



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:22 AM UTC

PDB ID : 9FQ6 / pdb_00009fq6
EMDB ID : EMD-50644
Title : Structure of the complete Vaccinia DNA-dependent RNA polymerase complex assembly intermediate 4
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2024-06-14
Resolution : 2.50 Å(reported)
Based on initial model : 6rfl

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

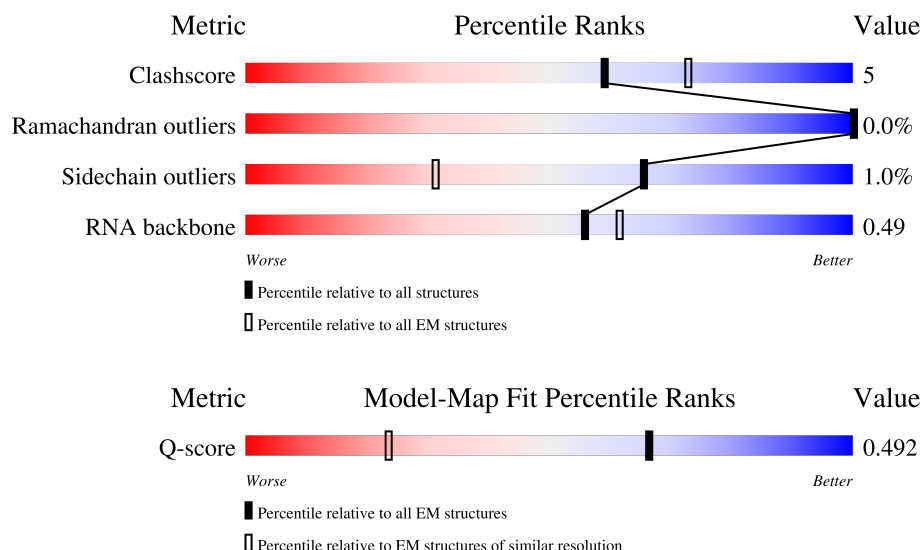
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1286	
2	B	1164	
3	C	305	

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Mol	Chain	Length	Quality of chain
4	E	185	 91% 8% .
5	F	164	 65% 32% .
6	G	161	 84% 15% .
7	I	795	 14% 86% 11% . .
8	J	63	 81% 16% .
9	L	287	 99% 85% 14% .
10	O	844	 95% 86% 14%
11	Q	129	 16% 81% 15% .
11	R	129	 78% 22% .
12	S	259	 22% 59% 14% 27%
13	U	72	 12% 79% 18% .
14	Y	631	 48% 86% 10% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 102921 atoms, of which 51194 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1278	Total	C	H	N	O	S	0	0
			20643	6610	10368	1690	1929	46		

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

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

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 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	159	Total	C	H	N	O	S	0	0
			2460	782	1219	205	248	6		

- Molecule 7 is a protein called RNA polymerase-associated transcription-specificity factor RAP94.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	773	Total	C	H	N	O	S	0	0
			12934	4210	6488	1025	1190	21		

- Molecule 8 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

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

- Molecule 9 is a protein called mRNA-capping enzyme regulatory subunit OPG124.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	284	Total	C	H	N	O	S	0	0
			4678	1492	2358	385	430	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	235	ASN	ASP	variant	UNP P20980

- Molecule 10 is a protein called mRNA-capping enzyme catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	844	Total	C	H	N	O	S	0	0
			13715	4399	6884	1123	1290	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	8	PHE	SER	variant	UNP P20979
O	202	THR	LYS	variant	UNP P20979

- Molecule 11 is a protein called Core protein OPG073.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms							AltConf	Trace
12	S	189	Total	C	H	N	O	P	S	0	0
			3004	950	1473	248	325	3	5		

- Molecule 13 is a RNA chain called URQ-UUG1-1 tRNA (72-MER).

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

- Molecule 14 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Y	609	Total	C	H	N	O	S	0	0
			9883	3152	4966	837	903	25		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Mg 1	0
15	U	3	Total 3	Mg 3	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

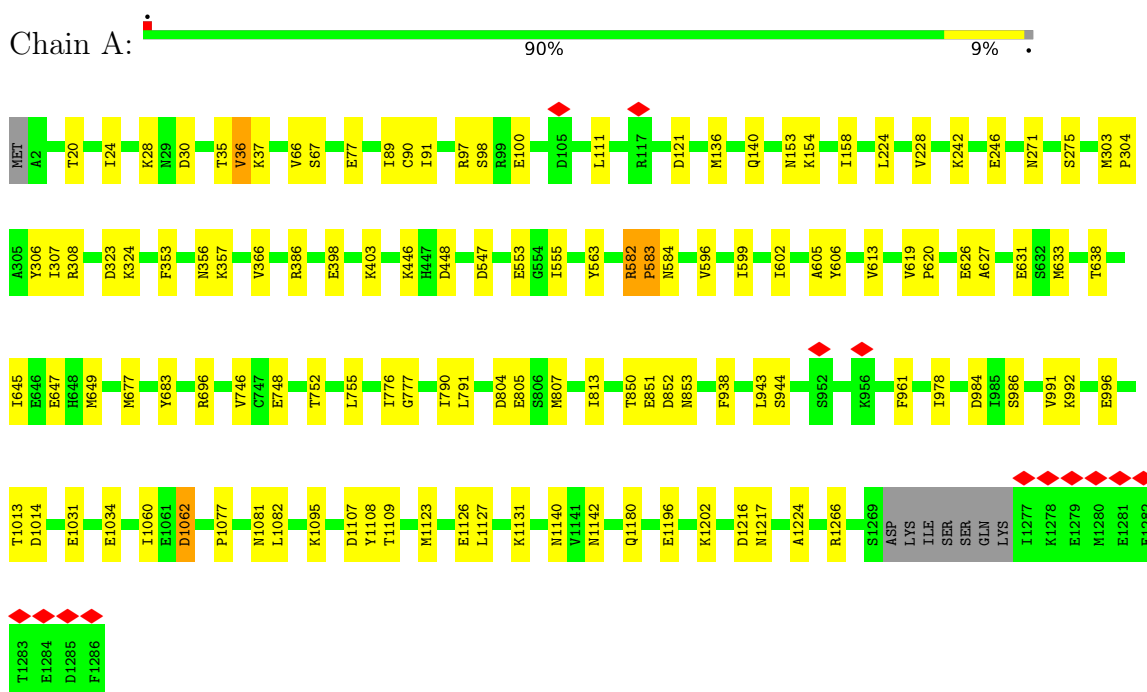
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total 2	O 2	0
17	B	2	Total 2	O 2	0
17	F	1	Total 1	O 1	0
17	I	1	Total 1	O 1	0
17	L	2	Total 2	O 2	0
17	S	2	Total 2	O 2	0
17	Y	1	Total 1	O 1	0

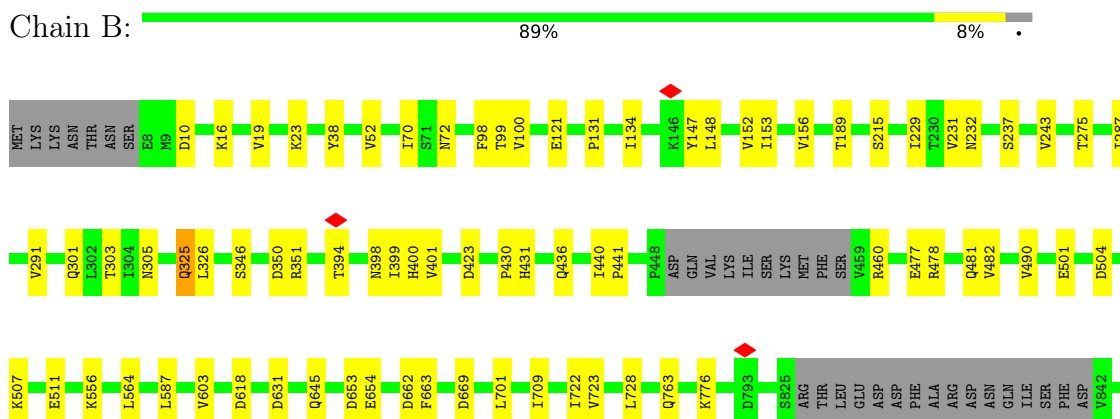
3 Residue-property plots

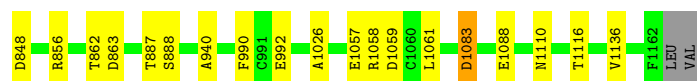
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase 147 kDa polypeptide

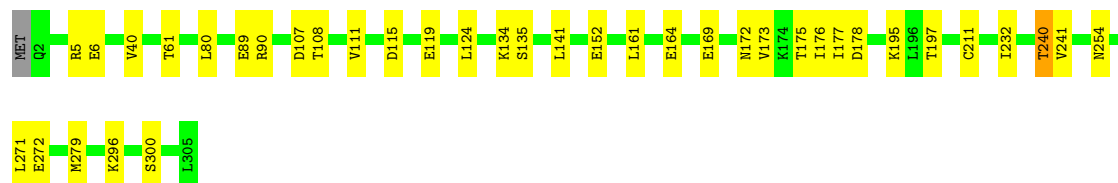
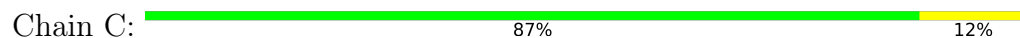


