



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:25 AM UTC

PDB ID : 9K13 / pdb_00009k13
EMDB ID : EMD-61963
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 2U scaffold at 3.04 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

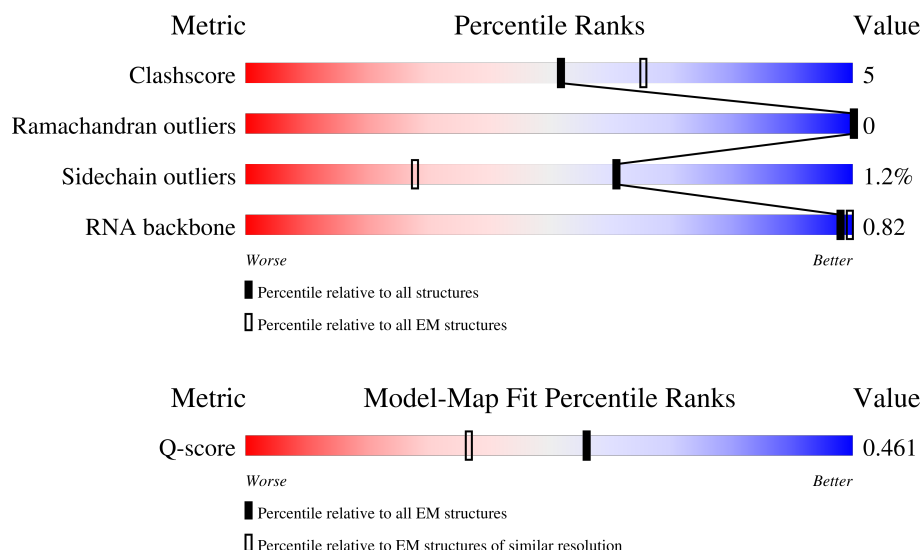
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.04 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.





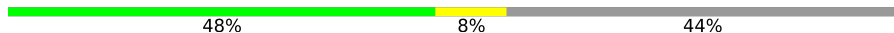







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	T	34	
2	N	34	
3	P	20	

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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 23483 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	17	Total	C	N	O	P	0	0
			345	164	64	100	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	19	Total	C	N	O	P	0	0
			392	186	72	115	19		

- 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*AP*CP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	8	Total	C	N	O	P	0	0
			171	76	30	57	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	844	Total	C	N	O	S	0	0
			6608	4175	1136	1253	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	

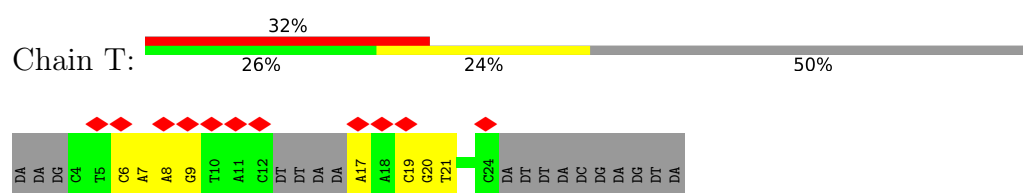
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

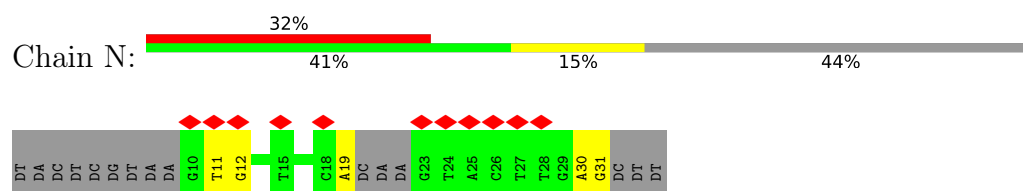
3 Residue-property plots [i](#)

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.

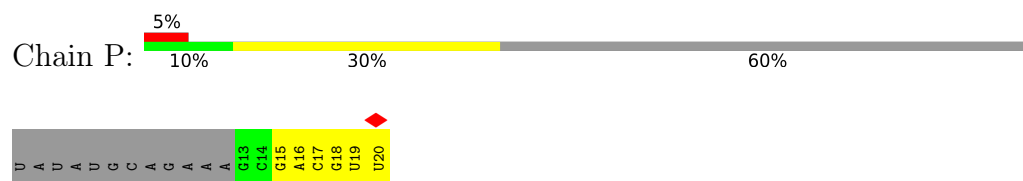
- Molecule 1: DNA (34-MER)



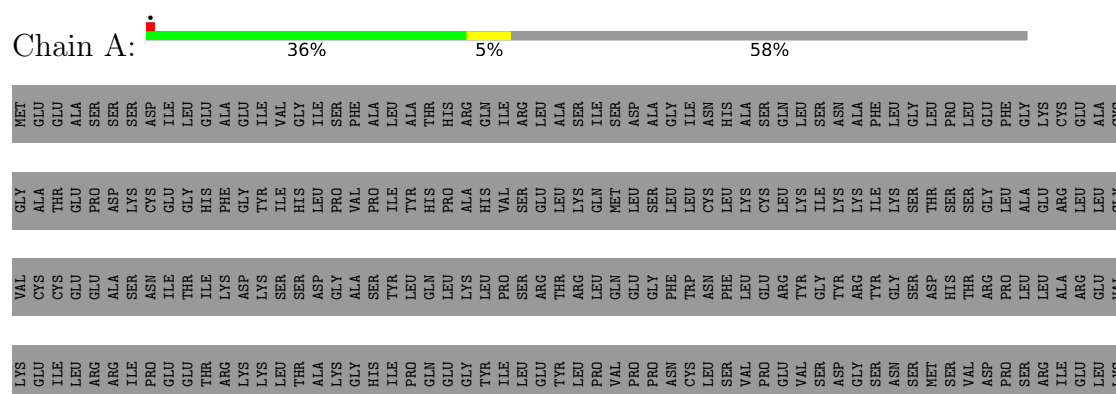
- Molecule 2: DNA (34-MER)



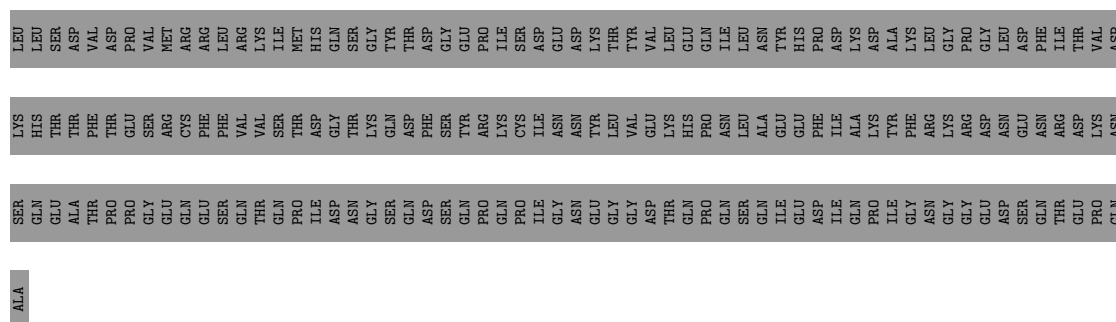
- Molecule 3: RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*GP*AP*CP*GP*UP*U)-3')



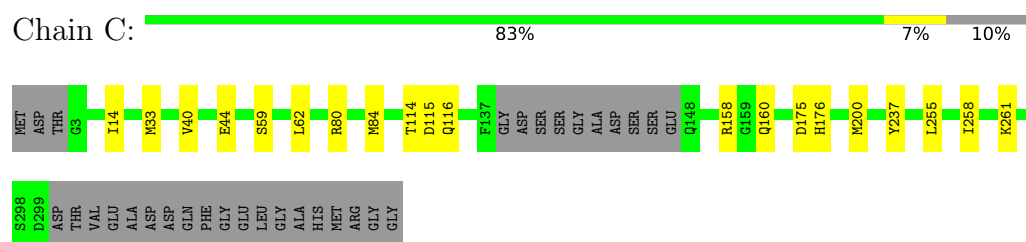
- Molecule 4: DNA-directed RNA polymerase V largest subunit



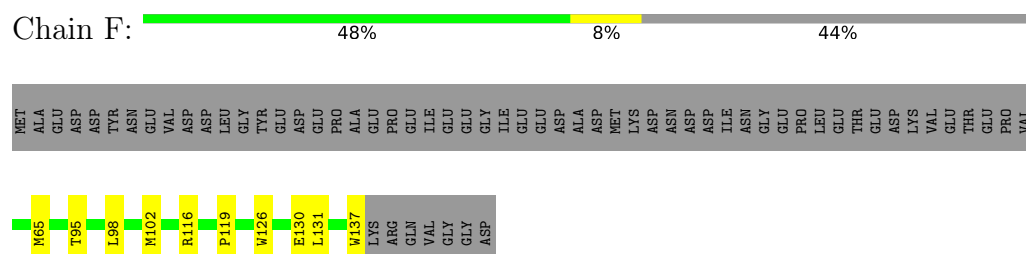




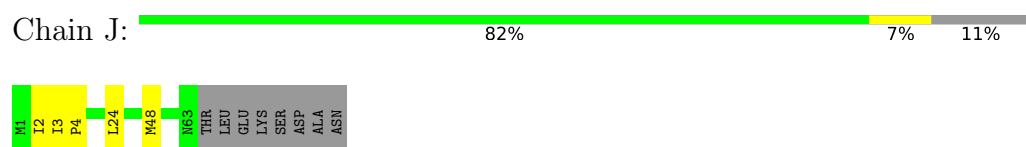
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



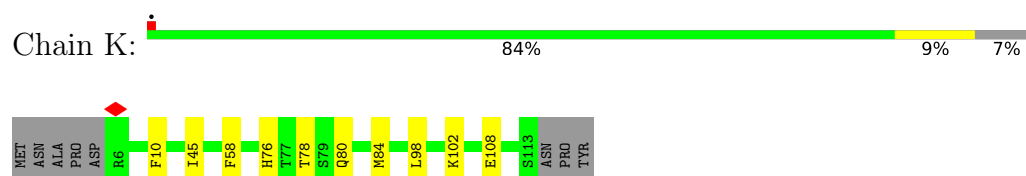
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



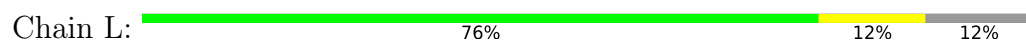
- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10



