



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:48 AM UTC

PDB ID : 9FPY / pdb_00009fpy
EMDB ID : EMD-50639
Title : Structure of the complete Vaccinia DNA-dependent RNA polymerase complex assembly intermediate 3
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2024-06-14
Resolution : 2.40 Å(reported)
Based on initial model : 6rfl

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:

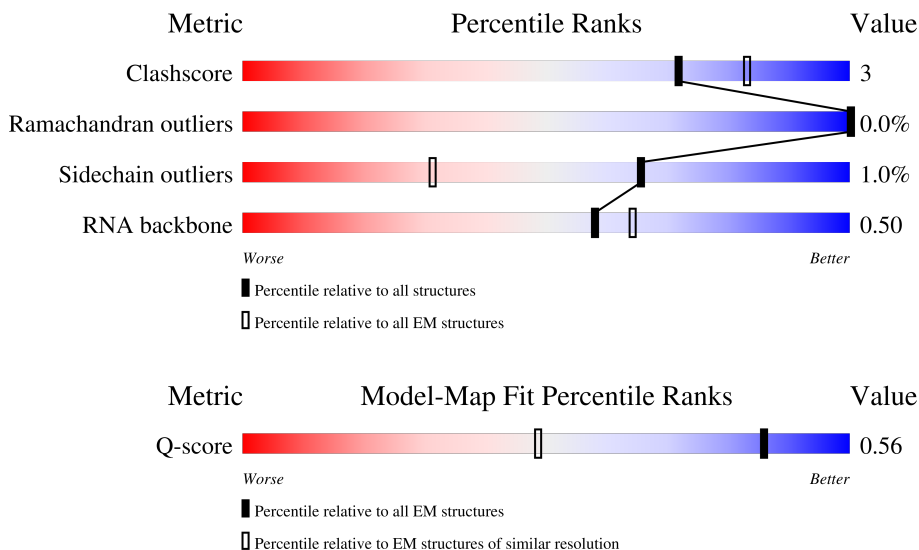
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.40 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	5628 (1.90 - 2.90)

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	C	305	
2	E	185	
3	G	161	

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Mol	Chain	Length	Quality of chain
4	J	63	
5	Q	129	
5	R	129	
6	U	72	
7	A	1286	
8	B	1164	
9	F	164	
10	I	795	
11	S	259	
12	Y	631	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 81451 atoms, of which 40427 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 DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	C	304	4946	1608	2462	399	464	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ASN	ASP	variant	UNP P21087

- Molecule 2 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	E	184	3041	966	1546	248	276	5	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	G	155	2404	766	1192	200	240	6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	J	61	1019	310	529	88	88	4	0	0

- Molecule 5 is a protein called Core protein OPG073.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	Q	124	2011	663	995	158	190	5	0	0
5	R	129	2109	689	1053	165	197	5	1	0

- Molecule 6 is a RNA chain called URQ-UUG1-1 tRNA (72-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	U	72	2405	714	808	275	533	75	3	0

- Molecule 7 is a protein called DNA-directed RNA polymerase 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	A	1268	20480	6556	10292	1679	1908	45	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P20504
A	489	GLU	LYS	variant	UNP P20504
A	1015	LYS	ARG	variant	UNP P20504

- Molecule 8 is a protein called DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	B	1129	18210	5794	9119	1554	1695	48	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	variant	UNP P68694
B	343	PHE	TYR	variant	UNP P68694

- Molecule 9 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	F	111	1844	588	926	158	169	3	0	0

- Molecule 10 is a protein called RNA polymerase-associated transcription-specificity factor RAP94.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	I	671	11277	3678	5660	898	1020	21	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
11	S	177	2846	903	1397	234	305	3	4	0	0

- Molecule 12 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	Y	545	8842	2819	4448	745	807	23	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	329	ASP	ASN	variant	UNP P20637

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
13	U	2	2	2	0
13	A	1	1	1	0
13	Y	1	1	1	0

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
14	A	2	2	2	0
14	B	1	1	1	0
14	I	1	1	1	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
15	A	2	2	2	0
15	B	2	2	2	0

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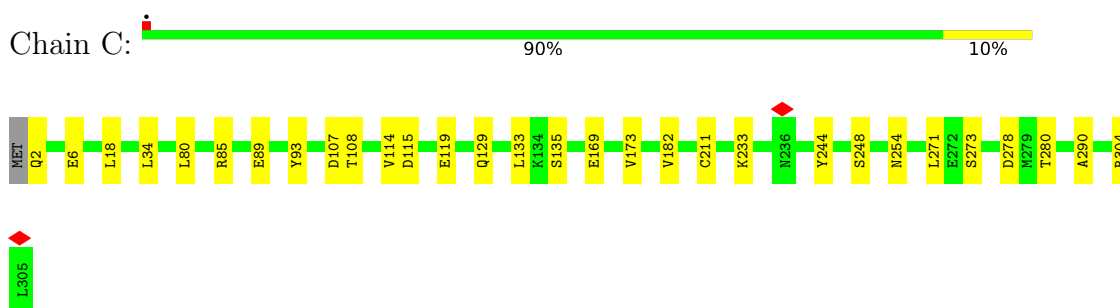
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Mol	Chain	Residues	Atoms		AltConf
15	F	1	Total 1	O 1	0
15	I	1	Total 1	O 1	0
15	S	2	Total 2	O 2	0
15	Y	1	Total 1	O 1	0

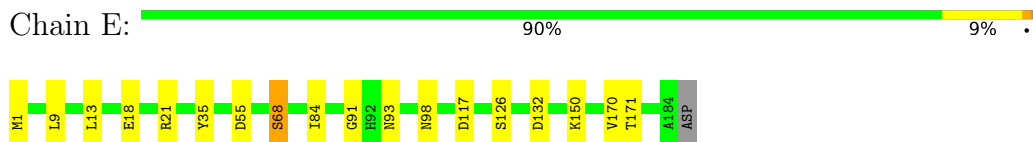
3 Residue-property plots [i](#)

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.

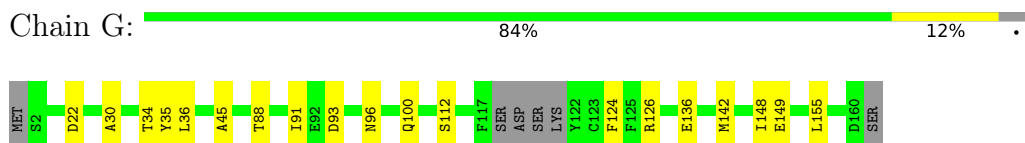
- Molecule 1: DNA-directed RNA polymerase 35 kDa subunit



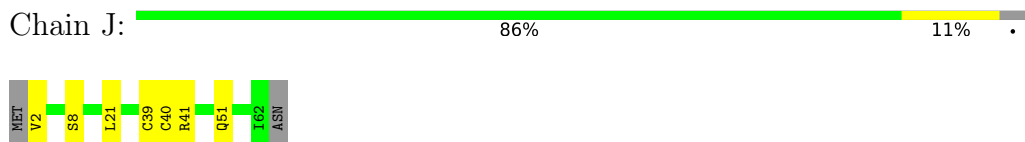
- Molecule 2: DNA-directed RNA polymerase 22 kDa subunit



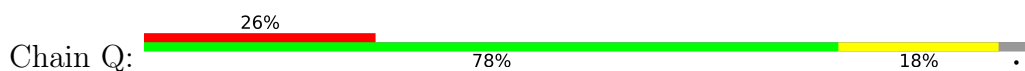
- Molecule 3: DNA-directed RNA polymerase 18 kDa subunit

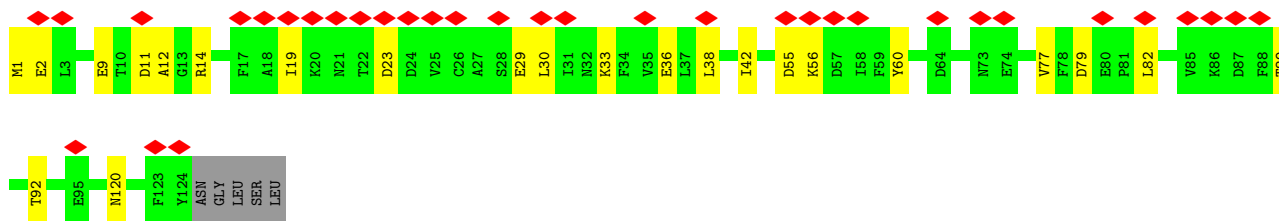


- Molecule 4: DNA-directed RNA polymerase 7 kDa subunit

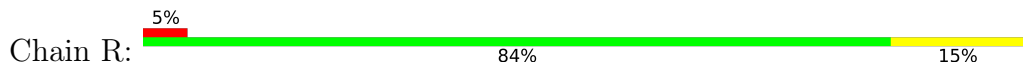


- Molecule 5: Core protein OPG073

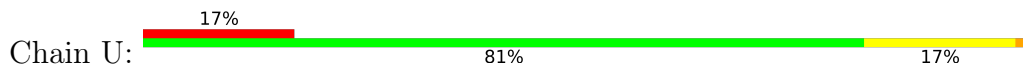




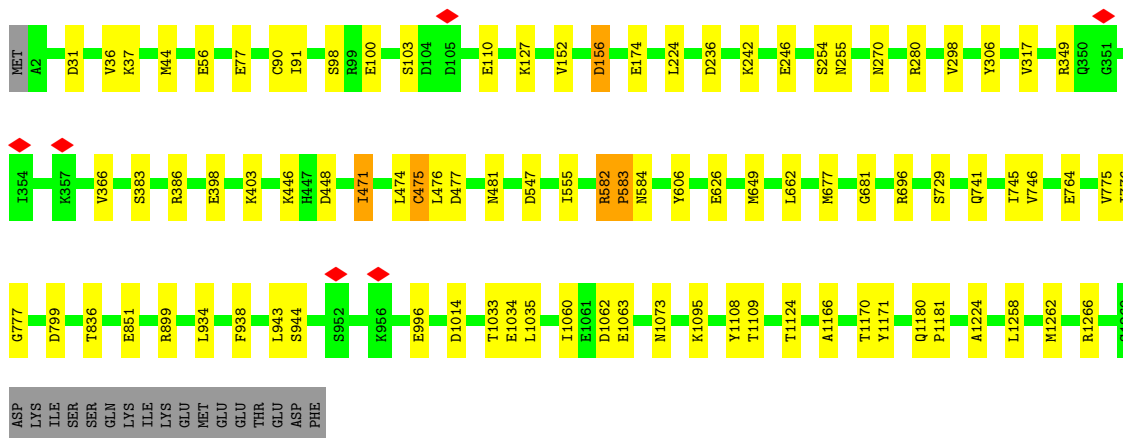
- Molecule 5: Core protein OPG073



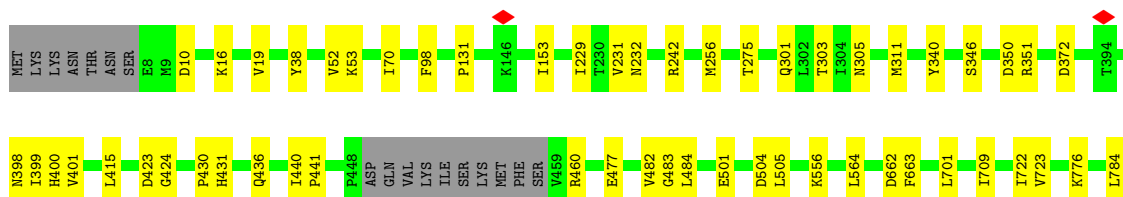
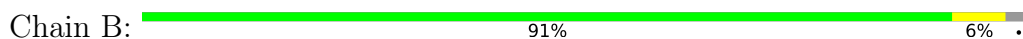
- Molecule 6: URQ-UUG1-1 tRNA (72-MER)



