



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 12:37 AM JST

PDB ID : 9IP3 / pdb\_00009ip3  
EMDB ID : EMD-60756  
Title : Cryo-EM structure of the RNA-dependent RNA polymerase complex in a compact conformation from Ebola virus  
Authors : Li, G.; Du, T.; Wang, J.; Wu, S.; Ru, H.  
Deposited on : 2024-07-10  
Resolution : 3.10 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.dev117  
MolProbity : 4.02b-467  
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) : 2.42

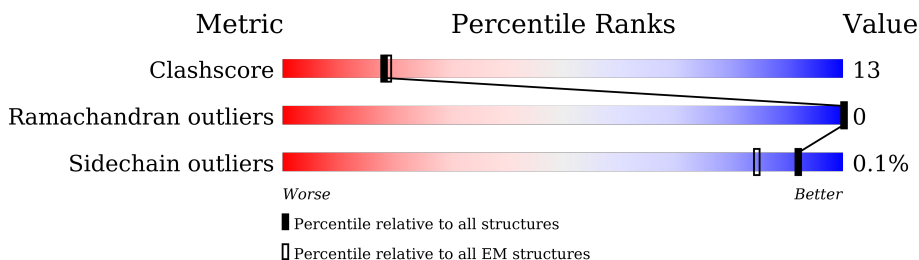
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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  $\geq 3$ , 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	1839	 5% 52% 22% 26%
2	B	657	 8% 25% 8% 67%
2	C	657	 7% 91%
2	D	657	 95%
2	E	657	 96%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13464 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,RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1365	10948	7034	1857	1998	59	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-428	MET	-	initiating methionine	UNP P0AEX9
A	-427	GLY	-	expression tag	UNP P0AEX9
A	-426	SER	-	expression tag	UNP P0AEX9
A	-425	GLY	-	expression tag	UNP P0AEX9
A	-424	TRP	-	expression tag	UNP P0AEX9
A	-423	SER	-	expression tag	UNP P0AEX9
A	-422	HIS	-	expression tag	UNP P0AEX9
A	-421	PRO	-	expression tag	UNP P0AEX9
A	-420	GLN	-	expression tag	UNP P0AEX9
A	-419	PHE	-	expression tag	UNP P0AEX9
A	-418	GLU	-	expression tag	UNP P0AEX9
A	-417	LYS	-	expression tag	UNP P0AEX9
A	-416	GLY	-	expression tag	UNP P0AEX9
A	-415	GLY	-	expression tag	UNP P0AEX9
A	-414	GLY	-	expression tag	UNP P0AEX9
A	-413	SER	-	expression tag	UNP P0AEX9
A	-412	GLY	-	expression tag	UNP P0AEX9
A	-411	GLY	-	expression tag	UNP P0AEX9
A	-410	GLY	-	expression tag	UNP P0AEX9
A	-409	SER	-	expression tag	UNP P0AEX9
A	-408	GLY	-	expression tag	UNP P0AEX9
A	-407	GLY	-	expression tag	UNP P0AEX9
A	-406	SER	-	expression tag	UNP P0AEX9
A	-405	ALA	-	expression tag	UNP P0AEX9
A	-404	TRP	-	expression tag	UNP P0AEX9
A	-403	SER	-	expression tag	UNP P0AEX9
A	-402	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-401	PRO	-	expression tag	UNP P0AEX9
A	-400	GLN	-	expression tag	UNP P0AEX9
A	-399	PHE	-	expression tag	UNP P0AEX9
A	-398	GLU	-	expression tag	UNP P0AEX9
A	-397	LYS	-	expression tag	UNP P0AEX9
A	-396	GLY	-	expression tag	UNP P0AEX9
A	-395	SER	-	expression tag	UNP P0AEX9
A	-394	ALA	-	expression tag	UNP P0AEX9
A	-393	SER	-	expression tag	UNP P0AEX9
A	-392	HIS	-	expression tag	UNP P0AEX9
A	-391	HIS	-	expression tag	UNP P0AEX9
A	-390	HIS	-	expression tag	UNP P0AEX9
A	-389	HIS	-	expression tag	UNP P0AEX9
A	-388	HIS	-	expression tag	UNP P0AEX9
A	-387	HIS	-	expression tag	UNP P0AEX9
A	-386	GLY	-	expression tag	UNP P0AEX9
A	-385	THR	-	expression tag	UNP P0AEX9
A	-384	LYS	-	expression tag	UNP P0AEX9
A	-383	THR	-	expression tag	UNP P0AEX9
A	-18	GLY	-	linker	UNP P0AEX9
A	-17	THR	-	linker	UNP P0AEX9
A	-16	ASP	-	linker	UNP P0AEX9
A	-15	TYR	-	linker	UNP P0AEX9
A	-14	ASP	-	linker	UNP P0AEX9
A	-13	ILE	-	linker	UNP P0AEX9
A	-12	PRO	-	linker	UNP P0AEX9
A	-11	THR	-	linker	UNP P0AEX9
A	-10	THR	-	linker	UNP P0AEX9
A	-9	LEU	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	VAL	-	linker	UNP P0AEX9
A	-6	LEU	-	linker	UNP P0AEX9
A	-5	PHE	-	linker	UNP P0AEX9
A	-4	GLN	-	linker	UNP P0AEX9
A	-3	GLY	-	linker	UNP P0AEX9
A	-2	PRO	-	linker	UNP P0AEX9
A	-1	GLY	-	linker	UNP P0AEX9
A	0	SER	-	linker	UNP P0AEX9
A	1401	SER	-	expression tag	UNP Q05318
A	1402	ARG	-	expression tag	UNP Q05318
A	1403	ASP	-	expression tag	UNP Q05318
A	1404	TYR	-	expression tag	UNP Q05318

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1405	LYS	-	expression tag	UNP Q05318
A	1406	ASP	-	expression tag	UNP Q05318
A	1407	ASP	-	expression tag	UNP Q05318
A	1408	ASP	-	expression tag	UNP Q05318
A	1409	ASP	-	expression tag	UNP Q05318
A	1410	LYS	-	expression tag	UNP Q05318

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein, Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total 1684	C 1056	N 297	O 322	S 9	1	0
2	C	56	Total 417	C 261	N 69	O 83	S 4	0	0
2	D	30	Total 231	C 147	N 36	O 44	S 4	0	0
2	E	24	Total 183	C 115	N 30	O 35	S 3	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-316	MET	-	initiating methionine	UNP P0AEX9
B	-315	GLY	-	expression tag	UNP P0AEX9
B	-314	SER	-	expression tag	UNP P0AEX9
B	-313	SER	-	expression tag	UNP P0AEX9
B	-312	HIS	-	expression tag	UNP P0AEX9
B	-311	HIS	-	expression tag	UNP P0AEX9
B	-310	HIS	-	expression tag	UNP P0AEX9
B	-309	HIS	-	expression tag	UNP P0AEX9
B	-308	HIS	-	expression tag	UNP P0AEX9
B	-307	HIS	-	expression tag	UNP P0AEX9
B	-306	GLY	-	expression tag	UNP P0AEX9
B	-305	THR	-	expression tag	UNP P0AEX9
B	-304	LYS	-	expression tag	UNP P0AEX9
B	-303	THR	-	expression tag	UNP P0AEX9
B	62	GLY	-	linker	UNP P0AEX9
B	63	THR	-	linker	UNP P0AEX9
B	64	ASP	-	linker	UNP P0AEX9
B	65	TYR	-	linker	UNP P0AEX9
B	66	ASP	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	67	ILE	-	linker	UNP P0AEX9
B	68	PRO	-	linker	UNP P0AEX9
B	69	THR	-	linker	UNP P0AEX9
B	70	THR	-	linker	UNP P0AEX9
B	71	GLU	-	linker	UNP P0AEX9
B	72	ASN	-	linker	UNP P0AEX9
B	73	LEU	-	linker	UNP P0AEX9
B	74	TYR	-	linker	UNP P0AEX9
B	75	PHE	-	linker	UNP P0AEX9
B	76	GLN	-	linker	UNP P0AEX9
B	77	GLY	-	linker	UNP P0AEX9
B	78	GLY	-	linker	UNP P0AEX9
B	79	SER	-	linker	UNP P0AEX9
C	-316	MET	-	initiating methionine	UNP P0AEX9
C	-315	GLY	-	expression tag	UNP P0AEX9
C	-314	SER	-	expression tag	UNP P0AEX9
C	-313	SER	-	expression tag	UNP P0AEX9
C	-312	HIS	-	expression tag	UNP P0AEX9
C	-311	HIS	-	expression tag	UNP P0AEX9
C	-310	HIS	-	expression tag	UNP P0AEX9
C	-309	HIS	-	expression tag	UNP P0AEX9
C	-308	HIS	-	expression tag	UNP P0AEX9
C	-307	HIS	-	expression tag	UNP P0AEX9
C	-306	GLY	-	expression tag	UNP P0AEX9
C	-305	THR	-	expression tag	UNP P0AEX9
C	-304	LYS	-	expression tag	UNP P0AEX9
C	-303	THR	-	expression tag	UNP P0AEX9
C	62	GLY	-	linker	UNP P0AEX9
C	63	THR	-	linker	UNP P0AEX9
C	64	ASP	-	linker	UNP P0AEX9
C	65	TYR	-	linker	UNP P0AEX9
C	66	ASP	-	linker	UNP P0AEX9
C	67	ILE	-	linker	UNP P0AEX9
C	68	PRO	-	linker	UNP P0AEX9
C	69	THR	-	linker	UNP P0AEX9
C	70	THR	-	linker	UNP P0AEX9
C	71	GLU	-	linker	UNP P0AEX9
C	72	ASN	-	linker	UNP P0AEX9
C	73	LEU	-	linker	UNP P0AEX9
C	74	TYR	-	linker	UNP P0AEX9
C	75	PHE	-	linker	UNP P0AEX9
C	76	GLN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	77	GLY	-	linker	UNP P0AEX9
C	78	GLY	-	linker	UNP P0AEX9
C	79	SER	-	linker	UNP P0AEX9
D	-316	MET	-	initiating methionine	UNP P0AEX9
D	-315	GLY	-	expression tag	UNP P0AEX9
D	-314	SER	-	expression tag	UNP P0AEX9
D	-313	SER	-	expression tag	UNP P0AEX9
D	-312	HIS	-	expression tag	UNP P0AEX9
D	-311	HIS	-	expression tag	UNP P0AEX9
D	-310	HIS	-	expression tag	UNP P0AEX9
D	-309	HIS	-	expression tag	UNP P0AEX9
D	-308	HIS	-	expression tag	UNP P0AEX9
D	-307	HIS	-	expression tag	UNP P0AEX9
D	-306	GLY	-	expression tag	UNP P0AEX9
D	-305	THR	-	expression tag	UNP P0AEX9
D	-304	LYS	-	expression tag	UNP P0AEX9
D	-303	THR	-	expression tag	UNP P0AEX9
D	62	GLY	-	linker	UNP P0AEX9
D	63	THR	-	linker	UNP P0AEX9
D	64	ASP	-	linker	UNP P0AEX9
D	65	TYR	-	linker	UNP P0AEX9
D	66	ASP	-	linker	UNP P0AEX9
D	67	ILE	-	linker	UNP P0AEX9
D	68	PRO	-	linker	UNP P0AEX9
D	69	THR	-	linker	UNP P0AEX9
D	70	THR	-	linker	UNP P0AEX9
D	71	GLU	-	linker	UNP P0AEX9
D	72	ASN	-	linker	UNP P0AEX9
D	73	LEU	-	linker	UNP P0AEX9
D	74	TYR	-	linker	UNP P0AEX9
D	75	PHE	-	linker	UNP P0AEX9
D	76	GLN	-	linker	UNP P0AEX9
D	77	GLY	-	linker	UNP P0AEX9
D	78	GLY	-	linker	UNP P0AEX9
D	79	SER	-	linker	UNP P0AEX9
E	-316	MET	-	initiating methionine	UNP P0AEX9
E	-315	GLY	-	expression tag	UNP P0AEX9
E	-314	SER	-	expression tag	UNP P0AEX9
E	-313	SER	-	expression tag	UNP P0AEX9
E	-312	HIS	-	expression tag	UNP P0AEX9
E	-311	HIS	-	expression tag	UNP P0AEX9
E	-310	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-309	HIS	-	expression tag	UNP P0AEX9
E	-308	HIS	-	expression tag	UNP P0AEX9
E	-307	HIS	-	expression tag	UNP P0AEX9
E	-306	GLY	-	expression tag	UNP P0AEX9
E	-305	THR	-	expression tag	UNP P0AEX9
E	-304	LYS	-	expression tag	UNP P0AEX9
E	-303	THR	-	expression tag	UNP P0AEX9
E	62	GLY	-	linker	UNP P0AEX9
E	63	THR	-	linker	UNP P0AEX9
E	64	ASP	-	linker	UNP P0AEX9
E	65	TYR	-	linker	UNP P0AEX9
E	66	ASP	-	linker	UNP P0AEX9
E	67	ILE	-	linker	UNP P0AEX9
E	68	PRO	-	linker	UNP P0AEX9
E	69	THR	-	linker	UNP P0AEX9
E	70	THR	-	linker	UNP P0AEX9
E	71	GLU	-	linker	UNP P0AEX9
E	72	ASN	-	linker	UNP P0AEX9
E	73	LEU	-	linker	UNP P0AEX9
E	74	TYR	-	linker	UNP P0AEX9
E	75	PHE	-	linker	UNP P0AEX9
E	76	GLN	-	linker	UNP P0AEX9
E	77	GLY	-	linker	UNP P0AEX9
E	78	GLY	-	linker	UNP P0AEX9
E	79	SER	-	linker	UNP P0AEX9