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



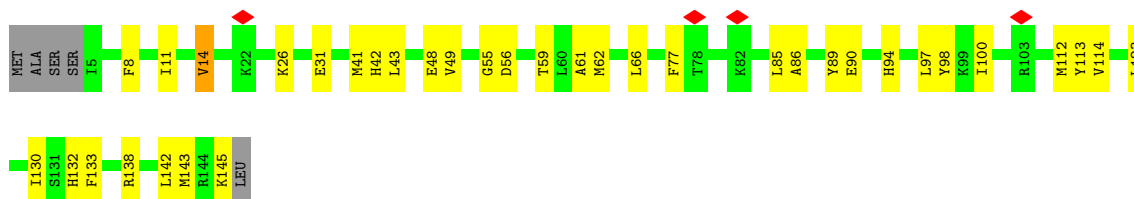
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12





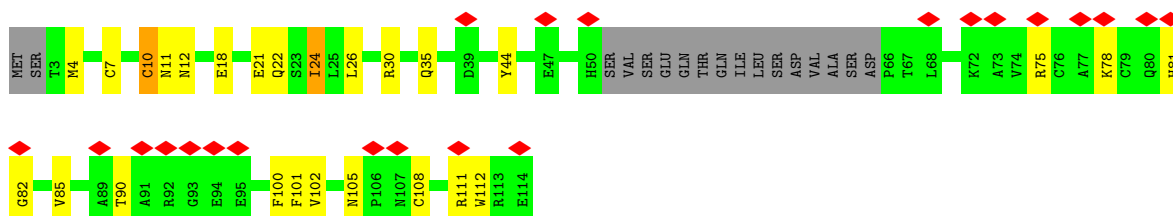
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H:



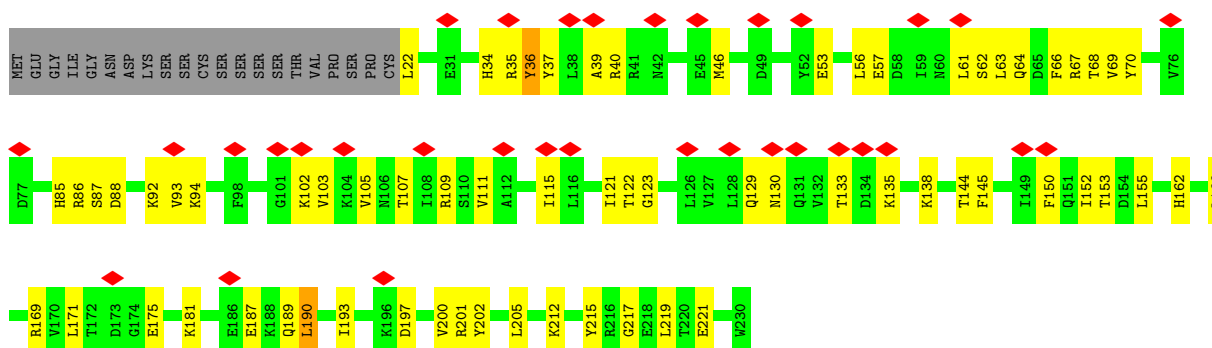
- Molecule 11: DNA-directed RNA polymerase subunit

Chain I:



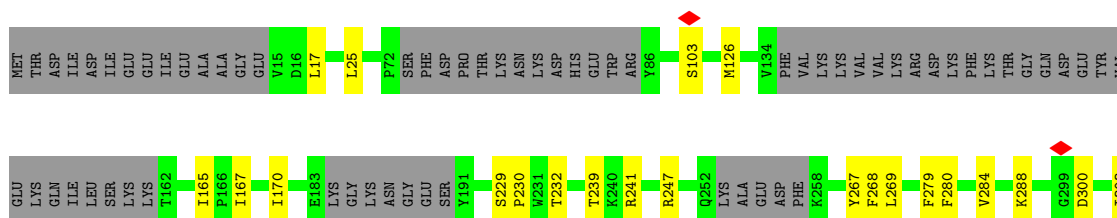
- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

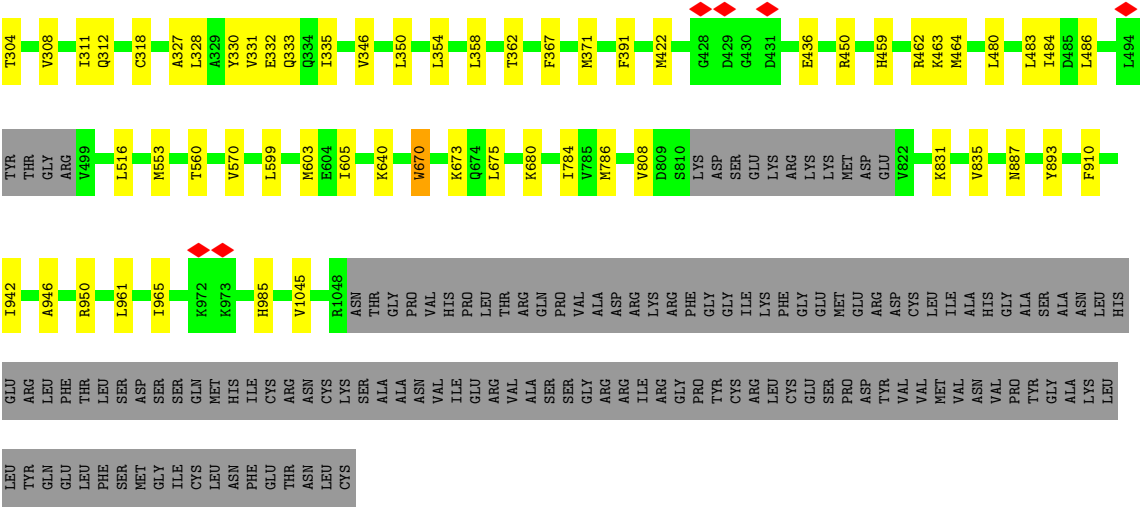
Chain E:



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

Chain B:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46670	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	0.140	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0118	Depositor
Map size (\AA)	328.5, 328.5, 328.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0/385	0.36	0/588
2	N	0.20	0/438	0.37	0/672
3	P	0.07	0/190	0.17	0/294
4	A	0.16	0/6720	0.42	0/9070
5	C	0.13	0/2286	0.37	0/3087
6	F	0.15	0/673	0.40	0/905
7	J	0.14	0/515	0.36	0/696
8	K	0.15	0/908	0.31	0/1224
9	L	0.15	0/369	0.37	0/493
10	H	0.15	0/1155	0.46	0/1557
11	I	0.14	0/804	0.42	1/1081 (0.1%)
12	E	0.14	0/1732	0.43	0/2332
13	B	0.14	0/7809	0.35	0/10524
All	All	0.15	0/23984	0.39	1/32523 (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($^{\circ}$)
11	I	24	ILE	N-CA-C	-5.43	108.56	113.71

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	345	0	192	8	0
2	N	392	0	216	3	0
3	P	171	0	87	5	0
4	A	6608	0	6661	85	0
5	C	2256	0	2269	18	0
6	F	660	0	669	9	0
7	J	507	0	512	4	0
8	K	890	0	883	9	0
9	L	365	0	364	4	0
10	H	1129	0	1128	23	0
11	I	787	0	736	20	0
12	E	1706	0	1759	48	0
13	B	7660	0	7600	47	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	23483	0	23076	252	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 5.

