



## wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 01:48 AM UTC

PDB ID : 9K16 / pdb\_00009k16  
EMDB ID : EMD-61966  
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 5U scaffold at 3.19 Angstrom  
Authors : Xie, G.; Du, X.; Du, J.  
Deposited on : 2024-10-16  
Resolution : 3.19 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](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:

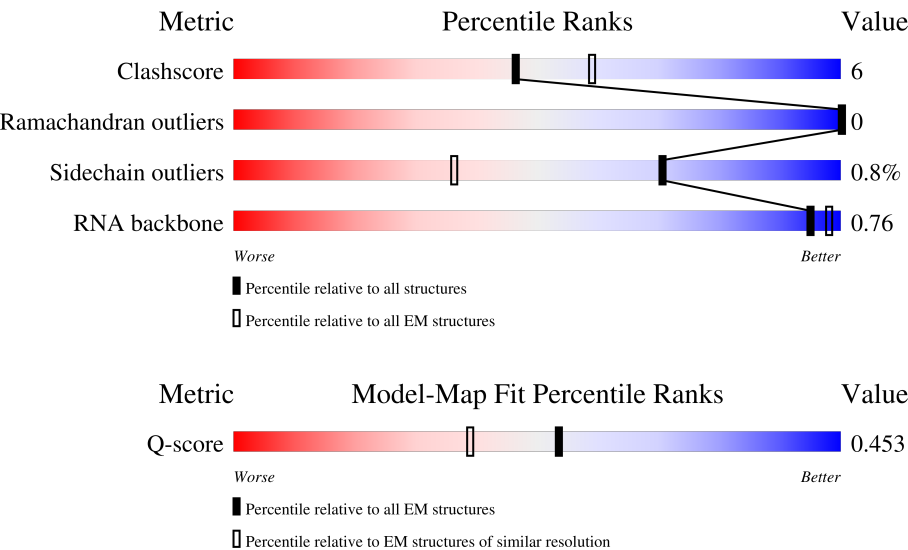
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.19 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.





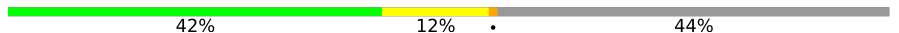







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14455 ( 2.69 - 3.69 )

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	T	34	<div><div>21% 9%21%71%</div></div>
2	N	34	<div><div>18% 32%18%50%</div></div>
3	P	20	<div><div>10% 15%85%</div></div>

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Mol	Chain	Length	Quality of chain
4	A	2032	
5	C	319	
6	F	144	
7	J	71	
8	K	116	
9	L	51	
10	H	146	
11	I	114	
12	E	230	
13	B	1169	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23179 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 DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	10	Total	C	N	O	P	0	0
			205	98	40	57	10		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	17	Total	C	N	O	P	0	0
			350	166	65	102	17		

- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*AP\*UP\*AP\*UP\*GP\*CP\*AP\*GP\*AP\*AP\*AP\*GP\*CP\*GP\*UP\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	843	Total	C	N	O	S	0	0
			6597	4170	1132	1251	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			660	420	114	122	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	45	Total	C	N	O	S	0	0
			365	224	70	67	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	97	Total	C	N	O	S	0	0
			787	482	150	143	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	967	Total	C	N	O	S	0	0
			7660	4827	1357	1432	44		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

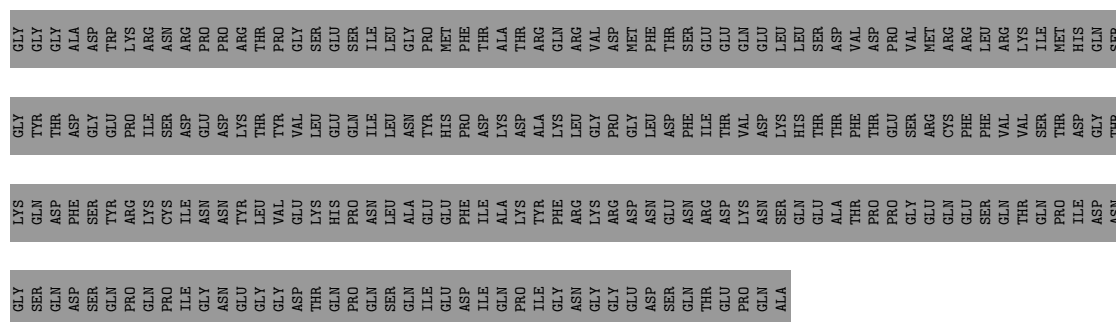
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0



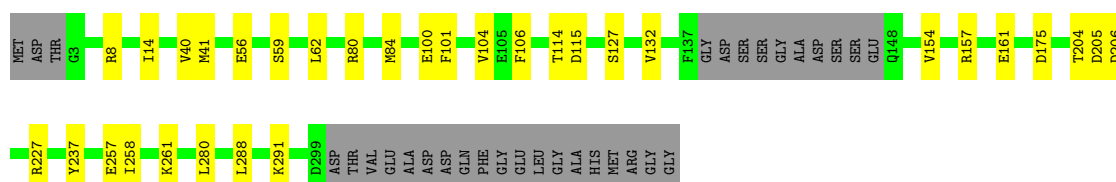


TRP	SER	GLU	TRP	TRP	GLY	SER	ALA	PRO	VAL	THR	ASP	K1082	C988	V899	Q698	H419	SER	ASP	VAL
GLY	THR	THR	TRP	GLY	GLU	SER	TRP	ASN	SER	GLU	SER	D1086	C989	V899	Q698	L446	SER	THR	LEU
TRP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1090	F991	K904	S707	D451	SER	GLY	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1099	R992	V906	D708	V455	LYS	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1102	S996	K909	K709	V465	ALA	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1114	D999	L916	L712	A465	LYS	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A1128	S1000	V917	M721	A467	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1132	D1001	M1002	M725	E468	ARG	SER	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1148	M1005	C1004	K728	D494	LYS	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1149	M1006	L1005	M518	P527	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1150	I1010	Y1023	T732	F542	LYS	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1155	Y1029	L1033	S735	V530	SER	GLU	GLU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1159	R1019	L1043	Y752	W539	HIS	HIS	HIS
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1167	Y1041	R1042	W785	F570	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	K1170	P1042	H938	E774	L545	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A1171	R1042	H940	P775	L567	MET	MET	MET
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1172	A1044	L941	L778	D575	ARG	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	I1048	K943	W789	Y382	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	I1049	E947	T800	Y385	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	S1052	G948	R592	R385	TVR	TVR	TVR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	P1053	W949	E596	R385	LEU	LEU	LEU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E1054	M953	E596	ASP	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	T1057	Y956	Q807	GLY	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	W1058	C960	F808	LYS	LYS	LYS	LYS
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	I1059	N965	R809	P644	PRO	PRO	PRO
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	R1060	N965	Y810	V646	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	L1062	S966	Q807	L649	ARG	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	H1063	L967	M836	R650	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	A1064	V968	L863	Q398	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	R1067	Q969	Y880	R402	ARG	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V1071	K972	P654	M405	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	L1072	K973	D655	N412	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	D1073	K974	E656	N413	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V1076	A975	L659	N413	LYS	LYS	LYS
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E1077	ASP	E660	ARG	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V1081	K980	A896	P415	SER	SER	SER
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	VAL	M981		K687	ASP	ASP	ASP