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

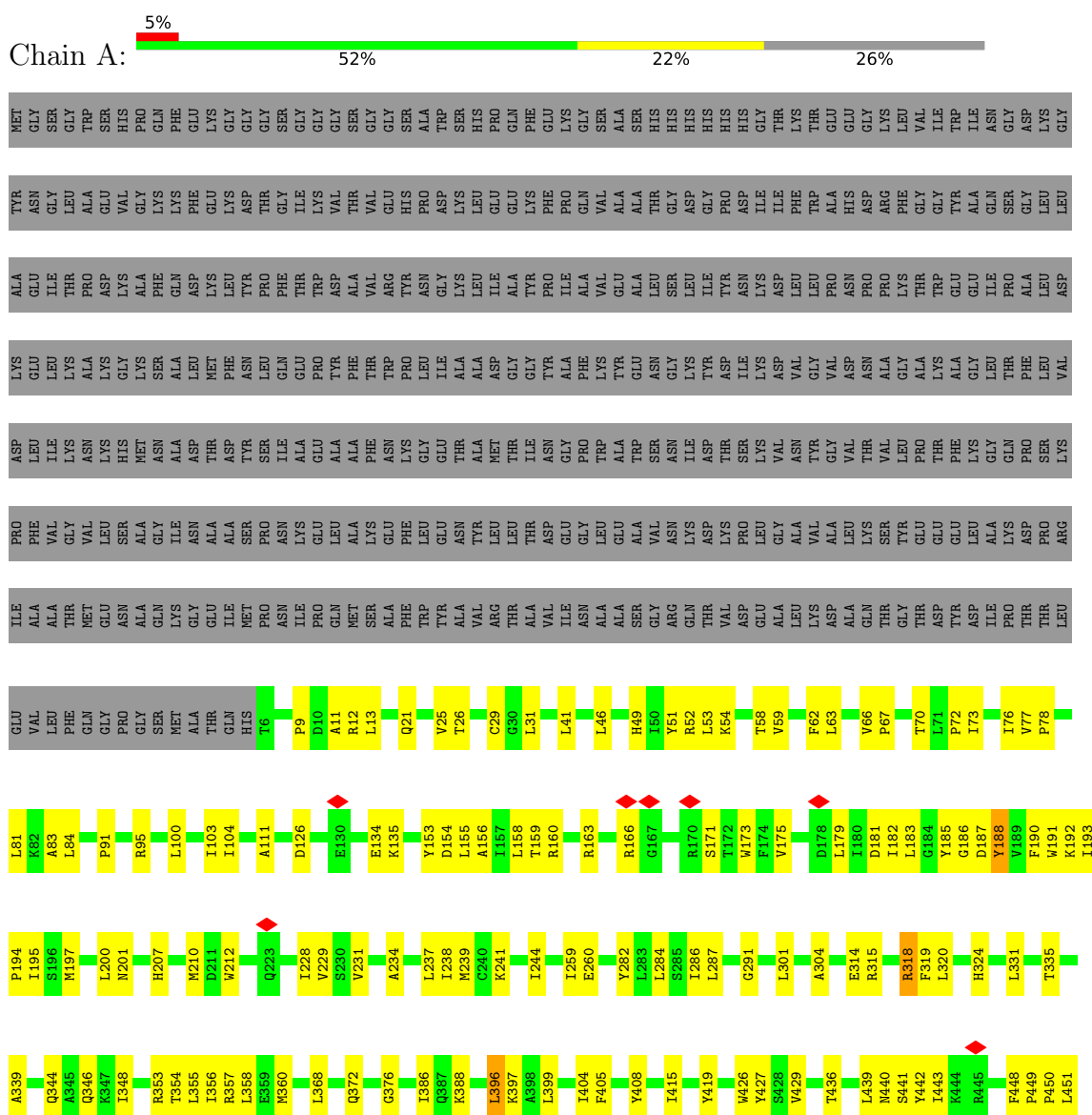
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

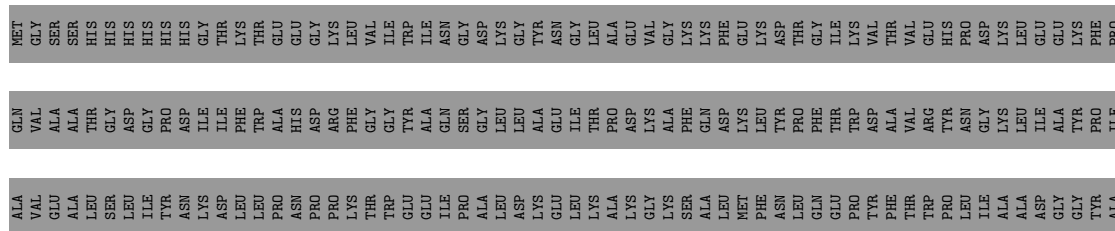
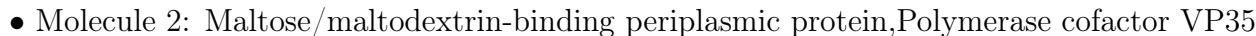


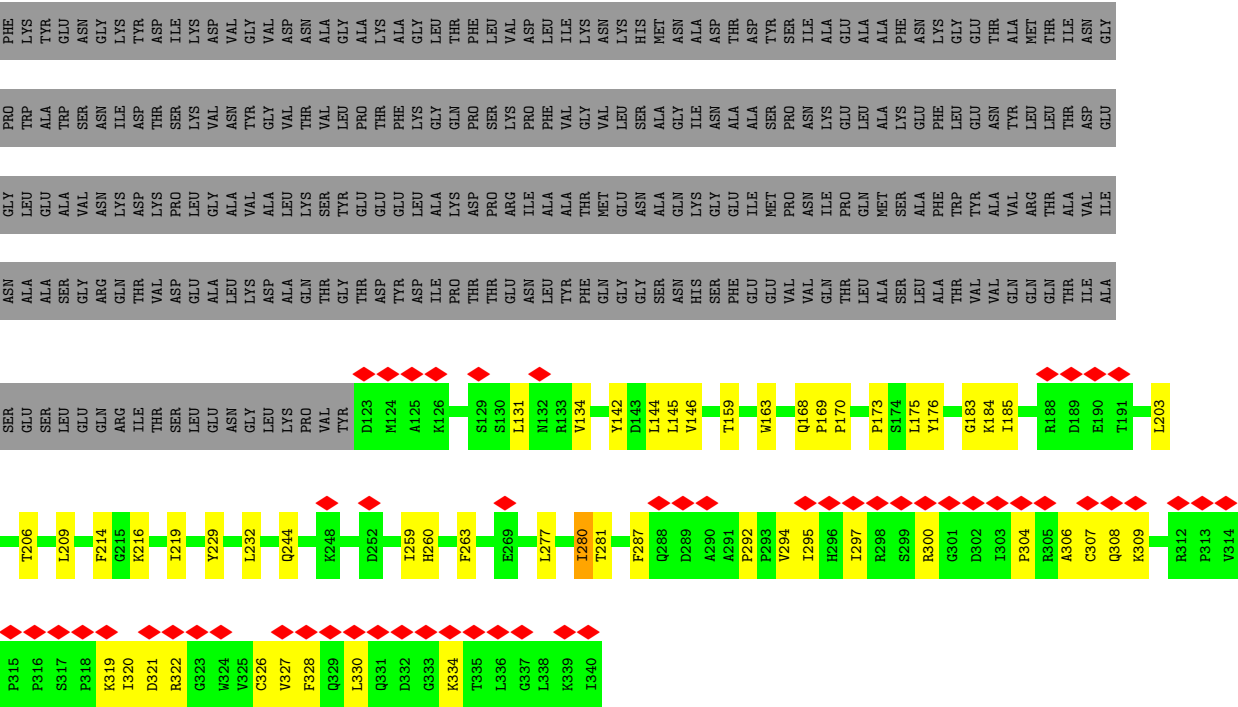
### 3 Residue-property plots

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.

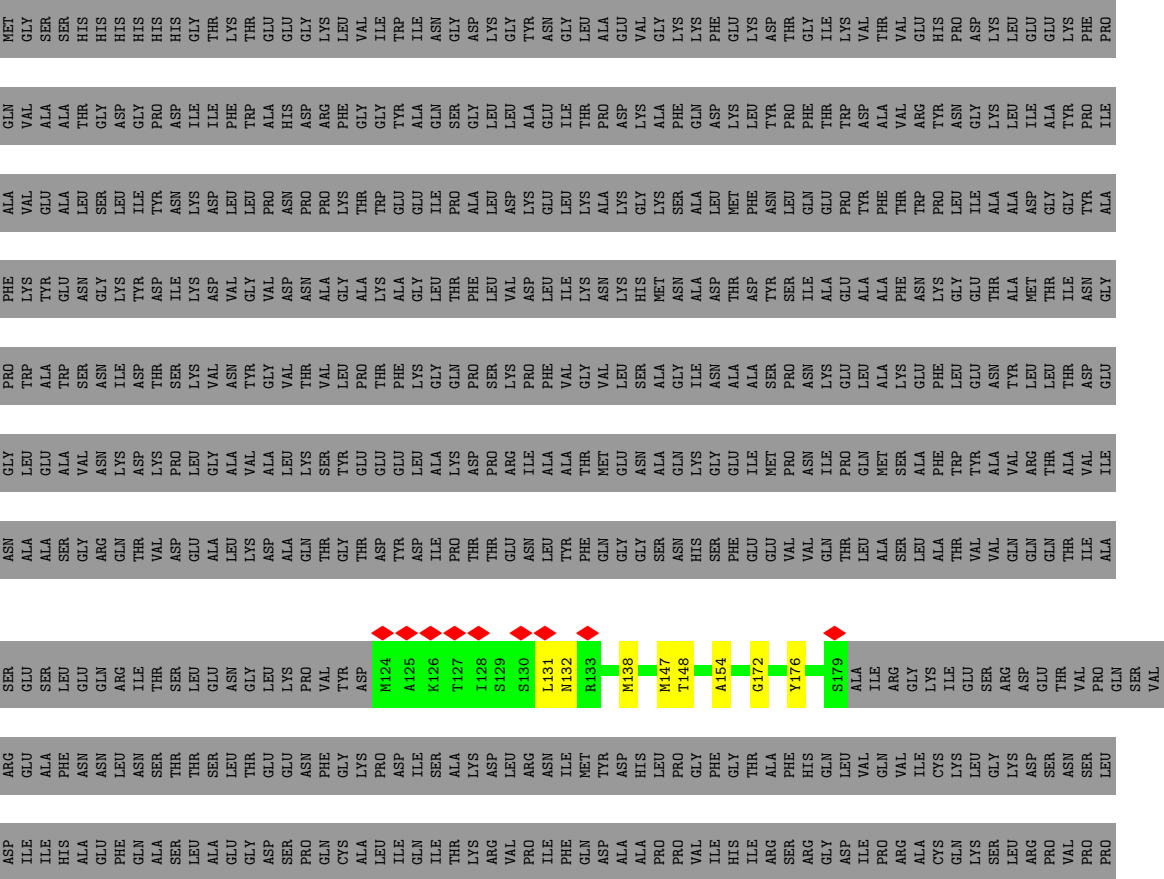
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,RNA-directed RNA polymerase L







● Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77587	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)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.838	Depositor
Minimum map value	-1.966	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.36	Depositor
Map size ( $\text{\AA}$ )	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.93, 0.93, 0.93	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.67	5/11220 (0.0%)	0.69	6/15233 (0.0%)
2	B	0.49	1/1719 (0.1%)	0.60	1/2333 (0.0%)
2	C	0.53	0/426	0.58	0/581
2	D	0.53	0/233	0.53	0/314
2	E	0.52	0/183	0.64	0/245
All	All	0.64	6/13781 (0.0%)	0.68	7/18706 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1381	TYR	CG-CD2	8.48	1.50	1.39
1	A	1085	TRP	CB-CG	-7.31	1.37	1.50
1	A	1381	TYR	CE1-CZ	6.44	1.47	1.38
2	B	163	TRP	CB-CG	-6.08	1.39	1.50
1	A	1143	TRP	CB-CG	-5.53	1.40	1.50
1	A	188	TYR	CB-CG	-5.52	1.43	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1381	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	A	1326	LEU	CB-CG-CD2	-7.31	98.57	111.00
1	A	972	LEU	CA-CB-CG	-6.53	100.28	115.30
1	A	1381	TYR	CB-CG-CD2	6.42	124.85	121.00
1	A	318	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	B	280	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	A	396	LEU	CB-CG-CD2	-5.55	101.56	111.00

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	10948	0	10919	304	0
2	B	1684	0	1684	44	0
2	C	417	0	406	11	0
2	D	231	0	242	2	0
2	E	183	0	193	7	0
3	A	1	0	0	0	0
All	All	13464	0	13444	349	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 13.

