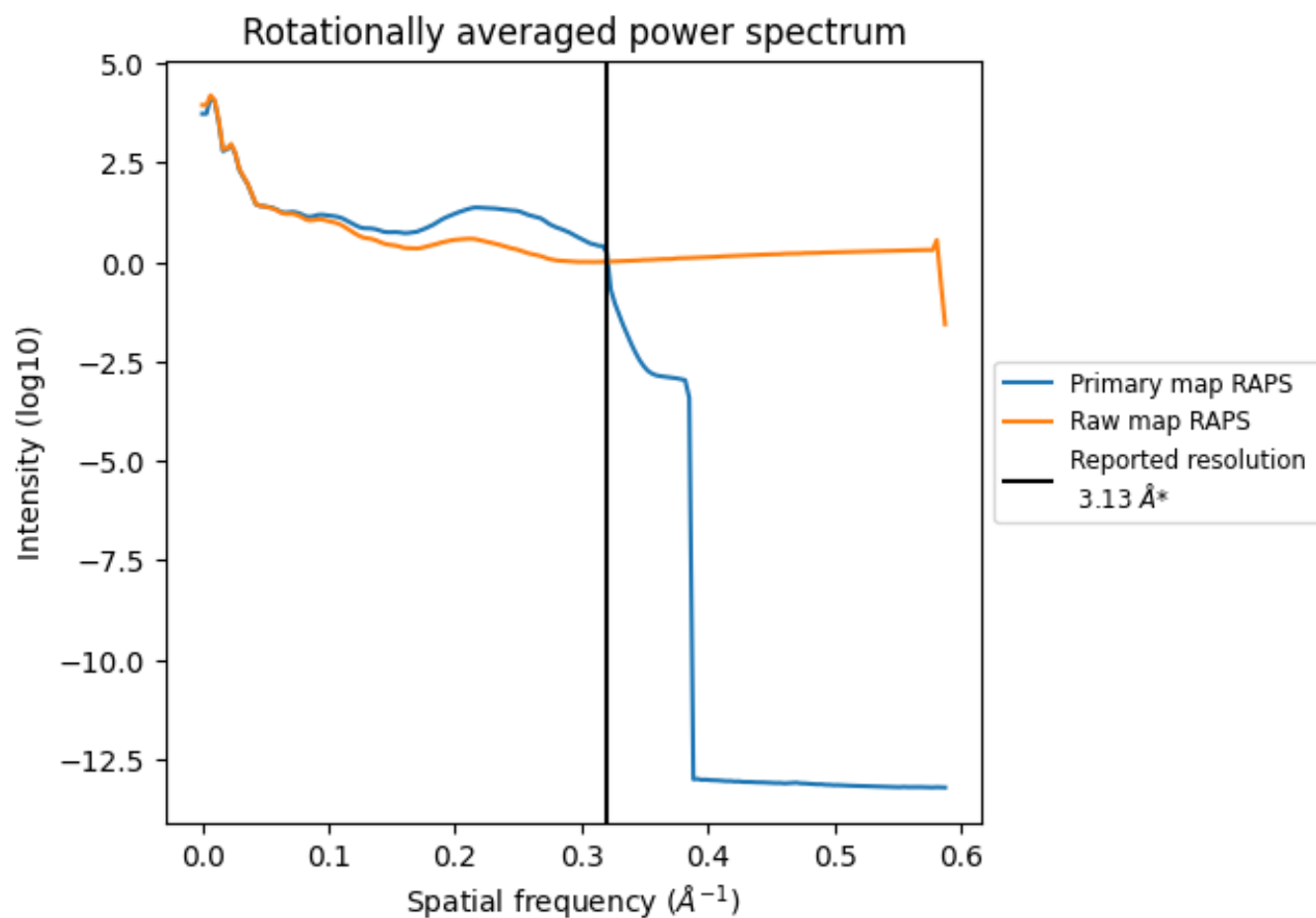
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