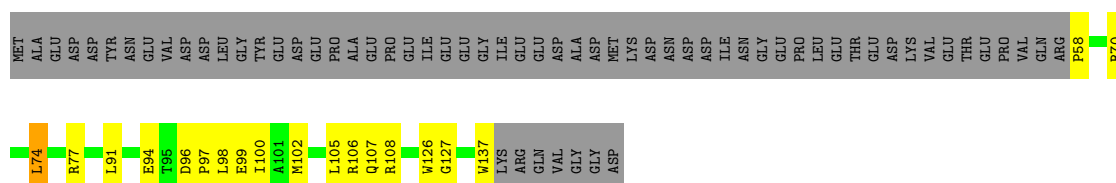
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain C: 80% 10% 10%



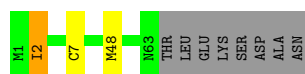
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain F: 42% 12% 44%



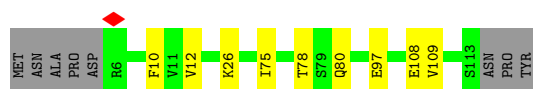
- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

Chain J: 85% 11%



- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

Chain K: 85% 8% 7%



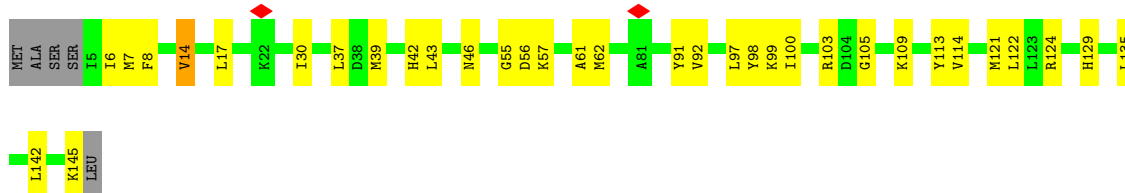
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L: 71% 18% 12%



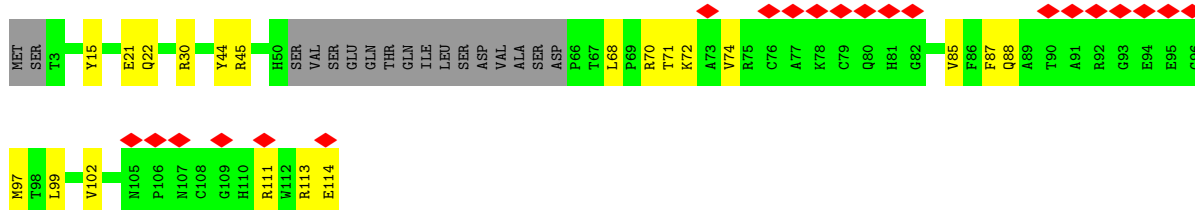
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H: 73% 23% ..



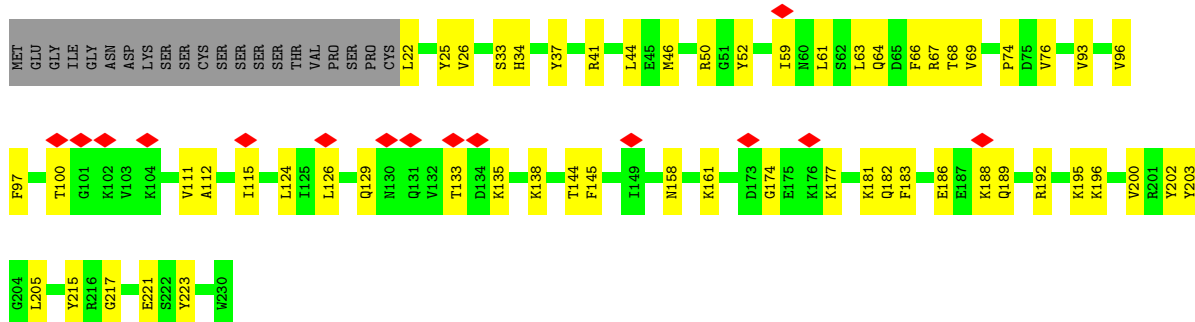
- Molecule 11: DNA-directed RNA polymerase subunit

Chain I: 18% 68% 18% 15%



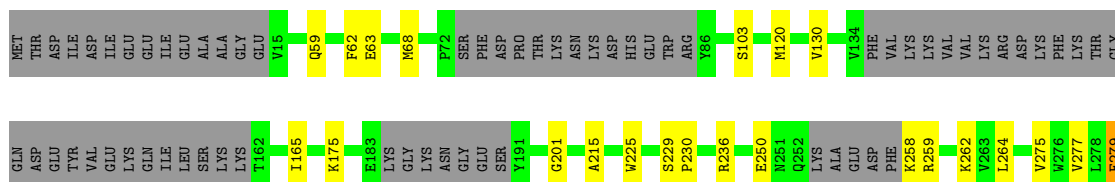
- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

Chain E: 7% 66% 25% 9%



- Molecule 13: DNA-directed RNA polymerase IV and V subunit 2

Chain B: 76% 7% 17%



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0143	Depositor
Map size (Å)	328.5, 328.5, 328.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	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: MG, 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	T	0.19	0/229	0.36	0/348
2	N	0.20	0/391	0.38	0/599
3	P	0.07	0/65	0.19	0/98
4	A	0.15	0/6710	0.41	1/9058 (0.0%)
5	C	0.13	0/2286	0.37	0/3087
6	F	0.15	0/673	0.43	0/905
7	J	0.16	0/515	0.38	0/696
8	K	0.15	0/908	0.33	0/1224
9	L	0.15	0/369	0.40	0/493
10	H	0.15	0/1155	0.44	0/1557
11	I	0.15	0/804	0.41	0/1081
12	E	0.16	0/1732	0.47	0/2332
13	B	0.14	0/7809	0.35	0/10524
All	All	0.15	0/23646	0.39	1/32002 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1002	MET	CB-CA-C	5.17	117.79	109.51

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	T	205	0	114	7	0
2	N	350	0	193	6	0
3	P	60	0	31	0	0
4	A	6597	0	6648	101	0
5	C	2256	0	2269	23	0
6	F	660	0	669	16	0
7	J	507	0	512	2	0
8	K	890	0	883	5	0
9	L	365	0	364	9	0
10	H	1129	0	1128	29	0
11	I	787	0	736	15	0
12	E	1706	0	1759	41	0
13	B	7660	0	7600	56	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23179	0	22906	281	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 6.