All (349) 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:849:SER:HA	1:A:1283:ASN:O	1.57	1.02
1:A:829:ILE:HG23	1:A:980:LEU:HD12	1.48	0.96
1:A:829:ILE:CG2	1:A:980:LEU:HD12	1.96	0.95
1:A:66:VAL:HG11	1:A:229:VAL:HG13	1.50	0.90
2:B:259:ILE:HG23	2:B:280:ILE:HD11	1.59	0.83
2:B:319:LYS:HD3	2:B:322:ARG:HB3	1.58	0.83
1:A:1375:ARG:HA	1:A:1381:TYR:CD1	2.16	0.81
2:B:287:PHE:HB3	2:B:320:ILE:HD11	1.64	0.79
1:A:803:LYS:HG3	1:A:804:LYS:HG3	1.64	0.78
1:A:1280:PHE:HE2	1:A:1315:ILE:HG21	1.48	0.76
1:A:815:SER:HB2	1:A:851:THR:HB	1.66	0.76
1:A:558:ASN:HD21	1:A:561:ARG:HB2	1.50	0.74
1:A:1247:ARG:HH11	1:A:1380:ILE:HG23	1.52	0.74
1:A:1021:LEU:O	1:A:1125:ARG:NH2	2.21	0.73
1:A:637:ASN:HD22	1:A:709:GLU:HA	1.53	0.72
1:A:499:GLU:HB3	1:A:679:TYR:CZ	2.26	0.70
1:A:1381:TYR:HD2	1:A:1382:ASP:H	1.38	0.70
1:A:1280:PHE:CE2	1:A:1315:ILE:HG21	2.27	0.70
1:A:673:TYR:CZ	1:A:694:PRO:HB2	2.28	0.69
1:A:1165:VAL:HG21	1:A:1319:VAL:HG11	1.74	0.69
1:A:49:HIS:HE2	1:A:166:ARG:HG2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ILE:HG21	1:A:980:LEU:HD12	1.75	0.68
2:B:300:ARG:NH1	2:B:308:GLN:OE1	2.22	0.68
1:A:429:VAL:HG21	1:A:443:ILE:HD13	1.77	0.67
2:B:142:TYR:HB3	2:E:138:MET:HE1	1.76	0.67
1:A:1156:ALA:HB2	1:A:1161:GLY:H	1.60	0.66
1:A:166:ARG:HG3	1:A:186:GLY:HA3	1.77	0.66
1:A:834:GLN:OE1	1:A:1081:ARG:NH2	2.28	0.66
1:A:1148:GLU:O	1:A:1343:ARG:NH2	2.24	0.66
1:A:479:SER:HA	1:A:482:ILE:HG22	1.79	0.65
1:A:111:ALA:HB2	1:A:859:ILE:HD11	1.79	0.64
1:A:201:ASN:HD22	1:A:210:MET:CE	2.10	0.64
1:A:439:LEU:N	1:A:460:GLU:OE1	2.31	0.64
1:A:1215:ALA:HB3	1:A:1382:ASP:HB2	1.79	0.64
1:A:388:LYS:HD2	1:A:559:VAL:HG13	1.80	0.64
2:B:277:LEU:O	2:B:280:ILE:HG22	1.98	0.64
2:B:319:LYS:HZ2	2:B:322:ARG:H	1.46	0.64
1:A:260:GLU:OE2	1:A:853:HIS:ND1	2.28	0.63
1:A:1208:LYS:HD3	1:A:1209:PRO:HD2	1.80	0.63
1:A:1164:PHE:HE1	1:A:1166:SER:HB2	1.64	0.63
1:A:415:ILE:HD13	1:A:585:LEU:HD11	1.81	0.63
1:A:852:ARG:NH1	1:A:1332:ARG:O	2.32	0.62
1:A:599:ARG:NH1	1:A:809:GLY:O	2.33	0.62
1:A:405:PHE:HA	2:B:144:LEU:HD13	1.82	0.61
1:A:318:ARG:HH11	2:B:216:LYS:N	1.99	0.61
1:A:1181:SER:O	1:A:1336:ALA:N	2.33	0.60
1:A:983:PHE:HE1	1:A:1073:ARG:HD2	1.66	0.60
1:A:973:ASN:HB3	1:A:1117:SER:HB2	1.83	0.60
1:A:1033:ASP:OD1	1:A:1037:ARG:NH1	2.34	0.60
1:A:740:MET:HG2	1:A:802:GLY:HA2	1.84	0.60
1:A:824:PRO:HG3	1:A:867:PHE:CE2	2.36	0.59
1:A:876:HIS:HD2	1:A:878:GLY:H	1.51	0.59
1:A:970:SER:O	1:A:1114:ARG:NH2	2.29	0.59
1:A:1294:VAL:HG21	1:A:1320:ILE:HG23	1.84	0.59
1:A:450:PRO:HB2	1:A:452:PRO:HD2	1.85	0.59
1:A:1144:LEU:HD11	1:A:1150:CYS:HB3	1.84	0.59
1:A:1167:VAL:HG21	1:A:1323:ALA:HB1	1.85	0.58
1:A:1247:ARG:NH1	1:A:1380:ILE:HG23	2.19	0.58
1:A:550:PHE:HB2	1:A:676:VAL:HG22	1.86	0.58
1:A:1015:MET:HB2	1:A:1369:LEU:HD11	1.86	0.58
2:B:145:LEU:HD11	2:B:175:LEU:HD21	1.86	0.57
1:A:605:LEU:HB3	1:A:624:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LEU:HD22	1:A:865:THR:HG23	1.86	0.57
1:A:179:LEU:HD12	1:A:194:PRO:HG2	1.84	0.57
1:A:1100:LEU:HD23	1:A:1112:ILE:HD11	1.87	0.56
1:A:1141:VAL:HG21	1:A:1326:LEU:HD13	1.87	0.56
1:A:1143:TRP:CZ2	1:A:1330:LYS:HD2	2.40	0.56
1:A:207:HIS:NE2	1:A:344:GLN:OE1	2.36	0.56
1:A:829:ILE:HG21	1:A:980:LEU:HB2	1.87	0.56
1:A:1246:ALA:HB2	1:A:1371:LEU:HB3	1.85	0.56
2:B:292:PRO:HB3	2:B:326:CYS:HA	1.86	0.56
1:A:91:PRO:HD2	1:A:175:VAL:HG22	1.87	0.56
1:A:1105:CYS:SG	1:A:1107:VAL:HG12	2.45	0.56
1:A:1381:TYR:CD2	1:A:1382:ASP:N	2.69	0.56
1:A:949:PHE:CZ	1:A:953:ILE:HD11	2.41	0.56
1:A:543:PRO:HG3	2:C:172:GLY:HA3	1.88	0.56
1:A:1229:VAL:HG12	1:A:1361:LEU:HB2	1.87	0.55
1:A:72:PRO:HB3	1:A:212:TRP:CZ2	2.41	0.55
1:A:851:THR:HG23	1:A:853:HIS:H	1.71	0.55
2:B:175:LEU:HD23	2:C:147:MET:HB3	1.89	0.55
1:A:324:HIS:CE1	1:A:356:ILE:HD13	2.42	0.54
1:A:58:THR:HG22	1:A:183:LEU:HD11	1.90	0.54
1:A:1375:ARG:HA	1:A:1381:TYR:CE1	2.42	0.54
1:A:399:LEU:HD13	1:A:404:ILE:HD11	1.90	0.54
1:A:1000:LEU:HD23	1:A:1379:LEU:HG	1.90	0.54
1:A:1313:ASN:HD21	1:A:1354:ARG:H	1.54	0.54
1:A:965:PHE:CZ	1:A:1028:SER:HB3	2.43	0.53
1:A:814:GLN:OE1	1:A:814:GLN:N	2.42	0.53
2:B:295:ILE:HB	2:B:328:PHE:HD1	1.74	0.53
1:A:187:ASP:OD1	1:A:187:ASP:N	2.40	0.53
1:A:962:ALA:HA	1:A:1121:ILE:HD13	1.89	0.53
2:E:138:MET:HA	2:E:141:LYS:HG3	1.91	0.53
1:A:643:GLU:OE1	1:A:643:GLU:N	2.38	0.53
1:A:126:ASP:OD1	1:A:1330:LYS:NZ	2.42	0.53
1:A:550:PHE:HB3	1:A:562:THR:HB	1.90	0.53
1:A:13:LEU:HD22	1:A:239:MET:HB3	1.91	0.52
1:A:645:THR:HG22	1:A:649:ILE:HG13	1.91	0.52
1:A:495:ASP:OD1	1:A:691:ARG:NH1	2.42	0.52
1:A:26:THR:HG22	1:A:231:VAL:HG21	1.91	0.52
1:A:831:ASP:OD2	1:A:872:LEU:CD2	2.58	0.52
1:A:1097:ALA:O	1:A:1101:THR:HG23	2.10	0.52
1:A:415:ILE:CD1	1:A:585:LEU:HD11	2.39	0.52
1:A:201:ASN:HD22	1:A:210:MET:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:VAL:O	1:A:991:THR:HG22	2.09	0.51
2:B:131:LEU:HD11	2:C:131:LEU:HD23	1.92	0.51
2:B:306:ALA:O	2:B:309:LYS:NZ	2.26	0.51
1:A:77:VAL:N	1:A:78:PRO:HD2	2.26	0.51
1:A:426:TRP:CD2	1:A:443:ILE:HG12	2.46	0.51
1:A:29:CYS:HB3	1:A:63:LEU:HD21	1.93	0.51
1:A:950:LEU:HB2	1:A:951:PRO:HD3	1.92	0.51
2:B:319:LYS:HD3	2:B:322:ARG:CB	2.33	0.51
1:A:396:LEU:C	1:A:396:LEU:HD23	2.30	0.51
1:A:927:ASP:HB3	1:A:930:THR:OG1	2.11	0.51
1:A:1267:ILE:O	1:A:1271:TYR:HB2	2.10	0.51
1:A:558:ASN:ND2	1:A:561:ARG:HB2	2.22	0.50
1:A:833:LEU:HD21	1:A:869:VAL:HG22	1.93	0.50
2:B:173:PRO:HA	2:C:148:THR:O	2.11	0.50
1:A:81:LEU:HG	1:A:244:ILE:HD11	1.93	0.50
1:A:1249:ASN:O	1:A:1250:LEU:HD22	2.11	0.50
1:A:903:LEU:O	1:A:913:SER:HB2	2.12	0.50
1:A:916:ASN:HB3	1:A:919:LYS:HG2	1.91	0.50
1:A:1030:PHE:CD1	1:A:1229:VAL:HG21	2.46	0.50
1:A:1205:PRO:HG3	1:A:1208:LYS:HE2	1.92	0.50
1:A:200:LEU:O	1:A:344:GLN:NE2	2.44	0.50
1:A:1250:LEU:CD2	1:A:1385:PRO:HG2	2.42	0.50
2:B:219:ILE:HD13	2:B:260:HIS:ND1	2.27	0.50
1:A:282:TYR:CZ	1:A:286:ILE:HD11	2.47	0.49
1:A:972:LEU:HD13	1:A:1113:LEU:CD2	2.42	0.49
1:A:442:TYR:OH	1:A:453:MET:SD	2.69	0.49
1:A:103:ILE:HD13	1:A:867:PHE:HB2	1.95	0.49
1:A:788:LYS:HB2	1:A:791:GLU:HG2	1.93	0.49
1:A:1112:ILE:HG13	1:A:1113:LEU:N	2.28	0.49
1:A:673:TYR:CE1	1:A:694:PRO:HB2	2.47	0.49
1:A:684:HIS:CE1	1:A:698:PRO:HG2	2.48	0.49
1:A:1164:PHE:CE1	1:A:1166:SER:HB2	2.47	0.49
1:A:1248:VAL:HB	1:A:1250:LEU:HD23	1.94	0.49
1:A:448:PHE:CG	1:A:449:PRO:HD2	2.48	0.49
1:A:757:ASP:HB3	1:A:760:GLU:HB3	1.93	0.49
1:A:1035:PHE:O	1:A:1038:THR:HG22	2.13	0.49
1:A:1247:ARG:HH11	1:A:1380:ILE:CG2	2.24	0.49
1:A:545:TYR:CE1	1:A:569:PRO:HG2	2.48	0.48
2:B:330:LEU:N	2:B:334:LYS:O	2.36	0.48
1:A:824:PRO:HG3	1:A:867:PHE:CD2	2.48	0.48
1:A:556:GLU:OE2	1:A:561:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:PRO:HD3	1:A:1260:PRO:HB3	1.96	0.48
1:A:1311:ASP:OD1	1:A:1311:ASP:N	2.46	0.48
1:A:95:ARG:NE	1:A:154:ASP:OD2	2.44	0.48
1:A:723:GLN:OE1	1:A:780:THR:HG22	2.13	0.48
1:A:991:THR:OG1	1:A:1061:ILE:O	2.27	0.48
1:A:360:MET:HE1	1:A:368:LEU:HD22	1.94	0.48
1:A:73:ILE:HD12	1:A:76:ILE:HB	1.95	0.48
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.69	0.48
1:A:852:ARG:HB3	1:A:1285:MET:HE1	1.94	0.48
1:A:1173:ILE:HG23	1:A:1186:THR:HB	1.96	0.48
2:B:287:PHE:CB	2:B:320:ILE:HD11	2.40	0.48
2:B:168:GLN:HB3	2:B:169:PRO:HD2	1.96	0.48
2:B:259:ILE:HG23	2:B:280:ILE:CD1	2.39	0.48
1:A:1120:HIS:CD2	1:A:1121:ILE:HG13	2.49	0.48
1:A:440:ASN:OD1	1:A:441:SER:N	2.47	0.47
2:E:124:MET:N	2:E:124:MET:SD	2.87	0.47
1:A:190:PHE:CD2	1:A:231:VAL:HG22	2.49	0.47
1:A:1229:VAL:HG13	1:A:1361:LEU:HD13	1.96	0.47
1:A:346:GLN:OE1	1:A:353:ARG:NH1	2.46	0.47
1:A:135:LYS:HD2	1:A:259:ILE:HD12	1.97	0.47
1:A:781:SER:HB3	2:B:206:THR:HG21	1.96	0.47
1:A:25:VAL:HG21	1:A:188:TYR:CG	2.50	0.47
1:A:66:VAL:HG13	1:A:228:ILE:HA	1.96	0.47
1:A:666:HIS:O	2:C:154:ALA:HB1	2.15	0.47
1:A:918:GLU:HG3	1:A:1136:ILE:HD11	1.97	0.47
1:A:1381:TYR:HD2	1:A:1382:ASP:N	2.10	0.47
1:A:73:ILE:HG13	1:A:77:VAL:HG23	1.97	0.47
1:A:1249:ASN:C	1:A:1250:LEU:HD22	2.35	0.47
1:A:9:PRO:HB3	1:A:163:ARG:HD3	1.97	0.47
1:A:372:GLN:HG2	1:A:557:LEU:HD12	1.96	0.47
1:A:479:SER:O	1:A:483:LYS:N	2.48	0.47
1:A:956:ASN:OD1	1:A:1093:ASP:HB2	2.15	0.47
1:A:12:ARG:NH1	1:A:821:ARG:O	2.48	0.46
1:A:1004:LEU:HB2	1:A:1377:ASN:HD21	1.80	0.46
2:B:146:VAL:HG11	2:E:141:LYS:HB3	1.96	0.46
1:A:582:ALA:HB2	1:A:714:LYS:HE2	1.96	0.46
1:A:52:ARG:NE	1:A:185:TYR:OH	2.48	0.46
2:B:183:GLY:C	2:B:185:ILE:H	2.18	0.46