- Molecule 2: DNA-directed RNA polymerase 133 kDa polypeptide

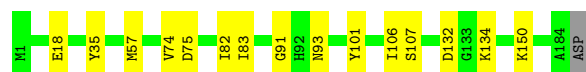




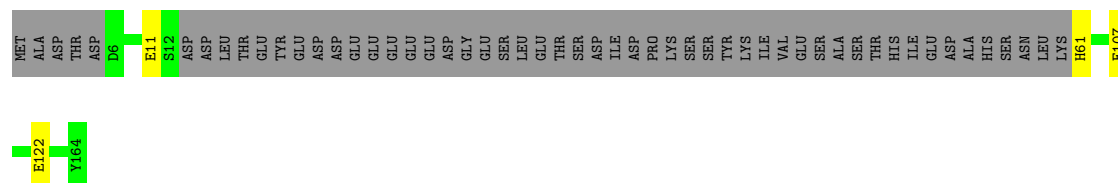
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit



- Molecule 4: DNA-directed RNA polymerase 22 kDa subunit



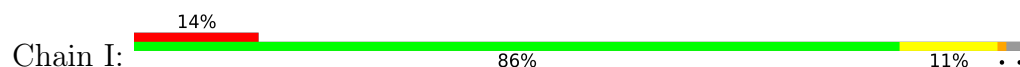
- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

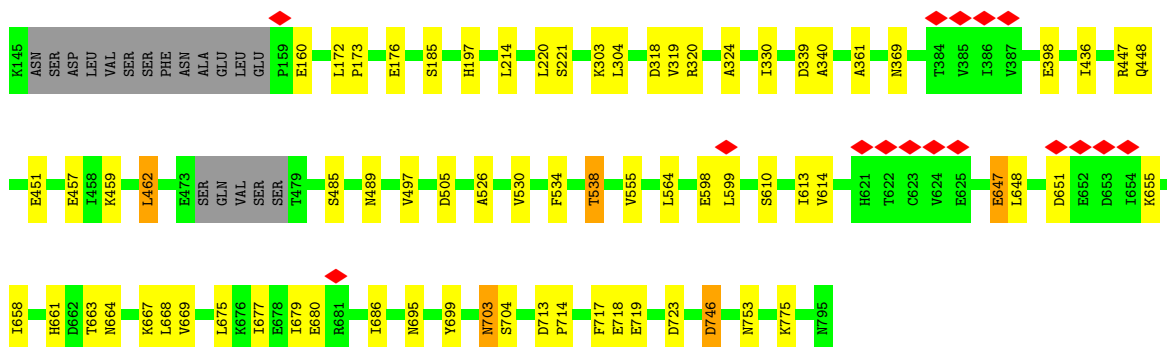


- Molecule 6: DNA-directed RNA polymerase 18 kDa subunit



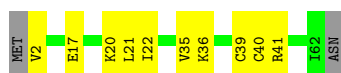
- Molecule 7: RNA polymerase-associated transcription-specificity factor RAP94





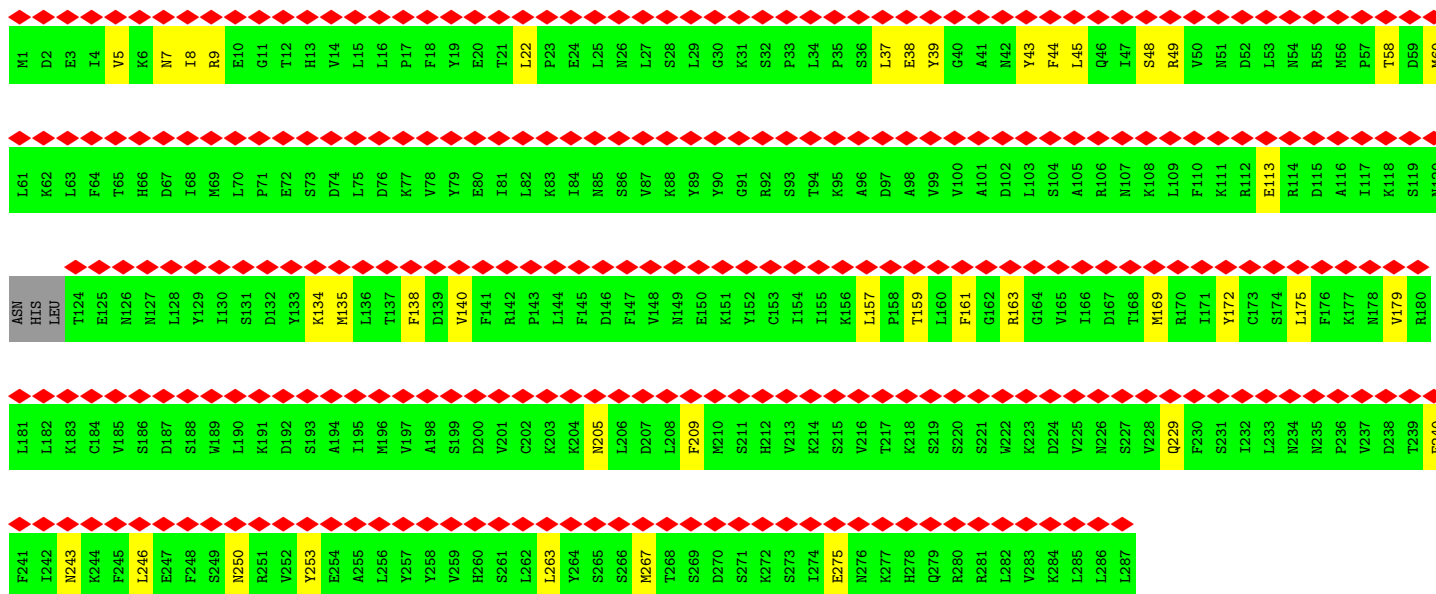
- Molecule 8: DNA-directed RNA polymerase 7 kDa subunit

Chain J: 81% 16%



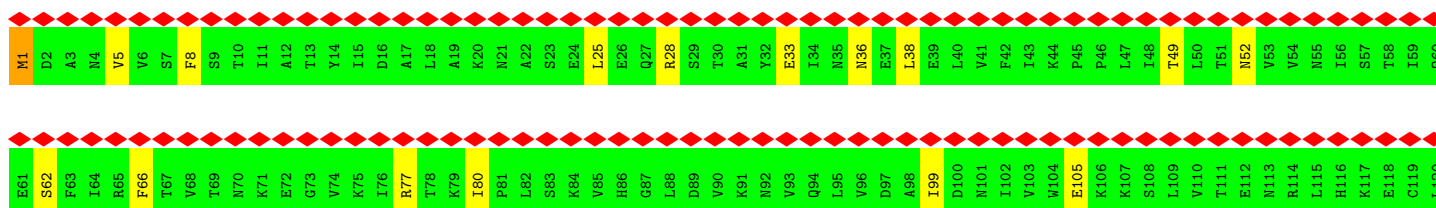
- Molecule 9: mRNA-capping enzyme regulatory subunit OPG124