The worst 5 of 281 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:N:10:DG:H22	13:B:463:LYS:HD3	1.46	0.81
12:E:100:THR:HA	12:E:129:GLN:HG2	1.70	0.73
4:A:938:HIS:HE2	4:A:1006:MET:HE3	1.54	0.72
11:I:68:LEU:HD11	11:I:87:PHE:HB2	1.73	0.70
4:A:592:LYS:HG3	4:A:596:GLU:HG3	1.74	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	833/2032 (41%)	805 (97%)	28 (3%)	0	100	100
5	C	283/319 (89%)	271 (96%)	12 (4%)	0	100	100
6	F	78/144 (54%)	73 (94%)	5 (6%)	0	100	100
7	J	61/71 (86%)	58 (95%)	3 (5%)	0	100	100
8	K	106/116 (91%)	103 (97%)	3 (3%)	0	100	100
9	L	43/51 (84%)	39 (91%)	4 (9%)	0	100	100
10	H	139/146 (95%)	126 (91%)	13 (9%)	0	100	100
11	I	93/114 (82%)	89 (96%)	4 (4%)	0	100	100
12	E	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
13	B	953/1169 (82%)	927 (97%)	26 (3%)	0	100	100
All	All	2796/4392 (64%)	2689 (96%)	107 (4%)	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	
4	A	748/1709 (44%)	741 (99%)	7 (1%)	70	81
5	C	253/276 (92%)	253 (100%)	0	100	100
6	F	72/128 (56%)	71 (99%)	1 (1%)	59	77
7	J	56/63 (89%)	55 (98%)	1 (2%)	51	74

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	98/105 (93%)	95 (97%)	3 (3%)	35	66
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	122 (99%)	1 (1%)	73	82
11	I	85/101 (84%)	85 (100%)	0	100	100
12	E	190/209 (91%)	187 (98%)	3 (2%)	55	75
13	B	846/1026 (82%)	842 (100%)	4 (0%)	81	85
All	All	2511/3790 (66%)	2491 (99%)	20 (1%)	70	82

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	203	TYR
13	B	279	PHE
13	B	670	TRP
13	B	291	VAL
4	A	1073	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	473	ASN
13	B	648	HIS
13	B	720	GLN
13	B	529	ASN
10	H	106	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	2/20 (10%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 7 ligands modelled in this entry, 7 are 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

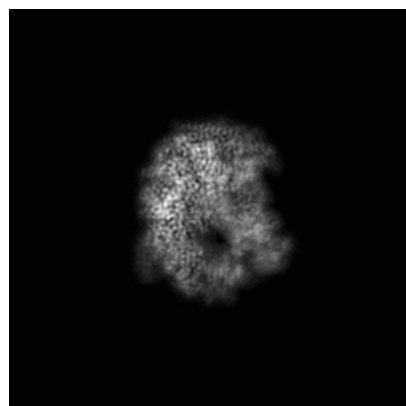
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61966. These allow visual inspection of the internal detail of the map and identification of artifacts.

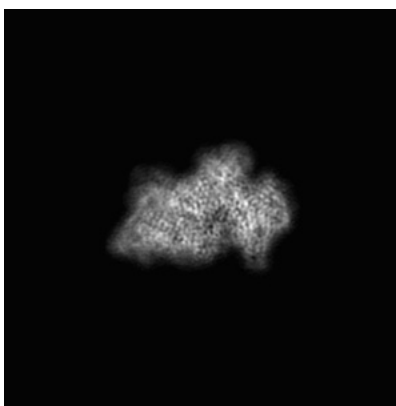
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

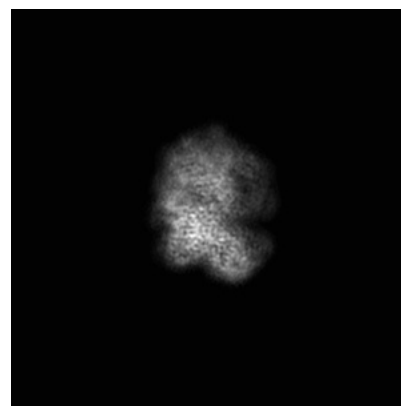
#### 6.1.1 Primary map



X

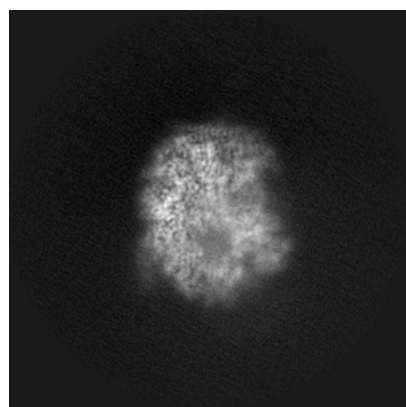


Y

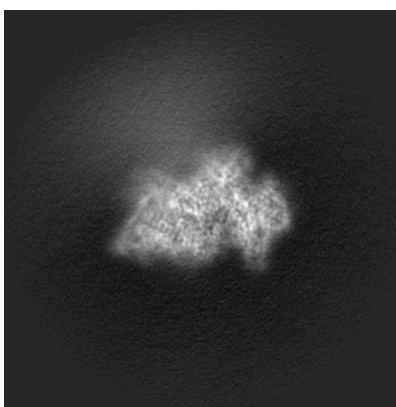


Z

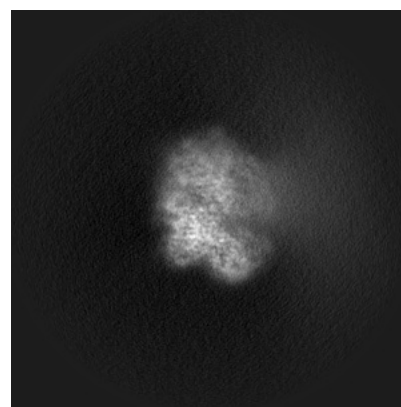
#### 6.1.2 Raw map



X



Y

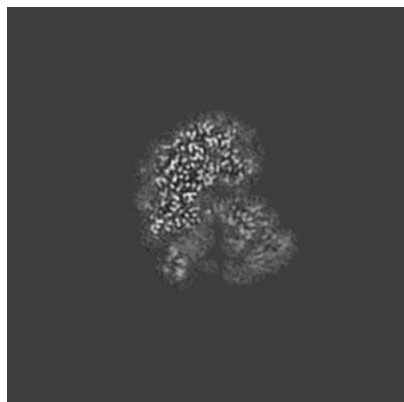


Z

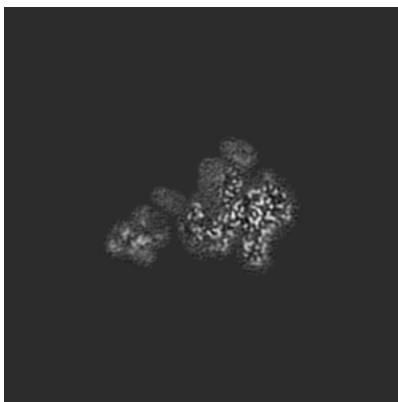
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