1:A:84:LEU:HD21	1:A:182:ILE:HD11	1.98	0.46
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.77	0.46
1:A:942:MET:HE2	1:A:943:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HG22	1:A:229:VAL:HG23	1.97	0.46
1:A:475:ILE:HG13	1:A:475:ILE:O	2.14	0.46
1:A:643:GLU:HB3	2:C:147:MET:HE3	1.97	0.46
1:A:160:ARG:HH12	1:A:825:LEU:HD13	1.81	0.46
2:B:297:ILE:HG13	2:B:330:LEU:HG	1.98	0.46
1:A:354:THR:O	1:A:358:LEU:HD22	2.15	0.46
1:A:1271:TYR:HA	1:A:1275:TYR:HB2	1.98	0.46
1:A:436:THR:HB	1:A:439:LEU:HB2	1.97	0.46
1:A:829:ILE:HG12	1:A:984:LEU:HD21	1.98	0.46
1:A:1167:VAL:HG22	1:A:1294:VAL:HG12	1.97	0.46
1:A:287:LEU:HD11	1:A:348:ILE:HD11	1.98	0.46
1:A:574:GLN:O	1:A:578:GLU:HG2	2.16	0.46
1:A:41:LEU:HD12	1:A:41:LEU:N	2.31	0.45
1:A:386:ILE:HG13	1:A:699:SER:O	2.16	0.45
1:A:488:ALA:HB1	1:A:547:ASN:OD1	2.16	0.45
1:A:553:LYS:NZ	1:A:563:PHE:HB3	2.31	0.45
1:A:76:ILE:HG23	1:A:193:ILE:HD13	1.98	0.45
1:A:879:PHE:HE1	1:A:1078:THR:HG21	1.81	0.45
1:A:1095:ILE:HD12	1:A:1095:ILE:H	1.82	0.45
1:A:1149:GLN:N	1:A:1149:GLN:OE1	2.49	0.45
1:A:703:GLY:HA3	2:C:176:TYR:CZ	2.52	0.45
1:A:557:LEU:HD23	1:A:557:LEU:HA	1.54	0.45
1:A:983:PHE:CE1	1:A:1073:ARG:HD2	2.50	0.45
1:A:396:LEU:CD1	2:B:169:PRO:HG3	2.46	0.45
1:A:912:LEU:HA	1:A:912:LEU:HD23	1.70	0.45
1:A:1027:MET:HG2	1:A:1030:PHE:H	1.81	0.45
1:A:831:ASP:HB3	1:A:876:HIS:CE1	2.52	0.45
1:A:13:LEU:O	1:A:555:LYS:NZ	2.40	0.45
1:A:497:VAL:O	1:A:679:TYR:HD1	2.00	0.45
1:A:1238:LEU:O	1:A:1241:LYS:HG2	2.17	0.45
1:A:1386:LEU:HD23	1:A:1390:LEU:HD11	1.99	0.45
1:A:451:LEU:N	1:A:452:PRO:HD2	2.31	0.45
1:A:372:GLN:HG2	1:A:557:LEU:CD1	2.48	0.44
1:A:1059:SER:HB3	1:A:1062:ILE:HB	1.99	0.44
2:B:263:PHE:HB2	2:B:280:ILE:HD12	1.98	0.44
1:A:201:ASN:HB2	1:A:339:ALA:O	2.17	0.44
1:A:950:LEU:HA	1:A:950:LEU:HD13	1.66	0.44
1:A:1238:LEU:O	1:A:1241:LYS:NZ	2.43	0.44
1:A:83:ALA:HB2	1:A:197:MET:HE1	1.99	0.44
1:A:1158:GLN:HB2	1:A:1159:PRO:HD3	1.98	0.44
1:A:534:TYR:CZ	1:A:569:PRO:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:TYR:HE2	2:C:148:THR:HG23	1.81	0.44
1:A:661:VAL:C	1:A:663:ASN:H	2.19	0.44
1:A:831:ASP:HB3	1:A:876:HIS:NE2	2.33	0.44
1:A:153:TYR:OH	1:A:824:PRO:HD2	2.17	0.44
2:B:142:TYR:O	2:B:146:VAL:HG23	2.18	0.44
2:B:209:LEU:HD13	2:B:214:PHE:HE1	1.83	0.44
1:A:21:GLN:HB3	1:A:680:TYR:CD2	2.53	0.44
1:A:171:SER:O	1:A:173:TRP:HD1	2.01	0.44
1:A:191:TRP:O	1:A:229:VAL:HA	2.18	0.44
1:A:814:GLN:HG2	1:A:814:GLN:O	2.18	0.44
1:A:1022:SER:HA	1:A:1125:ARG:NH1	2.33	0.44
1:A:484:ASP:OD1	1:A:515:ARG:NH2	2.50	0.43
2:B:319:LYS:HG2	2:B:320:ILE:N	2.33	0.43
1:A:73:ILE:HG13	1:A:73:ILE:O	2.18	0.43
1:A:1035:PHE:HA	1:A:1038:THR:HG22	1.99	0.43
1:A:1165:VAL:HG21	1:A:1319:VAL:CG1	2.47	0.43
1:A:1144:LEU:HD23	1:A:1144:LEU:HA	1.76	0.43
1:A:25:VAL:HG21	1:A:188:TYR:CD2	2.54	0.43
1:A:11:ALA:O	1:A:241:LYS:NZ	2.43	0.43
1:A:724:ILE:HD12	1:A:746:ILE:HG12	2.00	0.43
2:B:203:LEU:O	2:B:206:THR:HG22	2.18	0.43
1:A:526:PHE:HB3	1:A:998:ASN:HD21	1.84	0.43
1:A:649:ILE:HG21	1:A:663:ASN:HA	2.01	0.43
1:A:895:ASP:OD1	1:A:895:ASP:N	2.49	0.43
1:A:1252:VAL:O	1:A:1256:LEU:HG	2.19	0.43
1:A:62:PHE:HE1	1:A:181:ASP:HB3	1.83	0.43
1:A:631:THR:HB	1:A:787:LEU:HD11	2.00	0.43
1:A:890:LEU:O	1:A:892:LYS:N	2.44	0.43
1:A:1024:THR:HB	1:A:1025:PRO:HD3	2.00	0.43
2:E:127:THR:OG1	2:E:128:ILE:N	2.52	0.43
1:A:156:ALA:HA	1:A:159:THR:HG22	2.00	0.43
1:A:478:LEU:HD11	1:A:1379:LEU:HB3	2.00	0.43
1:A:515:ARG:HB3	1:A:517:PRO:HD2	2.00	0.43
1:A:947:ASP:OD1	1:A:947:ASP:N	2.52	0.43
1:A:949:PHE:CE2	1:A:953:ILE:HD11	2.54	0.43
1:A:1217:ARG:O	1:A:1221:GLU:HG3	2.19	0.43
1:A:1229:VAL:HG22	1:A:1267:ILE:HD11	2.00	0.43
1:A:134:GLU:N	1:A:134:GLU:OE1	2.51	0.42
1:A:789:PRO:HB3	2:B:214:PHE:CE1	2.54	0.42
1:A:811:GLN:H	1:A:1287:ASN:CG	2.15	0.42
1:A:66:VAL:CG1	1:A:67:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TRP:CE3	1:A:443:ILE:HG12	2.54	0.42
1:A:483:LYS:O	1:A:516:VAL:HG11	2.19	0.42
1:A:510:LYS:HE3	1:A:510:LYS:HB3	1.82	0.42
1:A:1166:SER:HB3	1:A:1295:SER:OG	2.20	0.42
1:A:1226:LEU:HD23	1:A:1226:LEU:HA	1.73	0.42
2:B:209:LEU:HD13	2:B:214:PHE:CE1	2.55	0.42
1:A:304:ALA:HB1	1:A:320:LEU:HB2	2.01	0.42
1:A:591:SER:O	1:A:738:ALA:HA	2.19	0.42
2:B:134:VAL:HG11	2:C:132:ASN:OD1	2.19	0.42
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.84	0.42
1:A:396:LEU:HD23	1:A:397:LYS:N	2.35	0.42
1:A:480:ILE:HG13	1:A:481:PHE:CD1	2.55	0.42
1:A:1348:LEU:HD22	1:A:1353:THR:HG21	2.01	0.42
1:A:472:THR:HB	1:A:532:LEU:HD11	2.01	0.42
1:A:495:ASP:OD1	1:A:495:ASP:N	2.51	0.42
1:A:931:SER:HA	1:A:1134:CYS:SG	2.60	0.42
1:A:1100:LEU:HD23	1:A:1112:ILE:CD1	2.49	0.42
2:D:137:GLU:O	2:D:141:LYS:HG2	2.18	0.42
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.86	0.42
1:A:234:ALA:O	1:A:238:ILE:HG12	2.20	0.42
1:A:552:LEU:HD23	1:A:562:THR:HG22	2.02	0.42
1:A:1141:VAL:HG21	1:A:1326:LEU:CD1	2.50	0.42
1:A:287:LEU:HD21	1:A:335:THR:HG22	2.01	0.42
1:A:728:GLU:HG3	1:A:733:PHE:O	2.20	0.42
1:A:155:LEU:HB3	1:A:237:LEU:HD11	2.02	0.42
1:A:239:MET:HE3	1:A:376:GLY:HA2	2.01	0.42
1:A:1215:ALA:CB	1:A:1382:ASP:HB2	2.49	0.42
2:B:159:THR:HA	2:B:170:PRO:HG3	2.01	0.42
2:B:294:VAL:HA	2:B:327:VAL:O	2.20	0.42
1:A:1071:LEU:HD12	1:A:1071:LEU:HA	1.85	0.41
1:A:357:ARG:NH2	2:B:232:LEU:O	2.53	0.41
1:A:634:GLU:HB2	1:A:742:ASP:HB3	2.02	0.41
1:A:909:LEU:HA	1:A:909:LEU:HD23	1.64	0.41
1:A:558:ASN:OD1	1:A:558:ASN:N	2.54	0.41
1:A:26:THR:HB	1:A:31:LEU:HB2	2.01	0.41
1:A:304:ALA:HB2	1:A:319:PHE:CD2	2.55	0.41
1:A:532:LEU:HD22	1:A:661:VAL:HG21	2.01	0.41
1:A:940:LEU:HD11	1:A:952:LEU:HD12	2.03	0.41
1:A:1024:THR:O	1:A:1126:PRO:HD2	2.21	0.41
2:B:229:TYR:OH	2:B:244:GLN:OE1	2.38	0.41
1:A:181:ASP:HB2	1:A:192:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HB3	1:A:679:TYR:CE1	2.55	0.41
2:B:229:TYR:O	2:B:232:LEU:N	2.47	0.41
2:B:281:THR:CG2	2:B:321:ASP:HB2	2.50	0.41
1:A:331:LEU:HD12	1:A:331:LEU:HA	1.80	0.41
1:A:787:LEU:HD12	1:A:787:LEU:HA	1.75	0.41
1:A:1000:LEU:HD21	1:A:1378:GLU:HG3	2.03	0.41
1:A:585:LEU:HD12	1:A:585:LEU:HA	1.68	0.41
1:A:737:SER:OG	1:A:744:GLN:NE2	2.43	0.41
1:A:859:ILE:HD13	1:A:859:ILE:HA	1.82	0.41
1:A:1268:VAL:HG23	1:A:1269:HIS:N	2.36	0.41
1:A:195:ILE:HD11	1:A:228:ILE:HB	2.02	0.41
1:A:483:LYS:HE3	1:A:483:LYS:HB3	1.84	0.41
1:A:824:PRO:O	1:A:825:LEU:HD23	2.21	0.41
1:A:852:ARG:HD3	1:A:1184:SER:HB3	2.02	0.41
1:A:1027:MET:HE3	1:A:1027:MET:HB2	1.93	0.41
1:A:159:THR:O	1:A:163:ARG:HG3	2.20	0.41
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.75	0.41
1:A:909:LEU:HD11	1:A:933:LEU:HD23	2.02	0.41
1:A:1178:PRO:HD2	1:A:1185:TRP:CD2	2.56	0.41
2:B:183:GLY:O	2:B:184:LYS:HG2	2.20	0.41
1:A:21:GLN:H	1:A:21:GLN:HG2	1.70	0.40
1:A:419:TYR:CE1	1:A:427:TYR:HB3	2.56	0.40
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.71	0.40
2:E:126:LYS:O	2:E:130:SER:N	2.36	0.40
1:A:53:LEU:HD22	1:A:59:VAL:HG21	2.03	0.40
1:A:408:TYR:HA	1:A:648:PHE:CE2	2.56	0.40
1:A:506:ASN:OD1	1:A:506:ASN:N	2.53	0.40
2:C:138:MET:SD	2:D:139:VAL:HG22	2.61	0.40
1:A:46:LEU:HA	1:A:46:LEU:HD23	1.85	0.40
1:A:1381:TYR:HD2	1:A:1382:ASP:C	2.25	0.40
1:A:51:TYR:O	1:A:54:LYS:HG2	2.22	0.40
1:A:73:ILE:O	1:A:77:VAL:HG23	2.21	0.40
1:A:100:LEU:HD11	1:A:104:ILE:HD11	2.02	0.40
1:A:284:LEU:HD23	1:A:291:GLY:HA3	2.03	0.40
1:A:314:GLU:HG2	1:A:315:ARG:N	2.37	0.40
1:A:396:LEU:HD21	2:C:148:THR:HB	2.03	0.40
1:A:793:PHE:HB2	1:A:795:HIS:CE1	2.56	0.40
1:A:936:LEU:HA	1:A:936:LEU:HD12	1.84	0.40
1:A:1044:LEU:HD13	1:A:1044:LEU:HA	1.86	0.40
2:B:304:PRO:HG2	2:B:307:CYS:HB2	2.04	0.40
2:E:131:LEU:HD23	2:E:131:LEU:HA	1.87	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	1357/1839 (74%)	1288 (95%)	69 (5%)	0	100	100
2	B	217/657 (33%)	208 (96%)	9 (4%)	0	100	100
2	C	54/657 (8%)	53 (98%)	1 (2%)	0	100	100
2	D	28/657 (4%)	27 (96%)	1 (4%)	0	100	100
2	E	22/657 (3%)	21 (96%)	1 (4%)	0	100	100
All	All	1678/4467 (38%)	1597 (95%)	81 (5%)	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	1218/1596 (76%)	1216 (100%)	2 (0%)	92	96
2	B	185/541 (34%)	185 (100%)	0	100	100
2	C	43/541 (8%)	43 (100%)	0	100	100
2	D	27/541 (5%)	27 (100%)	0	100	100
2	E	21/541 (4%)	21 (100%)	0	100	100
All	All	1494/3760 (40%)	1492 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	ARG
1	A	1270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	637	ASN
1	A	671	GLN
1	A	876	HIS

