



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 02:22 pm BST

PDB ID : 9SKC / pdb_00009skc
EMDB ID : EMD-53761
Title : Model of M. pneumoniae 30S iT-TC (stable, +fidaxomicin)
Authors : Dobbs, J.M.; Mahamid, J.
Deposited on : 2025-09-02
Resolution : 9.50 Å(reported)

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

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

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:

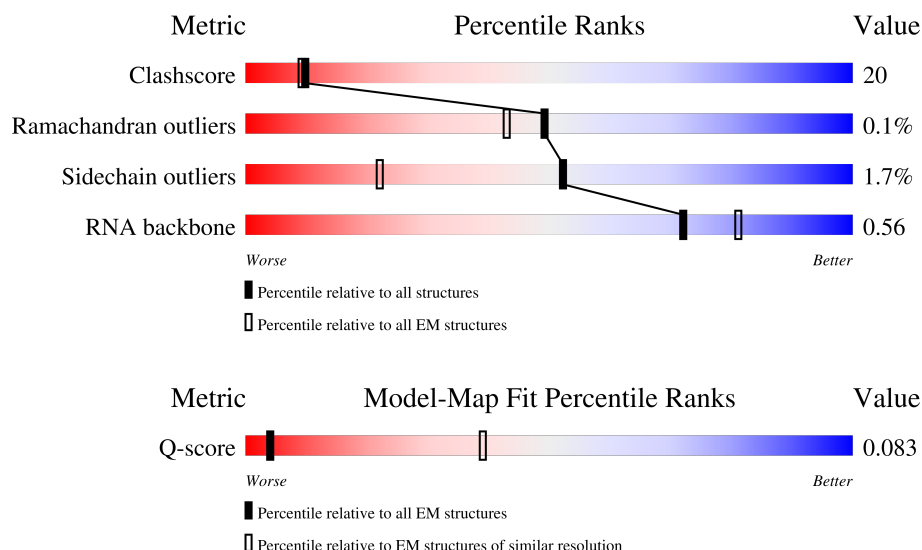
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 9.50 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	234 (9.00 - 10.00)

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	5	1505	
2	6	70	
3	A	249	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	215	
5	C	203	
6	D	153	
7	E	167	
8	F	154	
9	G	141	
10	H	128	
11	I	101	
12	J	114	
13	K	136	
14	L	118	
15	M	60	
16	N	83	
17	O	87	
18	P	83	
19	Q	65	
20	R	84	
21	S	77	
22	T	53	
23	U	65	
24	V	163	
25	W	1276	
26	X	327	
26	a	327	
27	Y	1391	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	Z	89	27% 73% 25%
29	b	366	35% 67% 31%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 84100 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	1492	Total	C	N	O	P	0	0
			31932	14270	5790	10380	1492		

- Molecule 2 is a RNA chain called Initiator fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	70	Total	C	N	O	P	0	0
			1494	667	267	491	69		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	249	Total	C	N	O	S	0	0
			1917	1224	331	355	7		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	215	Total	C	N	O	S	0	0
			1682	1063	308	306	5		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	203	Total	C	N	O	S	0	0
			1605	1015	306	280	4		

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	153	Total	C	N	O	S	0	0
			1153	731	222	197	3		

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	167	Total	C	N	O	S	0	0
			1211	762	219	229	1		

- Molecule 8 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	154	Total	C	N	O	S	0	0
			1231	777	234	215	5		

- Molecule 9 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	141	Total	C	N	O	S	0	0
			1103	720	192	189	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	128	Total	C	N	O	S	0	0
			993	634	184	174	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	101	Total	C	N	O	S	0	0
			803	518	141	143	1		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	114	Total	C	N	O	S	0	0
			828	514	153	155	6		

- Molecule 13 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	136	Total	C	N	O	S	0	0
			1055	667	209	177	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	118	Total	C	N	O	0	0
			922	576	186	160		

- Molecule 15 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	60	Total	C	N	O	S	0
			473	302	96	71	4	0

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	N	83	Total	C	N	O		0
			673	428	125	120		

- Molecule 17 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	O	87	Total	C	N	O	S	0
			690	445	128	115	2	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	83	Total	C	N	O		0
			675	425	135	115		

- Molecule 19 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Q	65	Total	C	N	O	S	0
			535	342	103	86	4	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	84	Total	C	N	O	S	0
			654	419	119	114	2	0

- Molecule 21 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	77	Total	C	N	O	0	0
			629	383	135	111		

- Molecule 22 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	53	Total	C	N	O	S	0	0
			439	275	93	70	1		

- Molecule 23 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	65	Total	C	N	O	S	0	0
			525	337	97	89	2		

- Molecule 24 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	163	Total	C	N	O	S	0	0
			1316	849	229	236	2		

- Molecule 25 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	1276	Total	C	N	O	S	0	0
			10085	6431	1752	1872	30		

- Molecule 26 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	308	Total	C	N	O	S	0	0
			2421	1550	407	454	10		
26	a	312	Total	C	N	O	S	0	0
			2452	1571	412	459	10		

- Molecule 27 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	1391	Total	C	N	O	S	0	0
			10948	6905	1892	2114	37		

- Molecule 28 is a protein called Probable DNA-directed RNA polymerase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	89	Total	C	N	O	S	0	0
			770	505	122	140	3		

- Molecule 29 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	366	Total	C	N	O	S	0	0
			2884	1834	479	562	9		

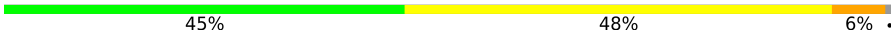
- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

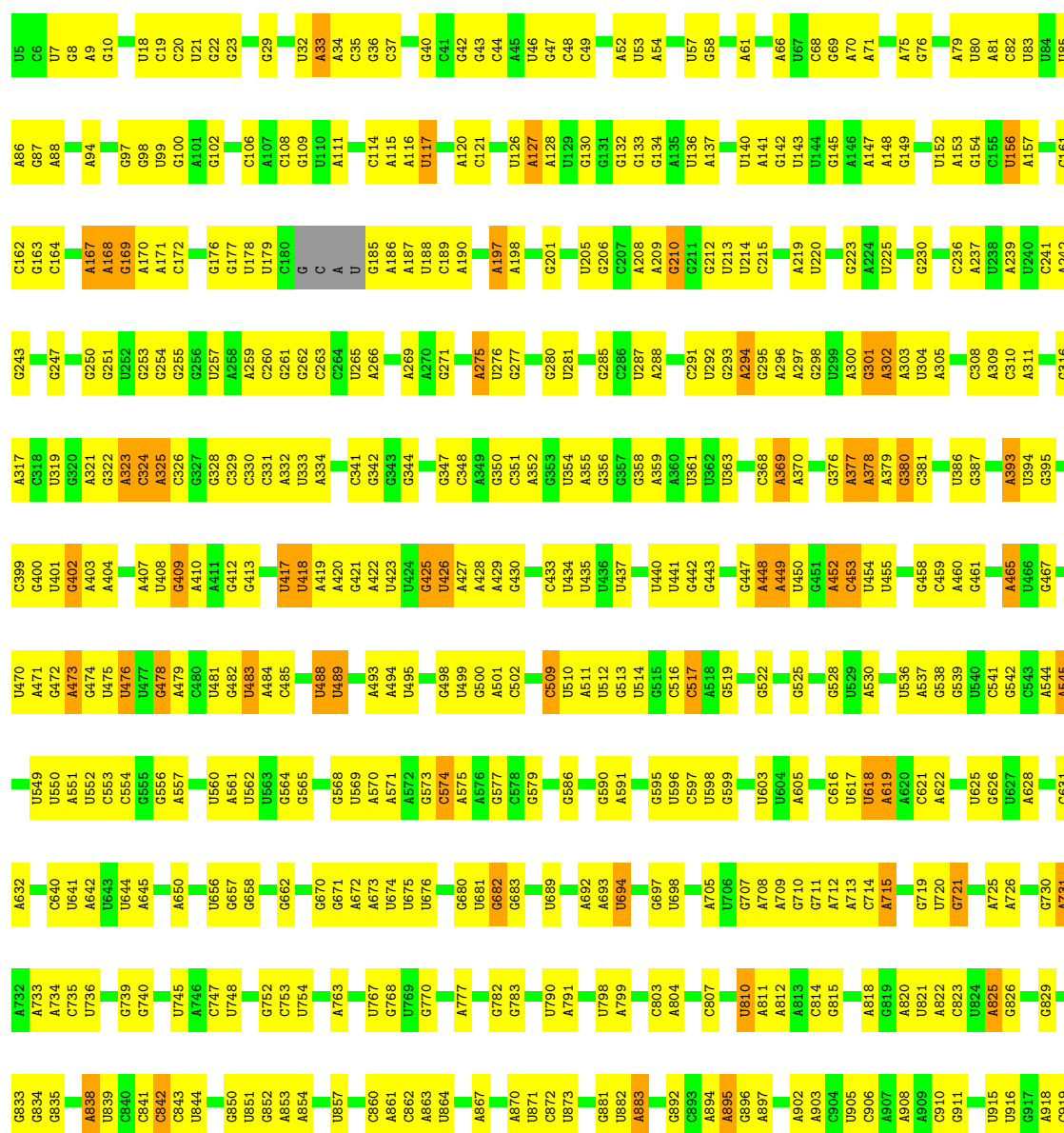
Mol	Chain	Residues	Atoms		AltConf
30	M	1	Total	Zn	0
			1	1	
30	Q	1	Total	Zn	0
			1	1	