- Molecule 7: DNA-directed RNA polymerase 147 kDa polypeptide

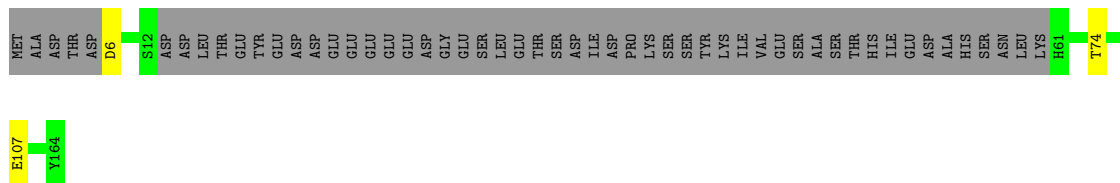


- Molecule 8: DNA-directed RNA polymerase 133 kDa polypeptide

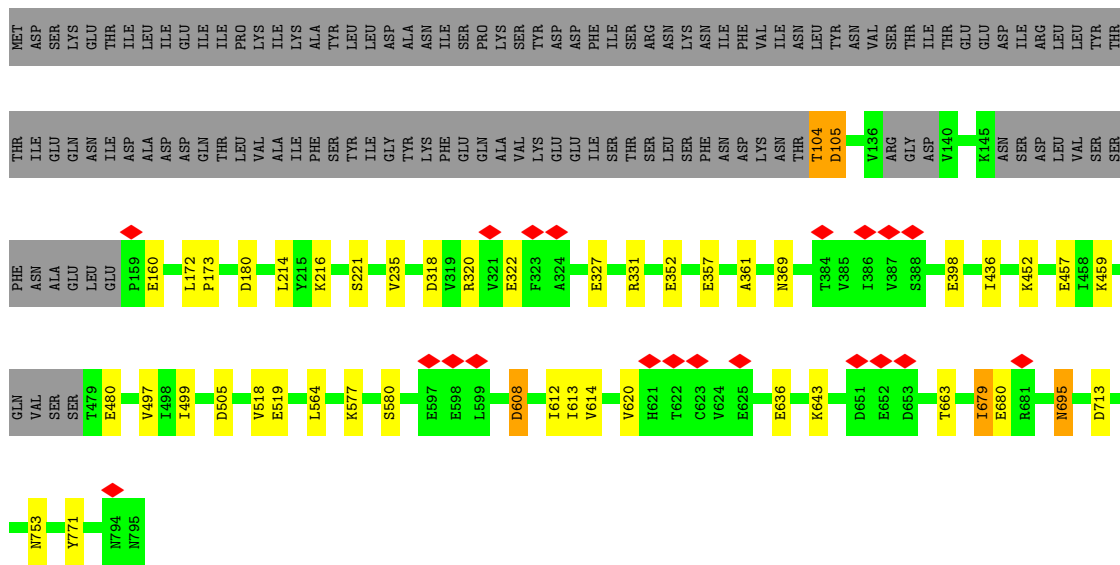




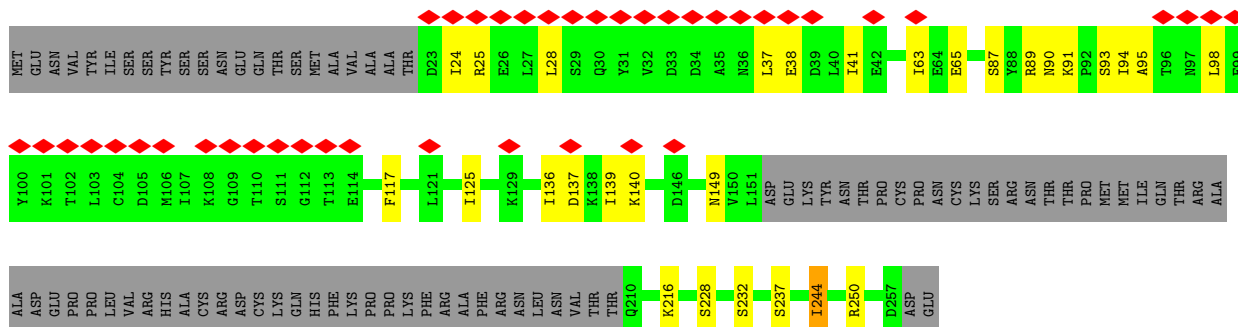
• Molecule 9: DNA-directed RNA polymerase 19 kDa subunit



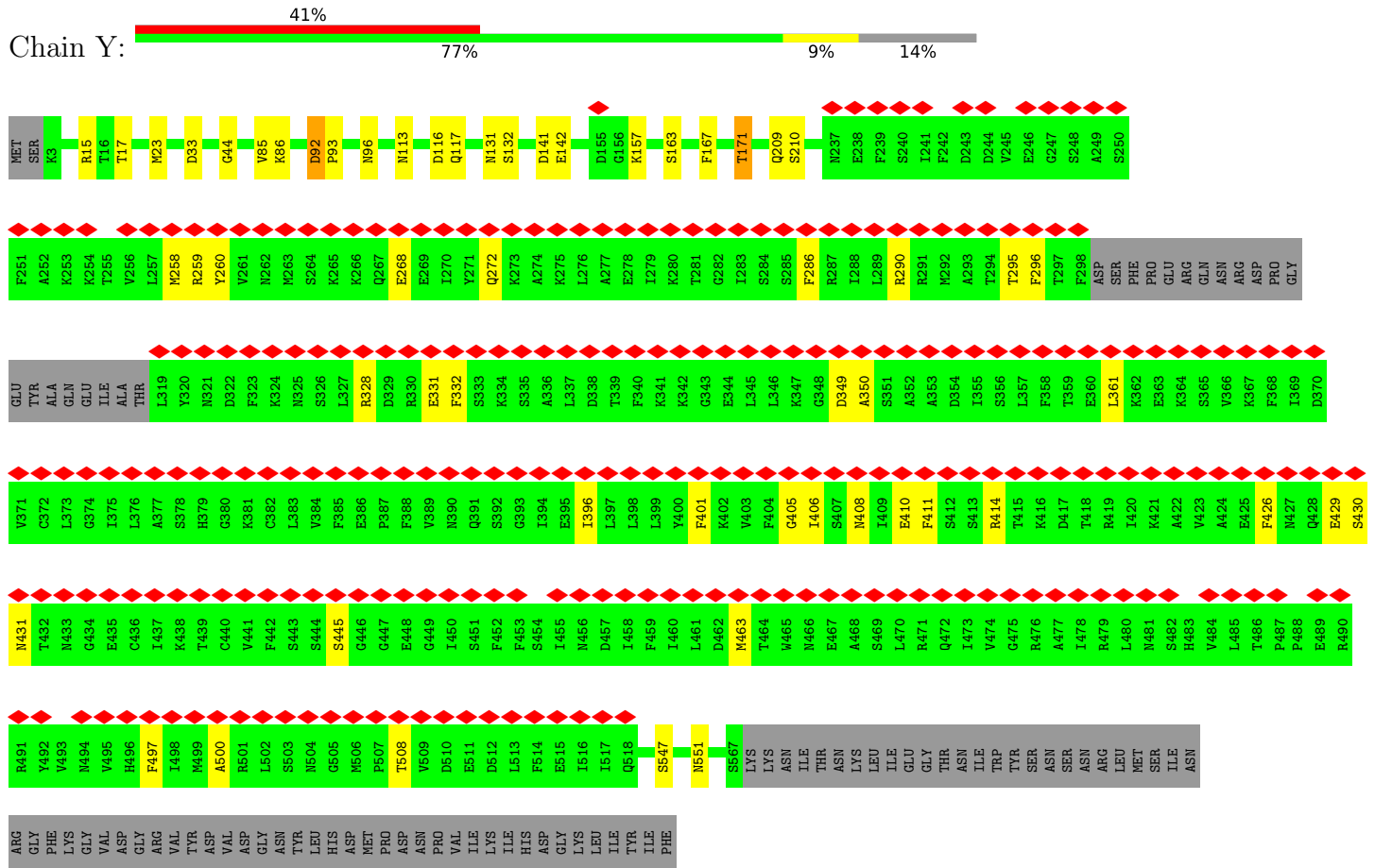
• Molecule 10: RNA polymerase-associated transcription-specificity factor RAP94



• Molecule 11: DNA-directed RNA polymerase 30 kDa polypeptide



• Molecule 12: Nucleoside triphosphatase I



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96385	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.941	Depositor
Minimum map value	-0.465	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	308.47998, 308.47998, 308.47998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9639999, 0.9639999, 0.9639999	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, 5MU, MG, OMC, 1MA, SEP

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	C	0.11	0/2540	0.27	0/3440
2	E	0.12	0/1522	0.28	0/2069
3	G	0.14	0/1230	0.29	0/1668
4	J	0.14	0/494	0.30	0/663
5	Q	0.10	0/1038	0.25	0/1406
5	R	0.12	0/1081	0.31	0/1463
6	U	0.08	0/1710	0.19	0/2661
7	A	0.13	0/10394	0.30	0/14052
8	B	0.12	0/9281	0.27	0/12537
9	F	0.14	0/933	0.32	0/1252
10	I	0.12	0/5748	0.27	0/7775
11	S	0.12	0/1442	0.35	0/1938
12	Y	0.09	0/4478	0.24	0/6029
All	All	0.12	0/41891	0.28	0/56953