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

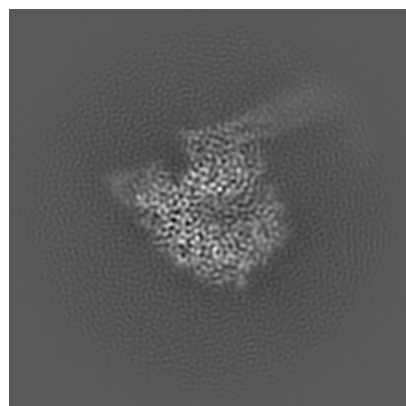
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60756. These allow visual inspection of the internal detail of the map and identification of artifacts.

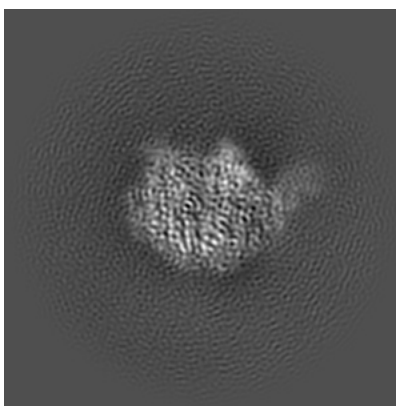
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

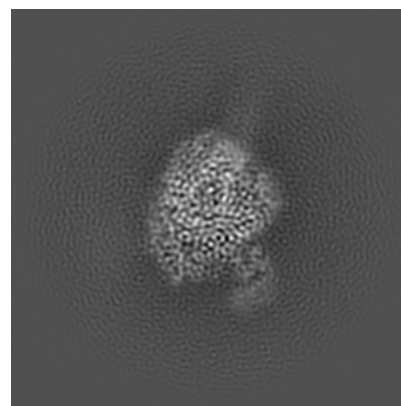
#### 6.1.1 Primary map



X

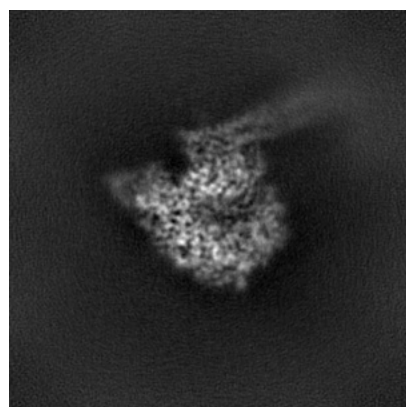


Y

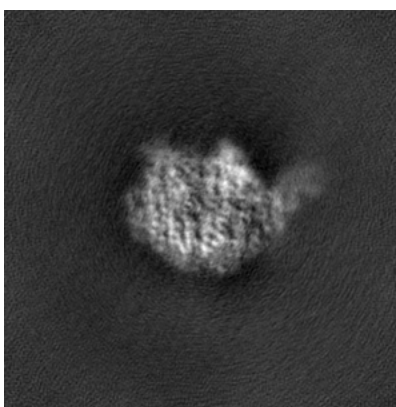


Z

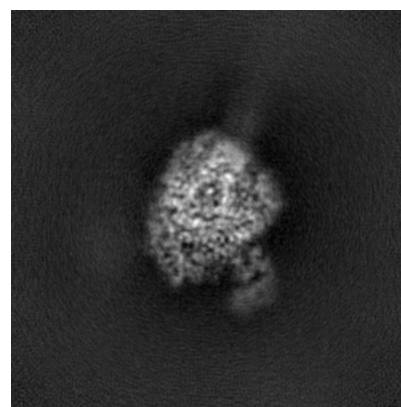
#### 6.1.2 Raw map



X



Y

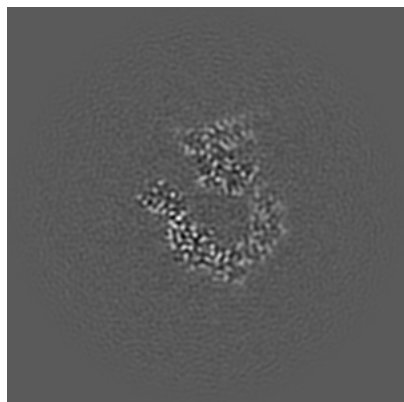


Z

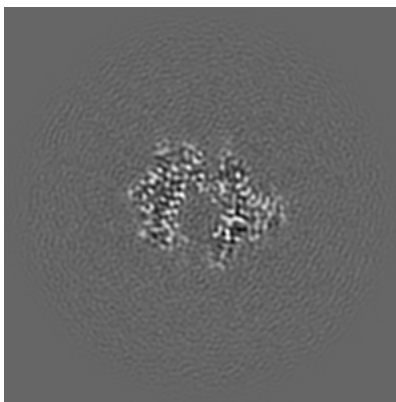
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