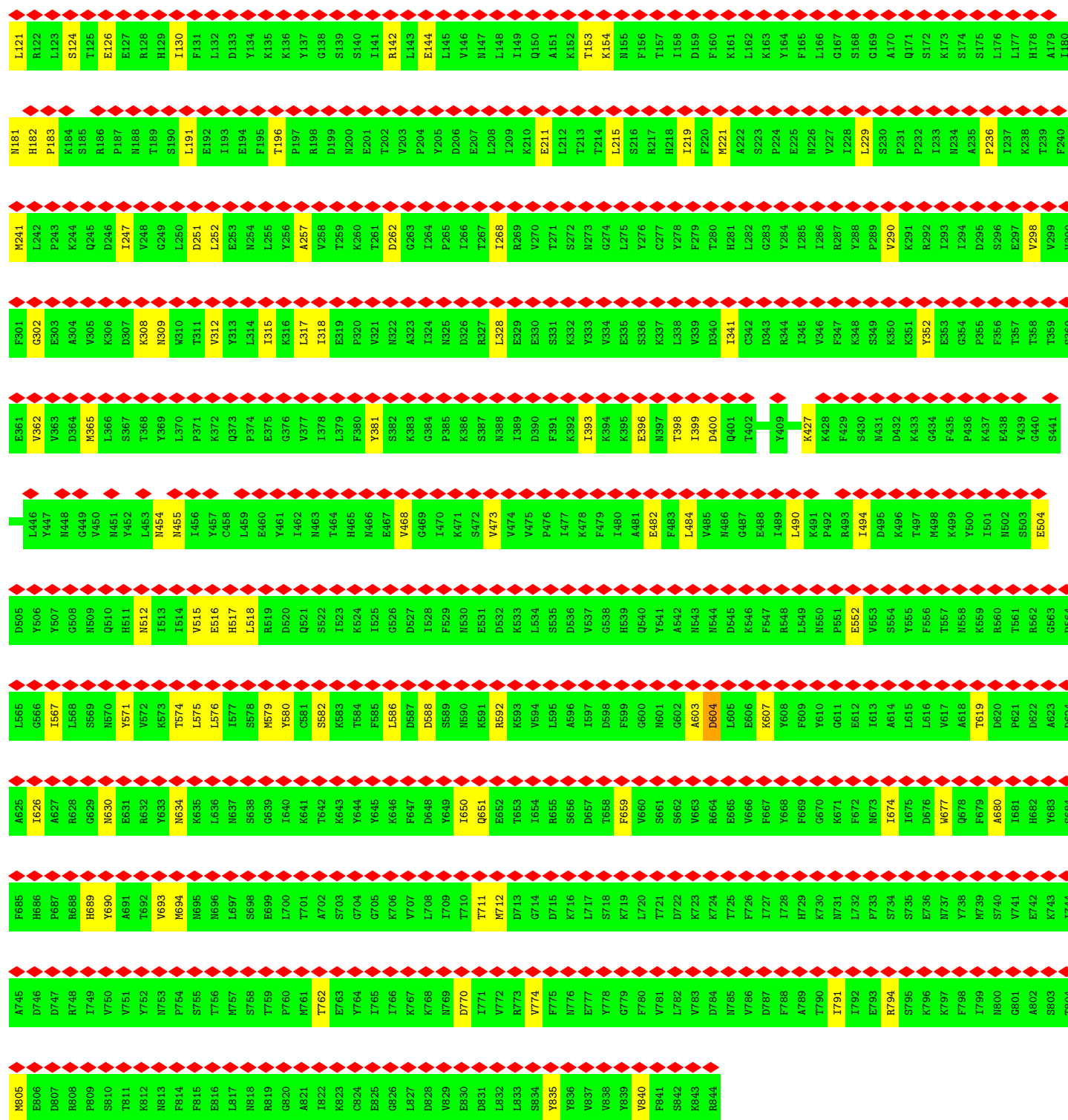
Chain L: 99% 85% 14%



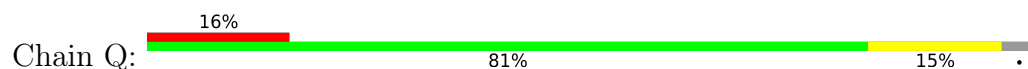
- Molecule 10: mRNA-capping enzyme catalytic subunit

Chain O: 95% 86% 14%



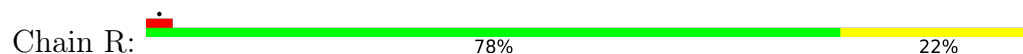


• Molecule 11: Core protein OPG073

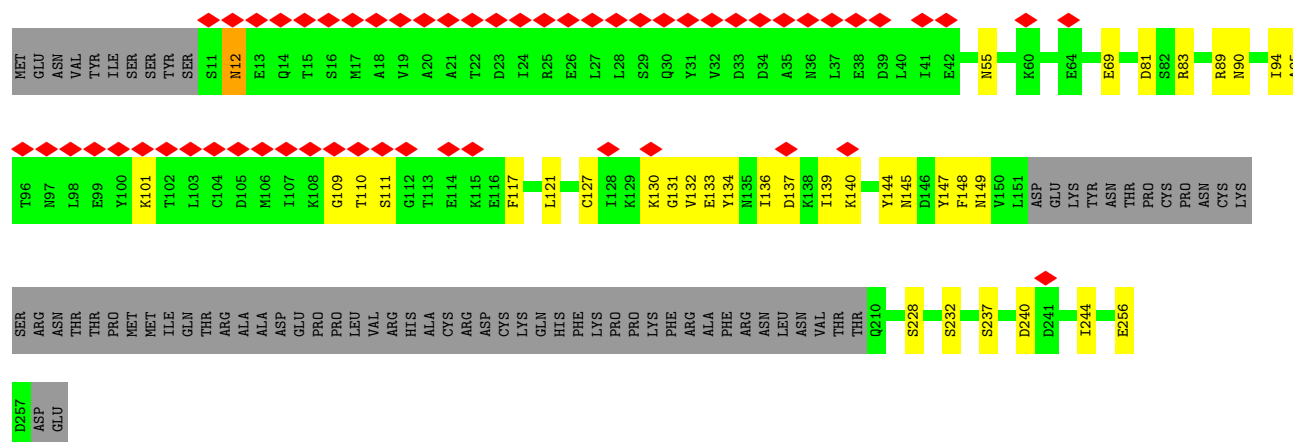




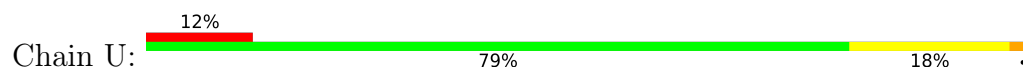
• Molecule 11: Core protein OPG073



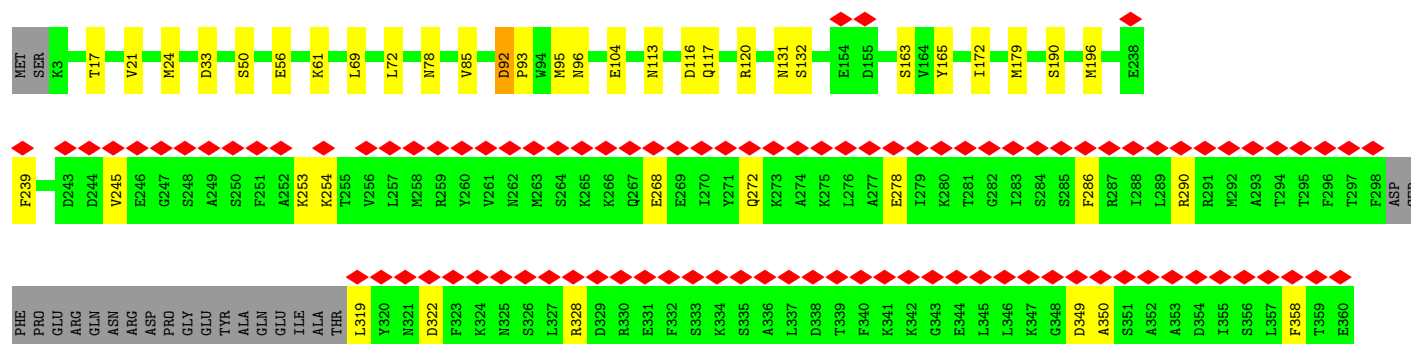
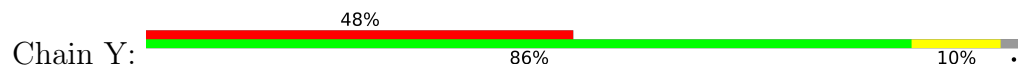
• Molecule 12: DNA-directed RNA polymerase 30 kDa polypeptide



• Molecule 13: URQ-UUG1-1 tRNA (72-MER)



• Molecule 14: Nucleoside triphosphatase I



I592	N593	R594	G595	F596	K597	G598	V599	D600	G601	R602	V603	Y604	D605	V606	D607	G608	M609	Y610	L611	H612	D613	M614	P615	D616	M617	P618	V619	D620	K621	L622	H623	D624	G625	K626	L627	T628	Y629	F630	F631																				
L361	K362	E363	K364	S365	V366	K367	F368	I369	D370	V371	C372	L373	G374	I375	L376	A377	S378	H379	G380	K381	C382	L383	V384	F385	E386	P387	F388	V389	N390	Q391	S392	G393	I394	E395	I396	L397	L398	L399	Y400	F401	K402	V403	F404	G405	I406	S407	N408	I409	E410	F411	S412	S413	R414	T415	K416	D417	T418	R419	L420
K421	A422	V423	A424	E425	F426	N427	Q428	E429	S430	N431	T432	N433	O434	E435	O436	L437	K438	T439	O440	V441	F442	S443	S444	S445	O446	O447	E448	O449	T450	S451	F452	F453	S454	T455	N456	D457	L458	F459	L460	L461	D462	M463	T464	M465	N466	E467	A468	S469	L470	R471	Q472	I473	R476	A477	I478	R479	L480	N481	
V484	L485	F489	R490	R491	H496	F497	L498	M499	A500	R501	L502	S503	N504	G505	M506	F507	T508	V509	D510	E511	D512	L513	F514	E515	I516	K520	D545	F546	S547	K568	K569	N570	T571	T572	N573	K574	L575	L576	E577	O578	T579	N580	I581	W582	Y583	S584	N585	S586	N587	L588	M590	S591							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171057	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	0.948	Depositor
Minimum map value	-0.487	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMC, ZN, 1MA, 5MU, 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	A	0.15	0/10481	0.31	0/14166
2	B	0.14	0/9281	0.29	0/12537
3	C	0.16	0/2540	0.33	0/3440
4	E	0.14	0/1522	0.30	0/2069
5	F	0.16	0/933	0.35	0/1252
6	G	0.15	0/1260	0.30	0/1709
7	I	0.13	0/6590	0.28	0/8918
8	J	0.17	0/494	0.35	0/663
9	L	0.15	0/2365	0.28	0/3189
10	O	0.10	0/6973	0.27	0/9433
11	Q	0.10	0/1038	0.28	0/1406
11	R	0.12	0/1081	0.33	0/1463
12	S	0.12	0/1524	0.31	0/2050
13	U	0.09	0/1710	0.20	0/2661
14	Y	0.11	0/5013	0.26	0/6750
All	All	0.13	0/52805	0.29	0/71706

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
1	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
1	A	582	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10275	10368	10388	81	0
2	B	9091	9119	9146	56	0
3	C	2484	2462	2470	27	0
4	E	1495	1546	1548	13	0
5	F	918	926	930	5	0
6	G	1241	1219	1222	18	0
7	I	6446	6488	6502	69	0
8	J	490	529	530	7	0
9	L	2320	2358	2363	34	0
10	O	6831	6884	6899	86	0
11	Q	1016	995	1007	15	0
11	R	1056	1053	1056	25	0
12	S	1531	1473	1473	29	0
13	U	1597	808	808	4	0
14	Y	4917	4966	4981	43	0
15	A	1	0	0	0	0
15	U	3	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
17	A	2	0	0	0	0
17	B	2	0	0	0	0
17	F	1	0	0	0	0
17	I	1	0	0	0	0
17	L	2	0	0	0	0
17	S	2	0	0	2	0
17	Y	1	0	0	0	0
All	All	51727	51194	51323	473	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.