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	582	ARG	Peptide

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	C	2484	2462	2470	18	0
2	E	1495	1546	1548	11	0
3	G	1212	1192	1194	14	0
4	J	490	529	530	5	0
5	Q	1016	995	1007	19	0
5	R	1056	1053	1056	20	0
6	U	1597	808	808	3	0
7	A	10188	10292	10312	58	0
8	B	9091	9119	9146	48	0
9	F	918	926	930	4	0
10	I	5617	5660	5674	38	0
11	S	1449	1397	1396	21	0
12	Y	4394	4448	4461	35	0
13	A	1	0	0	0	0
13	U	2	0	0	0	0
13	Y	1	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	I	1	0	0	0	0
15	A	2	0	0	1	0
15	B	2	0	0	0	0
15	F	1	0	0	0	0
15	I	1	0	0	0	0
15	S	2	0	0	0	0
15	Y	1	0	0	0	0
All	All	41024	40427	40532	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (275) 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)
3:G:148:ILE:HD12	3:G:148:ILE:O	1.76	0.85
7:A:446:LYS:NZ	7:A:547:ASP:OD1	2.11	0.84
10:I:636:GLU:N	10:I:636:GLU:OE1	2.10	0.84
7:A:56:GLU:OE1	7:A:56:GLU:N	2.10	0.83
7:A:98:SER:OG	7:A:100:GLU:OE1	1.96	0.83
7:A:110:GLU:OE1	7:A:110:GLU:N	2.14	0.81
10:I:104:THR:O	10:I:104:THR:OG1	2.01	0.77
8:B:1058:ARG:NH2	8:B:1059:ASP:OD1	2.18	0.76
5:R:64:ASP:O	5:R:67:SER:OG	2.03	0.76
7:A:649:MET:HG2	7:A:662:LEU:HD11	1.68	0.75
8:B:372:ASP:OD1	11:S:250:ARG:NH1	2.19	0.75
10:I:398:GLU:O	12:Y:547:SER:OG	2.05	0.75
1:C:89:GLU:N	1:C:89:GLU:OE1	2.20	0.74
8:B:477:GLU:N	8:B:477:GLU:OE1	2.21	0.74
5:R:39:SER:O	5:R:109:LYS:NZ	2.20	0.74
10:I:160:GLU:N	10:I:160:GLU:OE2	2.19	0.74
12:Y:406:ILE:O	12:Y:408:ASN:ND2	2.20	0.74
5:R:73:ASN:ND2	10:I:459:LYS:O	2.21	0.73
8:B:784:LEU:O	10:I:577:LYS:NZ	2.19	0.73
12:Y:268:GLU:O	12:Y:272:GLN:NE2	2.21	0.72
3:G:22:ASP:OD1	7:A:1266:ARG:NH2	2.22	0.72
7:A:91:ILE:O	7:A:91:ILE:HG23	1.88	0.72
5:Q:11:ASP:OD2	5:Q:89:THR:OG1	2.07	0.72
11:S:94:ILE:HG22	11:S:95:ALA:H	1.53	0.72
12:Y:286:PHE:O	12:Y:290:ARG:NH2	2.24	0.71
1:C:2:GLN:NE2	1:C:6:GLU:OE2	2.23	0.70
6:U:35:U:N3	12:Y:163:SER:OG	2.24	0.70
3:G:30:ALA:O	3:G:34:THR:HG22	1.91	0.70
12:Y:167:PHE:O	12:Y:171:THR:OG1	2.10	0.70
4:J:21:LEU:O	4:J:21:LEU:HD23	1.92	0.69
11:S:37:LEU:CD1	11:S:41:ILE:HD11	2.22	0.69
11:S:65:GLU:N	11:S:65:GLU:OE1	2.26	0.69
5:R:42:ILE:CG2	5:R:106:ILE:HD11	2.23	0.68
10:I:608:ASP:OD1	10:I:608:ASP:N	2.22	0.68
10:I:620:VAL:O	10:I:620:VAL:HG22	1.94	0.68
12:Y:410:GLU:OE1	12:Y:414:ARG:NH2	2.27	0.68
7:A:156:ASP:OD1	7:A:156:ASP:N	2.26	0.67
8:B:776:LYS:NZ	8:B:848:ASP:OD2	2.27	0.66
11:S:244:ILE:HD12	11:S:244:ILE:O	1.95	0.66
12:Y:116:ASP:OD1	12:Y:117:GLN:N	2.28	0.66
5:Q:9:GLU:O	5:Q:92:THR:OG1	2.14	0.66
8:B:398:ASN:O	8:B:401:VAL:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:270:ASN:O	15:A:1401:HOH:O	2.13	0.65
12:Y:92:ASP:O	12:Y:96:ASN:ND2	2.29	0.65
5:Q:9:GLU:OE1	5:Q:92:THR:OG1	2.10	0.65
8:B:709:ILE:O	8:B:709:ILE:HG22	1.96	0.64
8:B:303:THR:OG1	8:B:305:ASN:O	2.14	0.64
5:Q:38:LEU:O	5:Q:42:ILE:N	2.28	0.63
11:S:139:ILE:HG22	11:S:140:LYS:H	1.63	0.63
10:I:614:VAL:HG12	10:I:614:VAL:O	1.99	0.62
2:E:91:GLY:O	2:E:150:LYS:NZ	2.34	0.61
7:A:31:ASP:O	7:A:31:ASP:OD2	2.18	0.61
7:A:582:ARG:O	7:A:584:ASN:N	2.33	0.61
7:A:317:VAL:HG12	7:A:317:VAL:O	2.00	0.61
7:A:606:TYR:OH	7:A:626:GLU:OE2	2.19	0.61
5:R:86:LYS:N	5:R:86:LYS:HE2	2.16	0.60
5:Q:120:ASN:ND2	5:R:100:GLU:OE2	2.35	0.60
7:A:127:LYS:HG3	7:A:127:LYS:O	2.02	0.60
3:G:34:THR:HG23	3:G:35:TYR:CD2	2.37	0.60
3:G:149:GLU:OE2	3:G:149:GLU:O	2.20	0.58
8:B:431:HIS:HB3	8:B:701:LEU:HD21	1.83	0.58
5:Q:77:VAL:HG22	5:Q:79:ASP:OD1	2.03	0.58
4:J:41:ARG:NH2	8:B:940:ALA:O	2.36	0.58
7:A:386:ARG:NH2	7:A:448:ASP:OD2	2.36	0.58
8:B:460:ARG:NH2	8:B:482:VAL:O	2.37	0.58
10:I:612:ILE:HD12	10:I:612:ILE:H	1.69	0.58
7:A:477:ASP:O	7:A:481:ASN:ND2	2.38	0.57
5:R:111:ASN:O	5:R:111:ASN:ND2	2.38	0.57
12:Y:411:PHE:O	12:Y:445:SER:OG	2.22	0.57
10:I:327:GLU:OE2	10:I:327:GLU:N	2.24	0.57
8:B:1029:ARG:NH1	8:B:1048:GLY:O	2.38	0.56
4:J:2:VAL:HG12	4:J:2:VAL:O	2.05	0.56
5:Q:55:ASP:OD1	5:Q:56:LYS:N	2.37	0.56
7:A:242:LYS:O	7:A:246:GLU:HG2	2.04	0.56
7:A:475:CYS:SG	7:A:476:LEU:N	2.78	0.56
12:Y:85:VAL:HG22	12:Y:86:LYS:H	1.71	0.56
8:B:887:THR:HG22	8:B:887:THR:O	2.06	0.56
12:Y:331:GLU:N	12:Y:331:GLU:OE1	2.39	0.56
8:B:722:ILE:HD12	8:B:723:VAL:HG23	1.87	0.56
1:C:6:GLU:N	1:C:6:GLU:OE1	2.39	0.56
7:A:943:LEU:O	7:A:944:SER:OG	2.13	0.55
8:B:10:ASP:OD1	8:B:10:ASP:N	2.40	0.55
5:R:25:VAL:HG21	5:R:29:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:NH1	1:C:93:TYR:O	2.39	0.55
12:Y:429:GLU:O	12:Y:430:SER:OG	2.21	0.55
10:I:452:LYS:HD2	10:I:452:LYS:C	2.32	0.54
7:A:127:LYS:O	7:A:127:LYS:CG	2.56	0.54
8:B:52:VAL:HG23	8:B:53:LYS:H	1.73	0.54
8:B:423:ASP:OD1	8:B:424:GLY:N	2.40	0.54
5:R:25:VAL:HG11	5:R:29:GLU:OE2	2.08	0.54
8:B:662:ASP:OD1	8:B:663:PHE:N	2.41	0.54
5:R:42:ILE:HG21	5:R:106:ILE:HD11	1.90	0.53
12:Y:33:ASP:OD1	12:Y:33:ASP:N	2.41	0.53
12:Y:131:ASN:OD1	12:Y:132:SER:N	2.42	0.53
7:A:1060:ILE:N	7:A:1060:ILE:HD12	2.23	0.53
2:E:21:ARG:NH2	2:E:55:ASP:OD2	2.41	0.53
8:B:796:ASN:OD1	8:B:796:ASN:N	2.40	0.53
7:A:934:LEU:O	7:A:1171:TYR:OH	2.27	0.53
8:B:556:LYS:NZ	8:B:564:LEU:O	2.41	0.53
10:I:361:ALA:O	10:I:369:ASN:ND2	2.43	0.52
11:S:37:LEU:HD13	11:S:41:ILE:HD11	1.91	0.52
7:A:851:GLU:OE1	7:A:899:ARG:NE	2.42	0.52
10:I:713:ASP:N	10:I:713:ASP:OD1	2.41	0.52
10:I:663:THR:HG23	10:I:680:GLU:OE1	2.10	0.52
5:R:25:VAL:HG22	5:R:26:CYS:H	1.75	0.52
7:A:174:GLU:OE1	7:A:174:GLU:N	2.42	0.51
7:A:799:ASP:OD1	11:S:216:LYS:NZ	2.43	0.51
10:I:695:ASN:OD1	10:I:695:ASN:N	2.43	0.51
11:S:24:ILE:HD13	11:S:117:PHE:HE2	1.75	0.51
10:I:457:GLU:OE1	10:I:457:GLU:N	2.43	0.51
7:A:91:ILE:O	7:A:91:ILE:CG2	2.57	0.51
3:G:148:ILE:HD12	3:G:148:ILE:C	2.35	0.51
5:R:20:LYS:HD2	5:R:20:LYS:C	2.36	0.51
7:A:1014:ASP:O	7:A:1073:ASN:ND2	2.43	0.51
5:Q:1:MET:HE3	5:Q:1:MET:N	2.26	0.51
4:J:39:CYS:SG	4:J:40:CYS:N	2.83	0.51
9:F:107:GLU:O	9:F:107:GLU:OE1	2.28	0.50
3:G:136:GLU:C	3:G:136:GLU:OE1	2.54	0.50
8:B:52:VAL:HG23	8:B:53:LYS:N	2.26	0.50
1:C:119:GLU:OE1	1:C:119:GLU:N	2.43	0.50
12:Y:258:MET:SD	12:Y:259:ARG:N	2.85	0.49
10:I:753:ASN:O	10:I:753:ASN:ND2	2.45	0.49
1:C:233:LYS:O	1:C:244:TYR:N	2.41	0.49
5:Q:33:LYS:NZ	5:Q:36:GLU:OE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:430:PRO:O	8:B:436:GLN:NE2	2.45	0.49
2:E:1:MET:HG3	2:E:84:ILE:HD12	1.93	0.49
1:C:278:ASP:OD2	1:C:280:THR:OG1	2.22	0.49
8:B:399:ILE:HG22	8:B:400:HIS:H	1.78	0.48
12:Y:426:PHE:O	12:Y:431:ASN:ND2	2.47	0.48
2:E:18:GLU:OE1	2:E:35:TYR:OH	2.29	0.48
7:A:996:GLU:O	7:A:1095:LYS:NZ	2.45	0.48
9:F:107:GLU:OE1	9:F:107:GLU:C	2.56	0.48
3:G:36:LEU:O	3:G:45:ALA:O	2.31	0.48
10:I:614:VAL:O	10:I:614:VAL:CG1	2.61	0.48
1:C:129:GLN:OE1	4:J:51:GLN:NE2	2.46	0.48
7:A:398:GLU:O	7:A:403:LYS:NZ	2.39	0.48
12:Y:328:ARG:HH12	12:Y:396:ILE:HG23	1.79	0.48
12:Y:463:MET:N	12:Y:463:MET:HE2	2.29	0.48