All (252) 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)
4:A:940:HIS:CE1	4:A:989:CYS:SG	2.63	0.92
4:A:885:ARG:HE	12:E:22:LEU:HB2	1.40	0.86
4:A:804:SER:HA	12:E:189:GLN:HB3	1.62	0.82
12:E:135:LYS:HA	12:E:138:LYS:HE3	1.71	0.73
1:T:17:DA:H61	3:P:20:U:H3	1.37	0.72
13:B:247:ARG:HH12	13:B:267:TYR:HB2	1.53	0.71
11:I:100:PHE:HE1	11:I:111:ARG:HB3	1.57	0.69
13:B:670:TRP:H	13:B:675:LEU:HD23	1.57	0.69
5:C:114:THR:HG22	5:C:116:GLN:H	1.58	0.68
8:K:78:THR:HG23	8:K:80:GLN:H	1.57	0.68
13:B:350:LEU:HD22	13:B:354:LEU:HD22	1.76	0.67
12:E:166:LEU:HD21	12:E:215:TYR:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:121:ILE:HG13	12:E:123:GLY:H	1.61	0.66
4:A:335:ASN:HB2	4:A:338:GLU:HG3	1.78	0.66
4:A:953:MET:HE3	4:A:953:MET:H	1.61	0.65
12:E:63:LEU:HD21	12:E:67:ARG:HH21	1.62	0.65
11:I:21:GLU:HG2	11:I:22:GLN:HG2	1.77	0.65
4:A:534:LYS:HB3	10:H:49:VAL:HG23	1.79	0.64
4:A:1096:LEU:HD11	12:E:35:ARG:HB2	1.80	0.63
13:B:247:ARG:NH1	13:B:267:TYR:HB2	2.14	0.63
11:I:78:LYS:HZ1	11:I:108:CYS:HA	1.64	0.62
12:E:85:HIS:CE1	12:E:88:ASP:H	2.17	0.62
4:A:1017:LEU:HD11	11:I:18:GLU:HB3	1.80	0.62
12:E:36:TYR:HB3	12:E:40:ARG:HH21	1.65	0.61
4:A:686:ILE:HD12	4:A:686:ILE:H	1.65	0.61
4:A:896:ALA:HB1	4:A:1048:ILE:HD13	1.81	0.60
6:F:61:THR:HB	6:F:116:ARG:HH11	1.66	0.60
4:A:904:LYS:HE2	4:A:1046:ALA:H	1.68	0.58
6:F:126:TRP:HE1	6:F:130:GLU:HB3	1.67	0.58
12:E:85:HIS:CE1	12:E:87:SER:H	2.22	0.58
4:A:363:LEU:HD23	4:A:366:LEU:HD12	1.86	0.57
4:A:951:ILE:HD11	4:A:1038:LYS:HD3	1.86	0.57
12:E:171:LEU:HD12	12:E:175:GLU:HB3	1.85	0.57
4:A:592:LYS:HB3	4:A:596:GLU:HG3	1.87	0.57
4:A:1133:SER:O	4:A:1137:ARG:HG2	2.04	0.57
12:E:121:ILE:HG13	12:E:122:THR:N	2.20	0.57
13:B:599:LEU:HD13	13:B:603:MET:HE1	1.87	0.56
4:A:1111:SER:HB3	4:A:1114:GLN:HG2	1.87	0.56
4:A:594:PRO:O	4:A:595:LYS:HD3	2.05	0.56
8:K:58:PHE:HB3	8:K:76:HIS:HB2	1.86	0.56
10:H:8:PHE:HB3	10:H:62:MET:HB2	1.87	0.56
12:E:107:THR:O	12:E:111:VAL:HG22	2.04	0.56
10:H:41:MET:HE2	10:H:43:LEU:HD22	1.87	0.56
4:A:502:MET:HE2	4:A:541:PHE:HB2	1.86	0.56
4:A:950:ASN:O	4:A:950:ASN:ND2	2.26	0.56
5:C:288:LEU:HD22	8:K:98:LEU:HD11	1.88	0.56
1:T:19:DC:H2'	1:T:20:DG:H8	1.70	0.56
11:I:85:VAL:HG13	11:I:102:VAL:HG13	1.87	0.55
5:C:33:MET:HE2	8:K:45:ILE:HD11	1.88	0.55
4:A:950:ASN:HD22	4:A:950:ASN:C	2.12	0.55
12:E:66:PHE:HA	12:E:69:VAL:HG12	1.87	0.55
12:E:94:LYS:HG2	12:E:121:ILE:HD13	1.89	0.55
12:E:187:GLU:HA	12:E:190:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1088:TRP:O	4:A:1092:ILE:HG22	2.06	0.55
13:B:335:ILE:HD12	13:B:346:VAL:HG12	1.89	0.55
4:A:895:SER:O	4:A:899:VAL:HG23	2.07	0.54
11:I:102:VAL:HB	11:I:111:ARG:HG2	1.88	0.54
13:B:961:LEU:O	13:B:965:ILE:HG23	2.06	0.54
4:A:918:GLU:HG3	4:A:991:PHE:CE2	2.42	0.54
4:A:412:ILE:HG21	4:A:446:LEU:HD21	1.88	0.54
4:A:964:ILE:HD12	4:A:1032:LEU:HD21	1.89	0.54
12:E:133:THR:HG22	12:E:135:LYS:H	1.72	0.54
10:H:61:ALA:HB3	10:H:142:LEU:HB2	1.90	0.54
11:I:75:ARG:HA	11:I:82:GLY:HA2	1.90	0.54
13:B:165:ILE:HD12	13:B:436:GLU:HG3	1.89	0.54
13:B:239:THR:HG22	13:B:241:ARG:H	1.72	0.53
4:A:542:PHE:HE1	4:A:570:PHE:HB3	1.74	0.53
1:T:8:DA:H2''	1:T:9:DG:C8	2.43	0.53
9:L:32:CYS:HB3	9:L:34:TYR:HD1	1.73	0.53
4:A:950:ASN:O	4:A:951:ILE:HD13	2.08	0.53
1:T:8:DA:H2''	1:T:9:DG:N7	2.24	0.53
5:C:33:MET:CE	8:K:45:ILE:HD11	2.39	0.52
4:A:1002:MET:HE3	4:A:1002:MET:H	1.73	0.52
4:A:950:ASN:HB2	11:I:90:THR:HG21	1.91	0.52
12:E:200:VAL:HG23	12:E:205:LEU:HB2	1.91	0.52
4:A:953:MET:H	4:A:953:MET:CE	2.21	0.52
4:A:553:LEU:HD22	4:A:588:ILE:HD11	1.92	0.52
4:A:1066:ARG:HG3	4:A:1067:ARG:N	2.25	0.52
4:A:362:TYR:HD1	6:F:95:THR:HG21	1.74	0.51
4:A:1123:CYS:O	4:A:1127:GLN:HG2	2.10	0.51
12:E:37:TYR:O	12:E:40:ARG:HG2	2.11	0.51
1:T:7:DA:C8	1:T:7:DA:H5'	2.46	0.51
13:B:126:MET:HG3	13:B:167:ILE:HG22	1.93	0.51
13:B:784:ILE:HG22	13:B:942:ILE:HG22	1.93	0.51
10:H:100:ILE:HG12	10:H:100:ILE:O	2.11	0.50
5:C:115:ASP:HB3	5:C:158:ARG:HH21	1.76	0.50
5:C:62:LEU:HD11	7:J:2:ILE:HD11	1.92	0.50
2:N:11:DT:H1'	2:N:12:DG:N7	2.26	0.50
13:B:229:SER:HB3	13:B:230:PRO:HD3	1.92	0.50
10:H:130:ILE:HG23	10:H:133:PHE:HD2	1.76	0.50
13:B:268:PHE:CE2	13:B:269:LEU:HD12	2.47	0.50
4:A:1089:ARG:HD3	12:E:153:THR:HG23	1.93	0.50
12:E:105:VAL:O	12:E:109:ARG:HG3	2.12	0.49
4:A:645:MET:HE2	4:A:649:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:885:ARG:NH1	4:A:886:CYS:HB2	2.28	0.49
13:B:280:PHE:HA	13:B:284:VAL:HG12	1.95	0.49
4:A:885:ARG:NE	12:E:22:LEU:HB2	2.18	0.49
13:B:300:ASP:HB3	13:B:303:ILE:HG12	1.94	0.49
13:B:553:MET:HE2	13:B:570:VAL:HG21	1.95	0.49
11:I:24:ILE:HB	11:I:26:LEU:HG	1.95	0.48
12:E:63:LEU:HD21	12:E:67:ARG:NH2	2.28	0.48
13:B:946:ALA:O	13:B:950:ARG:HG2	2.13	0.48
4:A:878:ILE:HD11	4:A:1110:TYR:HD1	1.78	0.48
10:H:142:LEU:HD12	10:H:142:LEU:H	1.77	0.48
12:E:36:TYR:HB3	12:E:40:ARG:NH2	2.28	0.48
13:B:450:ARG:HH11	13:B:450:ARG:HG2	1.78	0.48
4:A:792:THR:HG23	4:A:794:ASP:H	1.78	0.48
4:A:362:TYR:O	4:A:366:LEU:HG	2.13	0.48
10:H:98:TYR:CZ	10:H:113:TYR:HB3	2.49	0.48
12:E:39:ALA:HA	12:E:155:LEU:O	2.13	0.48
4:A:531:LYS:HD3	10:H:77:PHE:HE2	1.79	0.48
11:I:4:MET:HE2	13:B:304:THR:HG23	1.96	0.48
13:B:165:ILE:HG23	13:B:436:GLU:HG2	1.96	0.48
3:P:15:G:H2'	3:P:16:A:C8	2.49	0.47
4:A:868:PHE:CE2	4:A:870:ASN:HB3	2.49	0.47
4:A:879:LEU:HD13	4:A:1102:ILE:HD12	1.96	0.47
4:A:964:ILE:O	4:A:968:VAL:HG12	2.14	0.47
6:F:98:LEU:O	6:F:102:MET:HE3	2.15	0.47
10:H:97:LEU:HD21	10:H:100:ILE:HB	1.94	0.47
5:C:80:ARG:O	5:C:84:MET:HG3	2.14	0.47
5:C:176:HIS:CD2	9:L:51:ARG:HG3	2.49	0.47
13:B:367:PHE:O	13:B:371:MET:HG3	2.14	0.47
4:A:1162:LEU:HD12	4:A:1172:LEU:HB2	1.97	0.47
13:B:480:LEU:O	13:B:484:ILE:HG23	2.14	0.47
13:B:887:ASN:HB2	13:B:893:TYR:HE2	1.78	0.47
4:A:1029:TYR:CE2	4:A:1033:LEU:HD11	2.49	0.47
5:C:237:TYR:CZ	5:C:258:ILE:HD13	2.50	0.47
6:F:61:THR:HB	6:F:116:ARG:NH1	2.30	0.47
3:P:15:G:H2'	3:P:16:A:H8	1.80	0.47
4:A:879:LEU:HD22	4:A:1102:ILE:HD11	1.97	0.47
4:A:642:ILE:O	4:A:646:VAL:HG23	2.15	0.46
1:T:6:DC:H2''	1:T:7:DA:C8	2.50	0.46
12:E:135:LYS:HD2	12:E:138:LYS:NZ	2.30	0.46
4:A:1096:LEU:HD21	12:E:34:HIS:HB3	1.96	0.46
11:I:81:HIS:HD2	11:I:105:ASN:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:105:ASN:HB3	11:I:108:CYS:HB2	1.97	0.46
4:A:465:ALA:O	4:A:469:VAL:HG23	2.15	0.46
12:E:61:LEU:HD11	12:E:66:PHE:HD1	1.80	0.46
13:B:463:LYS:HD2	13:B:463:LYS:HA	1.70	0.46
7:J:3:ILE:HD12	7:J:4:PRO:HD2	1.98	0.46
13:B:459:HIS:HB3	13:B:462:ARG:O	2.15	0.46
12:E:169:ARG:HB2	12:E:212:LYS:HE3	1.97	0.46
13:B:831:LYS:HG3	13:B:835:VAL:H	1.79	0.46
12:E:150:PHE:HE1	12:E:201:ARG:HD3	1.81	0.46
13:B:327:ALA:O	13:B:331:VAL:HG23	2.15	0.46
4:A:885:ARG:HH11	4:A:886:CYS:HB2	1.80	0.46
4:A:1155:MET:HE3	4:A:1155:MET:HB2	1.80	0.46
4:A:950:ASN:ND2	4:A:950:ASN:C	2.72	0.45
4:A:1127:GLN:O	4:A:1131:ARG:HG3	2.15	0.45
10:H:66:LEU:HD12	10:H:85:LEU:HD13	1.97	0.45
4:A:643:SER:OG	4:A:644:PRO:HD3	2.15	0.45
4:A:686:ILE:HD12	4:A:686:ILE:N	2.29	0.45
12:E:46:MET:HA	12:E:202:TYR:CZ	2.51	0.45
13:B:232:THR:HG23	13:B:247:ARG:HB3	1.97	0.45
13:B:358:LEU:HD12	13:B:358:LEU:HA	1.86	0.45
5:C:261:LYS:HE3	5:C:261:LYS:HB2	1.77	0.45
4:A:323:SER:HA	4:A:457:LEU:O	2.17	0.45
11:I:11:ASN:HB3	13:B:288:LYS:HG2	1.98	0.45
3:P:16:A:H2'	3:P:17:C:C6	2.53	0.44
4:A:961:GLU:O	4:A:964:ILE:HG22	2.17	0.44
10:H:31:GLU:OE1	10:H:42:HIS:HB3	2.16	0.44
10:H:112:MET:HE2	10:H:123:LEU:HD23	2.00	0.44
4:A:1133:SER:HB2	12:E:219:LEU:HD22	1.99	0.44
12:E:197:ASP:HB3	12:E:200:VAL:HG12	1.98	0.44
4:A:510:LYS:O	4:A:514:GLN:HG3	2.18	0.44
11:I:26:LEU:HD22	11:I:35:GLN:HB2	2.00	0.44
5:C:297:LEU:HD23	8:K:84:MET:SD	2.57	0.44
4:A:675:LEU:HD21	4:A:684:ILE:HD11	1.99	0.44
4:A:900:ARG:HD2	4:A:900:ARG:O	2.18	0.44
12:E:56:LEU:HG	12:E:57:GLU:CD	2.43	0.44
12:E:135:LYS:HE2	12:E:135:LYS:HB3	1.91	0.44
4:A:890:TYR:HA	4:A:893:GLU:OE2	2.17	0.44
13:B:229:SER:CB	13:B:230:PRO:HD3	2.48	0.44
5:C:200:MET:HE2	5:C:255:LEU:HD11	2.00	0.43
10:H:85:LEU:HD12	10:H:86:ALA:N	2.33	0.43
11:I:75:ARG:HD2	11:I:75:ARG:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:10:CYS:HB3	11:I:12:ASN:OD1	2.18	0.43
10:H:26:LYS:HB3	10:H:48:GLU:OE2	2.19	0.43
10:H:56:ASP:HB3	10:H:145:LYS:HE2	2.01	0.43
12:E:66:PHE:HE2	12:E:70:TYR:HD2	1.66	0.43
4:A:591:GLU:HA	6:F:137:TRP:O	2.19	0.43
10:H:145:LYS:HA	10:H:145:LYS:HD3	1.84	0.43
11:I:30:ARG:NH2	13:B:312:GLN:HA	2.33	0.43
4:A:1037:ILE:HD13	4:A:1037:ILE:HA	1.89	0.43
4:A:916:LEU:HA	11:I:44:TYR:O	2.19	0.43
4:A:542:PHE:CE1	4:A:570:PHE:HB3	2.52	0.43
7:J:48:MET:HE3	7:J:48:MET:HB3	1.90	0.43
10:H:89:TYR:HB3	10:H:143:MET:O	2.19	0.43
13:B:328:LEU:HD12	13:B:328:LEU:H	1.84	0.43
5:C:285:ILE:HG21	8:K:102:LYS:HB2	2.01	0.43
10:H:97:LEU:HA	10:H:114:VAL:HG12	2.00	0.43
1:T:6:DC:C4	1:T:7:DA:N6	2.87	0.43
12:E:61:LEU:HD12	12:E:62:SER:O	2.18	0.43
4:A:395:LYS:HG2	4:A:398:GLN:HE22	1.84	0.42
11:I:101:PHE:HB2	11:I:112:TRP:CZ3	2.54	0.42
13:B:330:TYR:HA	13:B:333:GLN:HG2	2.01	0.42
10:H:14:VAL:HG22	10:H:55:GLY:H	1.82	0.42
2:N:19:DA:H5'	2:N:19:DA:H8	1.84	0.42
4:A:605:GLN:HB3	4:A:606:PRO:HD3	2.01	0.42
5:C:40:VAL:HG13	5:C:44:GLU:HB2	2.01	0.42
13:B:318:CYS:HB2	13:B:330:TYR:CD1	2.55	0.42
12:E:64:GLN:O	12:E:68:THR:HG23	2.19	0.42
4:A:726:LYS:NZ	4:A:726:LYS:HB2	2.35	0.42
4:A:1141:LYS:HB3	4:A:1141:LYS:HE2	1.82	0.42
2:N:30:DA:H2''	2:N:31:DG:C8	2.54	0.42
4:A:646:VAL:HG13	4:A:659:LEU:HD11	2.02	0.42
9:L:27:ILE:HG23	9:L:37:LEU:HD12	2.02	0.42
4:A:1161:MET:C	4:A:1162:LEU:HD23	2.45	0.41
4:A:362:TYR:CD1	6:F:95:THR:HG21	2.54	0.41
4:A:1066:ARG:HG3	4:A:1068:GLY:H	1.83	0.41
5:C:59:SER:O	5:C:160:GLN:HG2	2.20	0.41
10:H:94:HIS:HE1	10:H:138:ARG:HB3	1.84	0.41
13:B:483:LEU:HD12	13:B:483:LEU:HA	1.87	0.41
13:B:786:MET:HE1	13:B:910:PHE:CZ	2.55	0.41
1:T:20:DG:H2'	1:T:21:DT:C6	2.56	0.41
13:B:362:THR:HG23	13:B:560:THR:HB	2.03	0.41
4:A:792:THR:OG1	6:F:119:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:46:MET:HA	12:E:202:TYR:OH	2.21	0.41
12:E:129:GLN:HE22	12:E:152:ILE:HD13	1.86	0.41
4:A:674:MET:HE2	4:A:695:LEU:HG	2.03	0.41
4:A:973:LYS:HA	4:A:973:LYS:HD2	1.92	0.41
4:A:1026:ASN:OD1	4:A:1027:THR:HG23	2.21	0.41
5:C:14:ILE:HG13	8:K:108:GLU:HB3	2.02	0.41
10:H:11:ILE:HG22	10:H:59:THR:HB	2.01	0.41
12:E:217:GLY:O	12:E:221:GLU:HG3	2.20	0.41
13:B:603:MET:HE3	13:B:605:ILE:HD11	2.03	0.41
12:E:66:PHE:CE2	12:E:70:TYR:HD2	2.39	0.41
12:E:144:THR:HG23	12:E:145:PHE:CD2	2.56	0.41
13:B:463:LYS:HG3	13:B:464:MET:SD	2.60	0.41
3:P:18:G:H2'	3:P:19:U:C6	2.56	0.41
4:A:532:SER:HA	10:H:90:GLU:O	2.21	0.41
6:F:65:MET:HG3	6:F:131:LEU:HB2	2.02	0.41
9:L:35:ARG:HE	13:B:103:SER:HB2	1.85	0.41
12:E:102:LYS:HA	12:E:130:ASN:HD21	1.86	0.41
13:B:25:LEU:HD13	13:B:673:LYS:NZ	2.36	0.41
4:A:953:MET:HE3	4:A:953:MET:N	2.34	0.41
12:E:93:VAL:O	12:E:94:LYS:HD3	2.21	0.41
4:A:457:LEU:HD23	4:A:457:LEU:HA	1.87	0.40
12:E:34:HIS:HB2	12:E:67:ARG:HH22	1.86	0.40
4:A:499:LEU:HB3	4:A:577:LEU:HD21	2.04	0.40
12:E:53:GLU:HG2	12:E:86:ARG:HA	2.03	0.40
13:B:17:LEU:H	13:B:680:LYS:HE2	1.86	0.40
13:B:308:VAL:HA	13:B:311:ILE:HG22	2.02	0.40
13:B:516:LEU:HD23	13:B:516:LEU:HA	1.96	0.40
13:B:640:LYS:HD3	13:B:640:LYS:HA	1.75	0.40
12:E:92:LYS:HG3	12:E:121:ILE:HA	2.03	0.40
4:A:594:PRO:C	4:A:595:LYS:HD3	2.47	0.40
13:B:332:GLU:OE2	13:B:346:VAL:HG13	2.21	0.40
5:C:175:ASP:HA	8:K:10:PHE:CZ	2.57	0.40
5:C:297:LEU:HD12	5:C:297:LEU:HA	1.92	0.40
7:J:24:LEU:HD23	7:J:24:LEU:HA	1.91	0.40
11:I:7:CYS:HB3	11:I:12:ASN:H	1.86	0.40