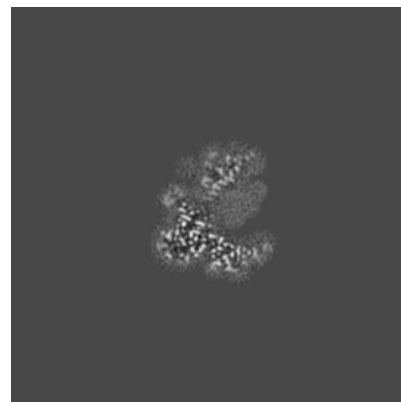
### 6.2.1 Primary map



X Index: 150

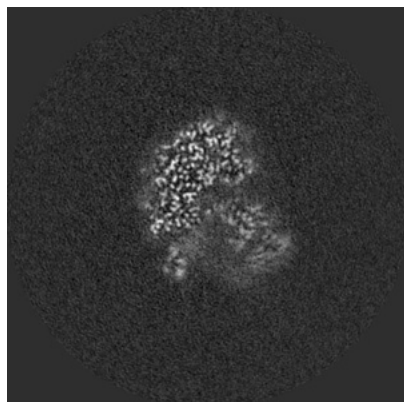


Y Index: 150

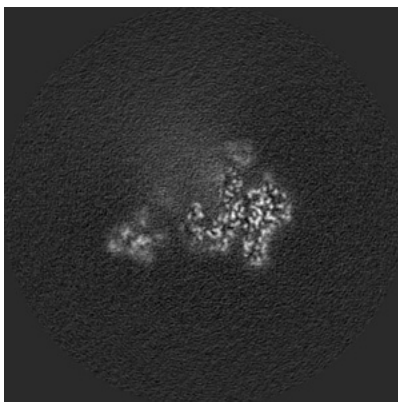


Z Index: 150

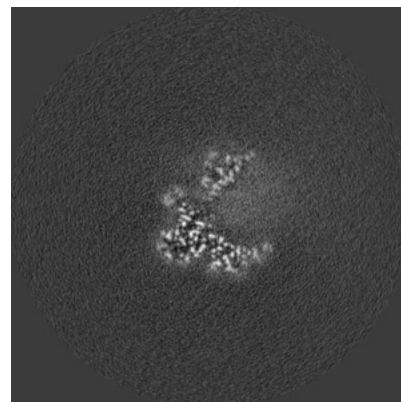
### 6.2.2 Raw map



X Index: 150



Y Index: 150

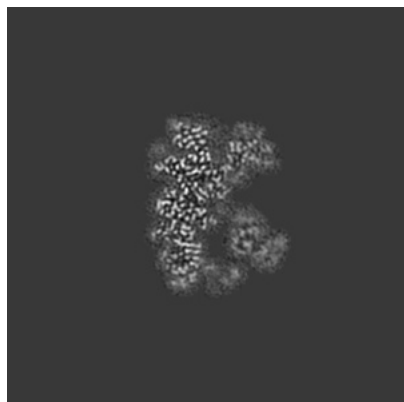


Z Index: 150

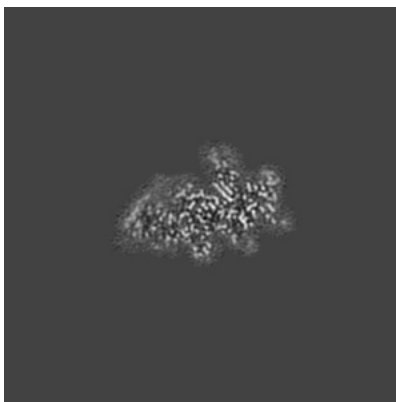
The images above show central slices of the map in three orthogonal directions.

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

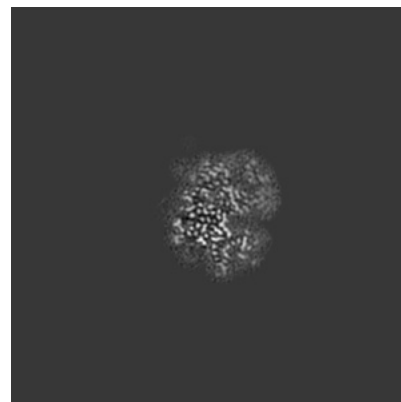
### 6.3.1 Primary map



X Index: 138

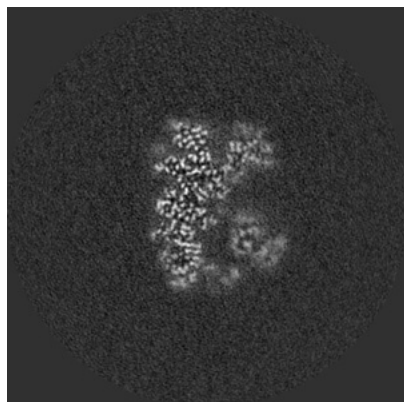


Y Index: 127

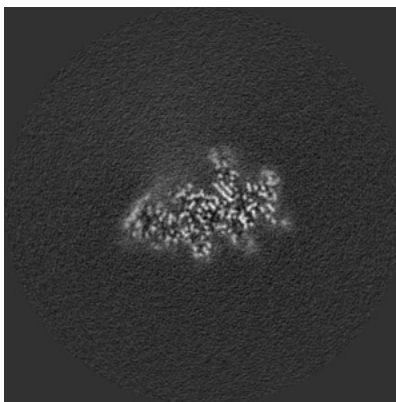


Z Index: 173

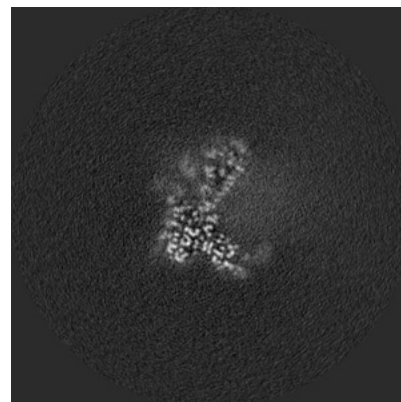
### 6.3.2 Raw map



X Index: 138



Y Index: 127

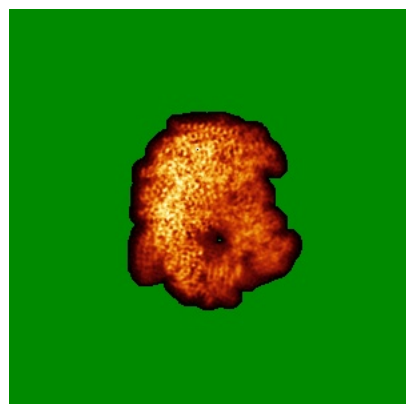


Z Index: 144

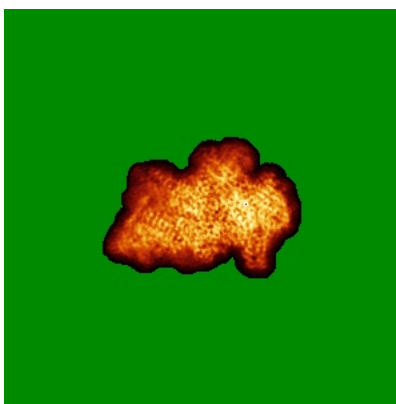
The images above show the largest variance slices of the map in three orthogonal directions.