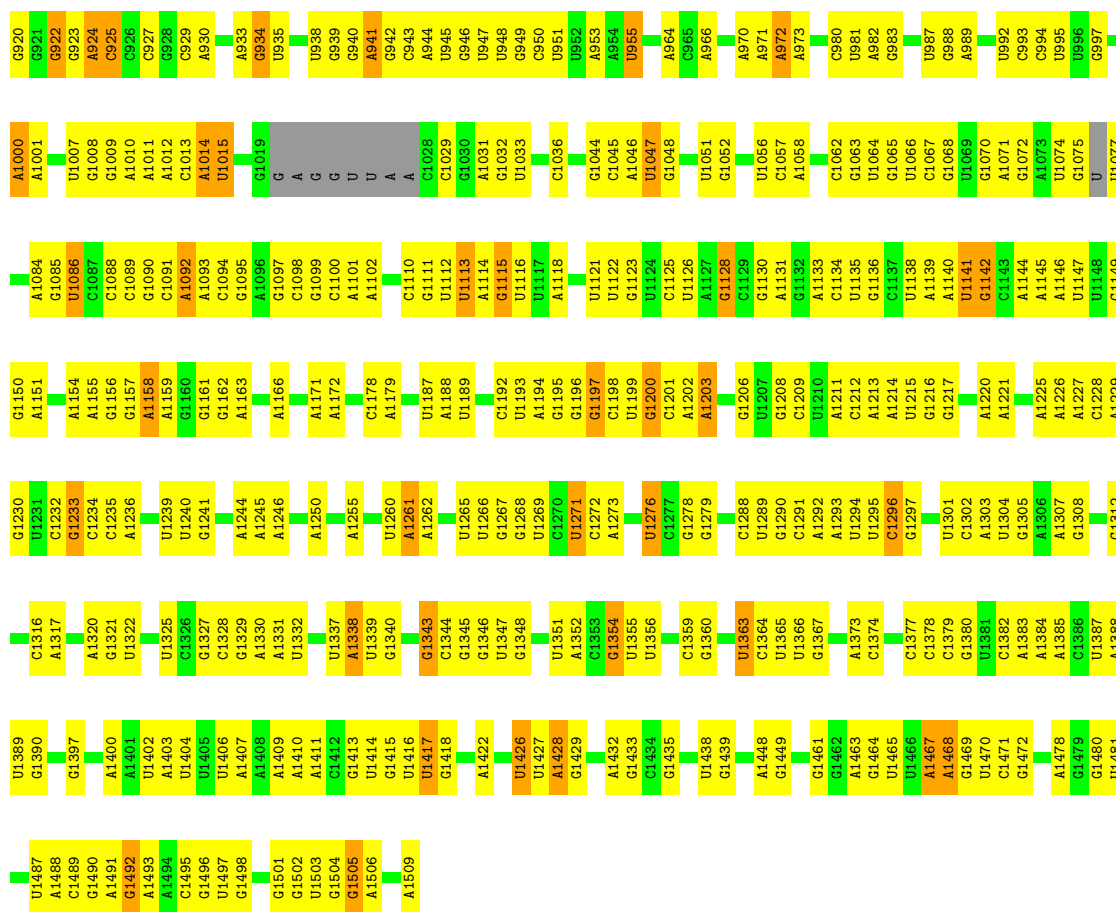
3 Residue-property plots

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

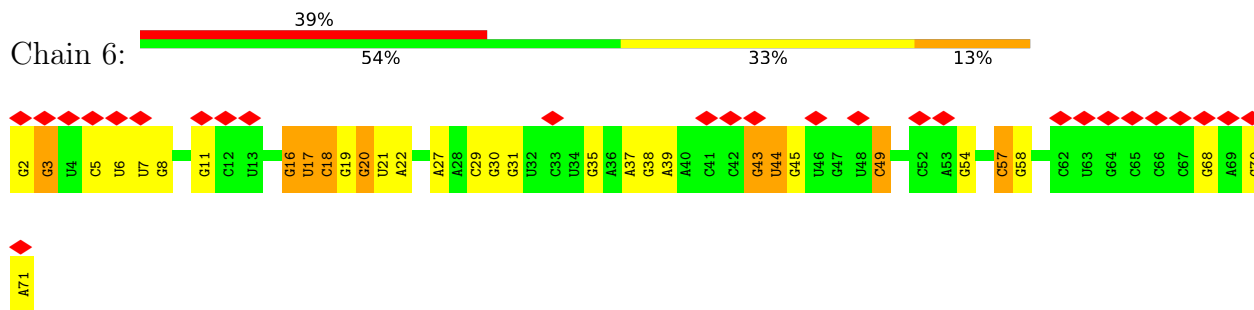
• Molecule 1: 16S ribosomal RNA

Chain 5: 

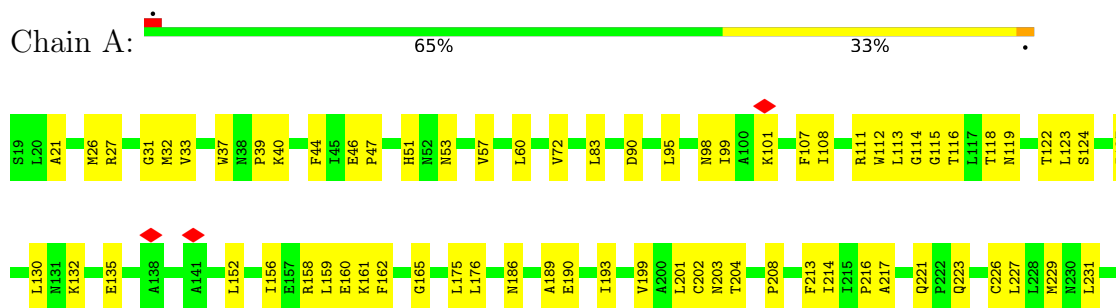


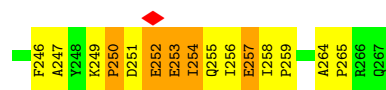


• Molecule 2: Initiator fMet-tRNA^{fMet}



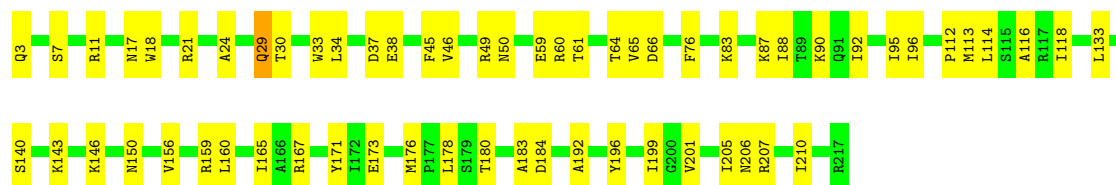
• Molecule 3: Small ribosomal subunit protein uS2





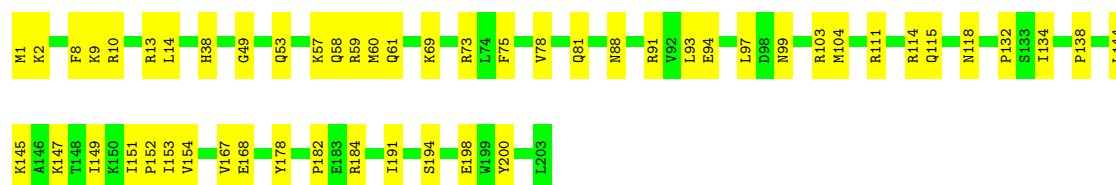
- Molecule 4: Small ribosomal subunit protein uS3

Chain B: 72% 28%



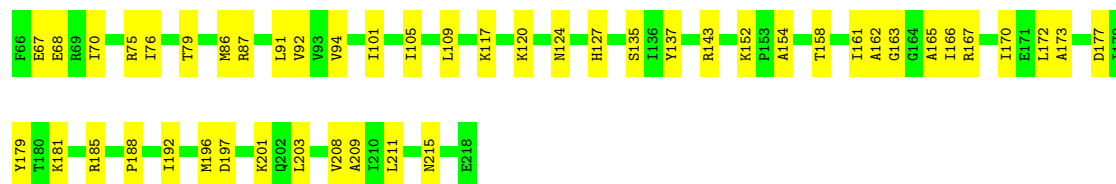
- Molecule 5: Small ribosomal subunit protein uS4