7:A:349:ARG:NH1	10:I:357:GLU:OE1	2.43	0.47
7:A:1124:THR:O	7:A:1124:THR:HG23	2.14	0.47
1:C:169:GLU:O	1:C:173:VAL:HG22	2.14	0.47
7:A:1180:GLN:N	7:A:1180:GLN:OE1	2.47	0.47
10:I:105:ASP:OD1	10:I:105:ASP:N	2.46	0.47
3:G:88:THR:O	3:G:100:GLN:N	2.45	0.47
7:A:776:ILE:HG23	7:A:777:GLY:H	1.79	0.47
8:B:350:ASP:OD1	8:B:351:ARG:N	2.48	0.47
9:F:6:ASP:OD1	9:F:6:ASP:C	2.57	0.47
12:Y:349:ASP:OD1	12:Y:350:ALA:N	2.44	0.47
1:C:107:ASP:OD1	1:C:108:THR:N	2.48	0.47
2:E:117:ASP:OD1	2:E:117:ASP:C	2.58	0.47
7:A:36:VAL:HG21	7:A:224:LEU:HB3	1.96	0.47
12:Y:15:ARG:NH1	12:Y:44:GLY:O	2.48	0.47
12:Y:85:VAL:HG22	12:Y:86:LYS:N	2.29	0.47
8:B:399:ILE:HG22	8:B:400:HIS:N	2.30	0.46
11:S:28:LEU:HD22	11:S:125:ILE:HD11	1.97	0.46
5:Q:14:ARG:NE	5:Q:82:LEU:HD22	2.30	0.46
5:R:45:ASP:OD2	5:R:46:GLN:N	2.48	0.46
10:I:663:THR:HG21	10:I:679:ILE:HB	1.97	0.46
6:U:15:A:H2'	6:U:58:A:H61	1.80	0.46
7:A:1033:THR:HG22	7:A:1034:GLU:N	2.30	0.46
8:B:862:THR:O	10:I:505:ASP:CB	2.64	0.46
1:C:80:LEU:HD23	1:C:80:LEU:C	2.41	0.46
7:A:298:VAL:HG12	7:A:298:VAL:O	2.14	0.46
7:A:764:GLU:OE2	8:B:1058:ARG:NH1	2.42	0.46
5:R:45:ASP:OD2	5:R:45:ASP:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:613:ILE:HD13	10:I:613:ILE:N	2.30	0.46
11:S:95:ALA:HB1	11:S:98:LEU:HD23	1.98	0.46
12:Y:141:ASP:OD1	12:Y:142:GLU:N	2.48	0.46
7:A:471:ILE:HG21	7:A:474:LEU:HD11	1.98	0.46
11:S:149:ASN:OD1	11:S:149:ASN:C	2.58	0.46
10:I:320:ARG:NH1	10:I:322:GLU:OE1	2.46	0.46
5:Q:19:ILE:HD11	5:Q:30:LEU:HD22	1.98	0.45
7:A:280:ARG:NH2	8:B:1076:ASP:OD1	2.49	0.45
12:Y:401:PHE:O	12:Y:405:GLY:N	2.49	0.45
8:B:990:PHE:O	8:B:992:GLU:N	2.48	0.45
12:Y:92:ASP:HB3	12:Y:93:PRO:HD3	1.98	0.45
5:R:25:VAL:HG22	5:R:26:CYS:N	2.31	0.45
8:B:242:ARG:HB3	10:I:739:TYR:CG	2.51	0.45
5:Q:2:GLU:N	5:Q:2:GLU:OE1	2.49	0.45
8:B:16:LYS:O	8:B:19:VAL:HG22	2.16	0.45
10:I:436:ILE:HG13	10:I:497:VAL:HG11	1.99	0.45
12:Y:157:LYS:N	12:Y:157:LYS:HD2	2.31	0.45
3:G:112:SER:OG	3:G:126:ARG:NH1	2.50	0.45
7:A:1033:THR:HG22	7:A:1034:GLU:H	1.82	0.45
7:A:696:ARG:O	8:B:346:SER:O	2.35	0.45
1:C:304:ARG:O	1:C:304:ARG:HG3	2.17	0.45
5:R:115:ILE:N	5:R:115:ILE:HD12	2.32	0.45
8:B:1067:ALA:O	8:B:1071:THR:HG22	2.17	0.44
1:C:133:LEU:HD23	1:C:133:LEU:O	2.17	0.44
9:F:74:THR:HG22	9:F:74:THR:O	2.17	0.44
11:S:93:SER:O	11:S:94:ILE:HD13	2.18	0.44
10:I:216:LYS:NZ	10:I:221:SER:OG	2.50	0.44
10:I:331:ARG:NH1	10:I:352:GLU:OE1	2.50	0.44
10:I:519:GLU:N	10:I:519:GLU:OE1	2.51	0.44
5:R:42:ILE:HB	5:R:106:ILE:HD11	1.99	0.44
12:Y:551:ASN:OD1	12:Y:551:ASN:N	2.50	0.44
5:R:12:ALA:O	5:R:85:VAL:HG11	2.17	0.44
8:B:256:MET:HE1	8:B:340:TYR:HB2	1.98	0.44
10:I:318:ASP:OD1	10:I:318:ASP:N	2.50	0.44
12:Y:295:THR:HG23	12:Y:296:PHE:CD1	2.53	0.44
5:R:106:ILE:O	5:R:107:ILE:HD13	2.18	0.43
1:C:254:ASN:HA	1:C:271:LEU:O	2.18	0.43
8:B:504:ASP:OD1	8:B:505:LEU:N	2.51	0.43
12:Y:85:VAL:O	12:Y:113:ASN:HA	2.18	0.43
5:Q:11:ASP:OD1	5:Q:12:ALA:N	2.51	0.43
7:A:677:MET:O	7:A:681:GLY:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:231:VAL:HG22	8:B:232:ASN:N	2.33	0.43
10:I:746:ASP:OD1	10:I:771:TYR:OH	2.37	0.43
11:S:90:ASN:OD1	11:S:91:LYS:N	2.41	0.43
11:S:63:ILE:HG22	11:S:65:GLU:OE1	2.19	0.43
8:B:981:SER:O	8:B:982:ASP:HB3	2.19	0.43
7:A:475:CYS:SG	7:A:477:ASP:N	2.91	0.43
5:Q:1:MET:O	5:Q:1:MET:SD	2.77	0.43
7:A:938:PHE:CD1	7:A:938:PHE:C	2.97	0.42
7:A:1062:ASP:O	7:A:1063:GLU:HB2	2.19	0.42
11:S:63:ILE:O	11:S:65:GLU:OE1	2.37	0.42
12:Y:332:PHE:HZ	12:Y:361:LEU:HD12	1.84	0.42
3:G:91:ILE:HD11	3:G:124:PHE:HB2	2.00	0.42
7:A:1258:LEU:O	7:A:1262:MET:HG3	2.19	0.42
11:S:244:ILE:O	11:S:244:ILE:CD1	2.66	0.42
11:S:139:ILE:HG22	11:S:140:LYS:N	2.32	0.42
8:B:38:TYR:OH	8:B:131:PRO:O	2.36	0.42
8:B:501:GLU:O	8:B:504:ASP:OD1	2.38	0.42
2:E:9:LEU:O	2:E:13:LEU:HG	2.20	0.42
5:R:42:ILE:CB	5:R:106:ILE:HD11	2.50	0.42
6:U:17:G:N1	6:U:54:U:O2	2.52	0.42
7:A:1035:LEU:HD12	7:A:1035:LEU:H	1.84	0.41
12:Y:258:MET:HG3	12:Y:260:TYR:CE2	2.55	0.41
7:A:254:SER:OG	7:A:255:ASN:N	2.53	0.41
10:I:564:LEU:HD12	10:I:564:LEU:N	2.35	0.41
12:Y:167:PHE:CE1	12:Y:171:THR:HG21	2.55	0.41
2:E:93:ASN:OD1	2:E:93:ASN:N	2.54	0.41
2:E:98:ASN:OD1	2:E:98:ASN:O	2.38	0.41
7:A:741:GLN:O	7:A:745:ILE:HG23	2.20	0.41
12:Y:500:ALA:O	12:Y:508:THR:OG1	2.36	0.41
5:Q:60:TYR:N	5:Q:60:TYR:CD1	2.87	0.41
8:B:440:ILE:HB	8:B:441:PRO:HD3	2.01	0.41
10:I:577:LYS:HA	10:I:580:SER:OG	2.20	0.41
1:C:115:ASP:OD1	1:C:115:ASP:C	2.63	0.41
5:Q:1:MET:HE3	5:Q:1:MET:H1	1.86	0.41
2:E:132:ASP:OD1	2:E:132:ASP:C	2.62	0.41
7:A:306:TYR:OH	8:B:1026:ALA:HB1	2.21	0.41
10:I:613:ILE:HG22	10:I:614:VAL:N	2.35	0.41
5:Q:82:LEU:HD23	5:Q:82:LEU:HA	1.95	0.41
7:A:582:ARG:O	7:A:583:PRO:C	2.64	0.41
8:B:709:ILE:O	8:B:709:ILE:CG2	2.67	0.41
12:Y:209:GLN:OE1	12:Y:210:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:SER:O	2:E:68:SER:OG	2.35	0.41
3:G:142:MET:N	3:G:155:LEU:O	2.44	0.41
5:Q:29:GLU:O	5:Q:33:LYS:HG2	2.20	0.41
2:E:170:VAL:HG23	2:E:171:THR:HG23	2.03	0.41
3:G:148:ILE:O	3:G:149:GLU:C	2.64	0.41
8:B:301:GLN:N	8:B:301:GLN:OE1	2.54	0.41
11:S:136:ILE:CG2	11:S:137:ASP:N	2.84	0.41
5:Q:23:ASP:N	5:Q:23:ASP:OD1	2.53	0.41
7:A:37:LYS:HG2	7:A:44:MET:HE1	2.03	0.41
7:A:1166:ALA:O	7:A:1170:THR:HG23	2.21	0.41
12:Y:258:MET:HE1	12:Y:497:PHE:HB2	2.01	0.41
7:A:1035:LEU:HD12	7:A:1035:LEU:N	2.36	0.40
8:B:483:GLY:O	8:B:484:LEU:HD12	2.20	0.40
10:I:172:LEU:HB2	10:I:173:PRO:HD3	2.03	0.40
11:S:89:ARG:NH1	11:S:90:ASN:O	2.53	0.40
8:B:70:ILE:HG23	8:B:98:PHE:CD1	2.56	0.40
8:B:311:MET:HE3	8:B:311:MET:HB2	1.98	0.40
1:C:34:LEU:HD12	1:C:182:VAL:CG1	2.50	0.40
7:A:383:SER:OG	8:B:1057:GLU:OE2	2.30	0.40
10:I:214:LEU:HD11	10:I:221:SER:HB3	2.03	0.40
11:S:25:ARG:NH2	11:S:38:GLU:OE2	2.54	0.40
7:A:1108:TYR:C	7:A:1109:THR:HG22	2.46	0.40
10:I:180:ASP:OD1	10:I:180:ASP:N	2.54	0.40
1:C:18:LEU:HD11	1:C:290:ALA:HB1	2.03	0.40
1:C:114:VAL:HG12	1:C:115:ASP:N	2.36	0.40
3:G:93:ASP:N	3:G:96:ASN:OD1	2.52	0.40
7:A:1180:GLN:HB2	7:A:1181:PRO:HD3	2.03	0.40
7:A:1224:ALA:HB2	8:B:1136:VAL:HG13	2.03	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	C	302/305 (99%)	281 (93%)	21 (7%)	0	100	100
2	E	182/185 (98%)	177 (97%)	5 (3%)	0	100	100
3	G	151/161 (94%)	147 (97%)	4 (3%)	0	100	100
4	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
5	Q	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
5	R	128/129 (99%)	123 (96%)	5 (4%)	0	100	100
7	A	1266/1286 (98%)	1195 (94%)	70 (6%)	1 (0%)	48	64
8	B	1123/1164 (96%)	1066 (95%)	57 (5%)	0	100	100
9	F	107/164 (65%)	104 (97%)	3 (3%)	0	100	100
10	I	663/795 (83%)	632 (95%)	31 (5%)	0	100	100
11	S	170/259 (66%)	150 (88%)	20 (12%)	0	100	100
12	Y	541/631 (86%)	513 (95%)	28 (5%)	0	100	100
All	All	4814/5271 (91%)	4563 (95%)	250 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	583	PRO