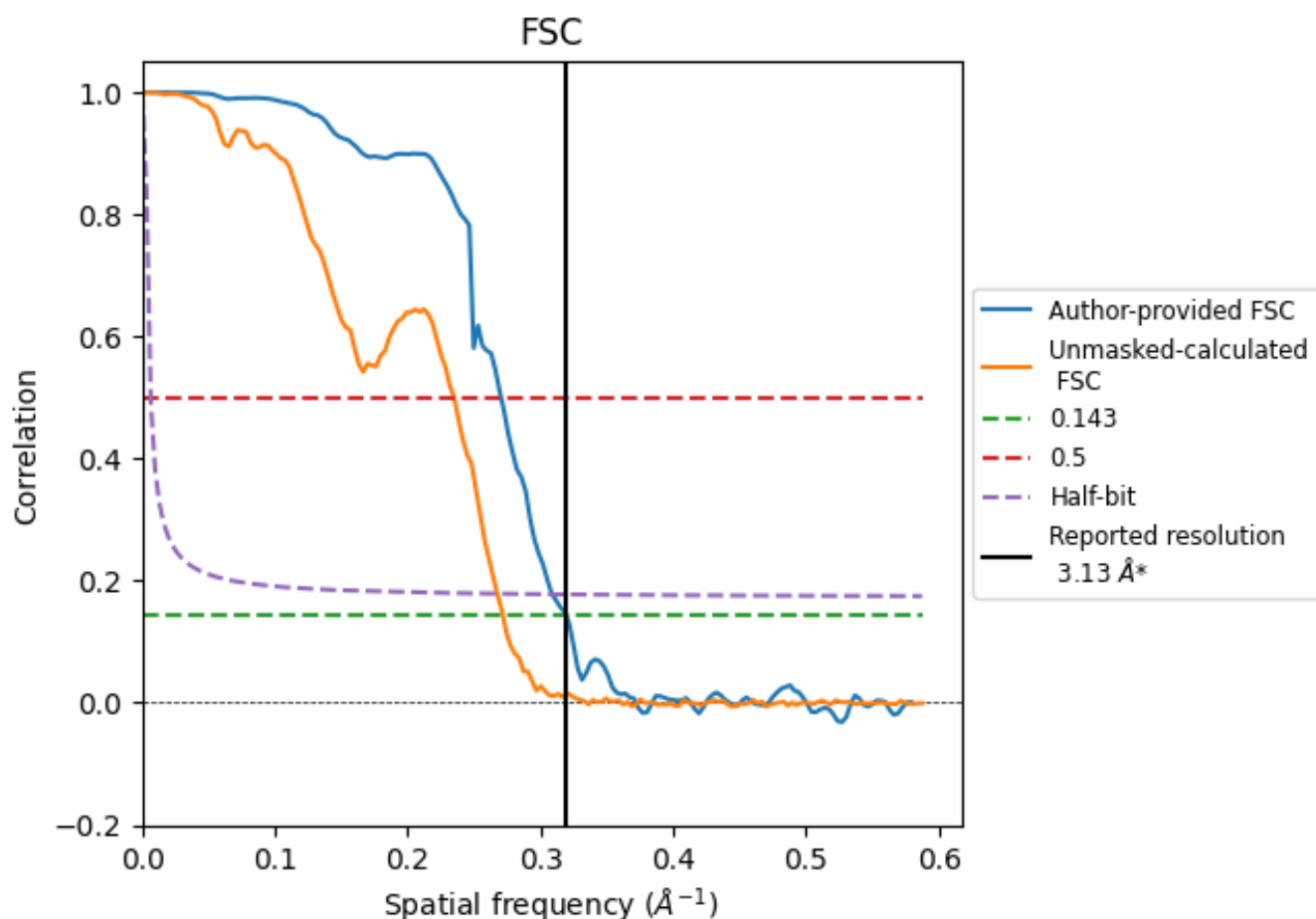


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

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 0.319 \AA^{-1}

8.2 Resolution estimates [i](#)

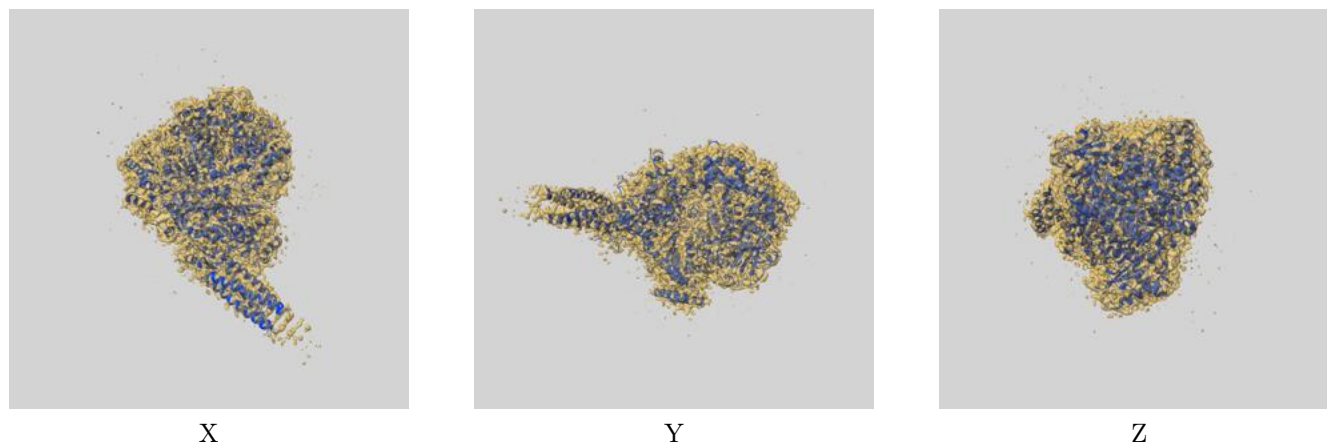
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.70	3.24