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	834/2032 (41%)	796 (95%)	38 (5%)	0	100	100
5	C	283/319 (89%)	277 (98%)	6 (2%)	0	100	100
6	F	78/144 (54%)	71 (91%)	7 (9%)	0	100	100
7	J	61/71 (86%)	58 (95%)	3 (5%)	0	100	100
8	K	106/116 (91%)	105 (99%)	1 (1%)	0	100	100
9	L	43/51 (84%)	40 (93%)	3 (7%)	0	100	100
10	H	139/146 (95%)	124 (89%)	15 (11%)	0	100	100
11	I	93/114 (82%)	87 (94%)	6 (6%)	0	100	100
12	E	207/230 (90%)	197 (95%)	10 (5%)	0	100	100
13	B	953/1169 (82%)	918 (96%)	35 (4%)	0	100	100
All	All	2797/4392 (64%)	2673 (96%)	124 (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	749/1709 (44%)	738 (98%)	11 (2%)	57	77
5	C	253/276 (92%)	252 (100%)	1 (0%)	84	87
6	F	72/128 (56%)	72 (100%)	0	100	100
7	J	56/63 (89%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	98/105 (93%)	98 (100%)	0	100	100
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	76
11	I	85/101 (84%)	84 (99%)	1 (1%)	63	79
12	E	190/209 (91%)	183 (96%)	7 (4%)	30	61
13	B	846/1026 (82%)	837 (99%)	9 (1%)	65	80
All	All	2512/3790 (66%)	2481 (99%)	31 (1%)	61	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	324	SER
4	A	343	MET
4	A	430	VAL
4	A	535	SER
4	A	541	PHE
4	A	649	LEU
4	A	864	CYS
4	A	950	ASN
4	A	981	MET
4	A	1049	ILE
4	A	1139	VAL
5	C	288	LEU
10	H	14	VAL
10	H	132	HIS
11	I	10	CYS
12	E	36	TYR
12	E	103	VAL
12	E	115	ILE
12	E	162	HIS
12	E	181	LYS
12	E	190	LEU
12	E	193	ILE
13	B	170	ILE
13	B	279	PHE
13	B	391	PHE
13	B	422	MET
13	B	486	LEU
13	B	670	TRP
13	B	808	VAL

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Mol	Chain	Res	Type
13	B	985	HIS
13	B	1045	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	1011	ASN
5	C	69	HIS
8	K	44	ASN
8	K	51	HIS
11	I	31	ASN
12	E	85	HIS
12	E	129	GLN
13	B	251	ASN
13	B	333	GLN
13	B	529	ASN
13	B	714	GLN
13	B	951	GLN
13	B	1039	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	7/20 (35%)	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

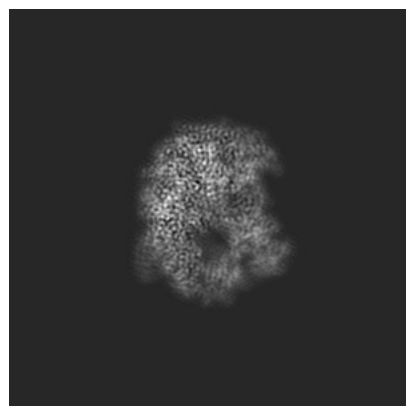
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61963. These allow visual inspection of the internal detail of the map and identification of artifacts.