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	C	286/287 (100%)	282 (99%)	4 (1%)	59	79
2	E	174/175 (99%)	172 (99%)	2 (1%)	65	82
3	G	138/144 (96%)	138 (100%)	0	100	100
4	J	60/62 (97%)	59 (98%)	1 (2%)	53	74
5	Q	117/121 (97%)	117 (100%)	0	100	100
5	R	122/121 (101%)	121 (99%)	1 (1%)	73	86
7	A	1139/1157 (98%)	1125 (99%)	14 (1%)	63	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	1030/1064 (97%)	1024 (99%)	6 (1%)	78	89
9	F	102/151 (68%)	102 (100%)	0	100	100
10	I	639/755 (85%)	629 (98%)	10 (2%)	55	76
11	S	162/237 (68%)	160 (99%)	2 (1%)	63	81
12	Y	496/573 (87%)	492 (99%)	4 (1%)	73	86
All	All	4465/4847 (92%)	4421 (99%)	44 (1%)	65	84

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	135	SER
1	C	211	CYS
1	C	248	SER
1	C	273	SER
2	E	68	SER
2	E	126	SER
4	J	8	SER
5	R	67	SER
7	A	77	GLU
7	A	90	CYS
7	A	103	SER
7	A	152	VAL
7	A	156	ASP
7	A	236	ASP
7	A	366	VAL
7	A	471	ILE
7	A	475	CYS
7	A	555	ILE
7	A	729	SER
7	A	746	VAL
7	A	775	VAL
7	A	836	THR
8	B	153	ILE
8	B	229	ILE
8	B	275	THR
8	B	415	LEU
8	B	796	ASN
8	B	1083	ASP
10	I	104	THR
10	I	105	ASP

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Mol	Chain	Res	Type
10	I	235	VAL
10	I	480	GLU
10	I	499	ILE
10	I	518	VAL
10	I	608	ASP
10	I	643	LYS
10	I	679	ILE
10	I	695	ASN
11	S	87	SER
11	S	244	ILE
12	Y	17	THR
12	Y	23	MET
12	Y	92	ASP
12	Y	171	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	ASN
1	C	129	GLN
1	C	167	ASN
1	C	245	ASN
1	C	260	ASN
2	E	70	ASN
2	E	125	ASN
2	E	167	ASN
3	G	63	ASN
3	G	157	ASN
4	J	51	GLN
4	J	53	ASN
5	Q	72	ASN
5	R	90	ASN
5	R	110	ASN
5	R	121	HIS
7	A	153	ASN
7	A	230	ASN
7	A	271	ASN
7	A	359	HIS
7	A	413	ASN
7	A	428	ASN
7	A	584	ASN
7	A	685	GLN

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Mol	Chain	Res	Type
7	A	686	GLN
7	A	822	GLN
7	A	828	GLN
7	A	994	ASN
8	B	61	ASN
8	B	101	ASN
8	B	295	HIS
8	B	320	ASN
8	B	387	ASN
8	B	714	HIS
8	B	754	GLN
8	B	766	GLN
8	B	779	GLN
8	B	789	ASN
8	B	967	GLN
8	B	1082	GLN
8	B	1132	ASN
9	F	65	HIS
9	F	115	HIS
10	I	271	HIS
10	I	284	HIS
10	I	341	ASN
10	I	405	HIS
10	I	424	GLN
10	I	431	ASN
10	I	501	ASN
10	I	515	ASN
10	I	621	HIS
10	I	703	ASN
11	S	55	ASN
12	Y	35	GLN
12	Y	144	HIS
12	Y	166	ASN
12	Y	189	ASN
12	Y	208	HIS
12	Y	540	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	U	68/72 (94%)	10 (14%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	U	16	U
6	U	17	G
6	U	34	5MU
6	U	35	U
6	U	37	A
6	U	46	A
6	U	48	C
6	U	60	C
6	U	71	C
6	U	72	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SEP	S	232	11	8,9,10	1.60	1 (12%)	7,12,14	1.32	1 (14%)
6	OMC	U	32	6	19,22,23	0.50	0	25,31,34	0.62	0
11	SEP	S	237	11	8,9,10	1.59	1 (12%)	7,12,14	1.42	1 (14%)
6	5MU	U	34	6	19,22,23	0.36	0	27,32,35	0.60	0
11	SEP	S	228	11	8,9,10	1.58	1 (12%)	7,12,14	1.31	1 (14%)
6	1MA	U	57	6	21,25,26	0.41	0	30,37,40	0.75	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SEP	S	232	11	-	0/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMC	U	32	6	-	0/9/27/28	0/2/2/2
11	SEP	S	237	11	-	0/6/8/10	-
6	5MU	U	34	6	-	1/7/25/26	0/2/2/2
11	SEP	S	228	11	-	2/6/8/10	-
6	1MA	U	57	6	-	0/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	S	232	SEP	P-O1P	3.49	1.61	1.50
11	S	228	SEP	P-O1P	3.48	1.61	1.50
11	S	237	SEP	P-O1P	3.47	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	237	SEP	OG-CB-CA	3.01	111.08	108.14
11	S	232	SEP	OG-CB-CA	2.95	111.01	108.14
11	S	228	SEP	OG-CB-CA	2.75	110.82	108.14
6	U	57	1MA	N1-C6-N6	2.24	125.34	119.71

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	34	5MU	O4'-C4'-C5'-O5'
11	S	228	SEP	CB-OG-P-O1P
11	S	228	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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.

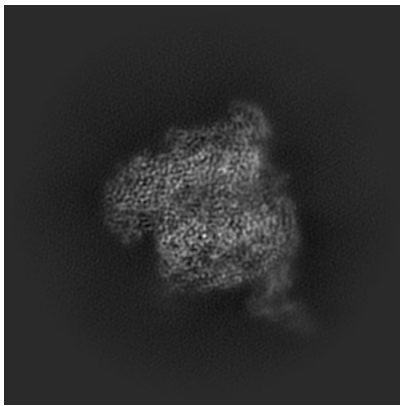
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50639. These allow visual inspection of the internal detail of the map and identification of artifacts.

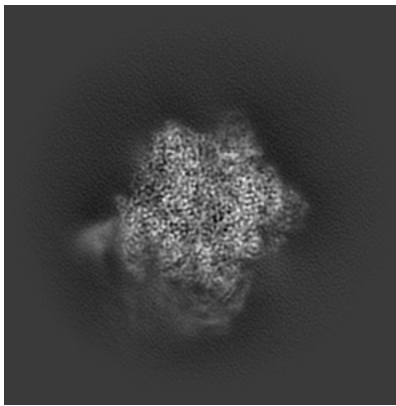
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

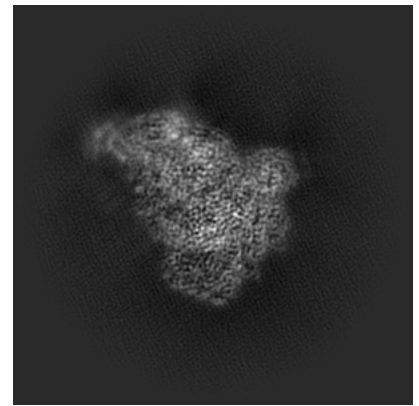
6.1.1 Primary map



X

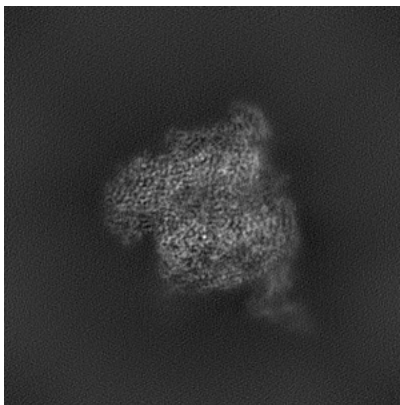


Y

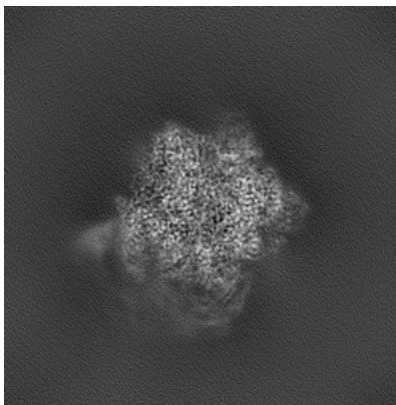


Z

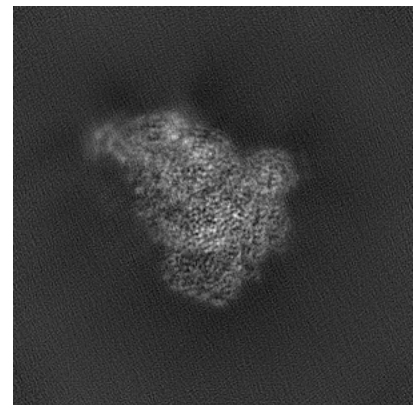
6.1.2 Raw map



X



Y

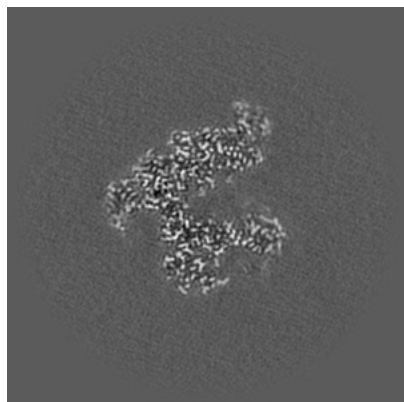


Z

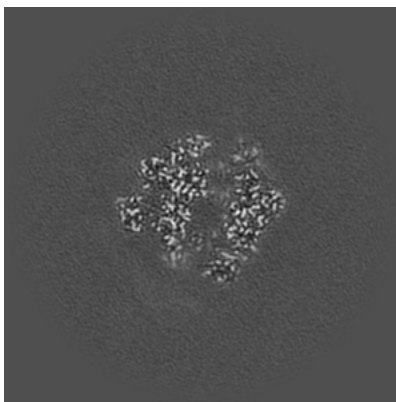
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

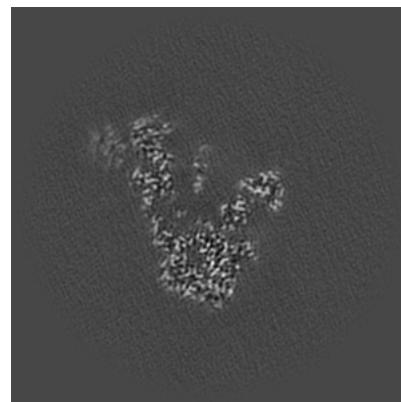
6.2.1 Primary map



X Index: 160

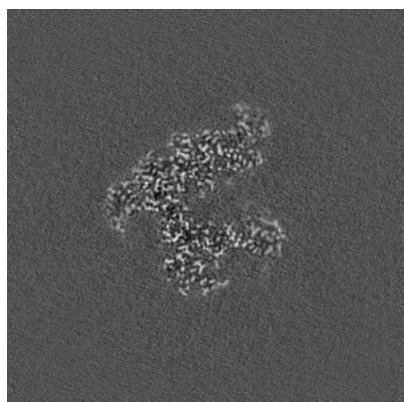


Y Index: 160

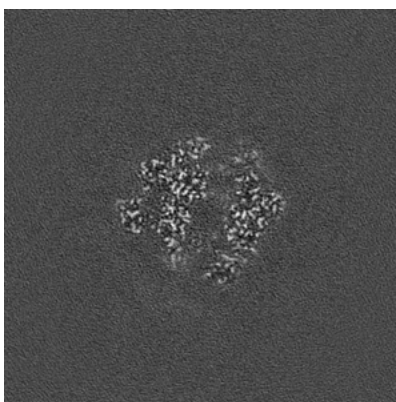


Z Index: 160

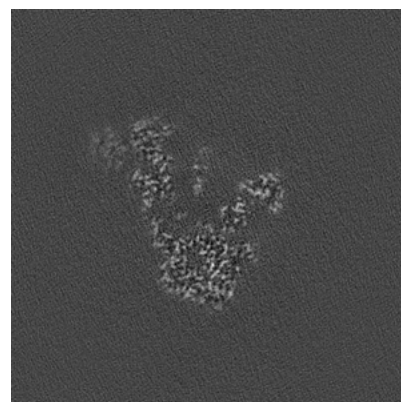
6.2.2 Raw map



X Index: 160



Y Index: 160

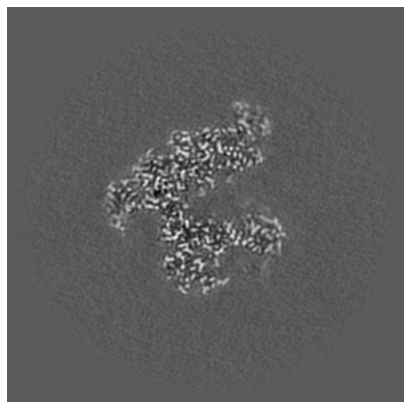


Z Index: 160

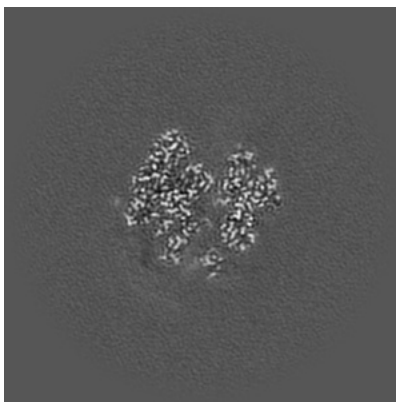
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