Unmasked-calculated*	3.68	4.26	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

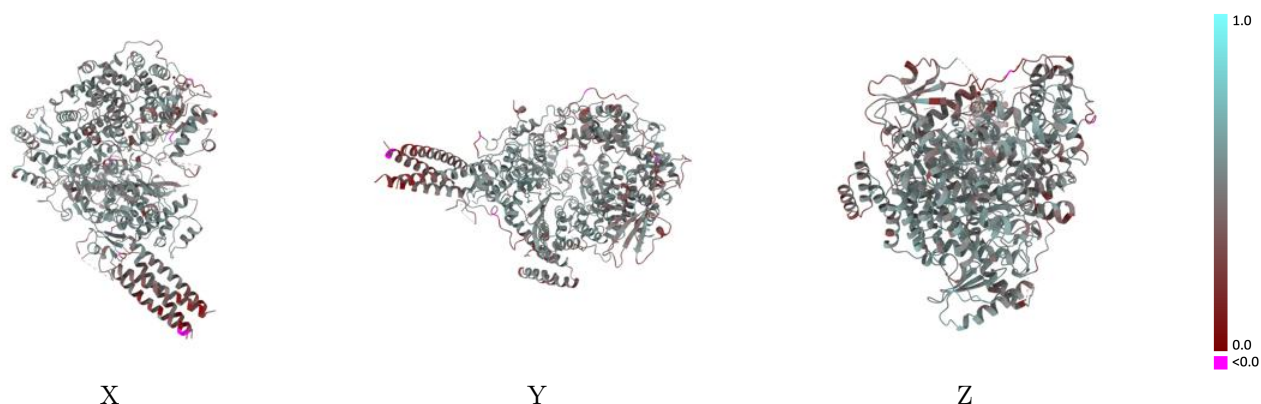
This section contains information regarding the fit between EMDB map EMD-65367 and PDB model 9VUL. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



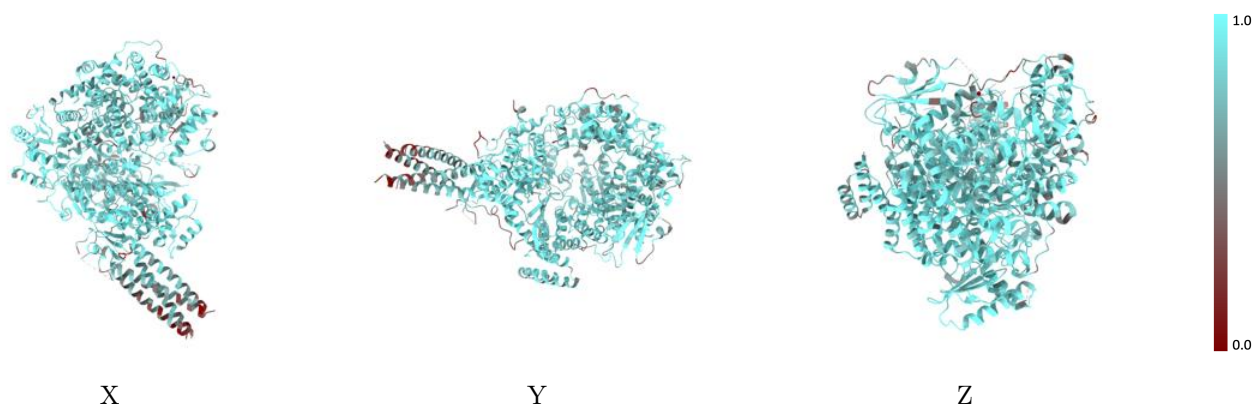
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