Chain C: 74% 26%



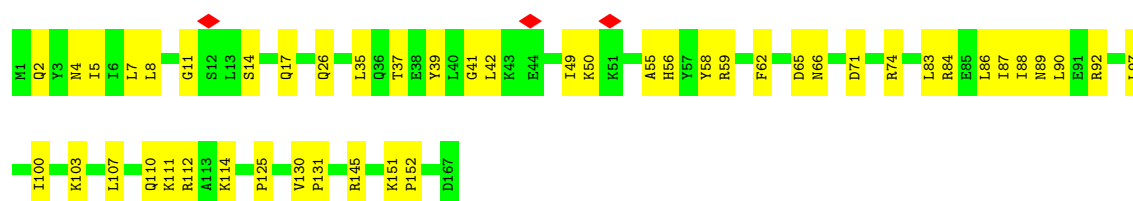
- Molecule 6: Small ribosomal subunit protein uS5

Chain D: 69% 31%



- Molecule 7: Small ribosomal subunit protein bS6

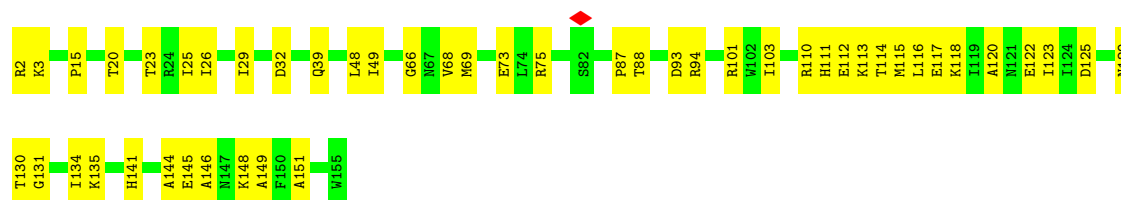
Chain E: 72% 28%



- Molecule 8: Small ribosomal subunit protein uS7

Chain F: 69% 31%

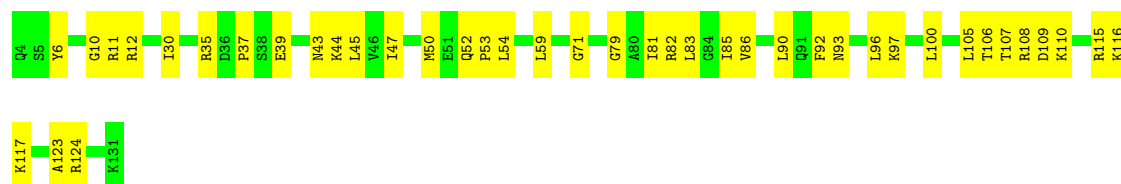




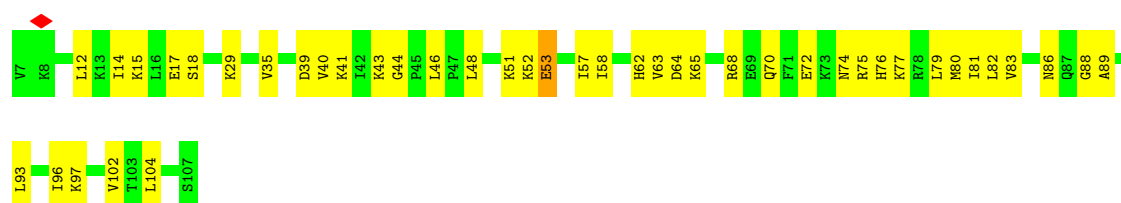
• Molecule 9: Small ribosomal subunit protein uS8



• Molecule 10: Small ribosomal subunit protein uS9



• Molecule 11: Small ribosomal subunit protein uS10

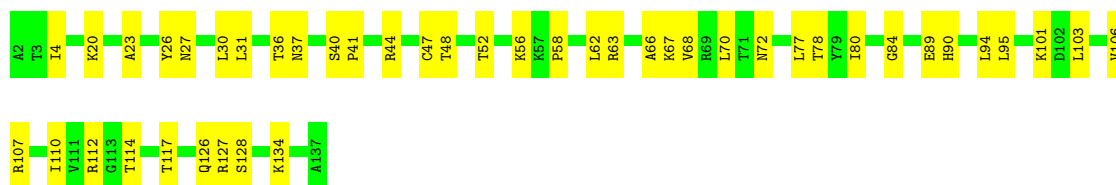


• Molecule 12: Small ribosomal subunit protein uS11

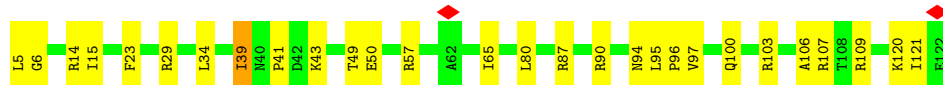
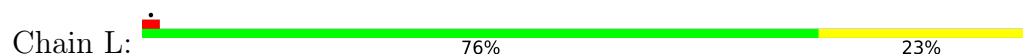


• Molecule 13: Small ribosomal subunit protein uS12





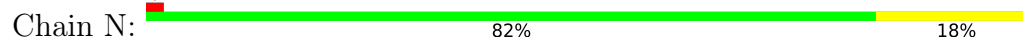
- Molecule 14: Small ribosomal subunit protein uS13



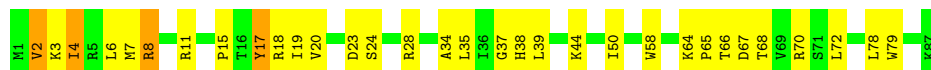
- Molecule 15: Small ribosomal subunit protein uS14



- Molecule 16: Small ribosomal subunit protein uS15



- Molecule 17: Small ribosomal subunit protein bS16



- Molecule 18: Small ribosomal subunit protein uS17



- Molecule 19: Small ribosomal subunit protein bS18



- Molecule 20: Small ribosomal subunit protein uS19

Chain R:  57% 39%



- Molecule 21: Small ribosomal subunit protein bS20

Chain S:  75% 25%



- Molecule 22: Small ribosomal subunit protein bS21

Chain T:  68% 28%



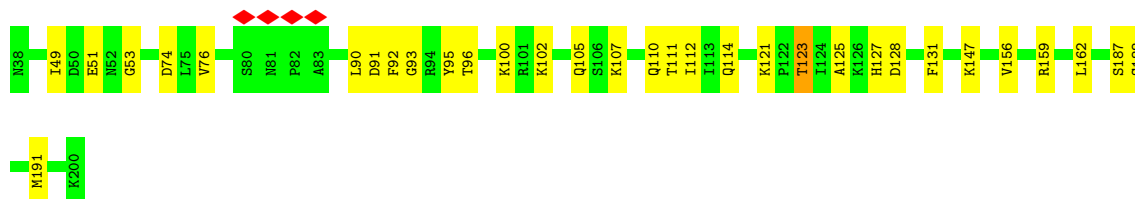
- Molecule 23: Translation initiation factor IF-1

Chain U:  20% 74% 26%



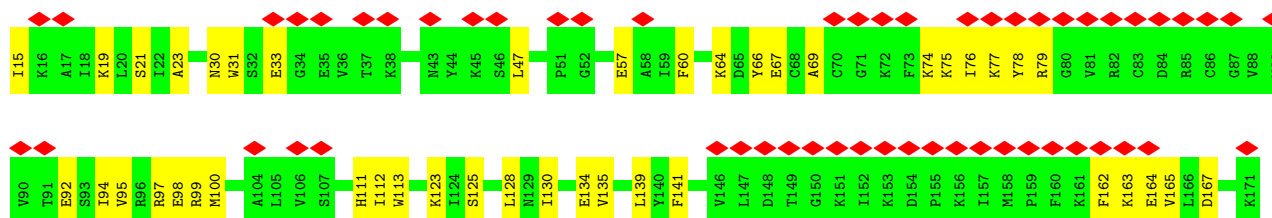
- Molecule 24: Translation initiation factor IF-3