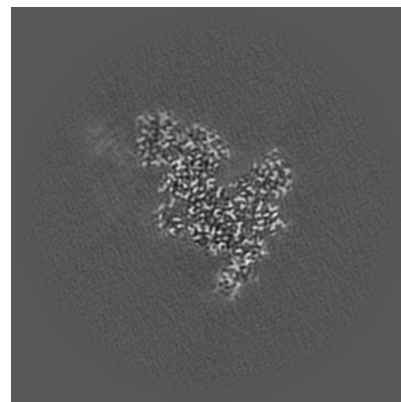
6.3.1 Primary map



X Index: 160

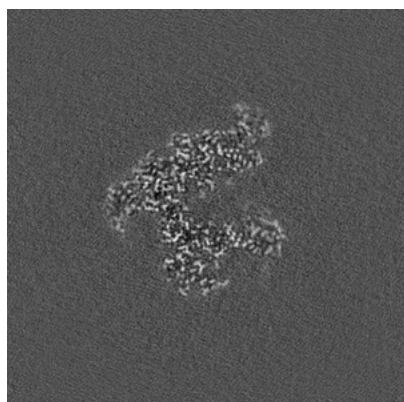


Y Index: 149

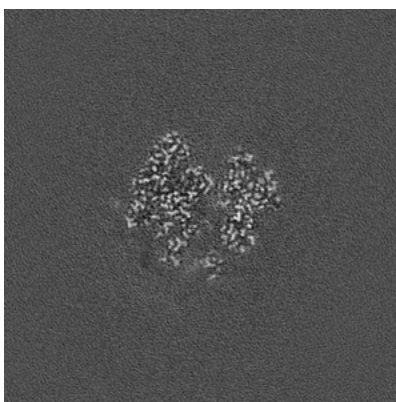


Z Index: 140

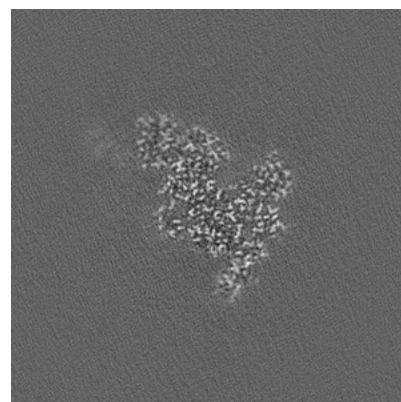
6.3.2 Raw map



X Index: 160



Y Index: 149

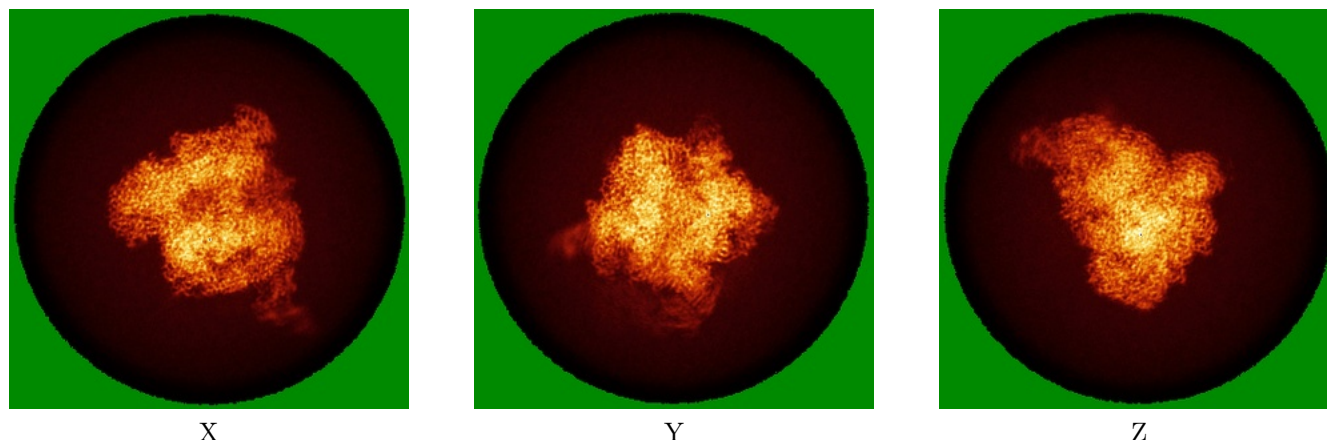


Z Index: 140

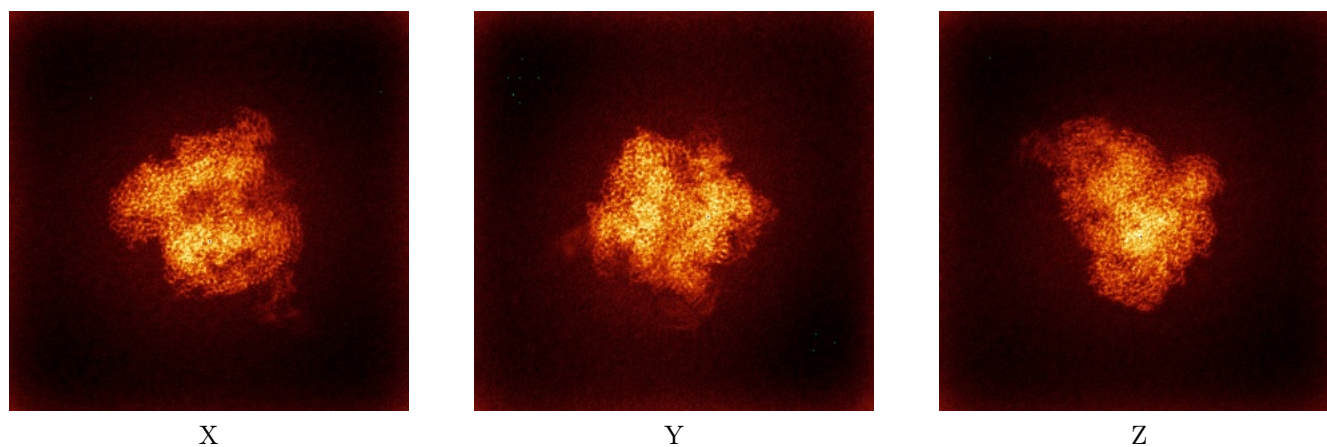
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



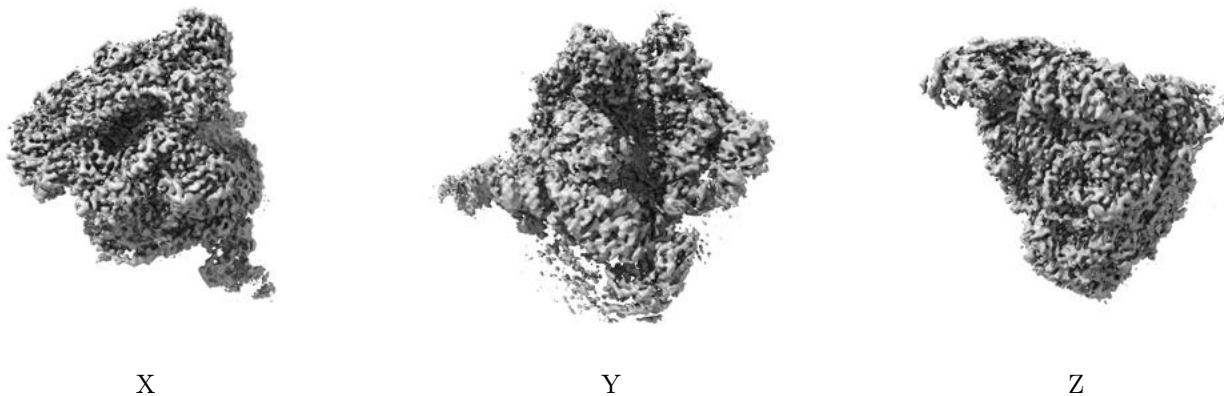
6.4.2 Raw map



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.

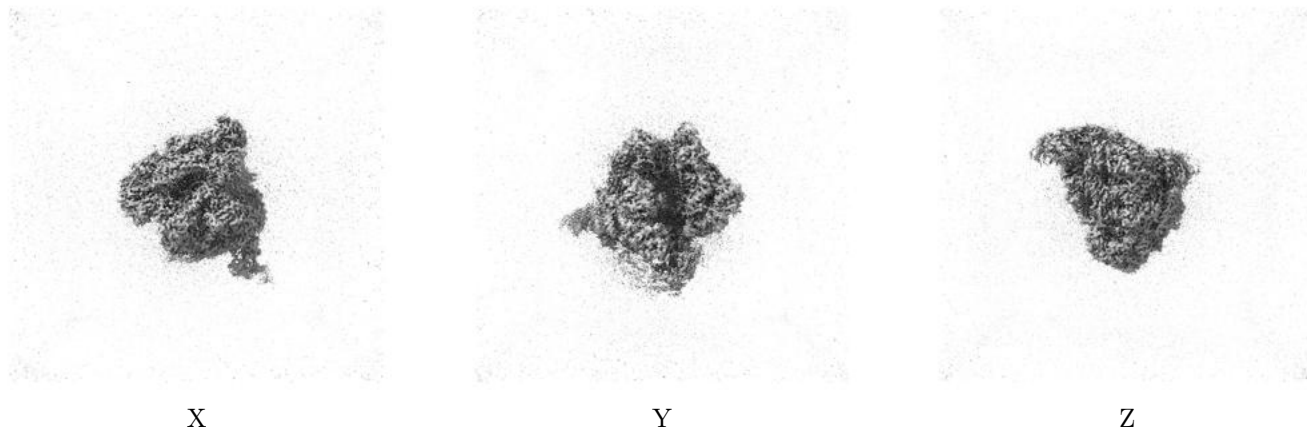
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