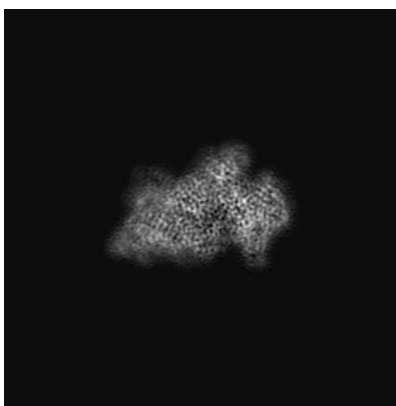
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

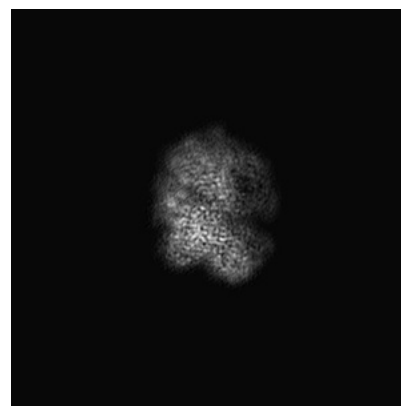
6.1.1 Primary map



X

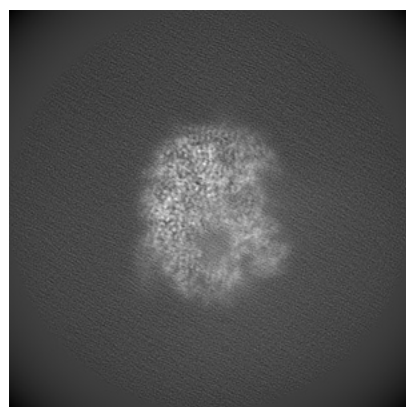


Y

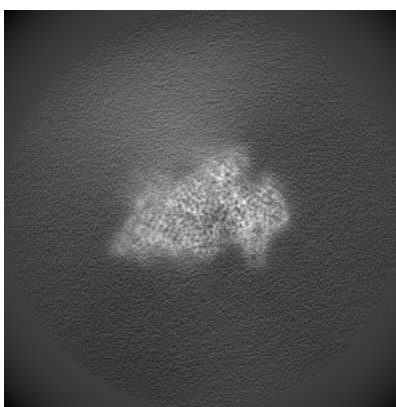


Z

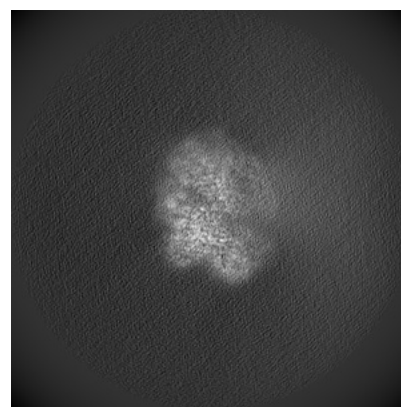
6.1.2 Raw map



X



Y



Z

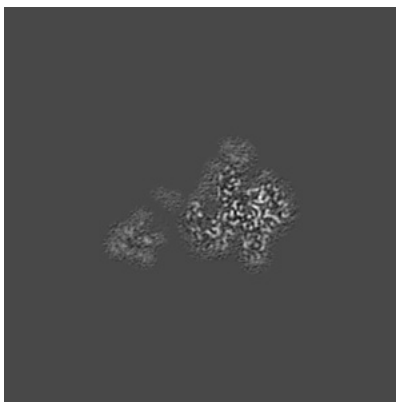
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

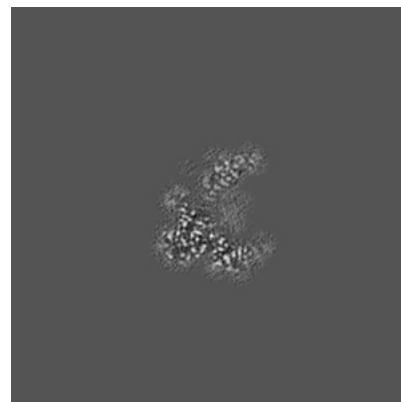
6.2.1 Primary map



X Index: 150

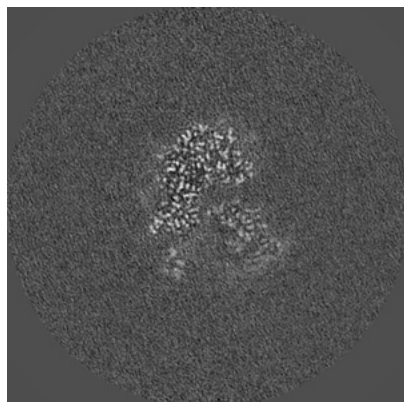


Y Index: 150

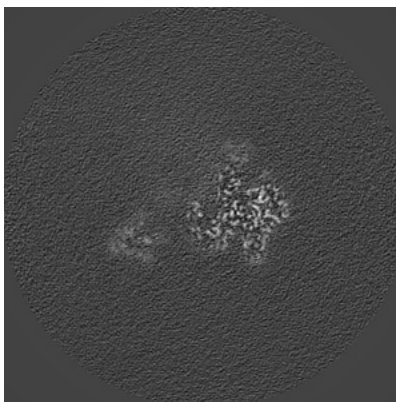


Z Index: 150

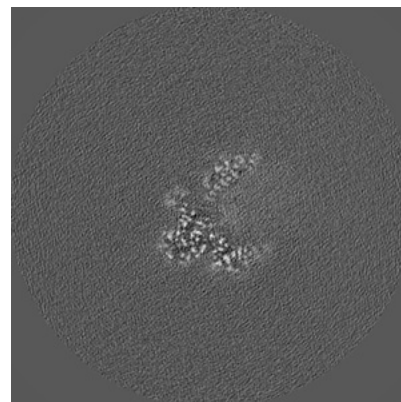
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

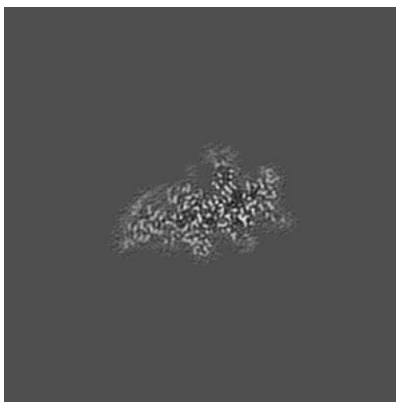
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

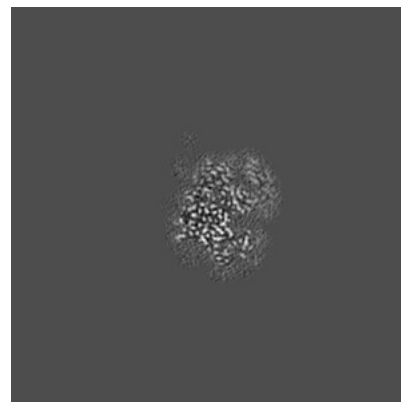
6.3.1 Primary map



X Index: 156

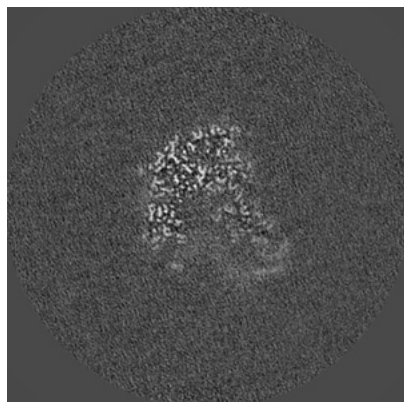


Y Index: 128

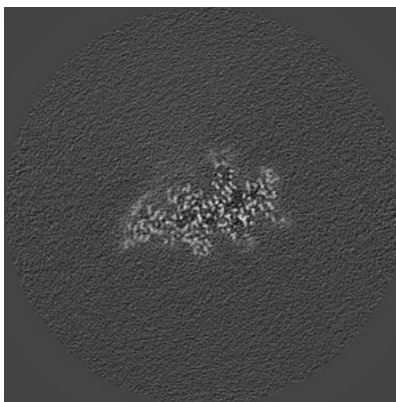


Z Index: 172

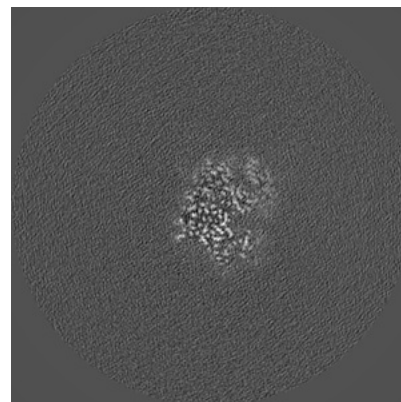
6.3.2 Raw map



X Index: 156



Y Index: 128

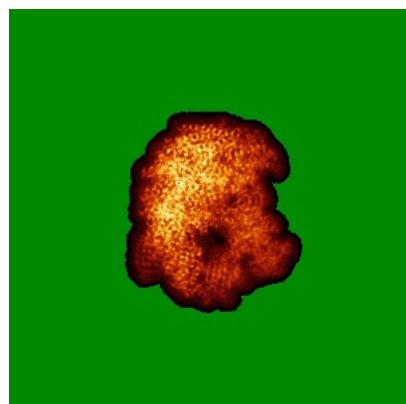


Z Index: 172

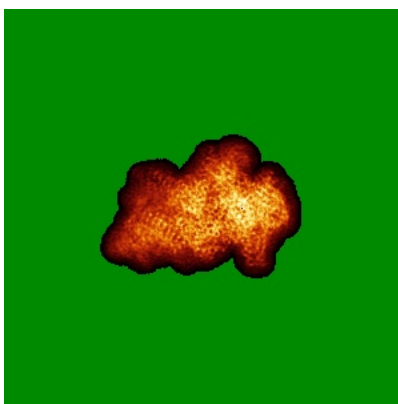
The images above show the largest variance slices of the map in three orthogonal directions.