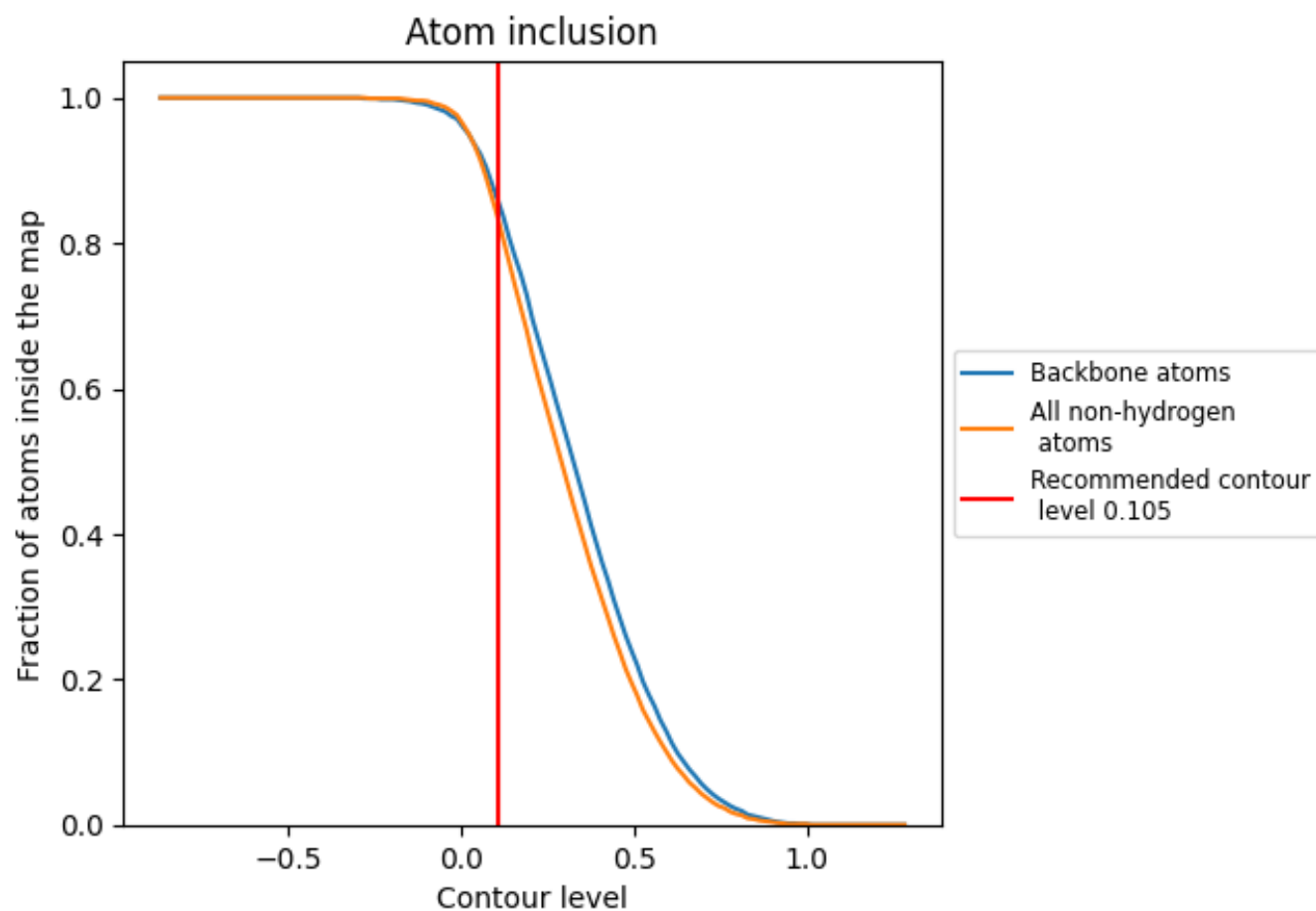
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8390	<div></div> 0.4790
A	<div></div> 0.6850	<div></div> 0.3990
B	<div></div> 0.5510	<div></div> 0.3410
C	<div></div> 0.6640	<div></div> 0.4040
D	<div></div> 0.6920	<div></div> 0.3840
L	<div></div> 0.8740	<div></div> 0.4970