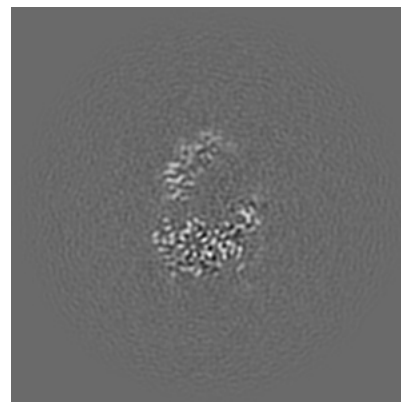
### 6.2.1 Primary map



X Index: 128

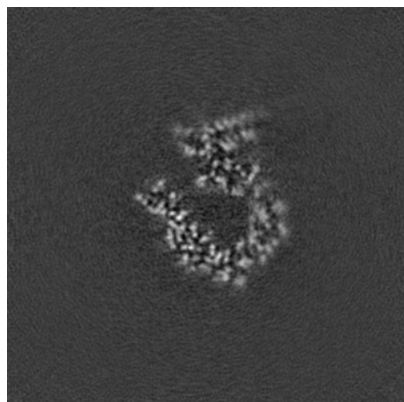


Y Index: 128

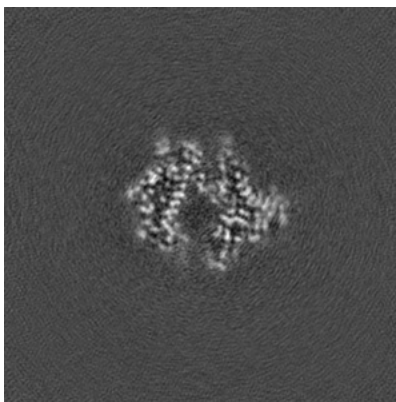


Z Index: 128

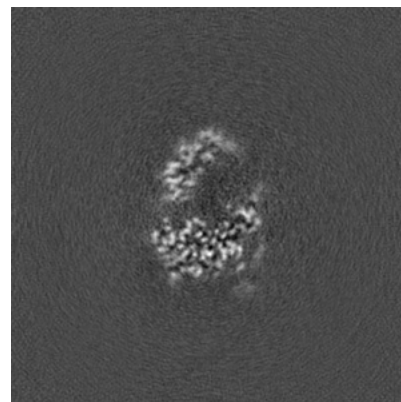
### 6.2.2 Raw map



X Index: 128



Y Index: 128

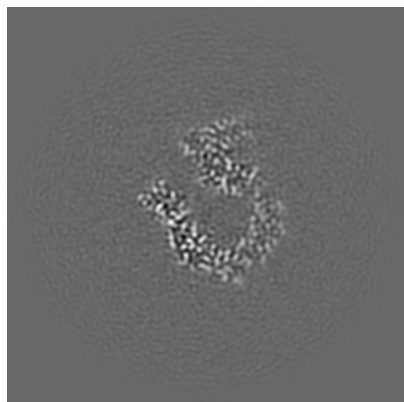


Z Index: 128

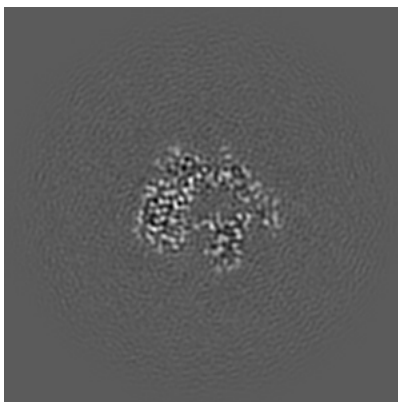
The images above show central slices of the map in three orthogonal directions.

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

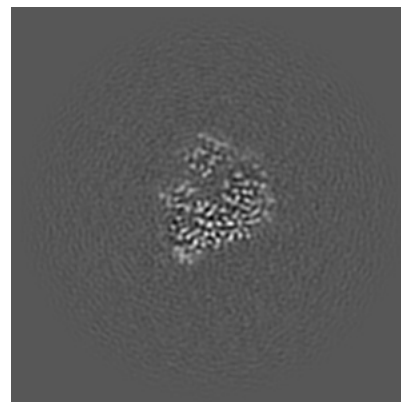
### 6.3.1 Primary map



X Index: 127

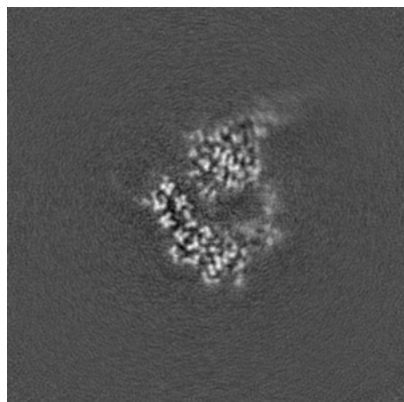


Y Index: 120

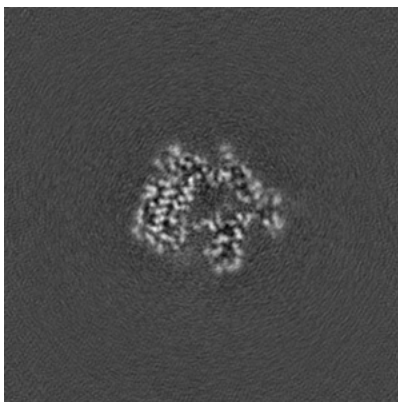


Z Index: 106

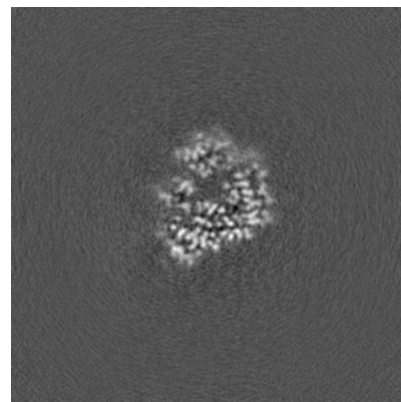
### 6.3.2 Raw map



X Index: 136



Y Index: 120



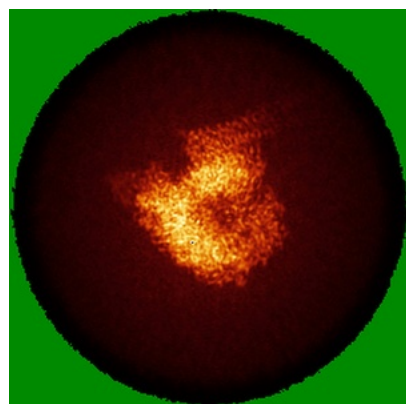
Z Index: 107

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

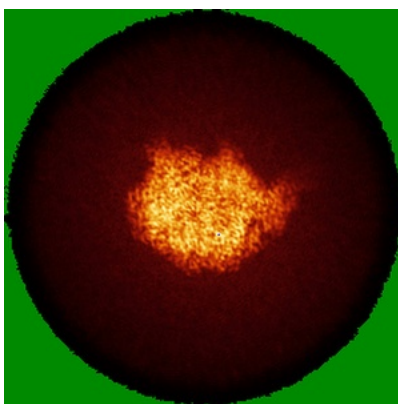


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

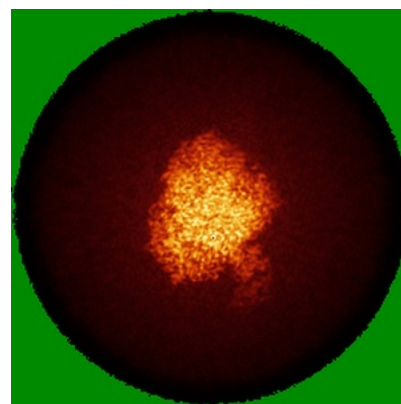
### 6.4.1 Primary map



X

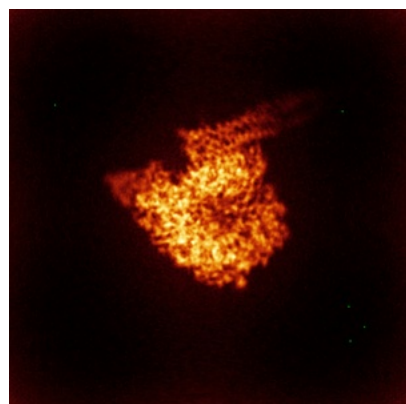


Y

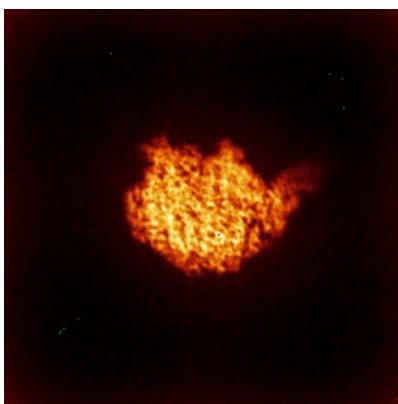


Z

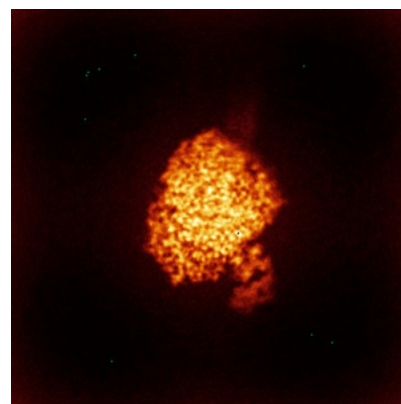
### 6.4.2 Raw map



X



Y

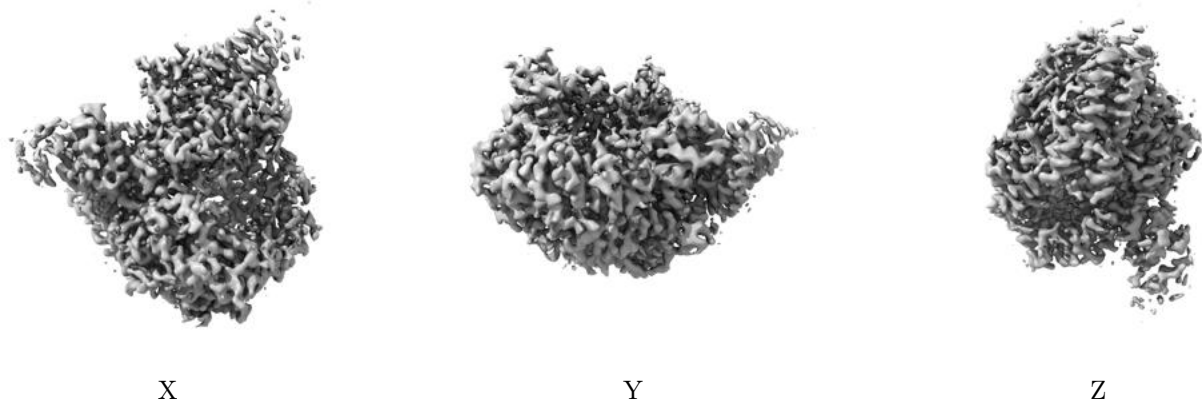


Z

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.

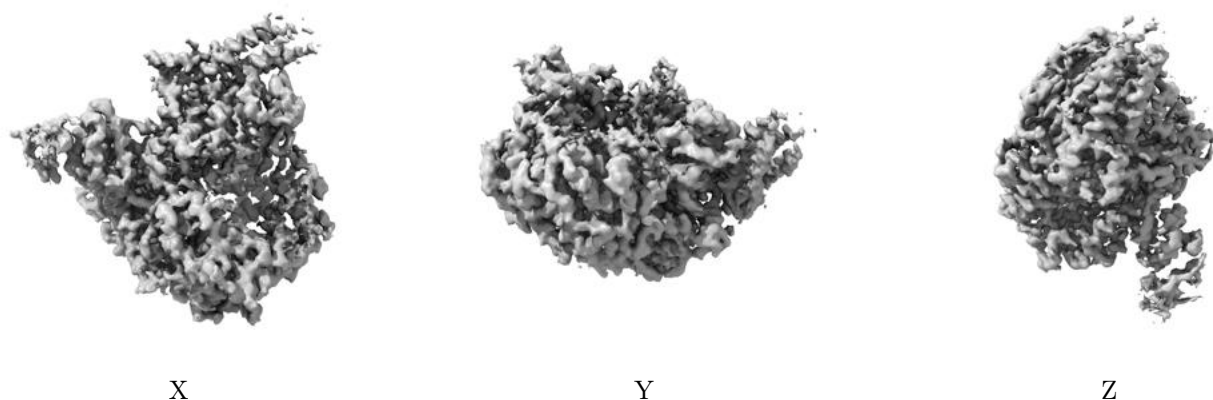
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. 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.