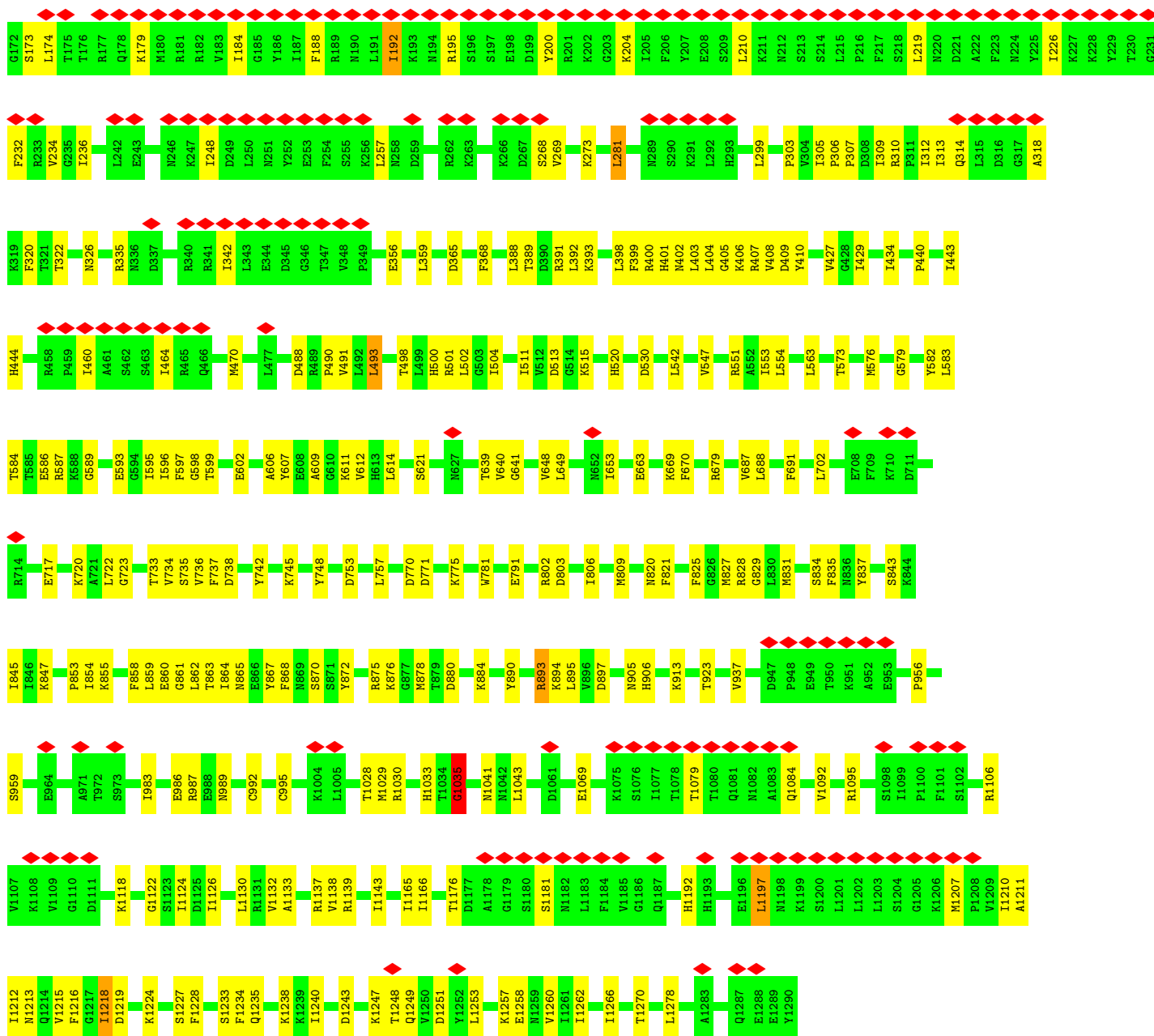
Chain V:  80% 19%



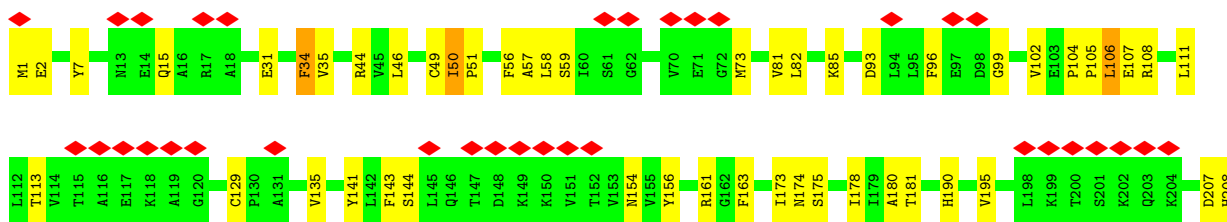
- Molecule 25: DNA-directed RNA polymerase subunit beta'