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

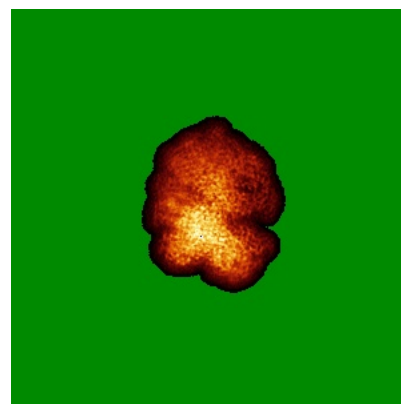
6.4.1 Primary map



X

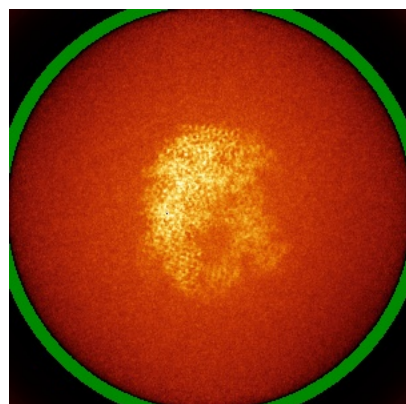


Y

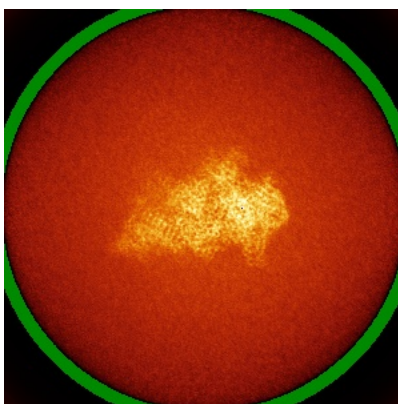


Z

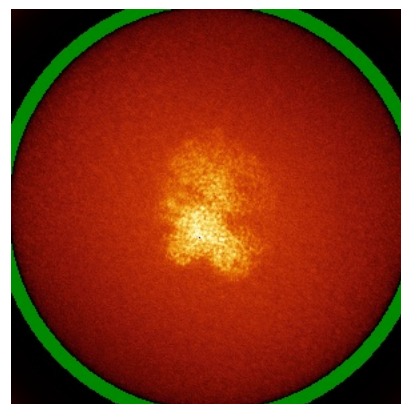
6.4.2 Raw map



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](#)

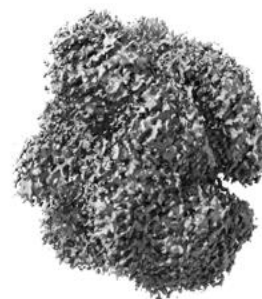
6.5.1 Primary map



X



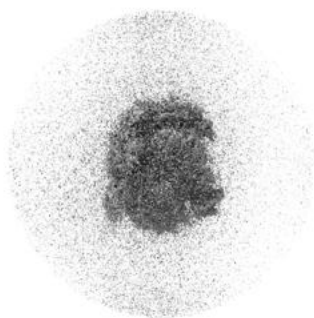
Y



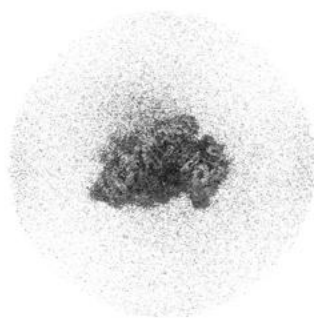
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

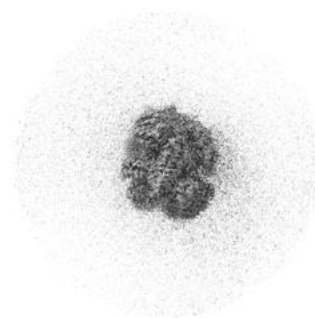
6.5.2 Raw map



X



Y



Z

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.

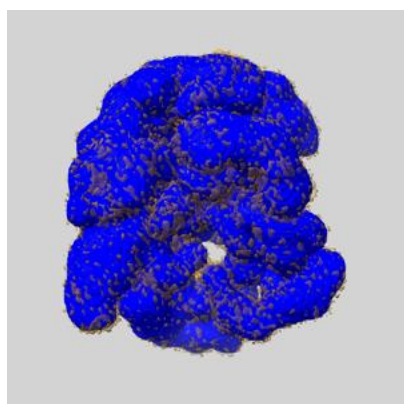
6.6 Mask visualisation [i](#)

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

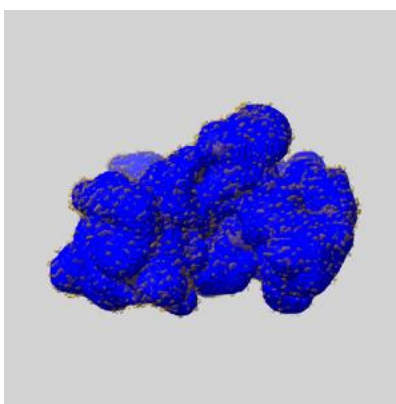
A mask typically either:

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

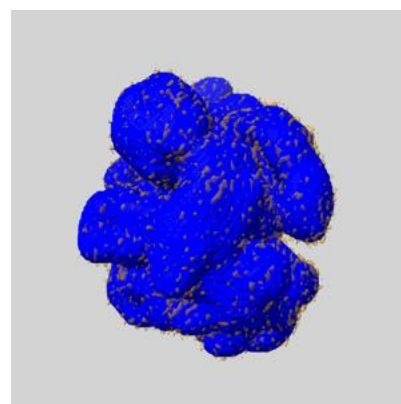
6.6.1 emd_61963_msk_1.map [i](#)