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

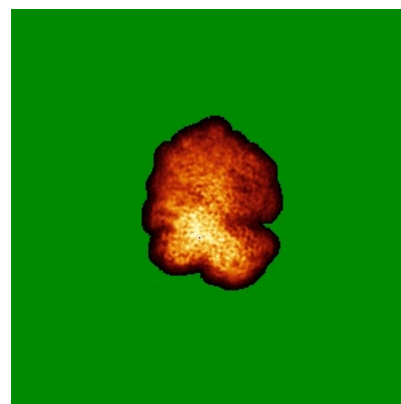
### 6.4.1 Primary map



X

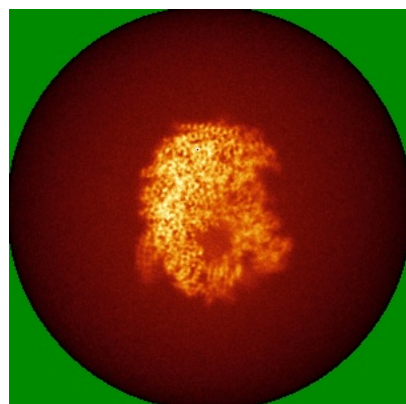


Y

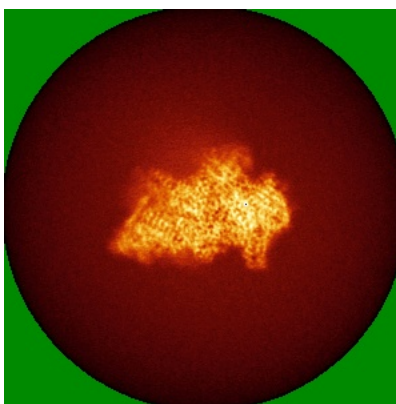


Z

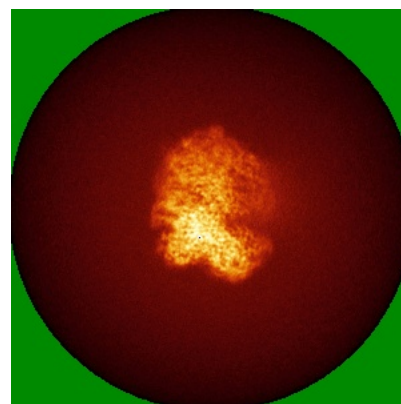
### 6.4.2 Raw map



X



Y

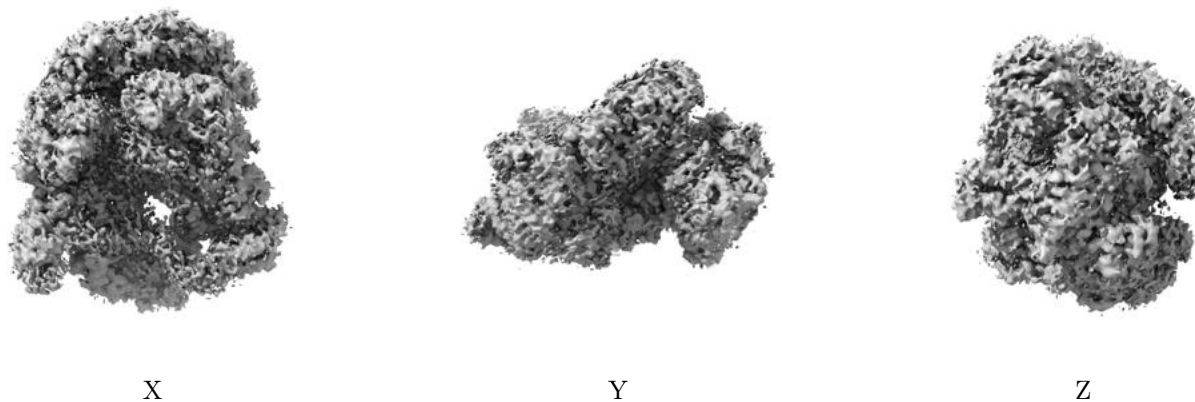


Z

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.

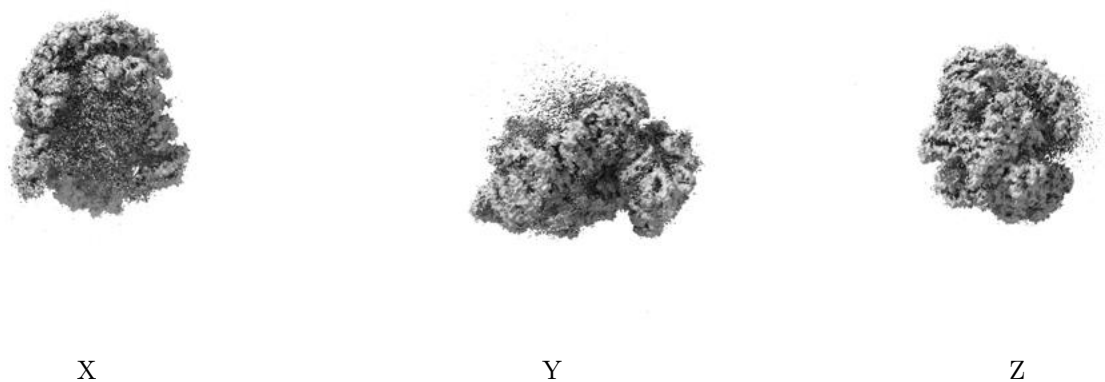
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0143. 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.

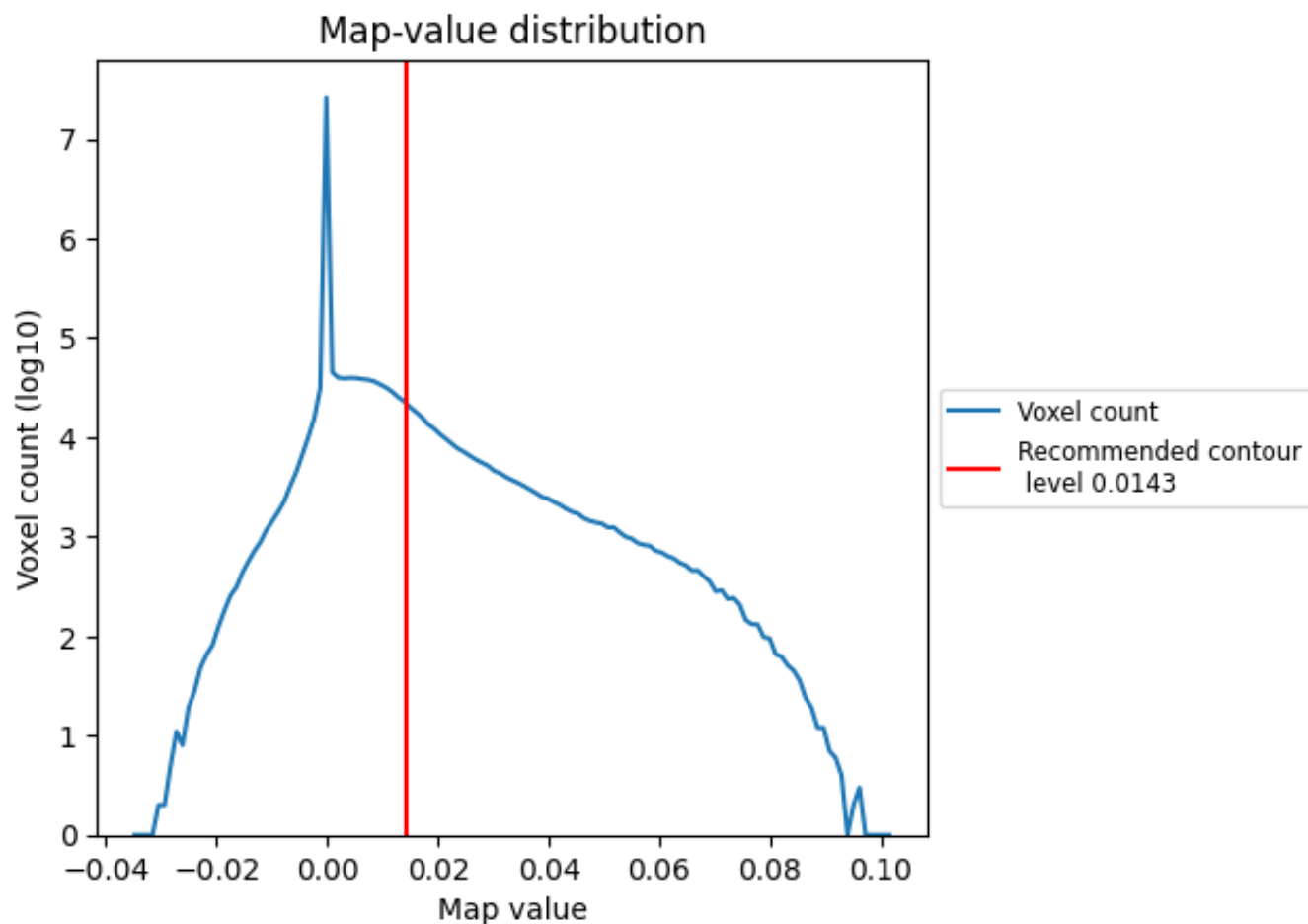
## 6.6 Mask visualisation [i](#)

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.