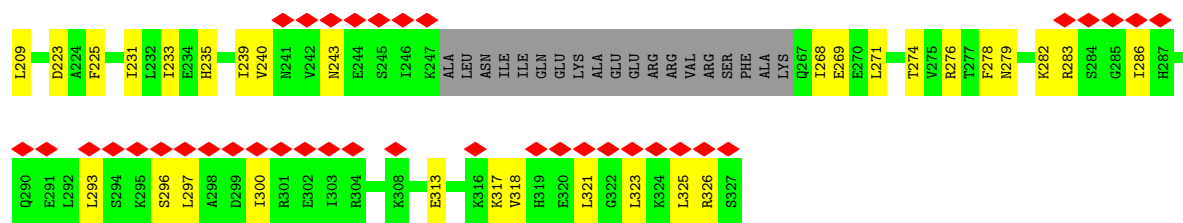
Chain W:  18% 76% 23%



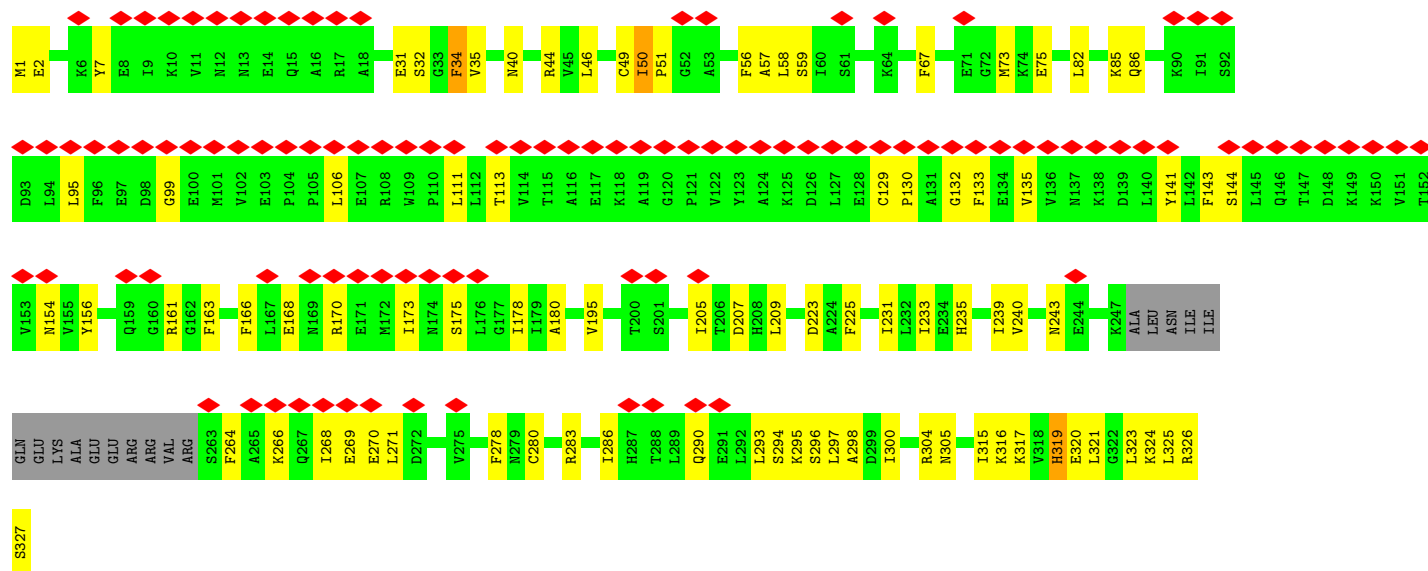


• Molecule 26: DNA-directed RNA polymerase subunit alpha

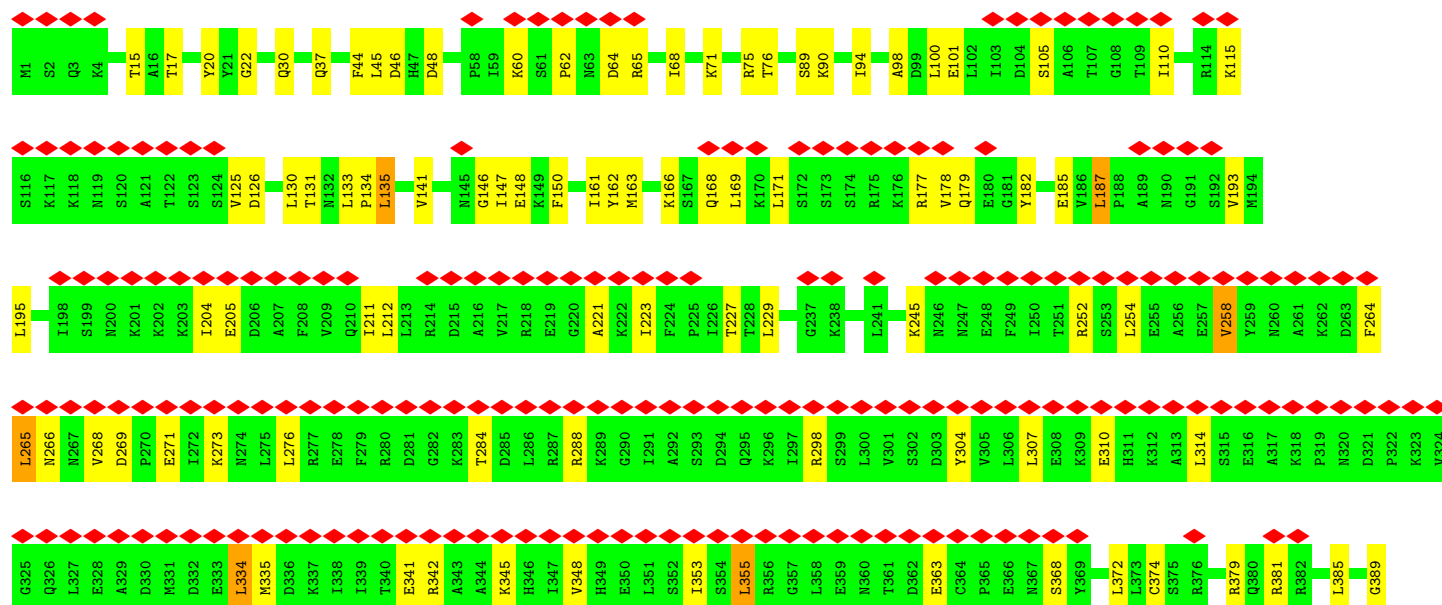
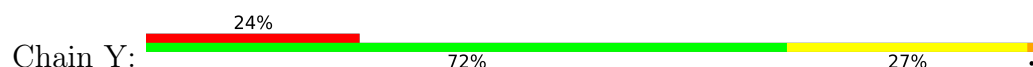


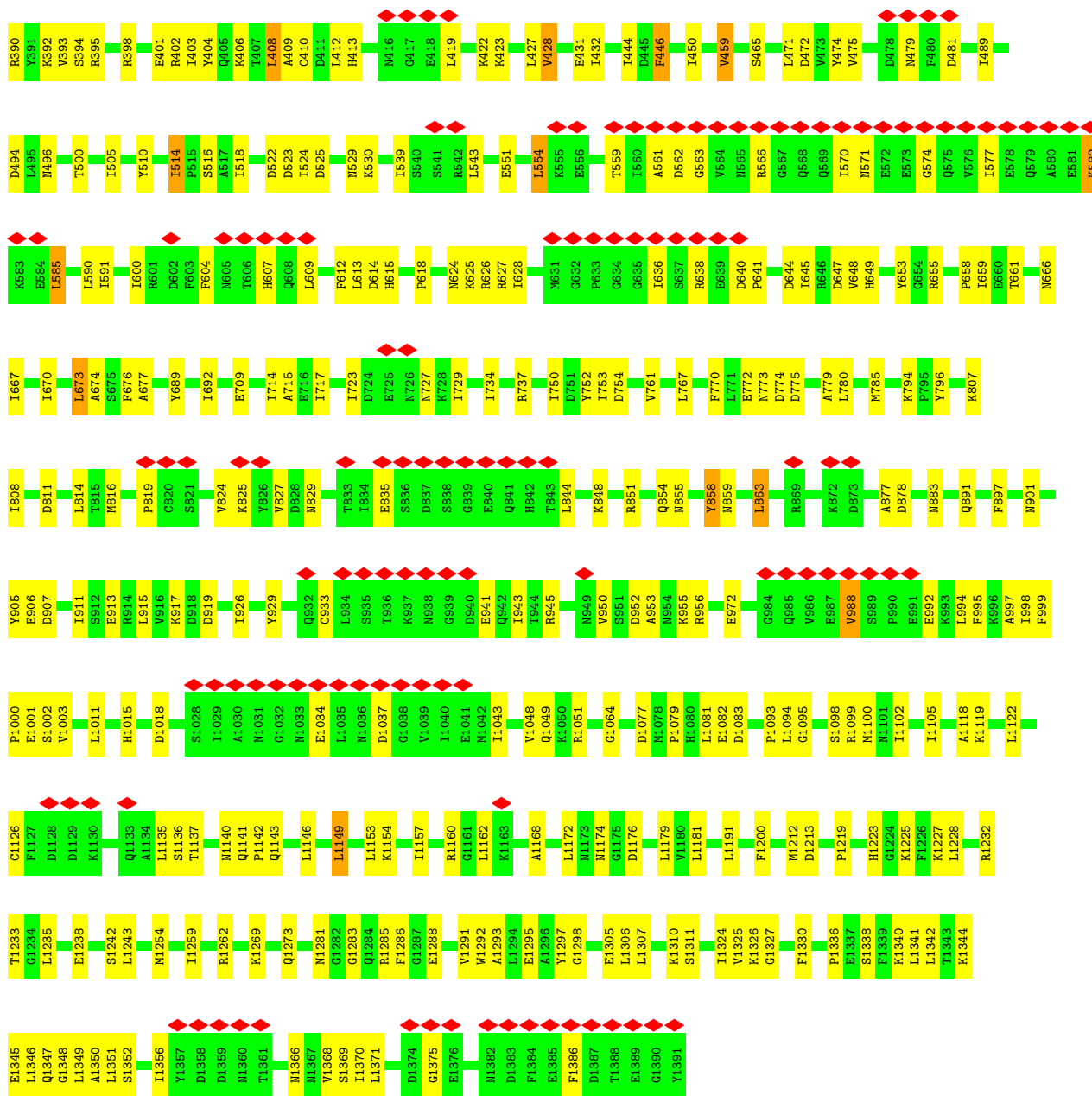


• Molecule 26: DNA-directed RNA polymerase subunit alpha

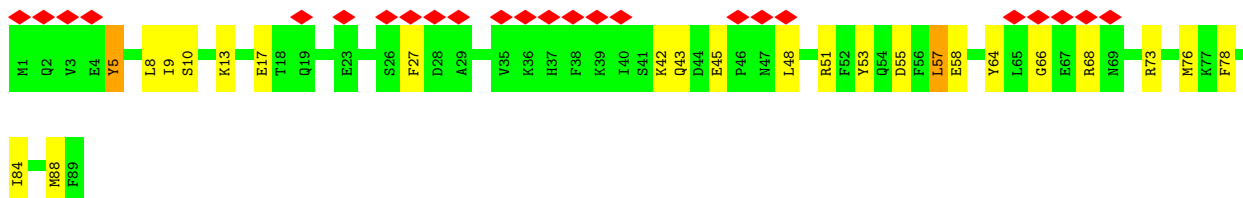
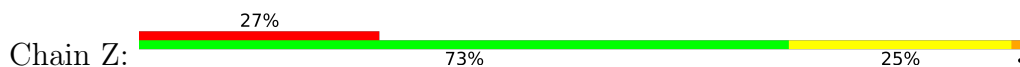