X



Y

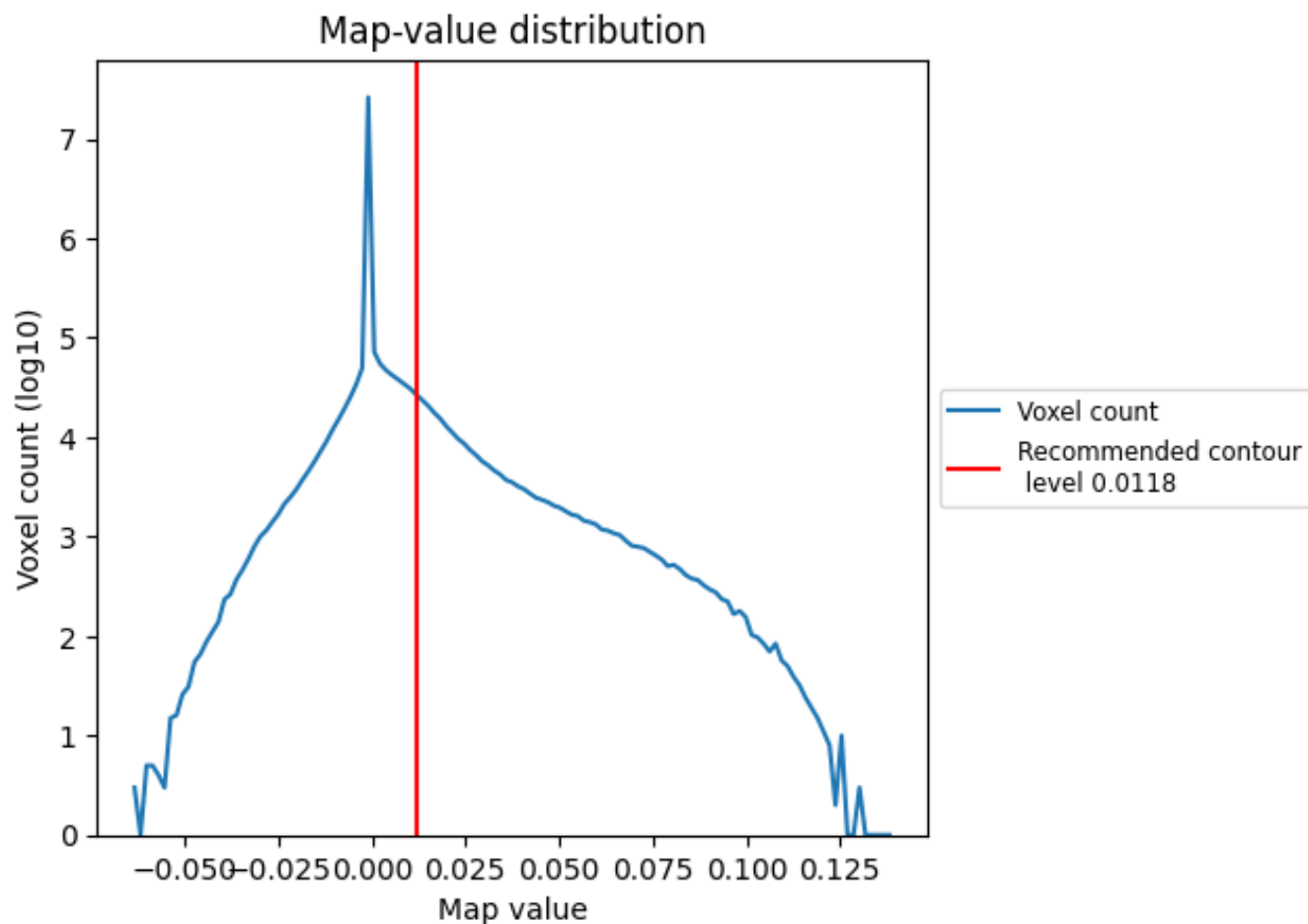


Z

7 Map analysis [i](#)

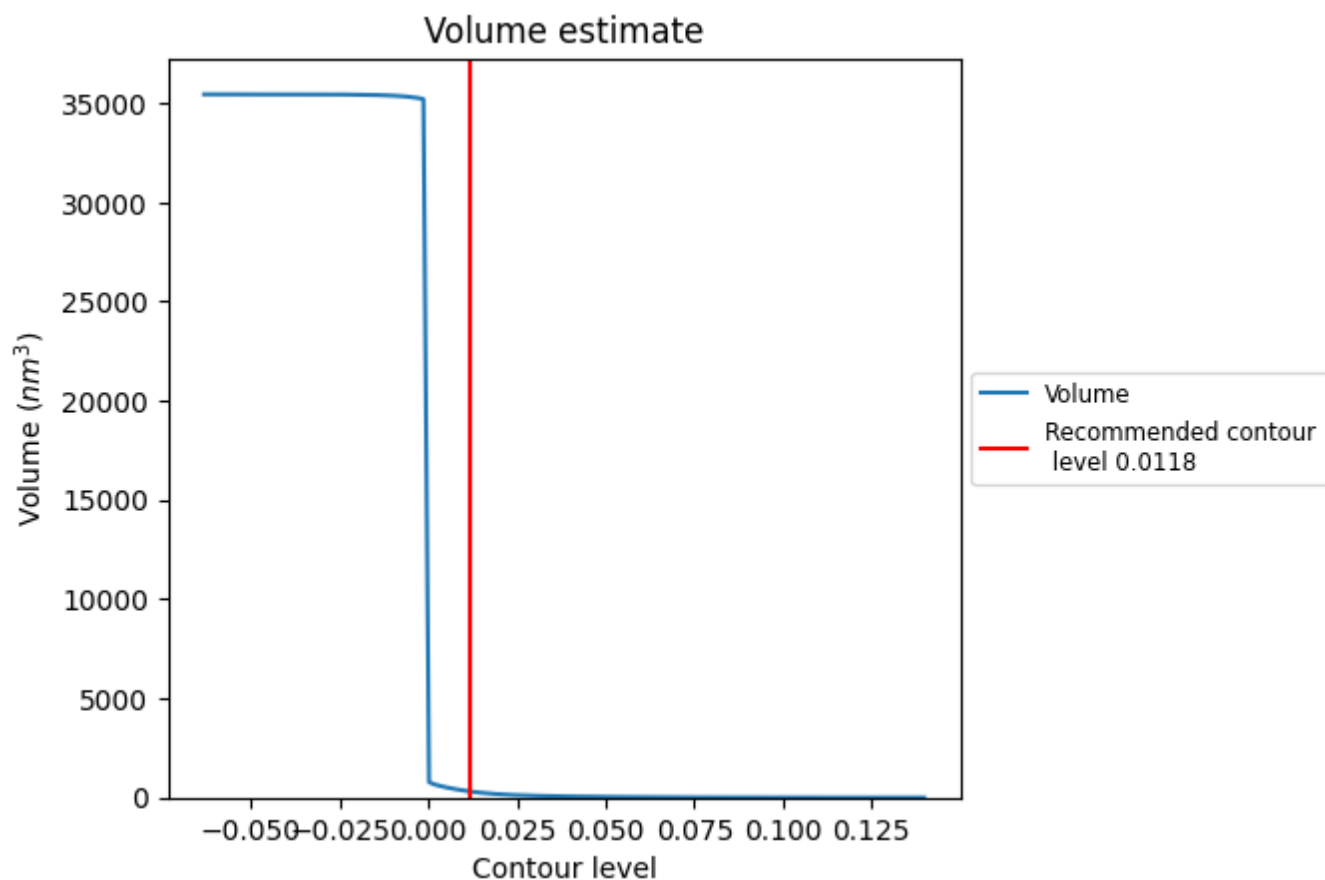
This section contains the results of statistical analysis of the map.

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.

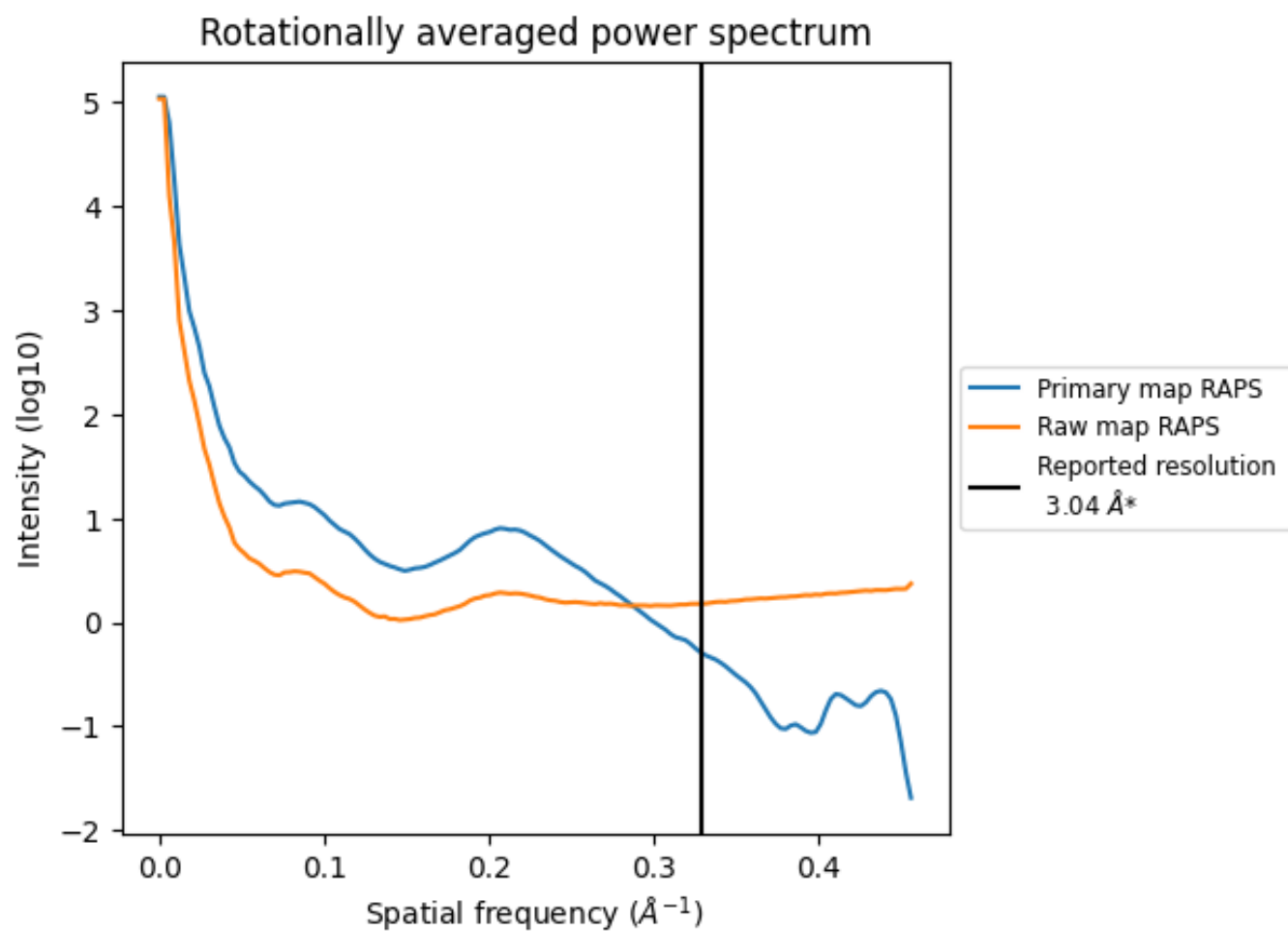
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm^3 ; this corresponds to an approximate mass of 277 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 ⓘ