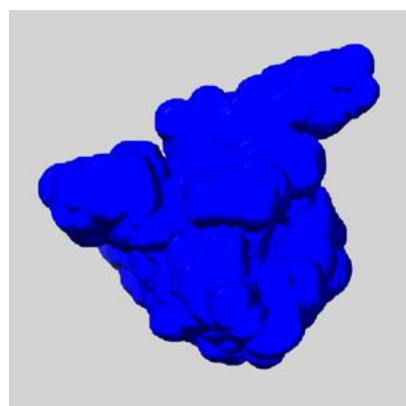
## 6.6 Mask visualisation [i](#)

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

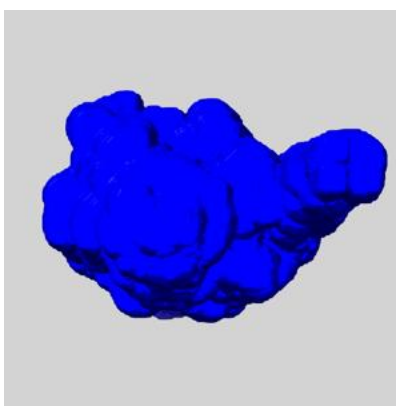
A mask typically either:

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

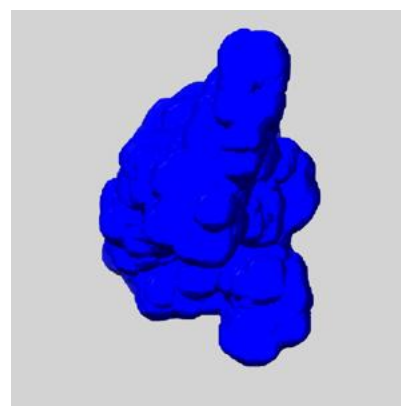
### 6.6.1 emd\_60756\_msk\_1.map [i](#)



X



Y

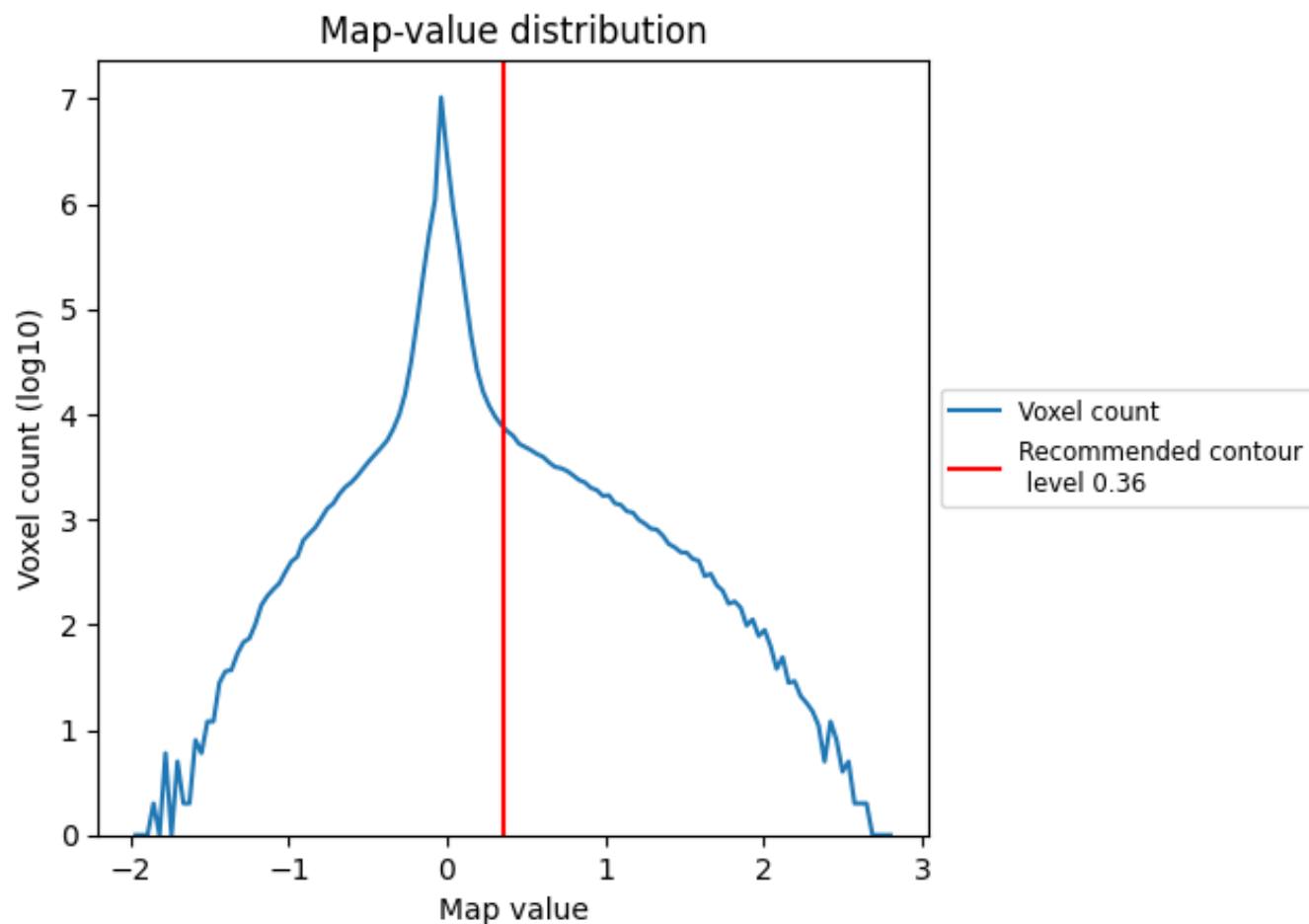


Z

## 7 Map analysis [i](#)

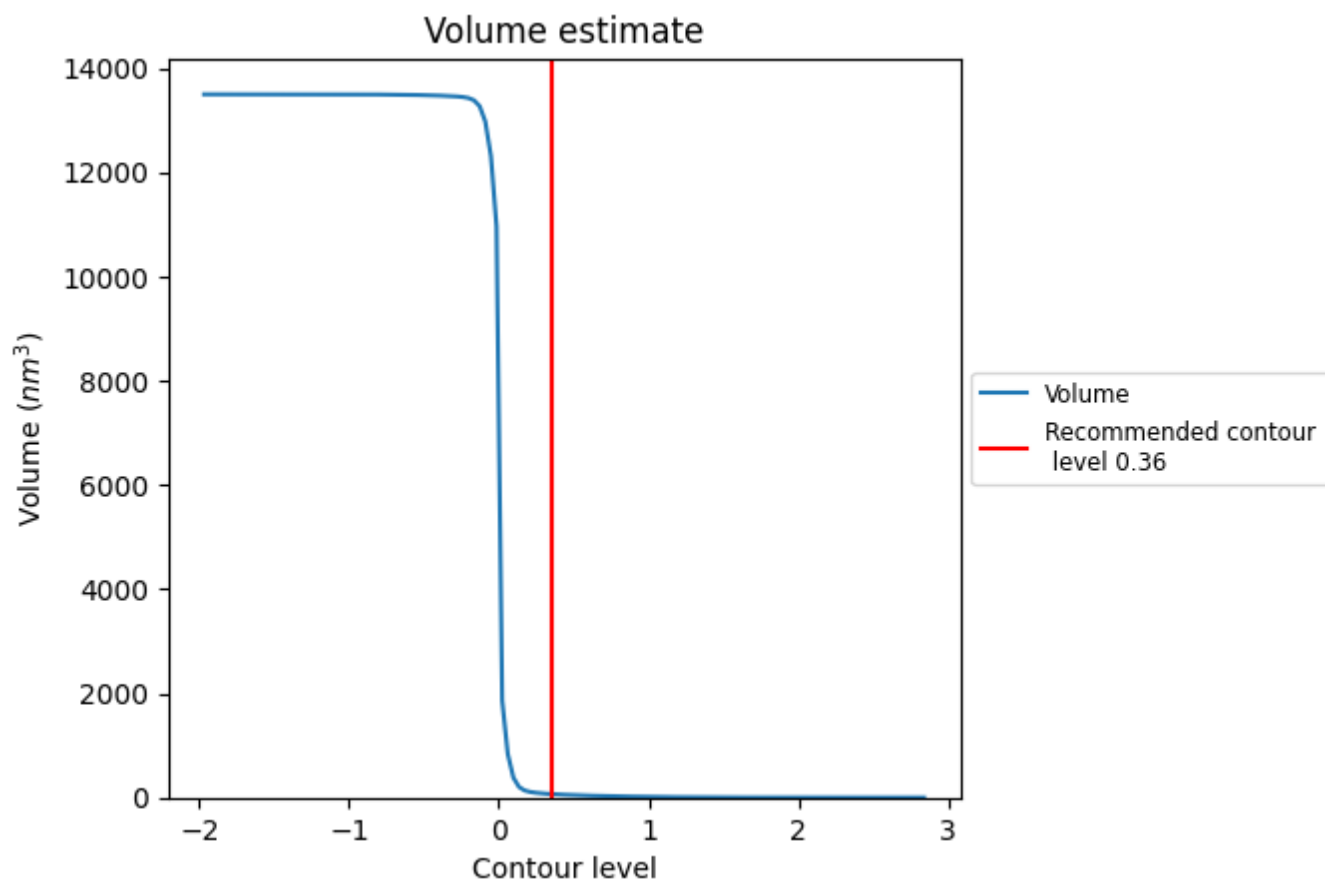
This section contains the results of statistical analysis of the map.

### 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.

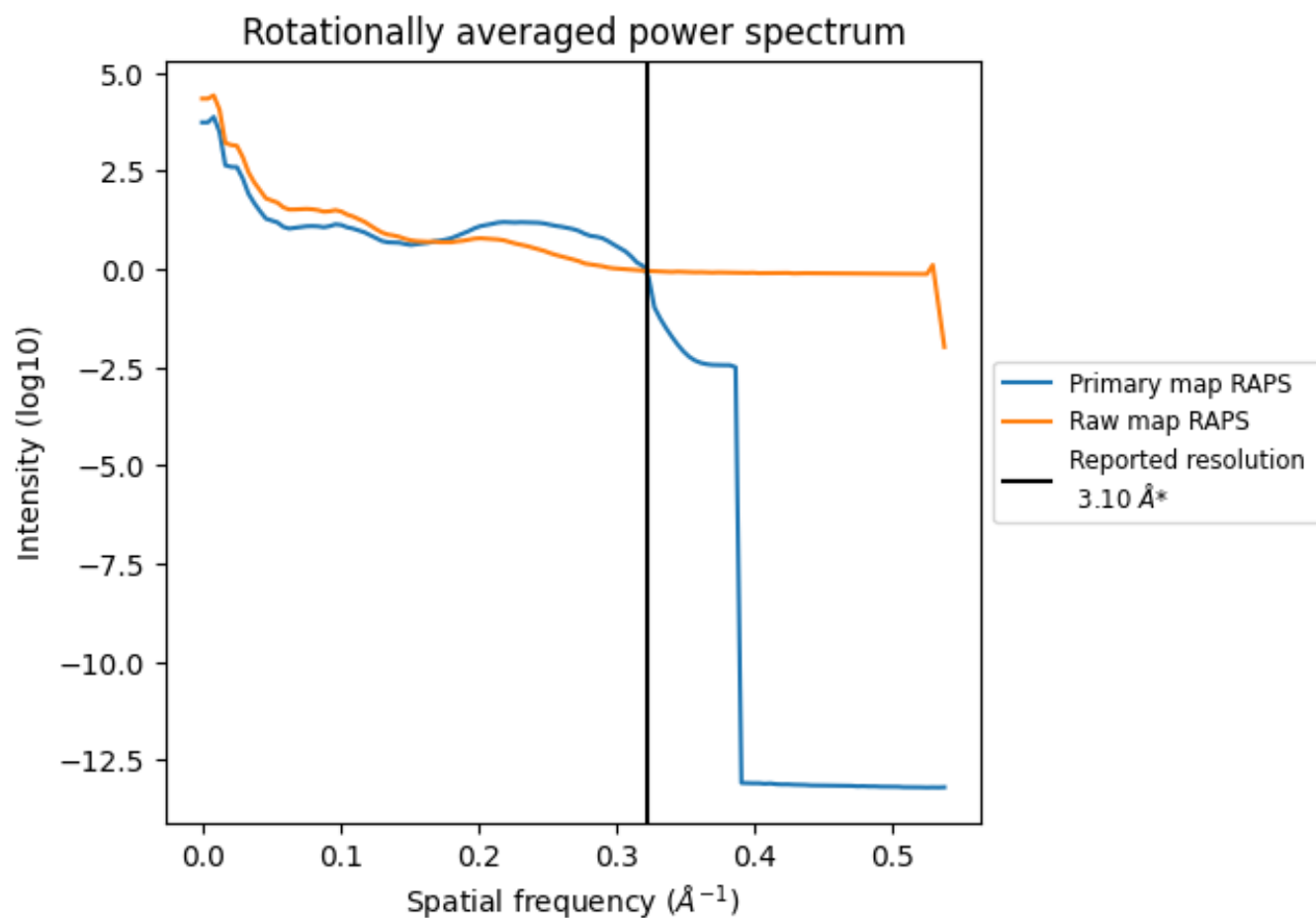
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm<sup>3</sup>; this corresponds to an approximate mass of 59 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 ⓘ