• Molecule 27: DNA-directed RNA polymerase subunit beta

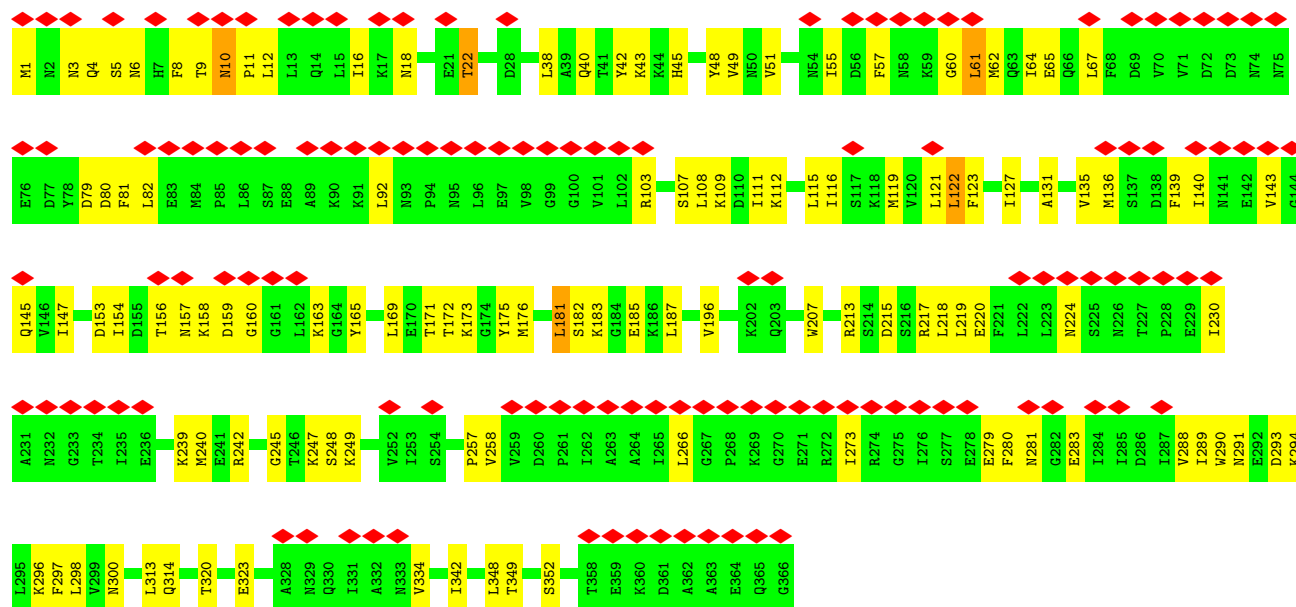




- Molecule 28: Probable DNA-directed RNA polymerase subunit delta



- Molecule 29: Transcription termination/antitermination protein NusA



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	1689	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 ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.017	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0, 2.0, 2.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	5	0.26	2/35753 (0.0%)	0.27	6/55734 (0.0%)
2	6	0.10	0/1670	0.29	0/2603
3	A	0.33	0/1951	0.67	5/2652 (0.2%)
4	B	0.14	0/1705	0.40	0/2304
5	C	0.15	0/1635	0.40	0/2202
6	D	0.15	0/1168	0.43	0/1568
7	E	0.16	0/1229	0.45	0/1670
8	F	0.15	0/1250	0.46	0/1682
9	G	0.16	0/1119	0.47	0/1508
10	H	0.17	0/1009	0.51	0/1354
11	I	0.24	0/814	0.56	0/1096
12	J	0.14	0/843	0.36	0/1136
13	K	0.23	0/1073	0.59	0/1445
14	L	0.32	0/933	0.64	0/1254
15	M	0.50	1/482 (0.2%)	0.84	1/643 (0.2%)
16	N	0.13	0/679	0.37	0/907
17	O	0.39	0/703	0.80	1/945 (0.1%)
18	P	0.14	0/684	0.40	0/913
19	Q	0.17	0/545	0.46	0/730
20	R	0.41	0/670	0.87	1/904 (0.1%)
21	S	0.15	0/631	0.42	0/838
22	T	0.45	0/442	0.86	0/582
23	U	0.71	0/531	1.07	0/709
24	V	0.68	0/1336	1.14	1/1793 (0.1%)
25	W	0.71	0/10259	1.06	2/13846 (0.0%)
26	X	0.68	0/2458	1.00	0/3313
26	a	0.69	0/2490	1.00	0/3355
27	Y	0.70	0/11124	1.06	0/15014
28	Z	0.69	0/792	1.05	0/1065
29	b	0.70	0/2922	1.01	0/3944
All	All	0.46	3/88900 (0.0%)	0.68	17/127709 (0.0%)

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
25	W	0	1
27	Y	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	924	A	O3'-P	36.27	2.15	1.61
1	5	1363	U	O3'-P	24.57	1.98	1.61
15	M	60	SER	CA-CB	-6.62	1.47	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	924	A	OP2-P-O3'	-24.78	33.66	108.00
1	5	1363	U	O3'-P-O5'	-14.33	82.50	104.00
3	A	259	PRO	N-CA-C	-13.91	83.81	112.47
1	5	924	A	OP1-P-O3'	12.87	146.60	108.00
1	5	924	A	P-O3'-C3'	12.41	138.82	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	W	893	ARG	Sidechain
27	Y	858	TYR	Sidechain

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	5	31932	0	16039	727	0
2	6	1494	0	754	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1917	0	1891	84	0
4	B	1682	0	1733	54	0
5	C	1605	0	1603	49	0
6	D	1153	0	1231	34	0
7	E	1211	0	1108	41	0
8	F	1231	0	1285	37	0
9	G	1103	0	1215	55	0
10	H	993	0	1023	32	0
11	I	803	0	876	31	0
12	J	828	0	855	26	0
13	K	1055	0	1124	32	0
14	L	922	0	957	32	0
15	M	473	0	505	15	0
16	N	673	0	730	11	0
17	O	690	0	726	37	0
18	P	675	0	728	19	0
19	Q	535	0	559	15	0
20	R	654	0	629	30	0
21	S	629	0	681	19	0
22	T	439	0	467	11	0
23	U	525	0	564	61	0
24	V	1316	0	1378	120	0
25	W	10085	0	10375	752	0
26	X	2421	0	2495	138	0
26	a	2452	0	2522	216	0
27	Y	10948	0	11071	945	0
28	Z	770	0	738	54	0
29	b	2884	0	2937	451	0
30	M	1	0	0	0	0
30	Q	1	0	0	0	0
All	All	84100	0	68799	2974	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 20.

The worst 5 of 2974 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:57:C:C4	24:V:49:ILE:HD13	1.23	1.71
27:Y:999:PHE:CZ	29:b:108:LEU:HD23	1.23	1.70
27:Y:998:ILE:HG22	29:b:108:LEU:CD2	1.19	1.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:999:PHE:CE1	29:b:108:LEU:HD23	1.28	1.64
29:b:290:TRP:HE1	29:b:293:ASP:CB	1.07	1.62

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	
3	A	247/249 (99%)	227 (92%)	18 (7%)	2 (1%)	16	54
4	B	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
5	C	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
6	D	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
7	E	165/167 (99%)	145 (88%)	20 (12%)	0	100	100
8	F	152/154 (99%)	135 (89%)	17 (11%)	0	100	100
9	G	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
10	H	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
11	I	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
12	J	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
13	K	134/136 (98%)	117 (87%)	17 (13%)	0	100	100
14	L	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
15	M	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
16	N	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
17	O	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
18	P	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
19	Q	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
20	R	82/84 (98%)	75 (92%)	7 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
22	T	51/53 (96%)	45 (88%)	6 (12%)	0	100	100
23	U	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
24	V	157/163 (96%)	155 (99%)	2 (1%)	0	100	100
25	W	1274/1276 (100%)	1252 (98%)	21 (2%)	1 (0%)	48	83
26	X	304/327 (93%)	301 (99%)	3 (1%)	0	100	100
26	a	308/327 (94%)	305 (99%)	3 (1%)	0	100	100
27	Y	1389/1391 (100%)	1355 (98%)	33 (2%)	1 (0%)	48	83
28	Z	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
29	b	358/366 (98%)	350 (98%)	6 (2%)	2 (1%)	21	59
All	All	6371/6475 (98%)	6083 (96%)	282 (4%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	250	PRO
25	W	1035	GLY
27	Y	582	LYS
3	A	254	ILE
29	b	3	ASN

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	
3	A	200/220 (91%)	197 (98%)	3 (2%)	57	72
4	B	176/180 (98%)	175 (99%)	1 (1%)	78	83
5	C	164/181 (91%)	164 (100%)	0	100	100
6	D	117/123 (95%)	117 (100%)	0	100	100
7	E	107/150 (71%)	107 (100%)	0	100	100
8	F	128/131 (98%)	128 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	121/123 (98%)	121 (100%)	0	100	100
10	H	101/111 (91%)	100 (99%)	1 (1%)	68	78
11	I	93/95 (98%)	91 (98%)	2 (2%)	45	64
12	J	91/91 (100%)	91 (100%)	0	100	100
13	K	111/117 (95%)	111 (100%)	0	100	100
14	L	92/100 (92%)	89 (97%)	3 (3%)	33	55
15	M	47/47 (100%)	45 (96%)	2 (4%)	26	47
16	N	76/76 (100%)	76 (100%)	0	100	100
17	O	71/76 (93%)	66 (93%)	5 (7%)	14	35
18	P	73/73 (100%)	73 (100%)	0	100	100
19	Q	56/56 (100%)	56 (100%)	0	100	100
20	R	66/74 (89%)	59 (89%)	7 (11%)	6	21
21	S	70/70 (100%)	70 (100%)	0	100	100
22	T	43/49 (88%)	38 (88%)	5 (12%)	5	18
23	U	57/57 (100%)	57 (100%)	0	100	100
24	V	145/145 (100%)	144 (99%)	1 (1%)	76	81
25	W	1113/1113 (100%)	1100 (99%)	13 (1%)	63	75
26	X	269/285 (94%)	262 (97%)	7 (3%)	40	62
26	a	272/285 (95%)	265 (97%)	7 (3%)	40	62
27	Y	1213/1213 (100%)	1188 (98%)	25 (2%)	47	65
28	Z	83/83 (100%)	79 (95%)	4 (5%)	23	44
29	b	327/327 (100%)	322 (98%)	5 (2%)	57	72
All	All	5482/5651 (97%)	5391 (98%)	91 (2%)	52	69

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	Y	314	LEU
27	Y	1137	THR
27	Y	355	LEU
27	Y	554	LEU
28	Z	5	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
27	Y	1033	ASN
29	b	300	ASN
27	Y	1115	HIS
26	a	86	GLN
25	W	137	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	1488/1505 (98%)	232 (15%)	5 (0%)
2	6	69/70 (98%)	13 (18%)	1 (1%)
All	All	1557/1575 (98%)	245 (15%)	6 (0%)

5 of 245 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	7	U
1	5	10	G
1	5	32	U
1	5	33	A
1	5	40	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	838	A
1	5	1338	A
2	6	16	G
1	5	419	A
1	5	168	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	b	3
1	5	3
24	V	2

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	292:GLU	C	293:ASP	N	8.91
1	b	143:VAL	C	144:GLY	N	6.10
1	V	91:ASP	C	92:PHE	N	4.18
1	V	111:THR	C	112:ILE	N	3.16
1	b	215:ASP	C	216:SER	N	3.12

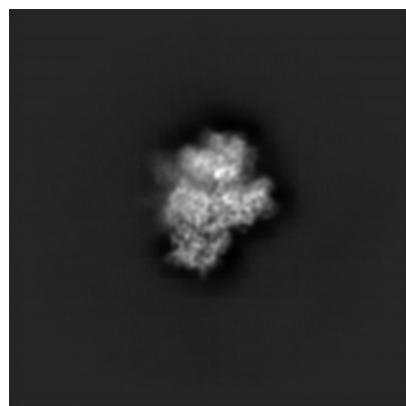
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53761. These allow visual inspection of the internal detail of the map and identification of artifacts.