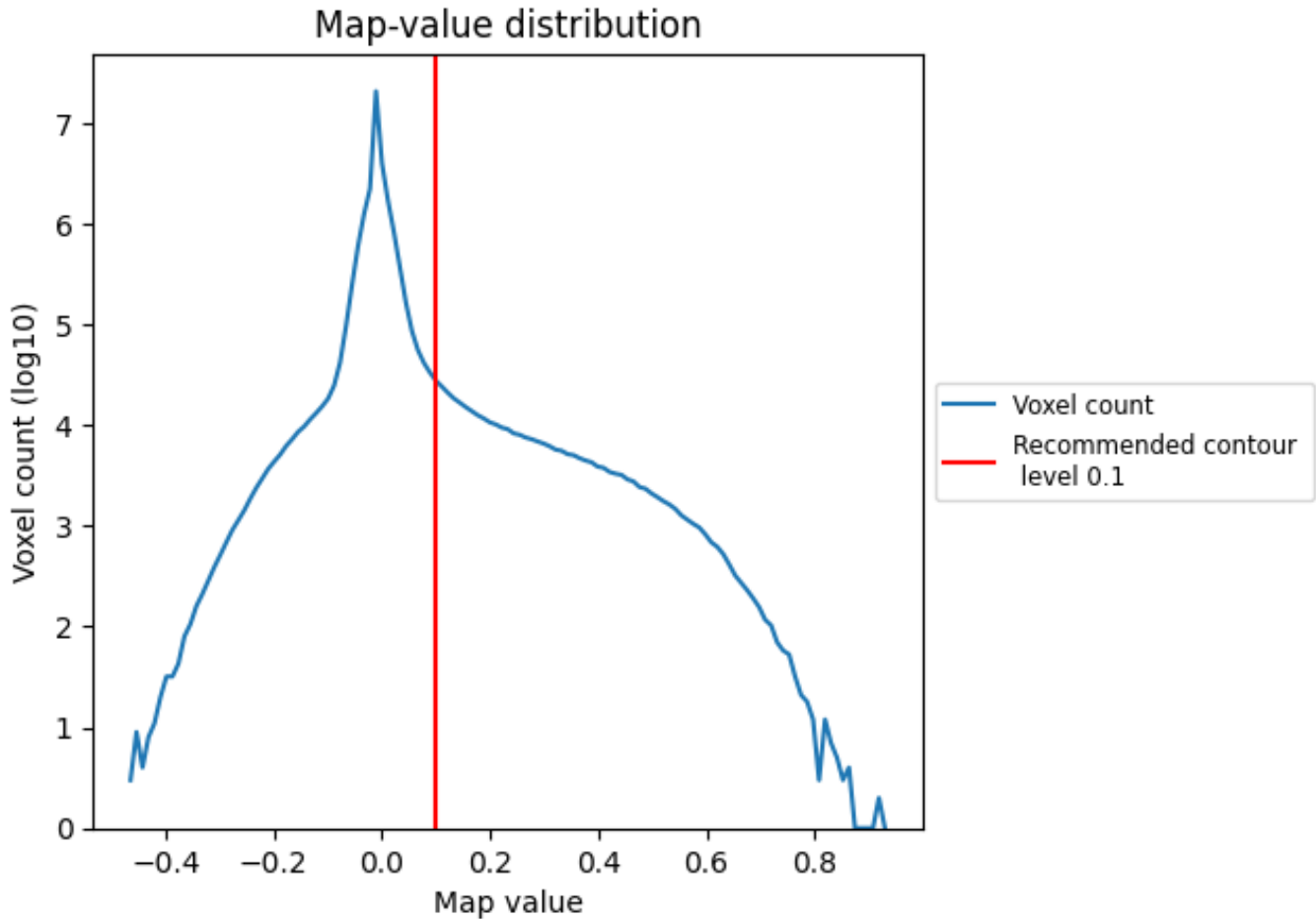
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

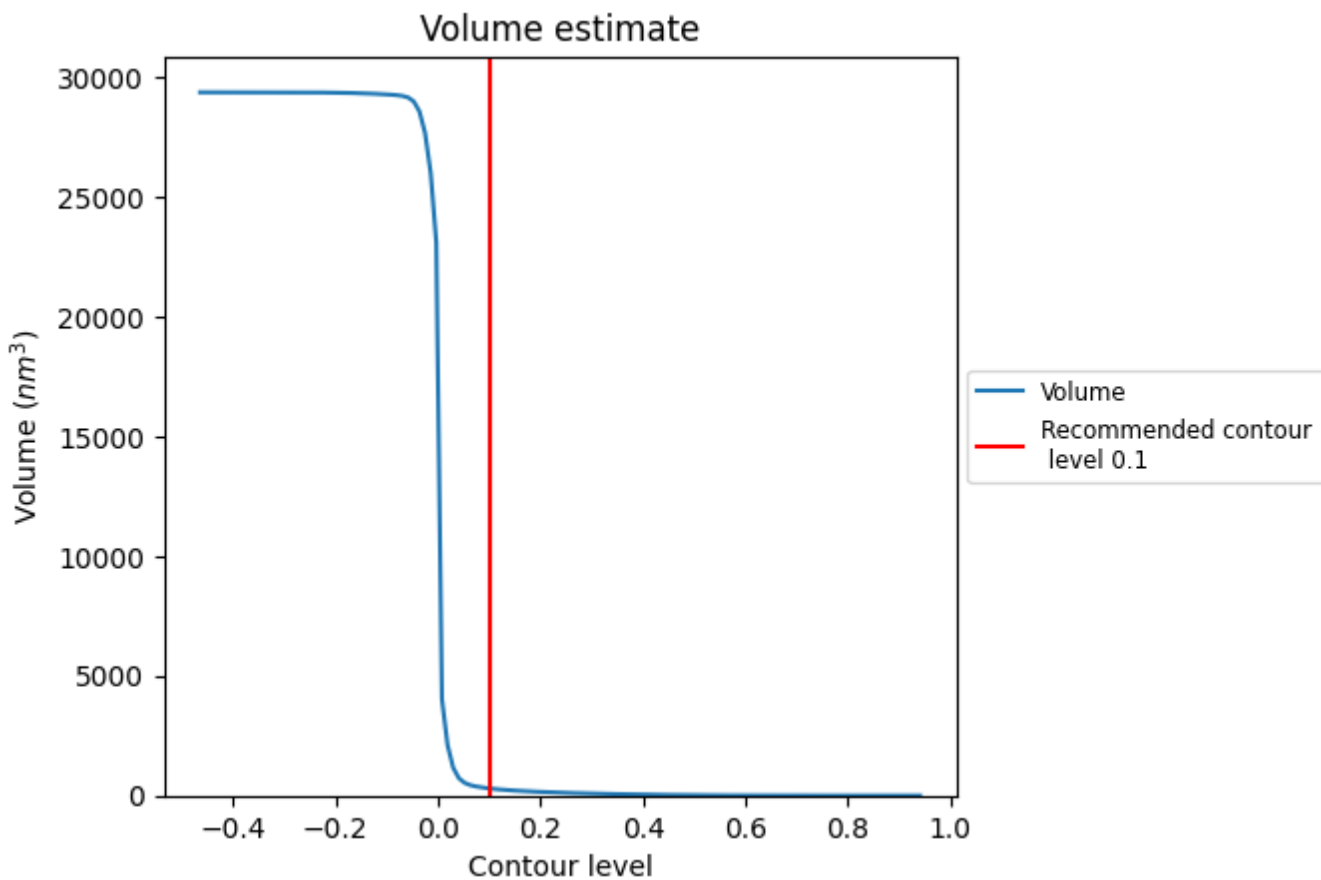
This section contains the results of statistical analysis of the map.

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.

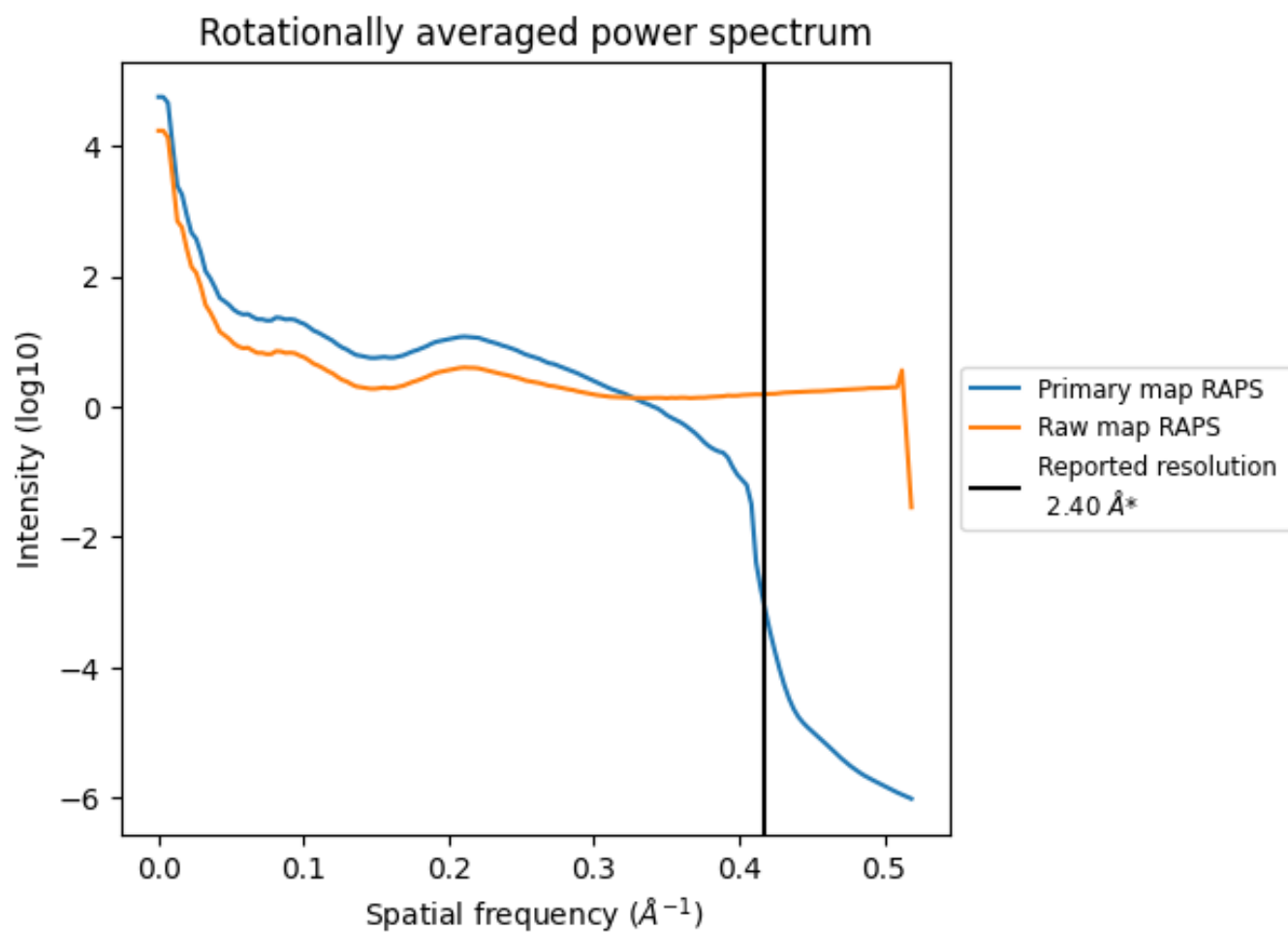
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm³; 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 i