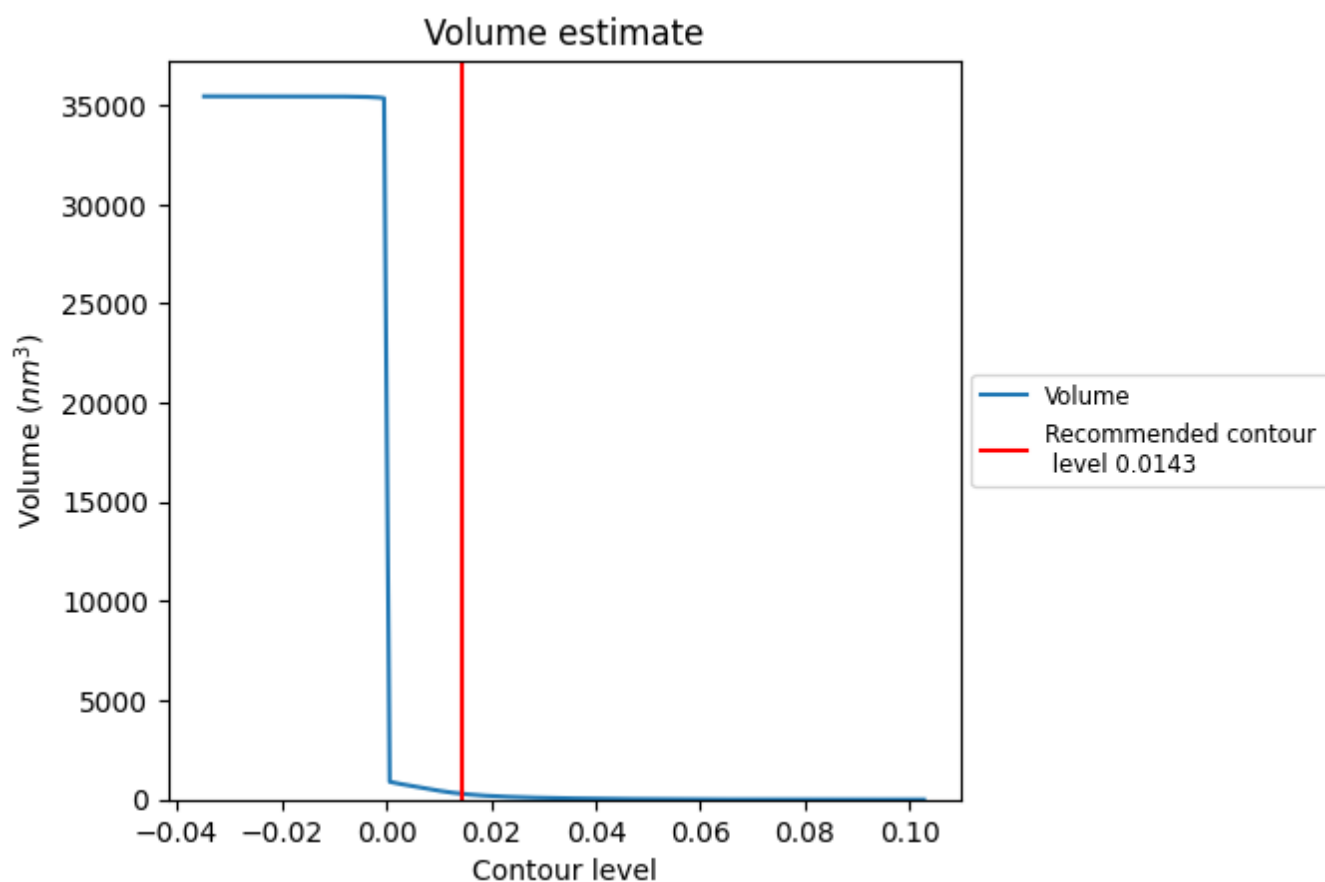
### 7.1 Map-value distribution [i](#)



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.



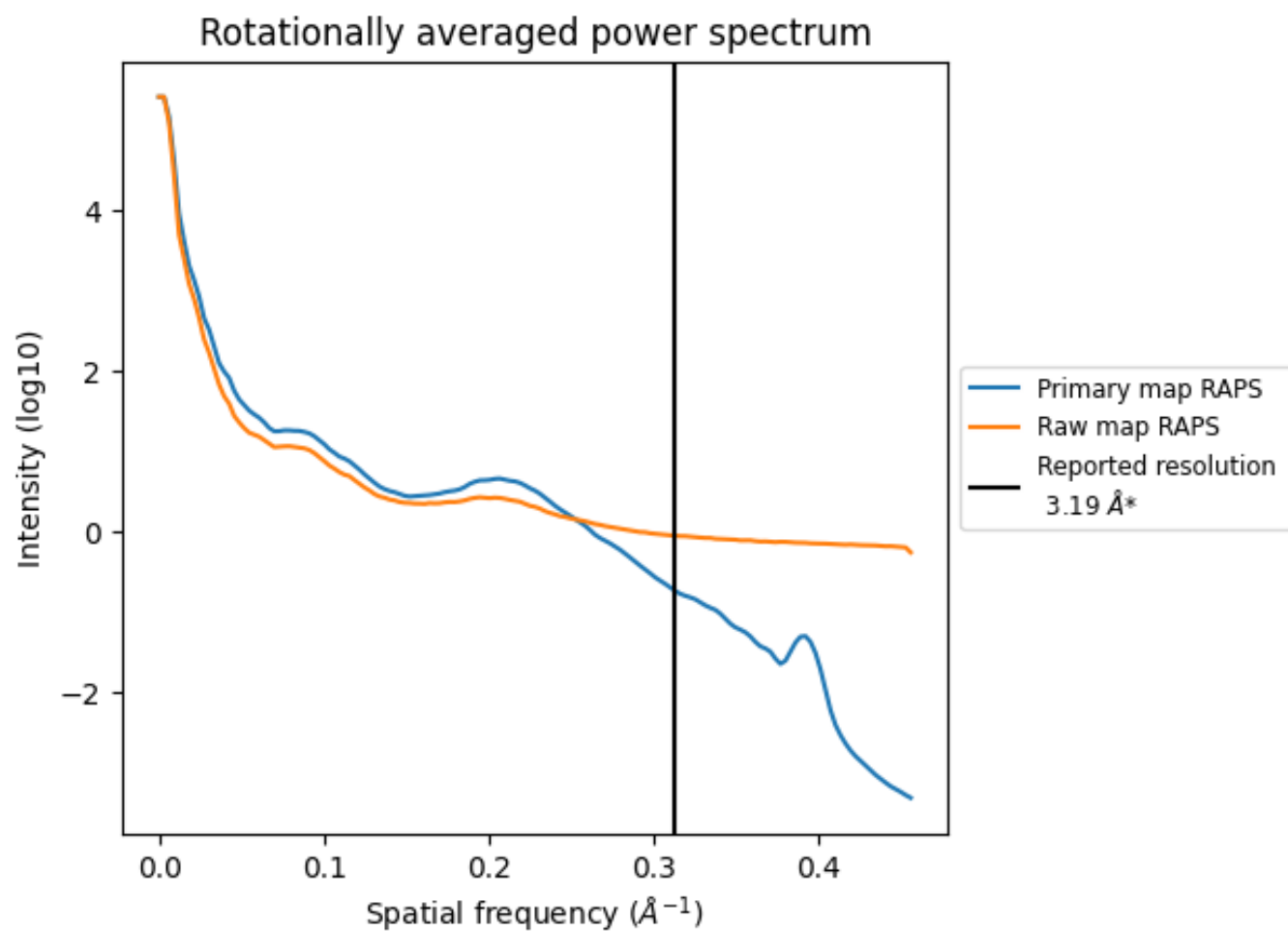
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297  $\text{nm}^3$ ; this corresponds to an approximate mass of 269 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 ⓘ