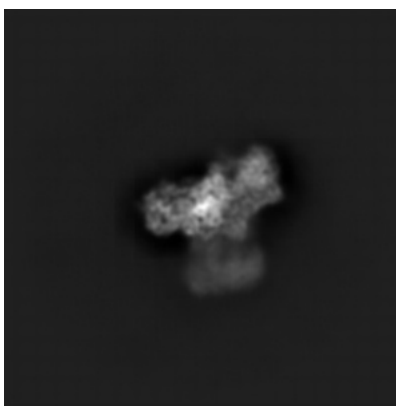
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

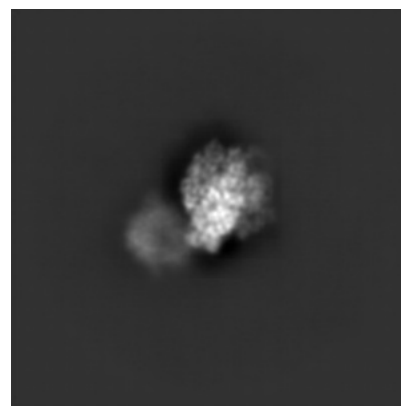
6.1.1 Primary map



X

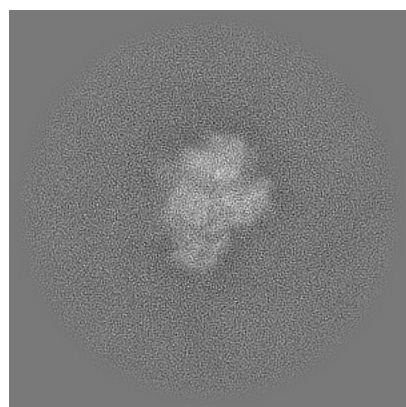


Y

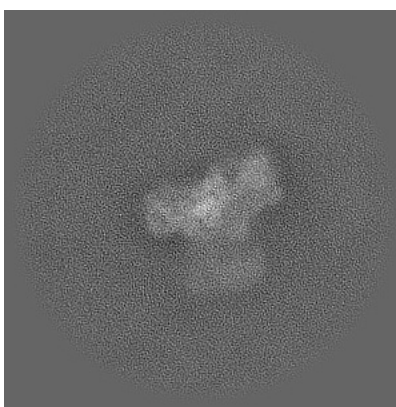


Z

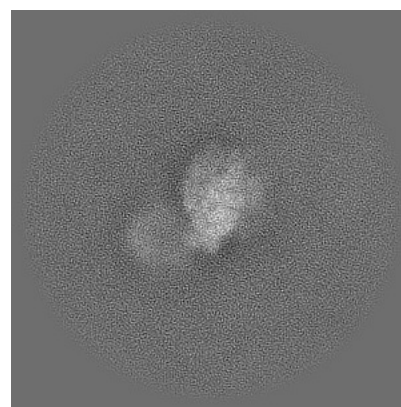
6.1.2 Raw map



X



Y

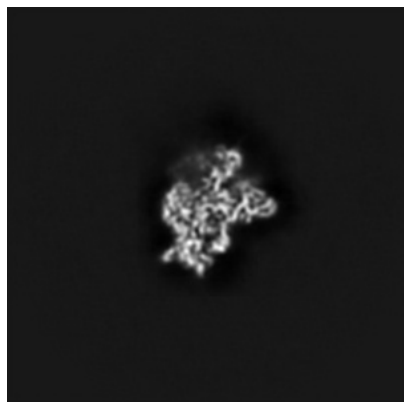


Z

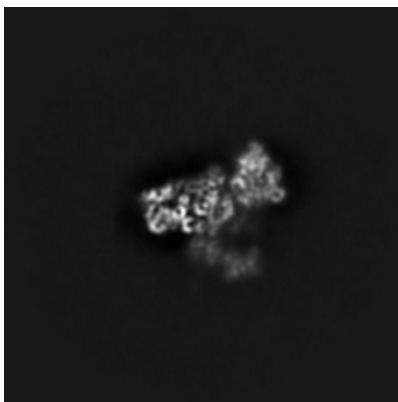
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

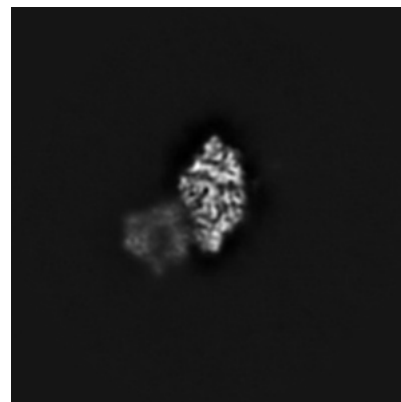
6.2.1 Primary map



X Index: 150

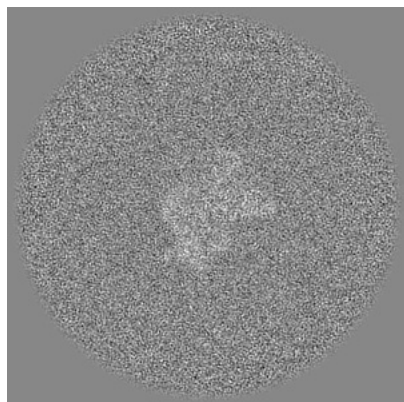


Y Index: 150

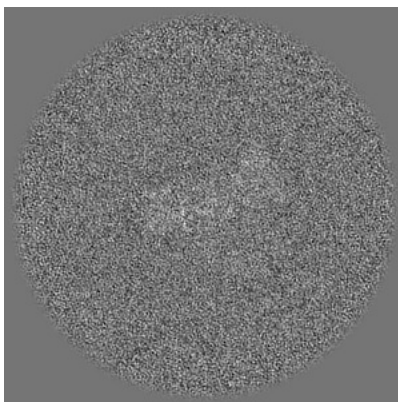


Z Index: 150

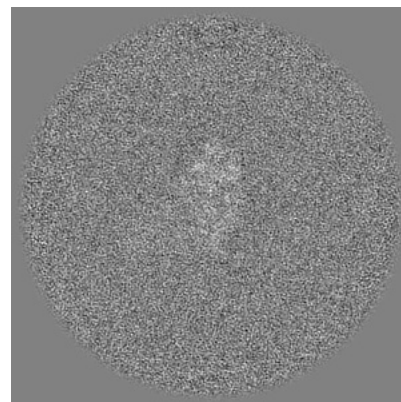
6.2.2 Raw map



X Index: 150



Y Index: 150

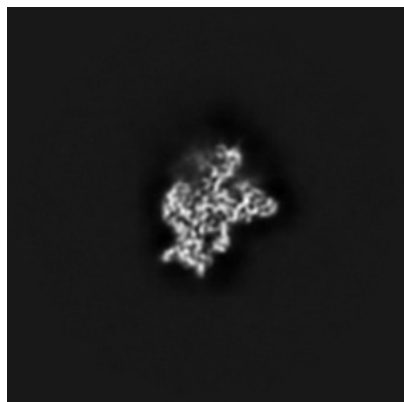


Z Index: 150

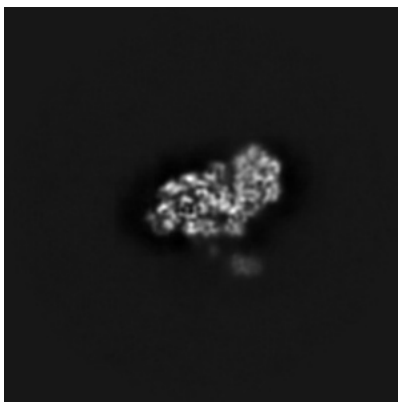
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