The worst 5 of 473 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)
9:L:43:TYR:OH	10:O:579:MET:N	1.98	0.97
6:G:136:GLU:OE2	6:G:136:GLU:N	2.07	0.88
10:O:588:ASP:O	10:O:592:ARG:NH2	2.08	0.86
1:A:446:LYS:NZ	1:A:547:ASP:OD1	2.07	0.86
14:Y:56:GLU:O	14:Y:61:LYS:NZ	2.12	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1274/1286 (99%)	1193 (94%)	80 (6%)	1 (0%)	48	68
2	B	1123/1164 (96%)	1054 (94%)	69 (6%)	0	100	100
3	C	302/305 (99%)	278 (92%)	24 (8%)	0	100	100
4	E	182/185 (98%)	176 (97%)	6 (3%)	0	100	100
5	F	107/164 (65%)	104 (97%)	3 (3%)	0	100	100
6	G	157/161 (98%)	144 (92%)	13 (8%)	0	100	100
7	I	765/795 (96%)	718 (94%)	47 (6%)	0	100	100
8	J	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
9	L	280/287 (98%)	272 (97%)	8 (3%)	0	100	100
10	O	842/844 (100%)	818 (97%)	24 (3%)	0	100	100
11	Q	122/129 (95%)	115 (94%)	7 (6%)	0	100	100
11	R	128/129 (99%)	120 (94%)	8 (6%)	0	100	100
12	S	182/259 (70%)	163 (90%)	19 (10%)	0	100	100
14	Y	605/631 (96%)	568 (94%)	37 (6%)	0	100	100
All	All	6128/6402 (96%)	5776 (94%)	351 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1149/1157 (99%)	1137 (99%)	12 (1%)	68	86
2	B	1030/1064 (97%)	1017 (99%)	13 (1%)	61	82
3	C	286/287 (100%)	279 (98%)	7 (2%)	43	70
4	E	174/175 (99%)	174 (100%)	0	100	100
5	F	102/151 (68%)	102 (100%)	0	100	100
6	G	142/144 (99%)	142 (100%)	0	100	100
7	I	735/755 (97%)	725 (99%)	10 (1%)	59	81
8	J	60/62 (97%)	60 (100%)	0	100	100
9	L	269/272 (99%)	268 (100%)	1 (0%)	84	93
10	O	774/774 (100%)	768 (99%)	6 (1%)	73	88
11	Q	117/121 (97%)	116 (99%)	1 (1%)	70	87
11	R	122/121 (101%)	121 (99%)	1 (1%)	73	88
12	S	171/237 (72%)	169 (99%)	2 (1%)	63	83
14	Y	554/573 (97%)	549 (99%)	5 (1%)	70	87
All	All	5685/5893 (96%)	5627 (99%)	58 (1%)	65	86

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	211	CYS
14	Y	78	ASN
7	I	197	HIS
14	Y	50	SER
11	Q	17	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
7	I	253	ASN
14	Y	408	ASN
8	J	57	GLN
14	Y	262	ASN
12	S	213	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	U	68/72 (94%)	11 (16%)	0

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	U	4	C
13	U	16	U
13	U	17	G
13	U	34	5MU
13	U	35	U

There are no RNA pucker outliers to report.

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

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	$\# Z > 2$
12	SEP	S	228	12	8,9,10	1.57	1 (12%)	7,12,14	1.34	1 (14%)
12	SEP	S	232	12	8,9,10	1.60	1 (12%)	7,12,14	1.28	1 (14%)
12	SEP	S	237	12	8,9,10	1.59	1 (12%)	7,12,14	1.36	1 (14%)
13	OMC	U	32	13	19,22,23	0.53	0	25,31,34	0.60	0
13	5MU	U	34	13	19,22,23	0.37	0	27,32,35	0.59	0
13	1MA	U	57	13	21,25,26	0.42	0	30,37,40	0.76	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
12	SEP	S	228	12	-	3/6/8/10	-
12	SEP	S	232	12	-	0/6/8/10	-
12	SEP	S	237	12	-	0/6/8/10	-
13	OMC	U	32	13	-	0/9/27/28	0/2/2/2
13	5MU	U	34	13	-	1/7/25/26	0/2/2/2
13	1MA	U	57	13	-	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)
12	S	232	SEP	P-O1P	3.49	1.61	1.50
12	S	237	SEP	P-O1P	3.46	1.61	1.50
12	S	228	SEP	P-O1P	3.43	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	237	SEP	OG-CB-CA	2.89	110.95	108.14
12	S	232	SEP	OG-CB-CA	2.81	110.88	108.14
12	S	228	SEP	OG-CB-CA	2.76	110.83	108.14
13	U	57	1MA	N1-C6-N6	2.23	125.31	119.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	S	228	SEP	CB-OG-P-O1P
12	S	228	SEP	CB-OG-P-O3P
13	U	34	5MU	O4'-C4'-C5'-O5'
12	S	228	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	57	1MA	1	0

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.

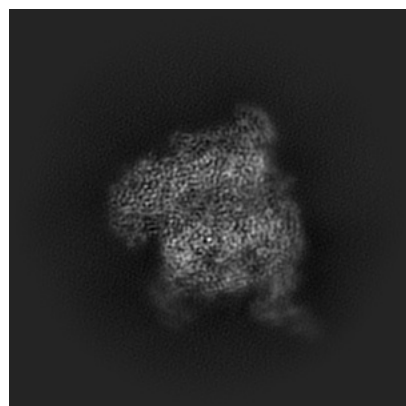
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50644. These allow visual inspection of the internal detail of the map and identification of artifacts.

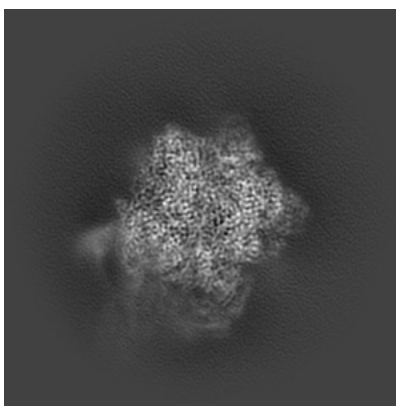
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

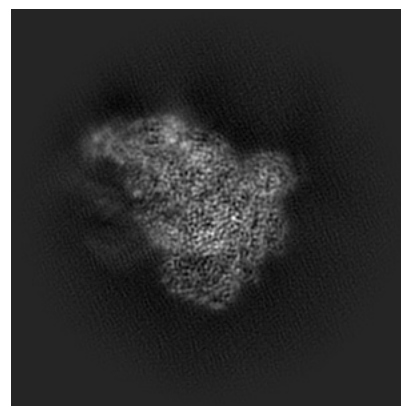
6.1.1 Primary map



X

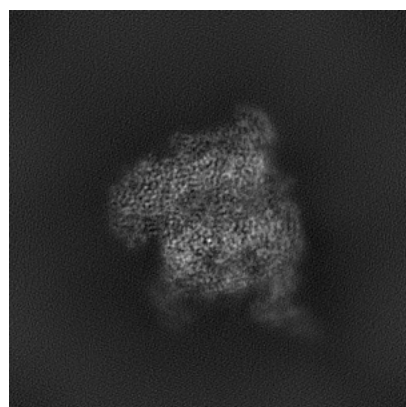


Y

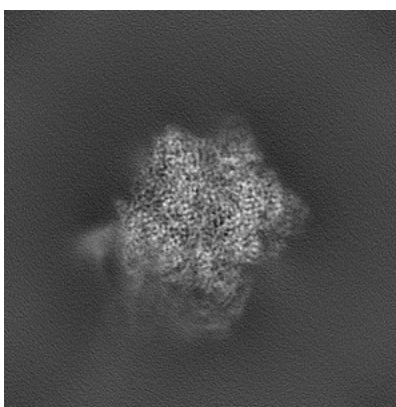


Z

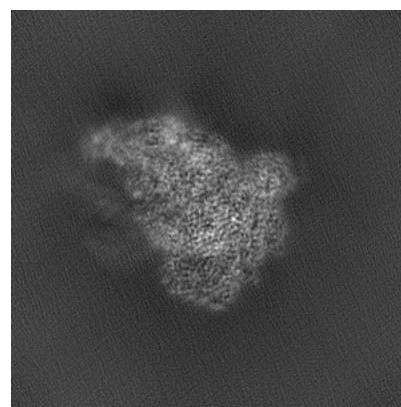
6.1.2 Raw map



X



Y

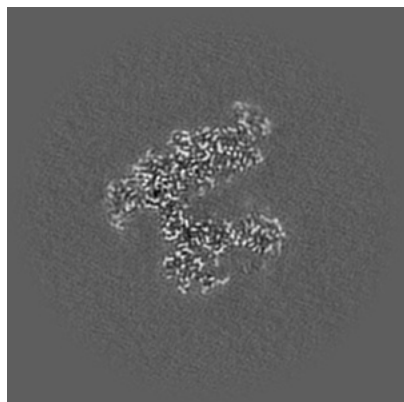


Z

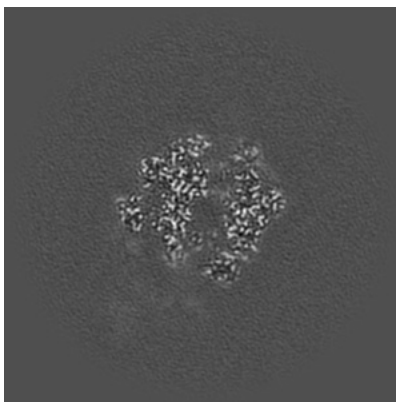
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