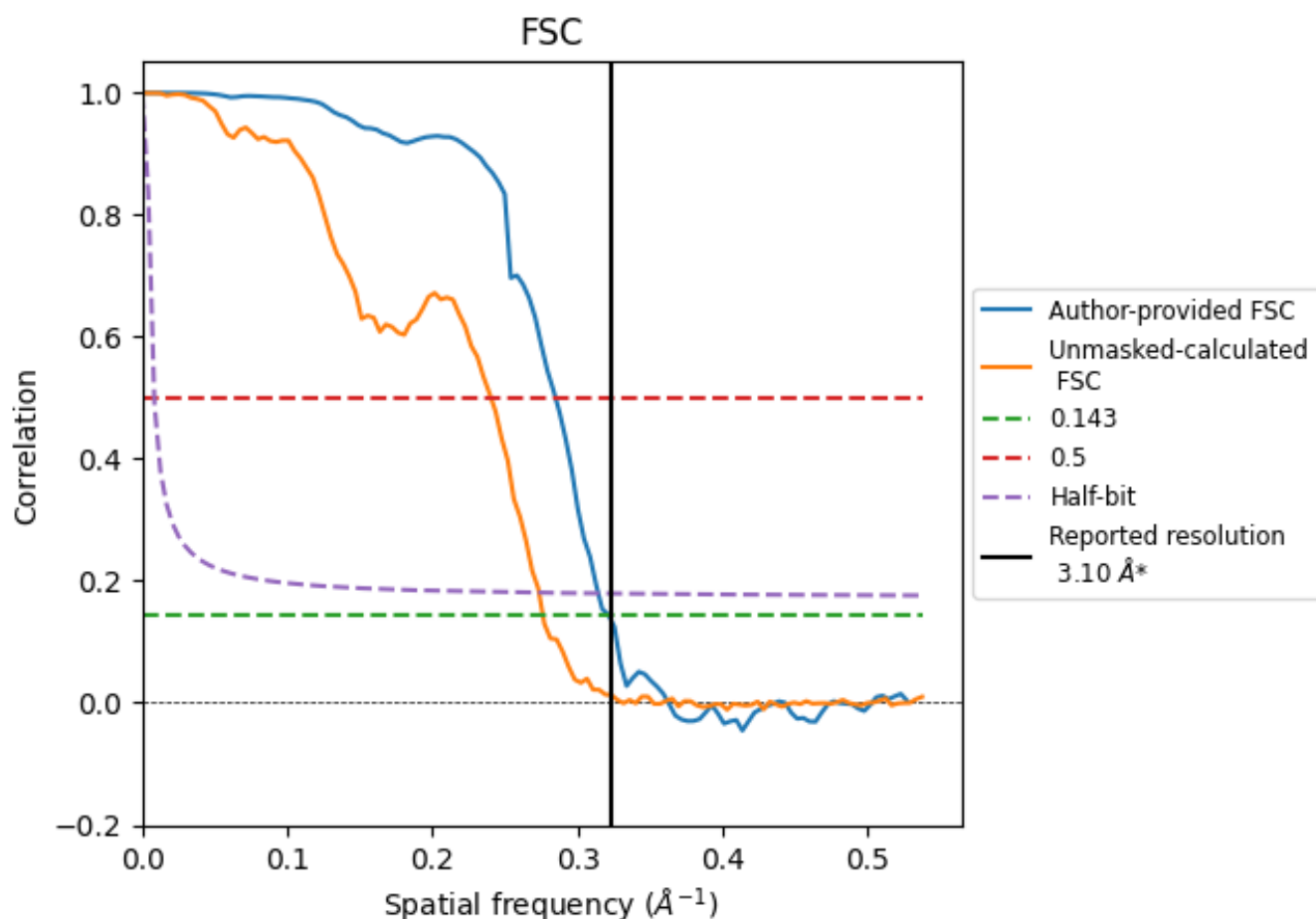


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

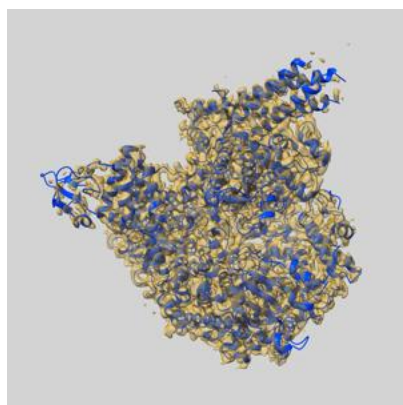
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.51	3.18
Unmasked-calculated*	3.62	4.16	3.66

\*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 3.62 differs from the reported value 3.1 by more than 10 %

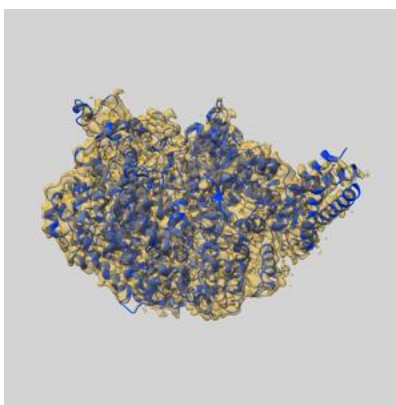
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60756 and PDB model 9IP3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

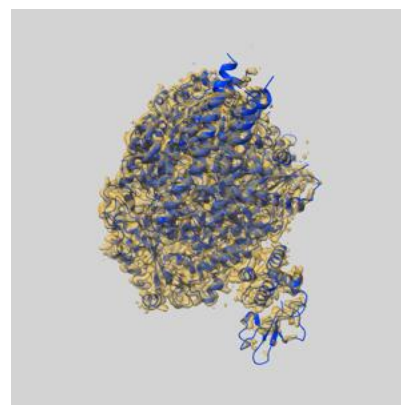
### 9.1 Map-model overlay [i](#)



X



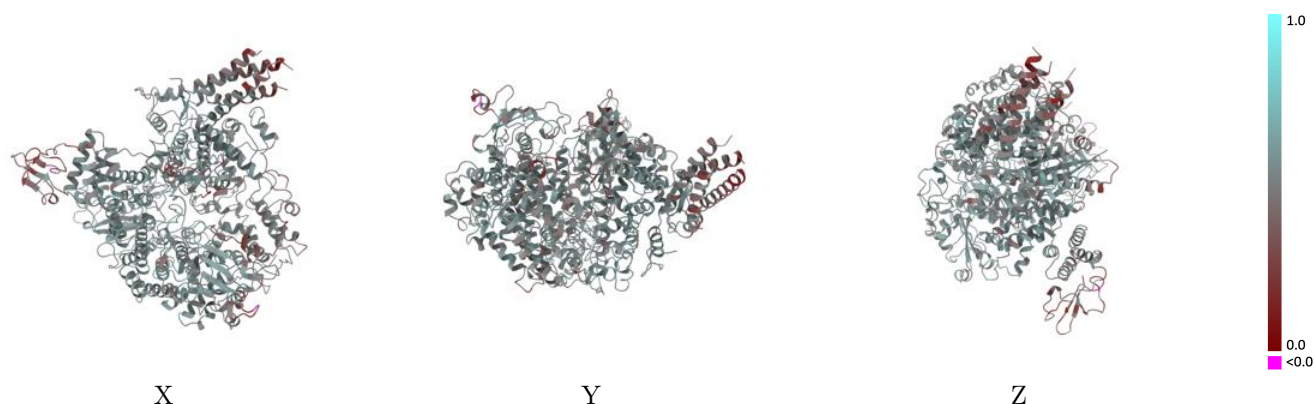
Y



Z

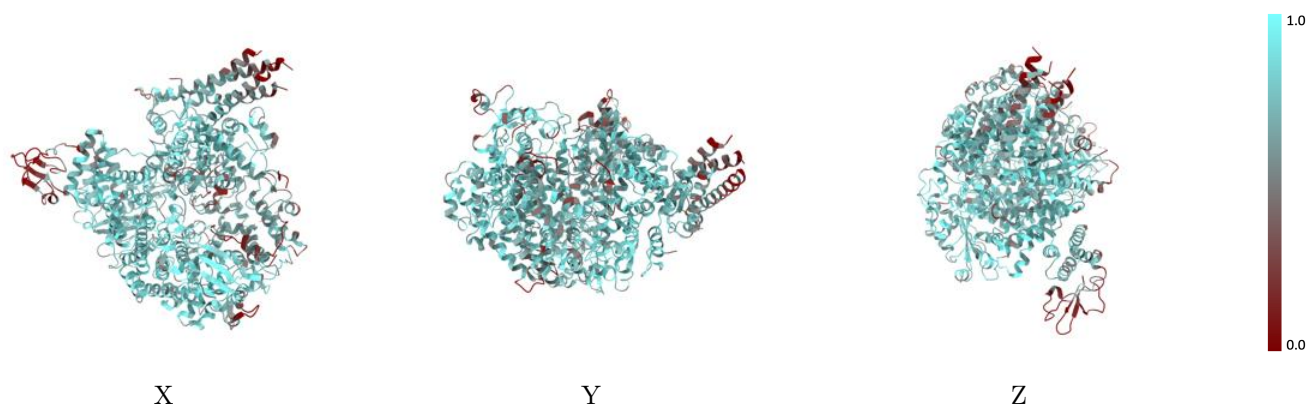
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

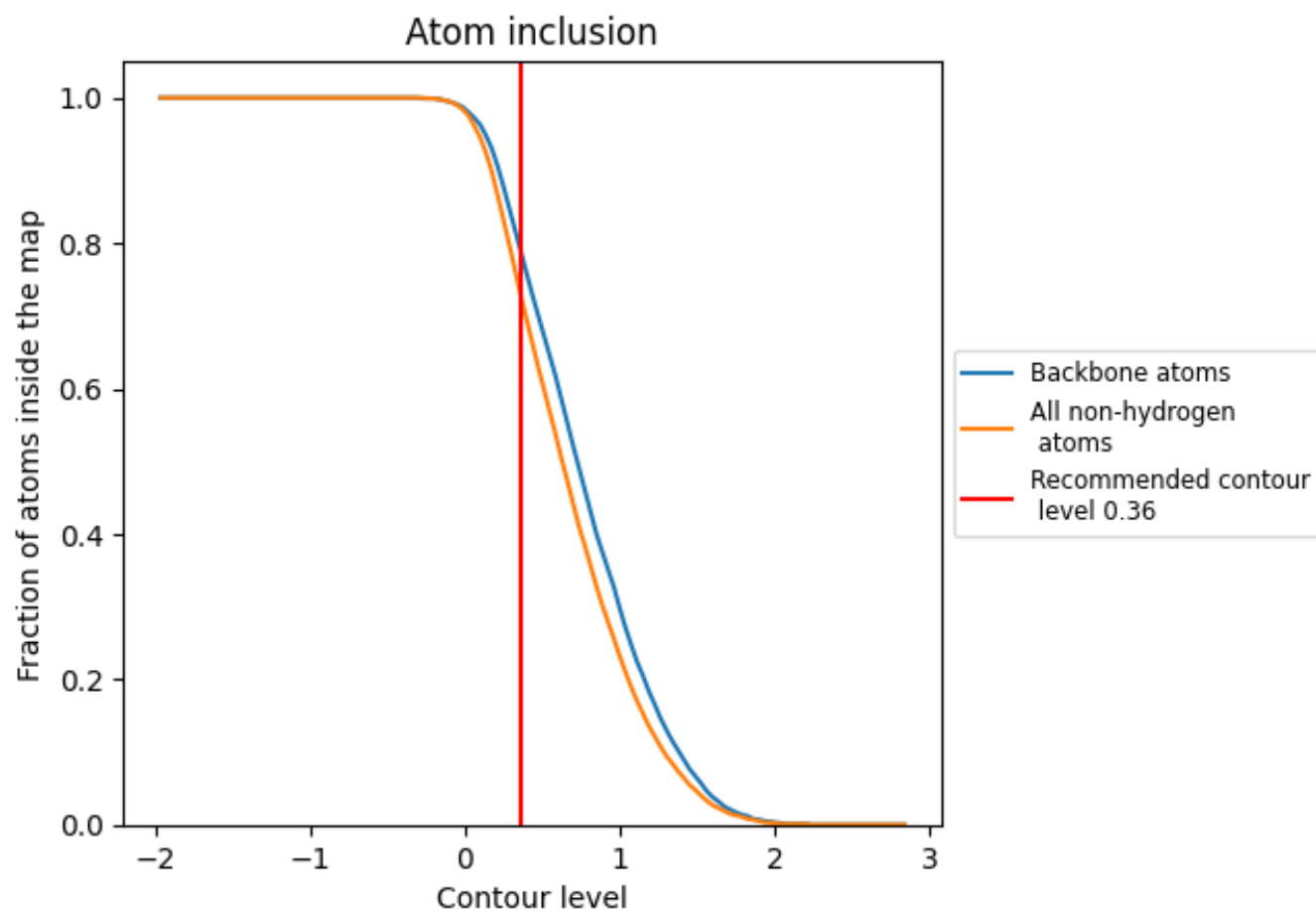
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.36).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7280	<div></div> 0.5070
A	<div></div> 0.7650	<div></div> 0.5200
B	<div></div> 0.5610	<div></div> 0.4540
C	<div></div> 0.6820	<div></div> 0.4970
D	<div></div> 0.4180	<div></div> 0.3790
E	<div></div> 0.5560	<div></div> 0.4040