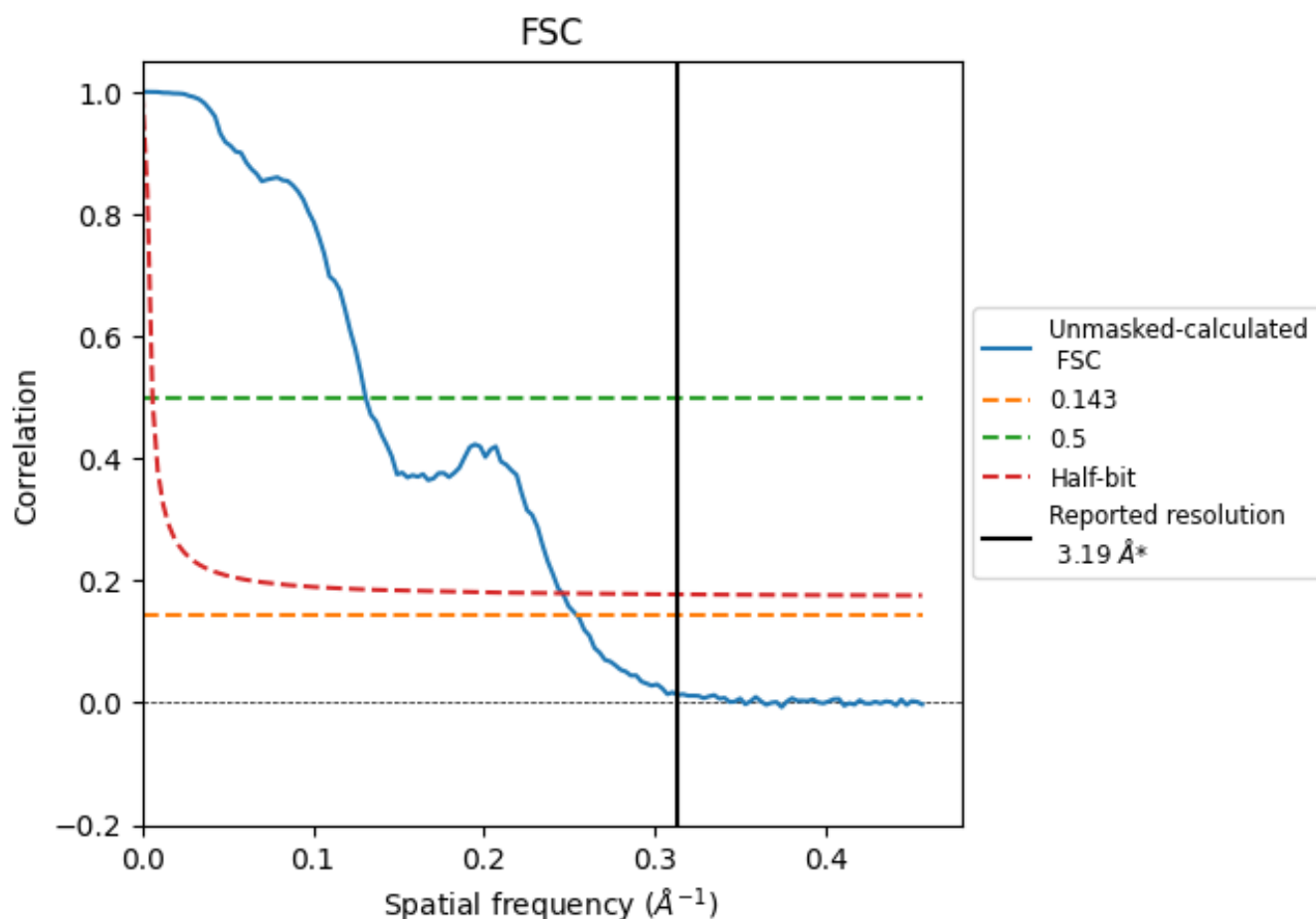


\*Reported resolution corresponds to spatial frequency of  $0.313 \text{ \AA}^{-1}$

## 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 0.313 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

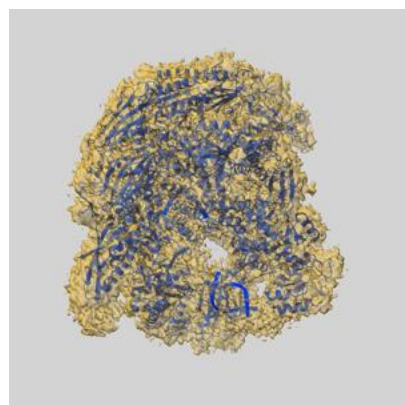
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	7.65	4.07

\*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 3.93 differs from the reported value 3.19 by more than 10 %

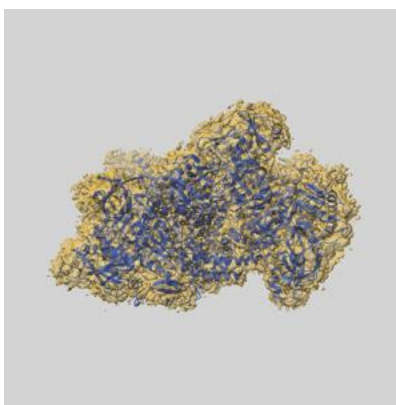
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61966 and PDB model 9K16. Per-residue inclusion information can be found in section [3](#) on page [8](#).