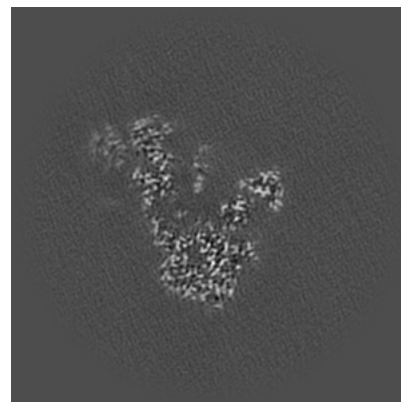
6.2.1 Primary map



X Index: 160

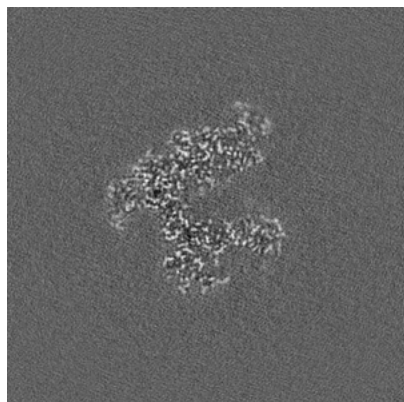


Y Index: 160

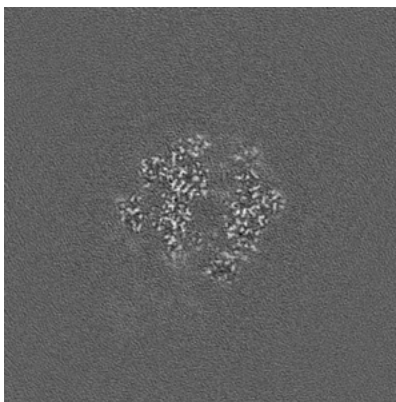


Z Index: 160

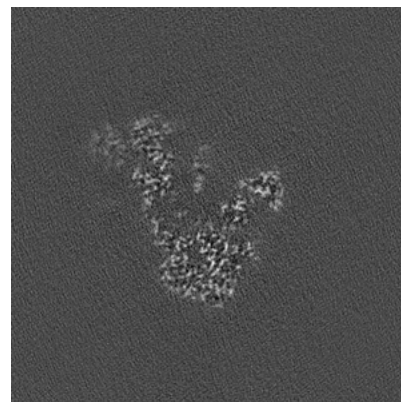
6.2.2 Raw map



X Index: 160



Y Index: 160

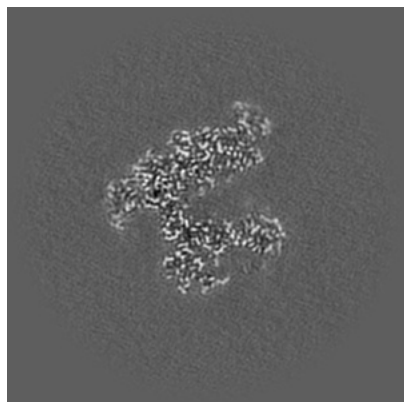


Z Index: 160

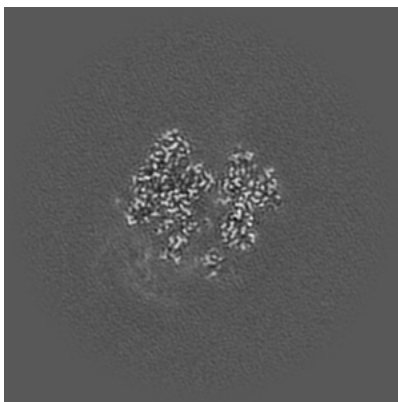
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

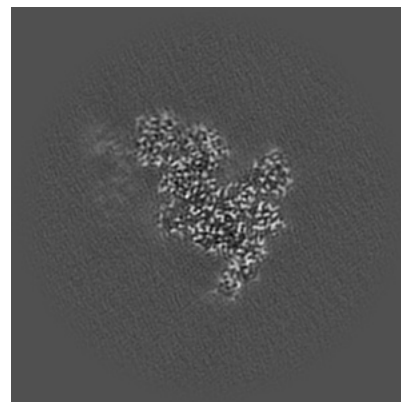
6.3.1 Primary map



X Index: 160

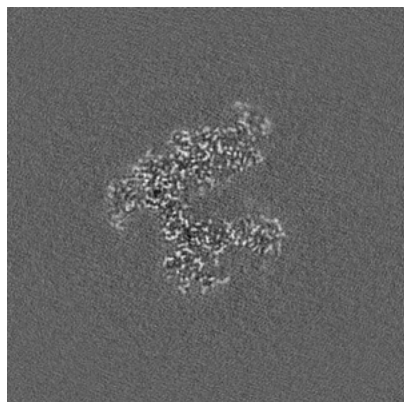


Y Index: 149

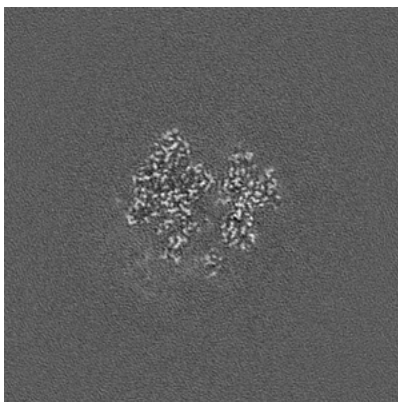


Z Index: 141

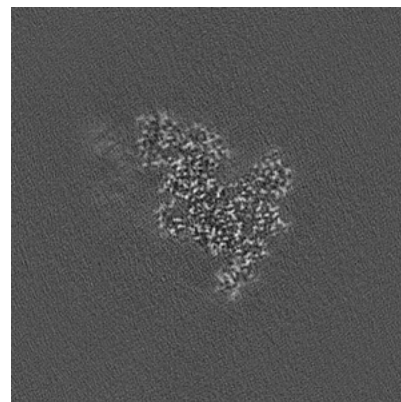
6.3.2 Raw map



X Index: 160



Y Index: 149

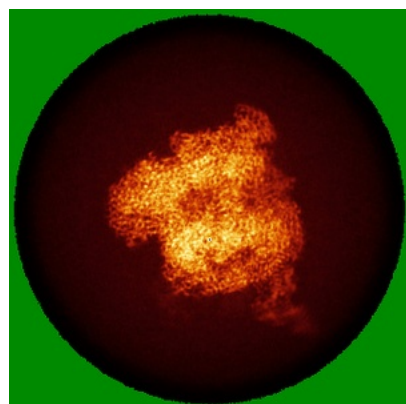


Z Index: 140

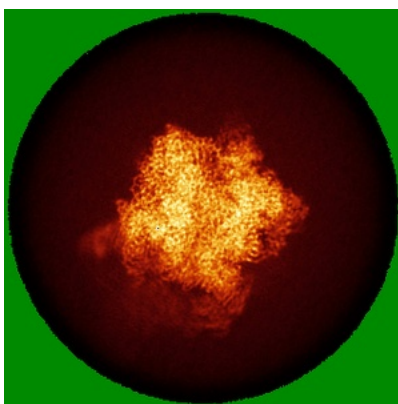
The images above show the largest variance slices of the map in three orthogonal directions.