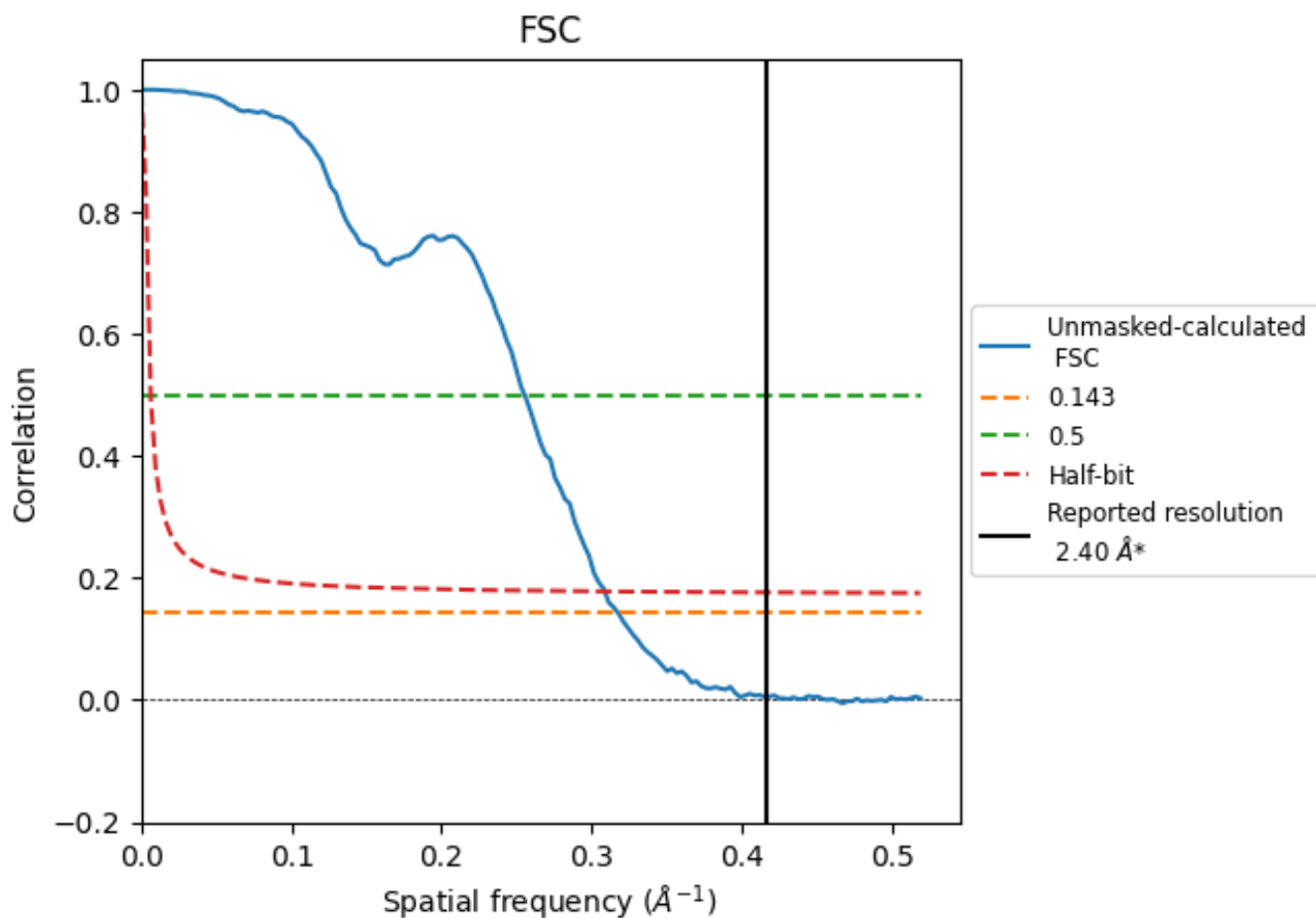


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

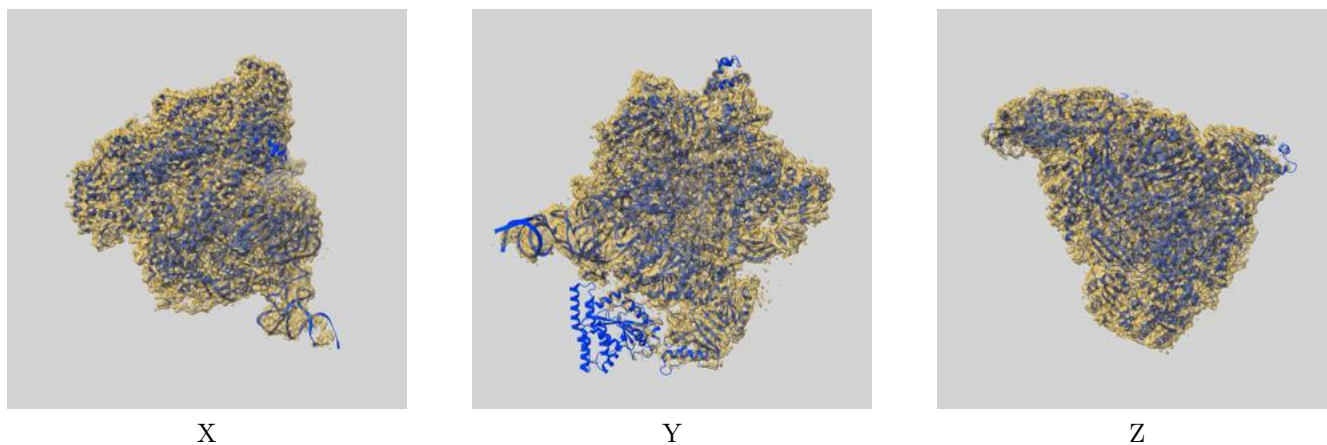
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.15	3.92	3.24

*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 3.15 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

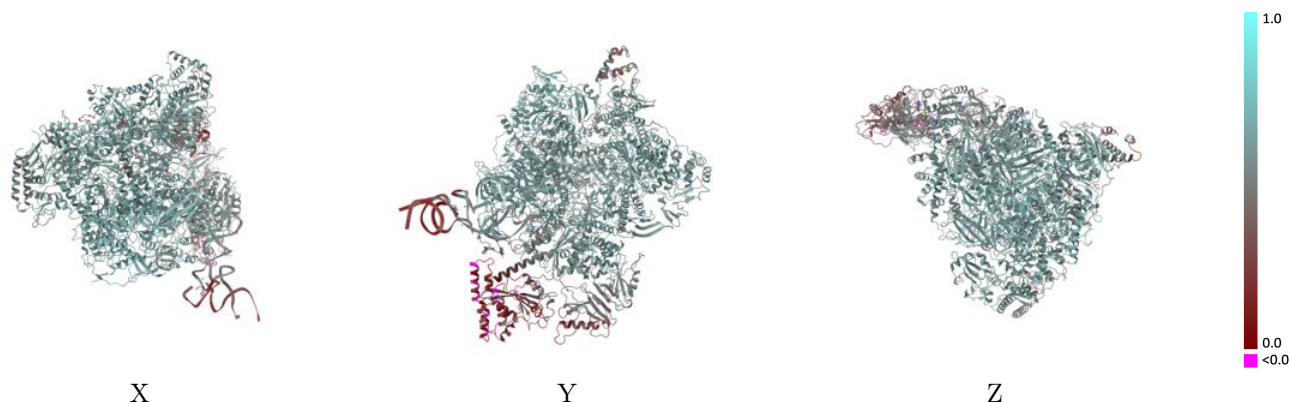
This section contains information regarding the fit between EMDB map EMD-50639 and PDB model 9FPY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



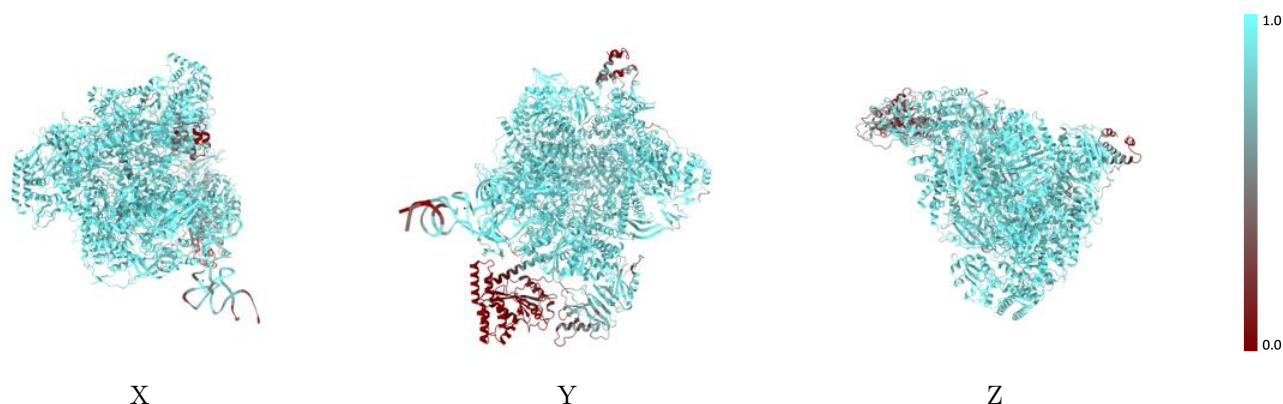
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



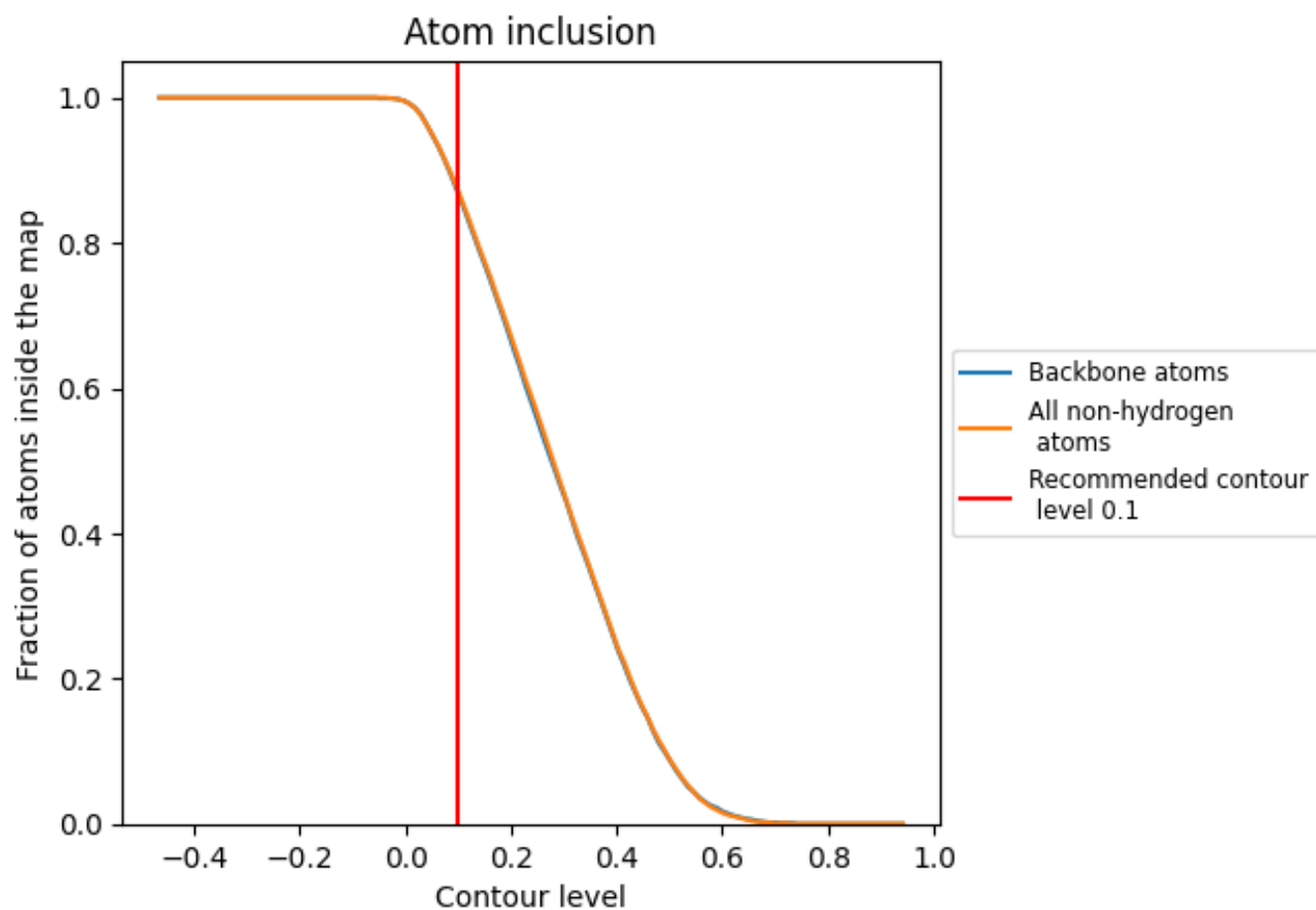
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.5600
A	 0.9530	 0.6070
B	 0.9670	 0.6180
C	 0.9400	 0.5680
E	 0.9800	 0.6180
F	 0.9710	 0.6290
G	 0.9380	 0.5920
I	 0.9110	 0.5740
J	 0.9580	 0.5880
Q	 0.5600	 0.4010
R	 0.8150	 0.5010
S	 0.6690	 0.4990
U	 0.7530	 0.3830
Y	 0.4960	 0.3960