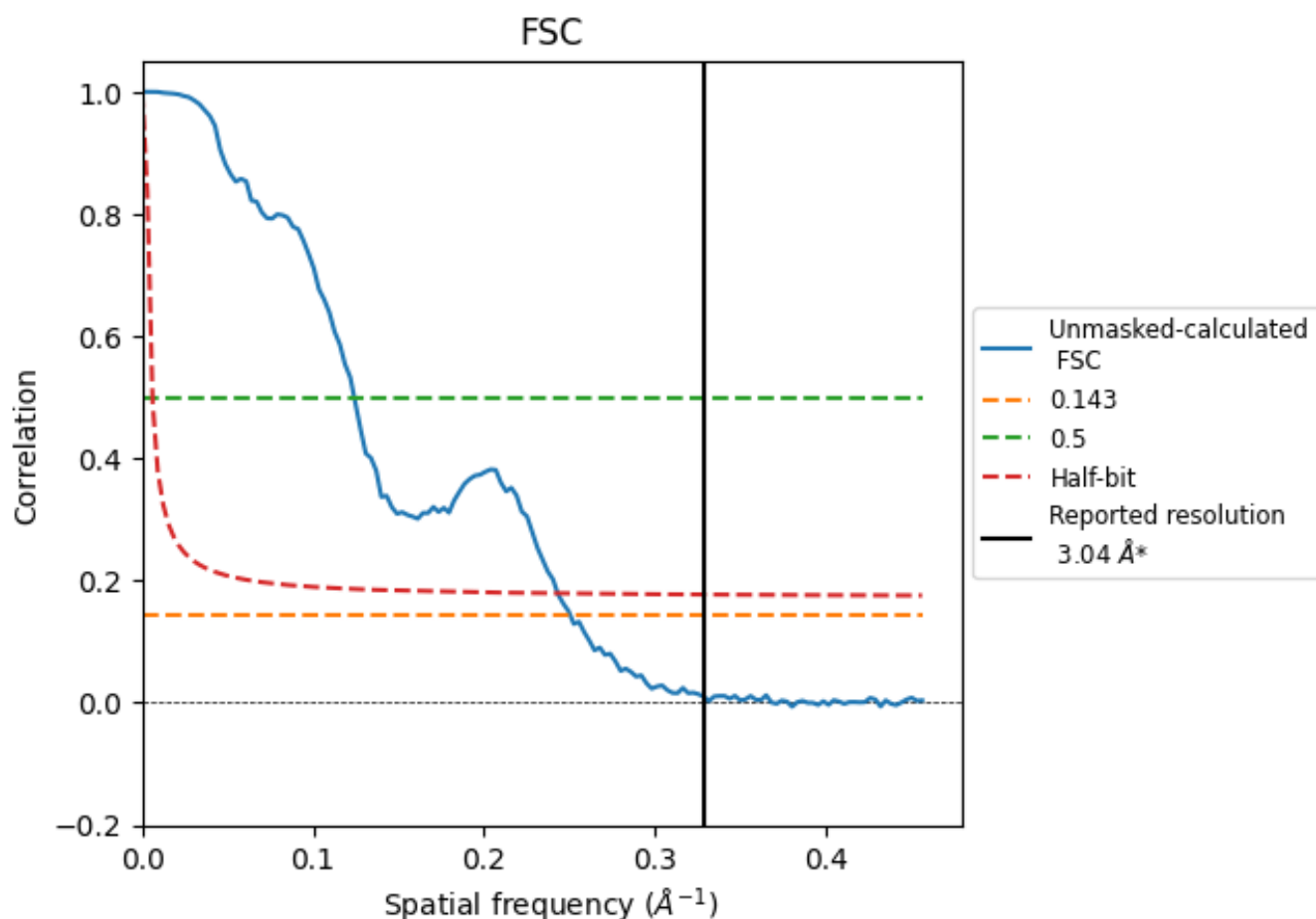


*Reported resolution corresponds to spatial frequency of 0.329 \AA^{-1}

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 0.329 Å⁻¹

8.2 Resolution estimates [i](#)

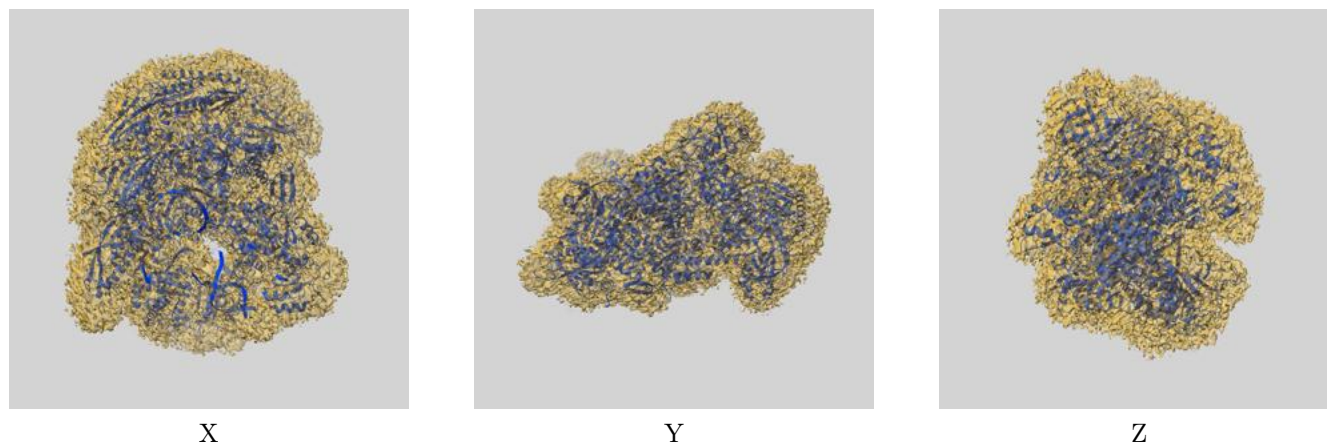
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	8.06	4.11

*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 3.99 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

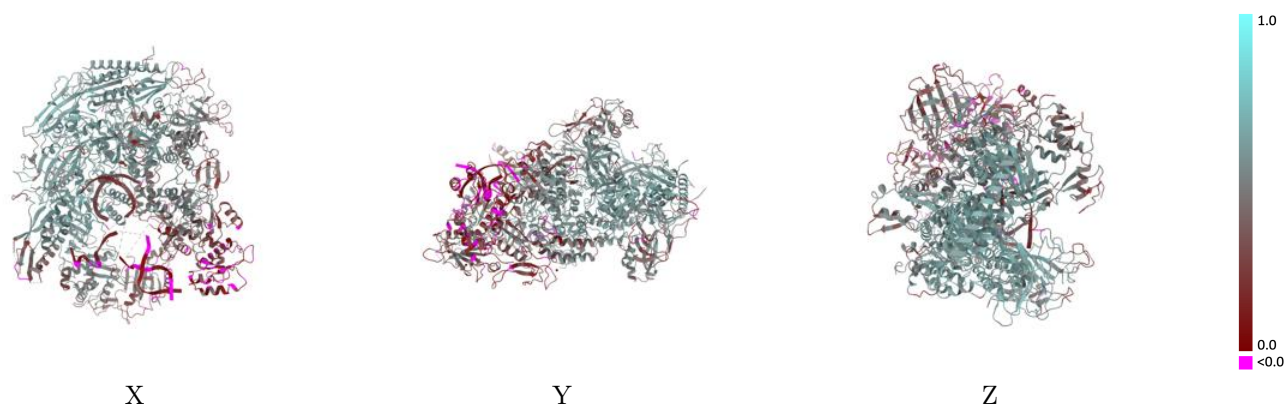
This section contains information regarding the fit between EMDB map EMD-61963 and PDB model 9K13. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



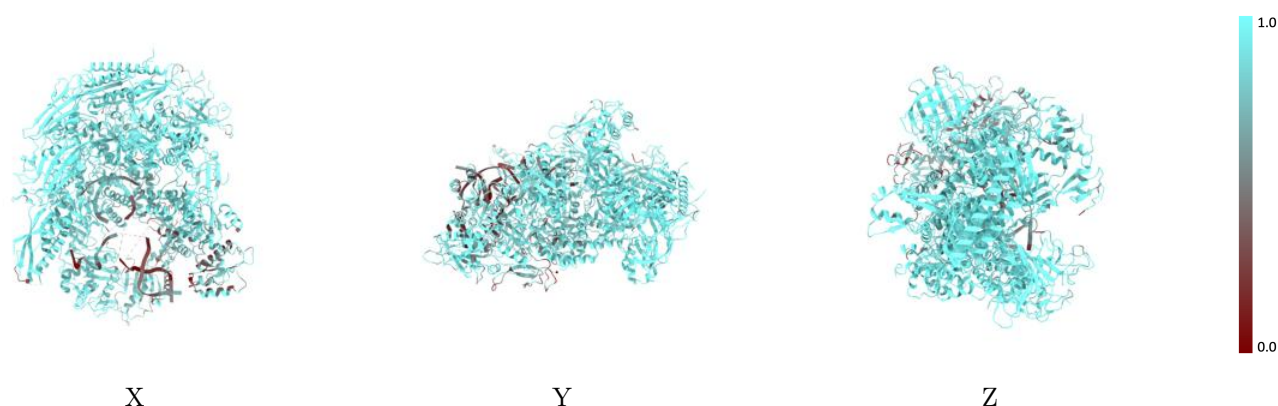
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



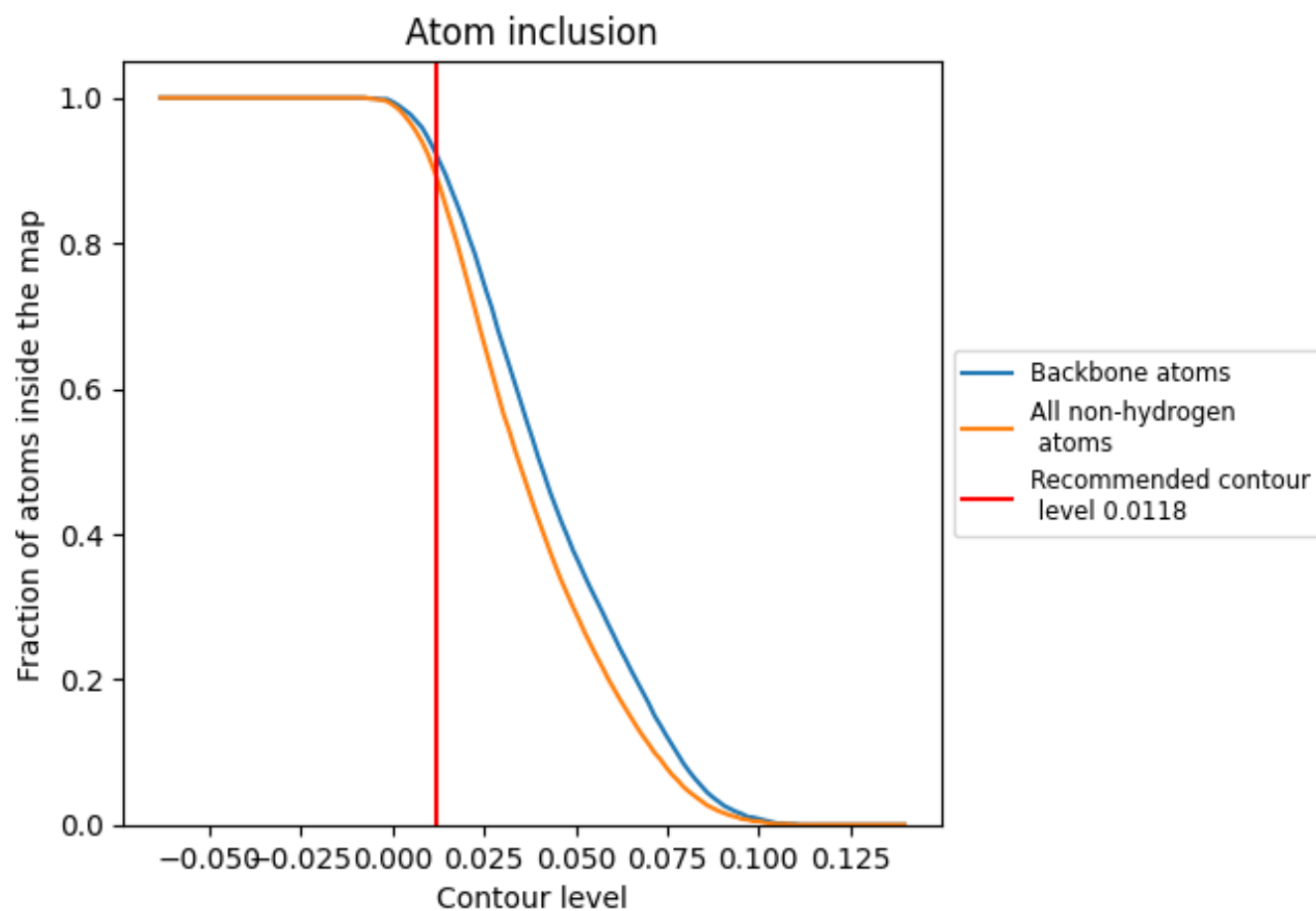
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.4610
A	 0.8920	 0.4390
B	 0.9660	 0.5570
C	 0.9810	 0.5760
E	 0.7110	 0.1790
F	 0.9110	 0.4150
H	 0.9070	 0.3890
I	 0.6900	 0.2480
J	 0.9960	 0.6170
K	 0.9550	 0.5640
L	 0.9630	 0.5310
N	 0.4160	 0.0840
P	 0.6080	 0.2980
T	 0.3650	 0.1120