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

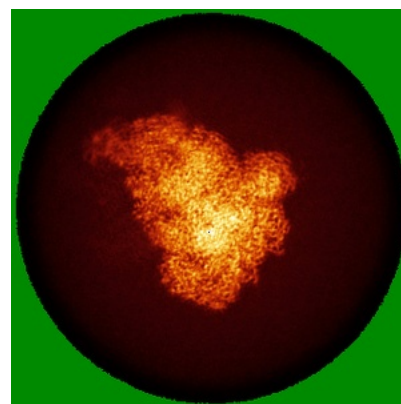
6.4.1 Primary map



X

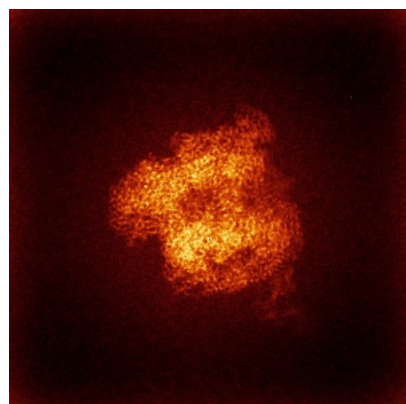


Y

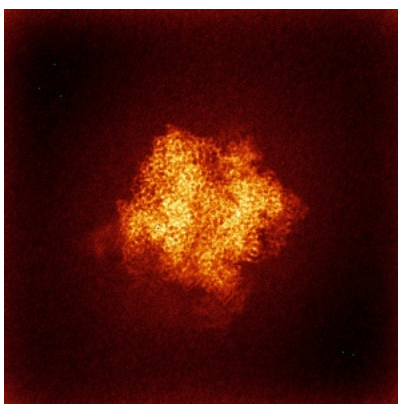


Z

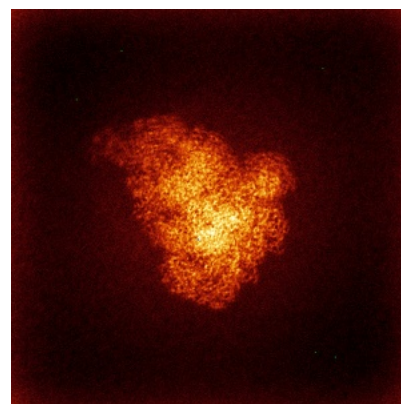
6.4.2 Raw map



X



Y

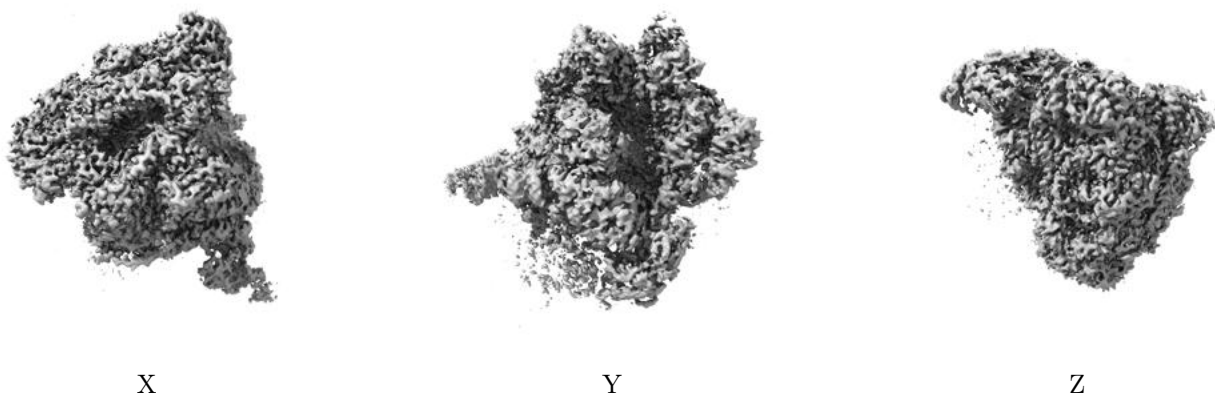


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

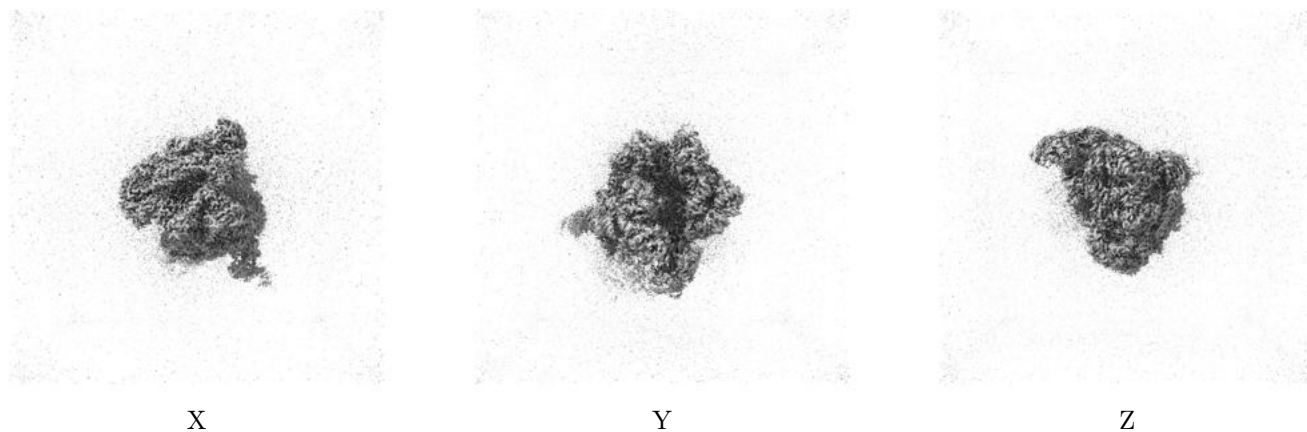
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

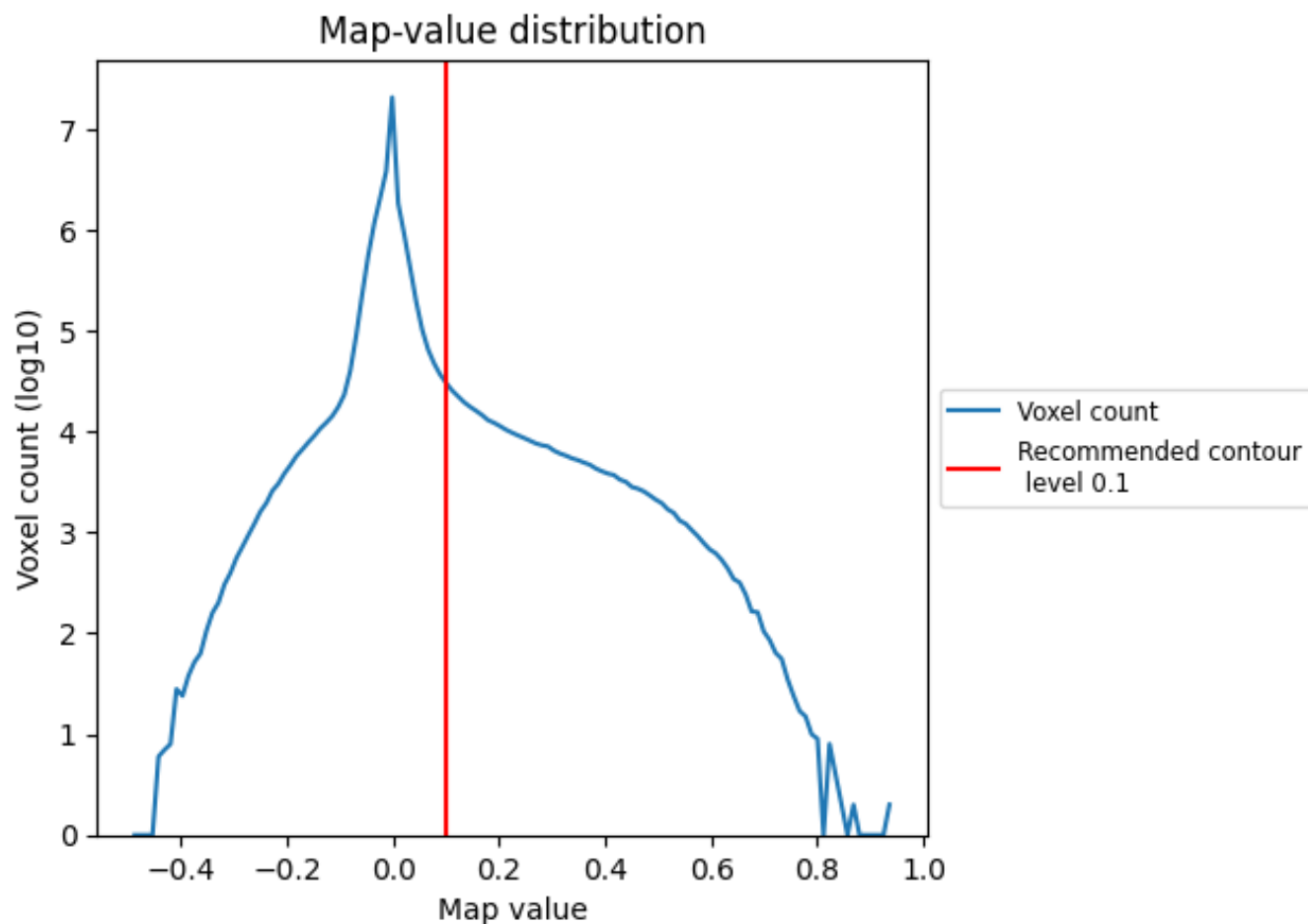
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

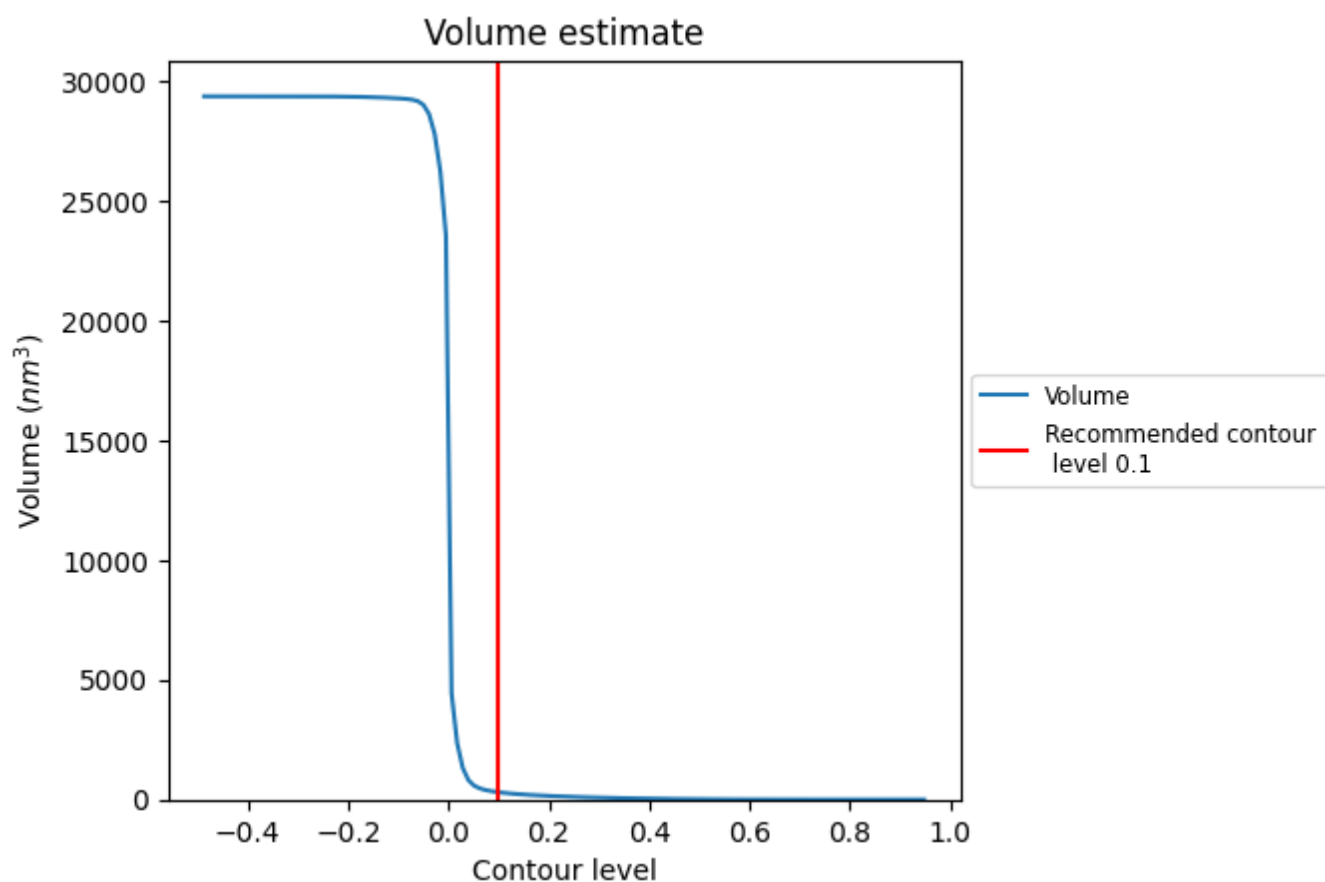
This section contains the results of statistical analysis of the map.