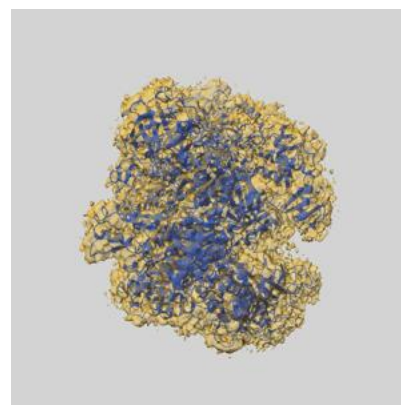
### 9.1 Map-model overlay [i](#)



X



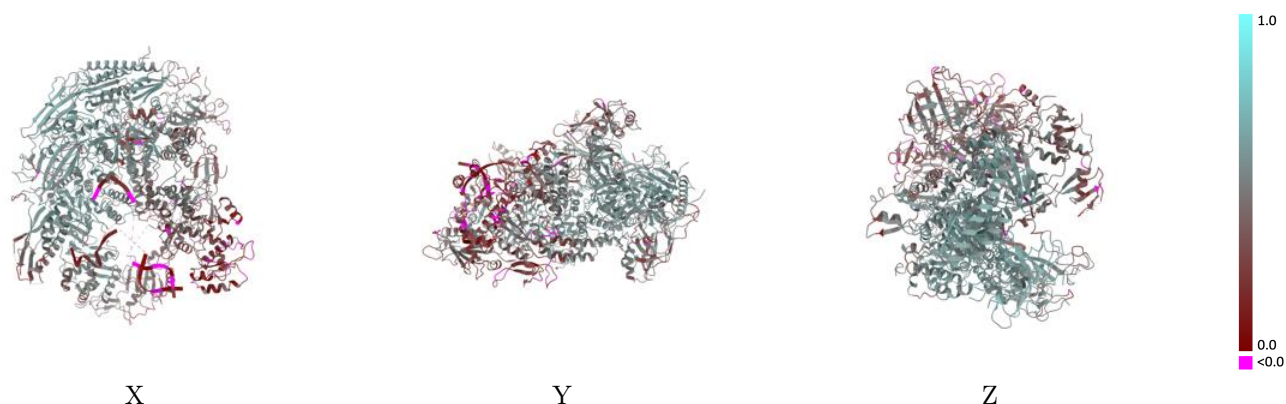
Y



Z

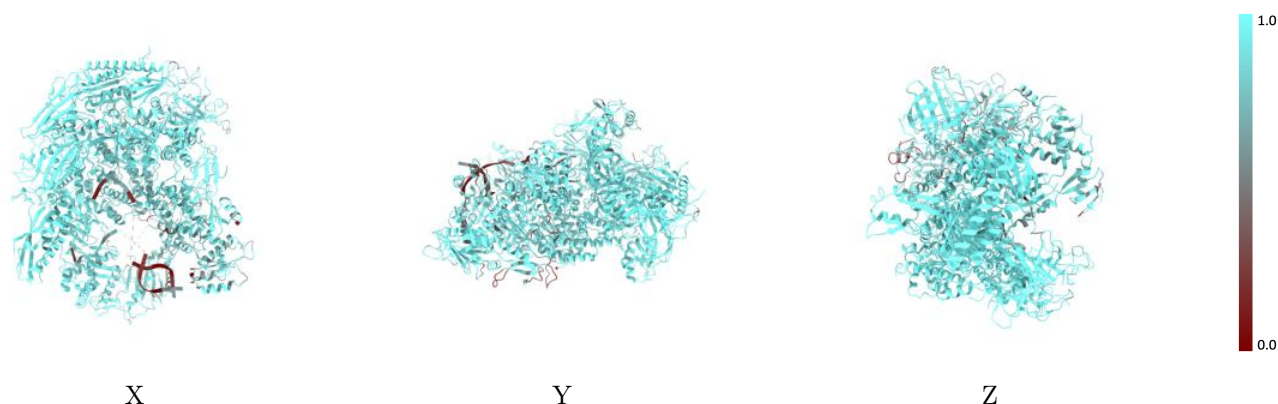
The images above show the 3D surface view of the map at the recommended contour level 0.0143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



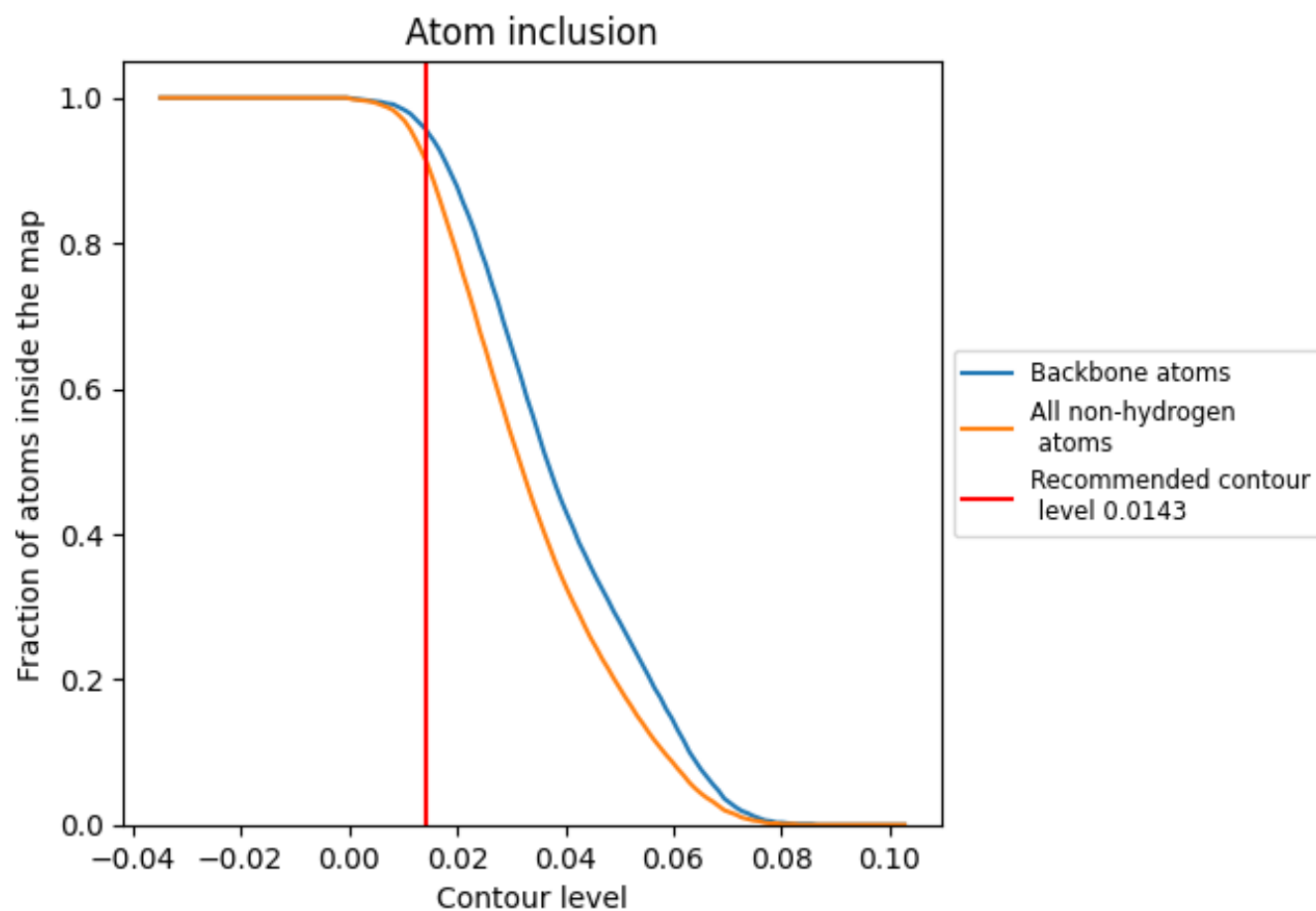
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0143).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.4530
A	 0.9080	 0.4250
B	 0.9750	 0.5400
C	 0.9860	 0.5540
E	 0.7970	 0.2130
F	 0.8730	 0.4050
H	 0.8950	 0.3920
I	 0.7260	 0.2840
J	 0.9960	 0.5860
K	 0.9680	 0.5440
L	 0.9770	 0.5110
N	 0.4910	 0.1090
P	 0.3170	 0.1070
T	 0.2390	 0.0100