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.

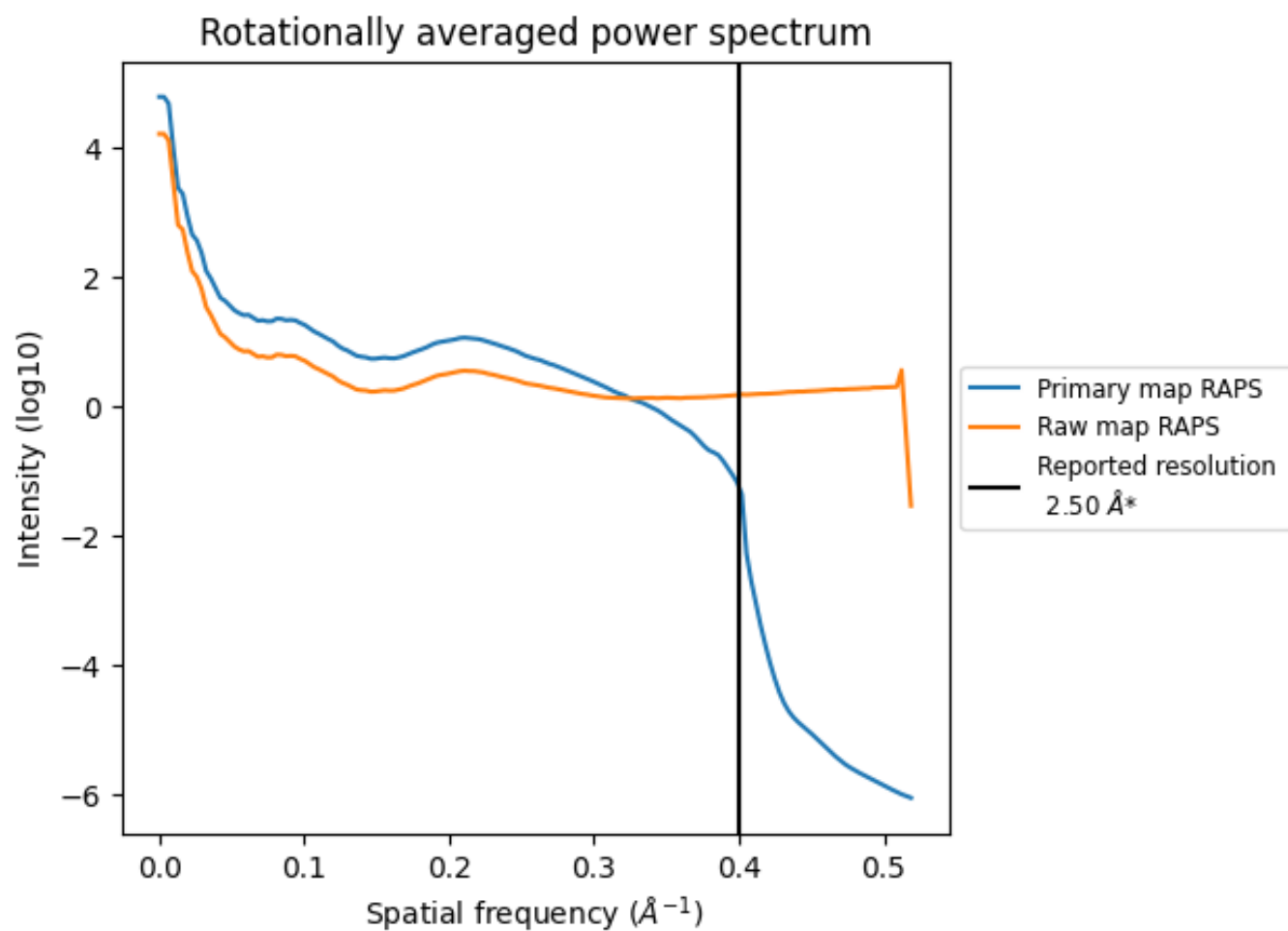
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 276 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 ⓘ

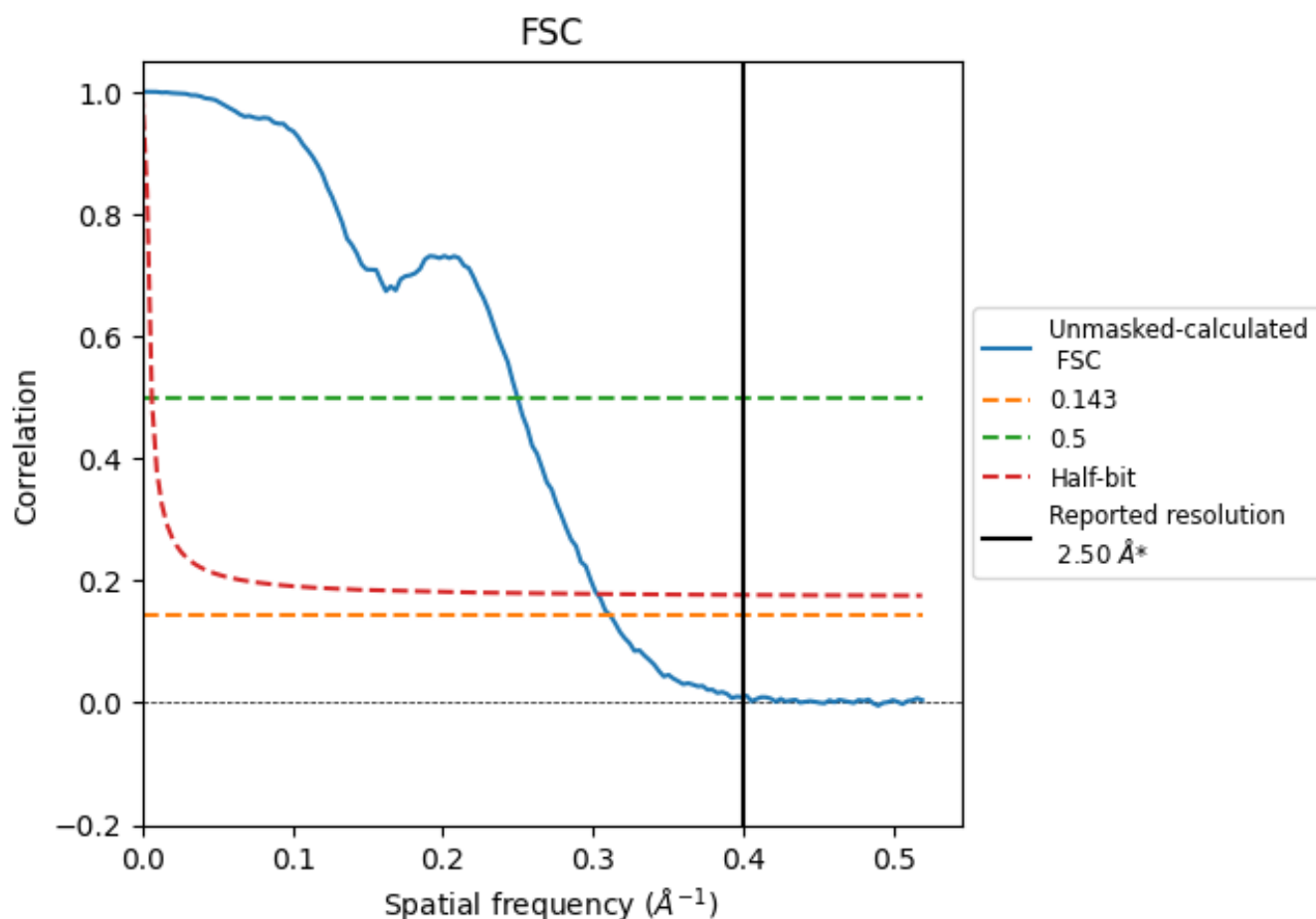


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

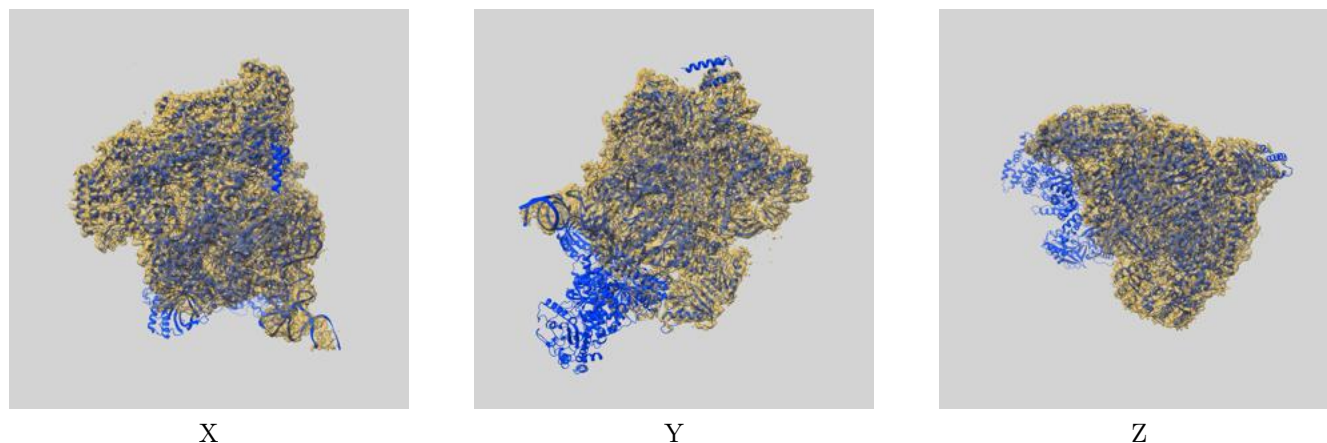
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	4.01	3.31

*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 3.21 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

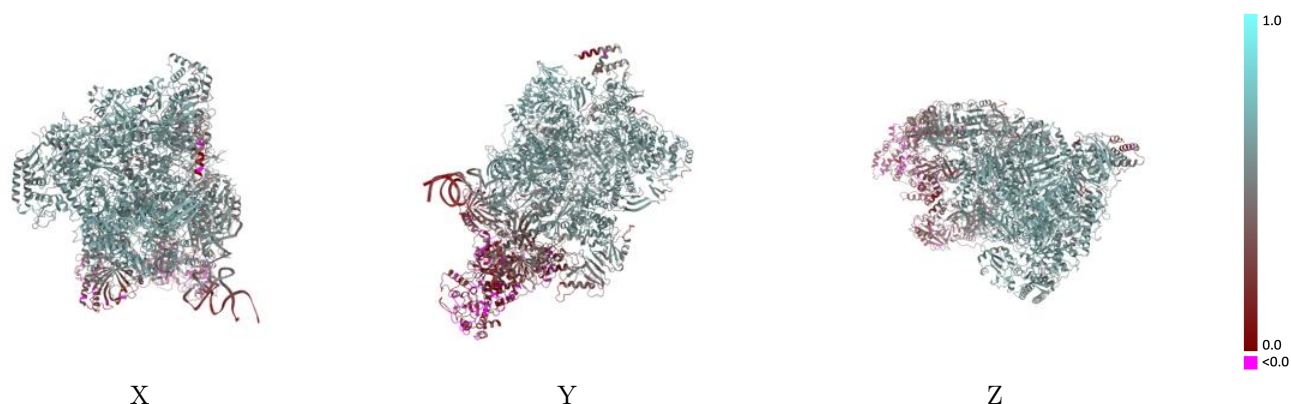
This section contains information regarding the fit between EMDB map EMD-50644 and PDB model 9FQ6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



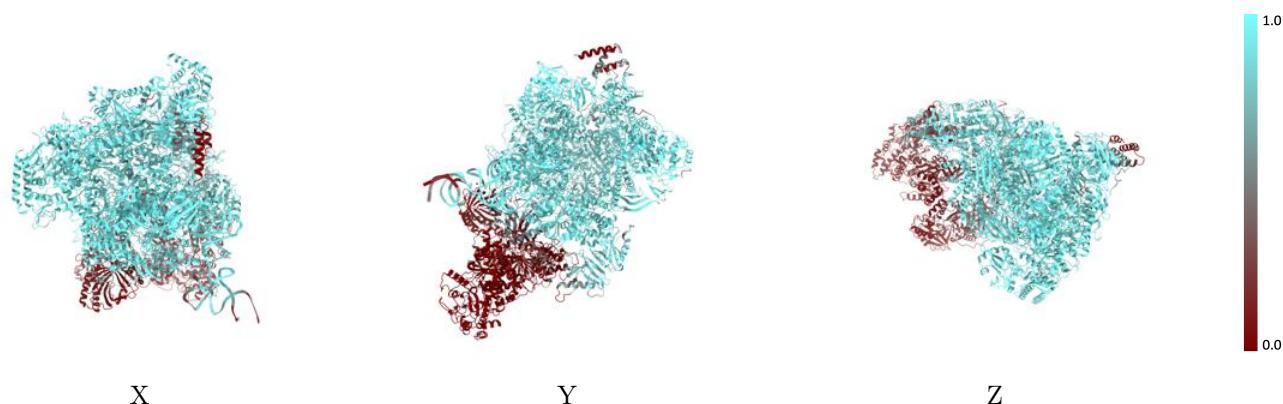
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



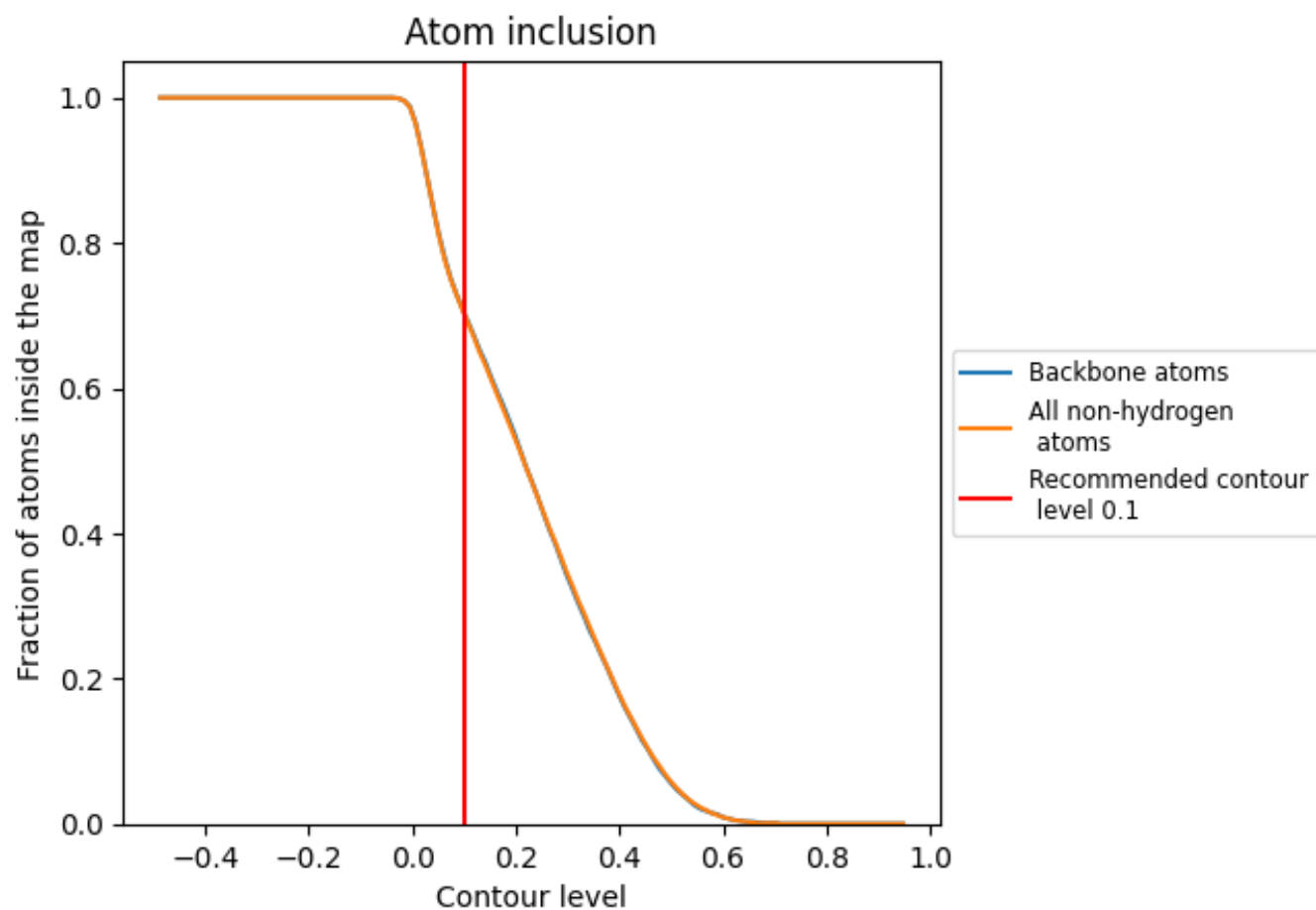
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.4920
A	0.9450	0.6000
B	0.9640	0.6150
C	0.9460	0.5690
E	0.9710	0.6130
F	0.9630	0.6260
G	0.9300	0.5770
I	0.7960	0.5210
J	0.9520	0.5830
L	0.0000	0.1380
O	0.0450	0.2590
Q	0.6390	0.4220
R	0.8420	0.5050
S	0.6020	0.4800
U	0.7630	0.3830
Y	0.4820	0.4090