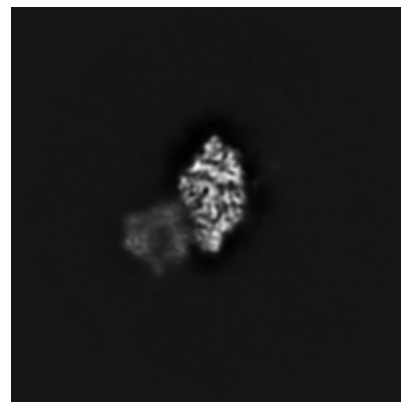
6.3.1 Primary map



X Index: 151

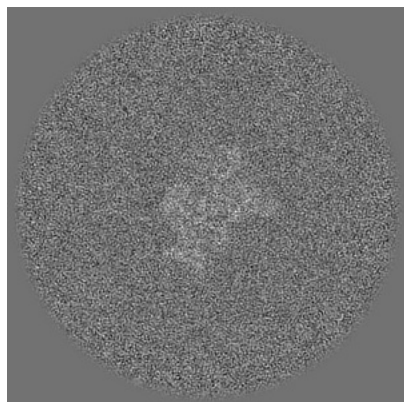


Y Index: 157

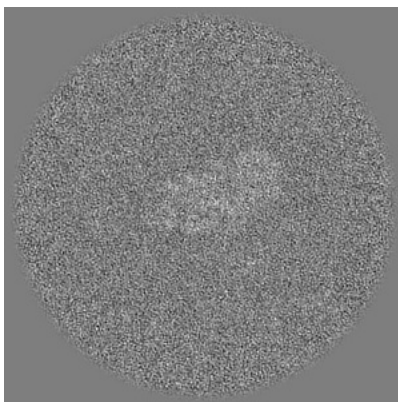


Z Index: 150

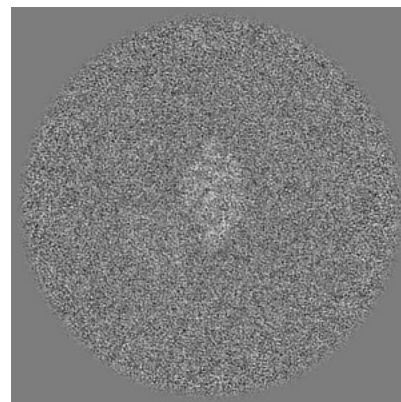
6.3.2 Raw map



X Index: 152



Y Index: 157

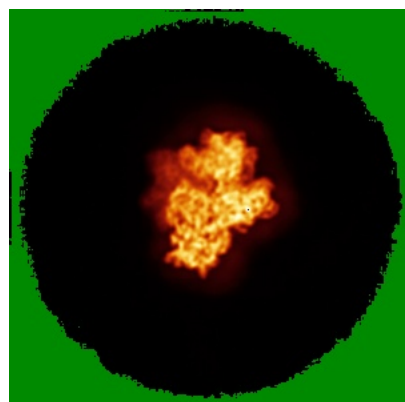


Z Index: 149

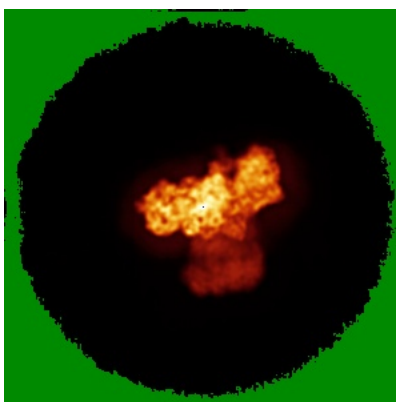
The images above show the largest variance slices of the map in three orthogonal directions.

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

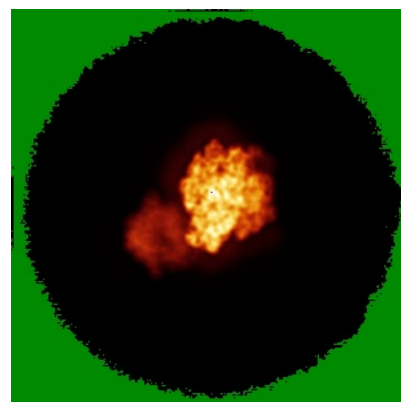
6.4.1 Primary map



X

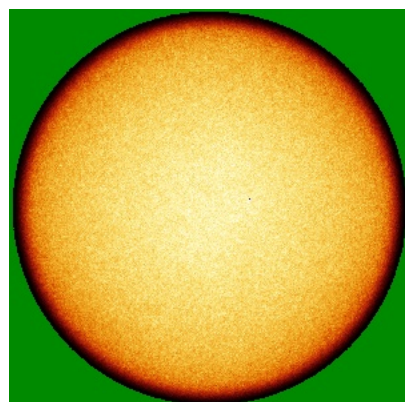


Y

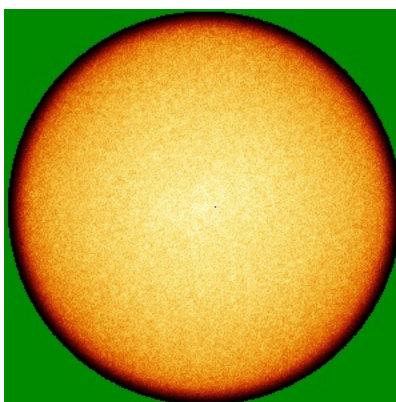


Z

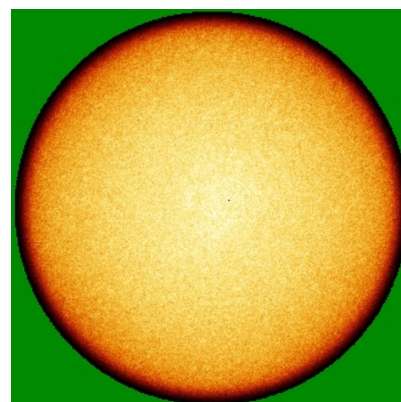
6.4.2 Raw map



X



Y

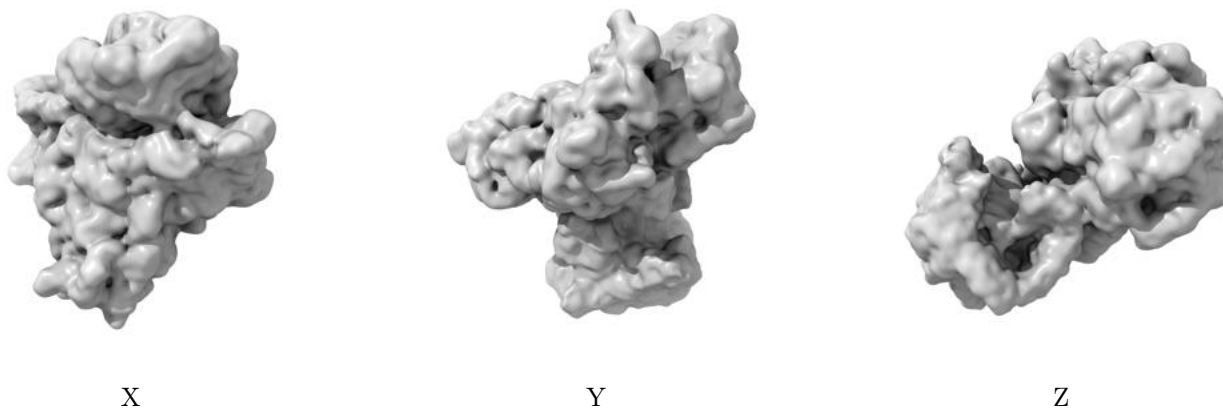


Z

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.

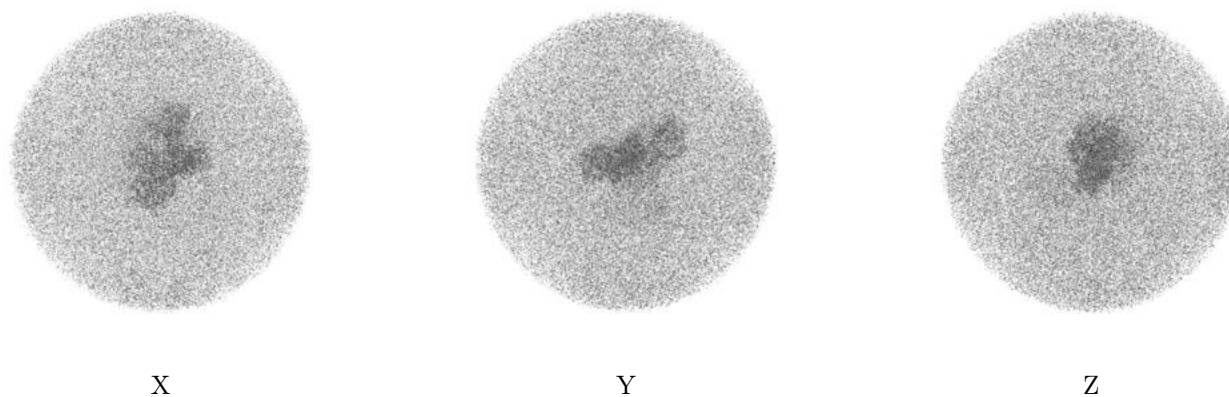
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0015. 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.

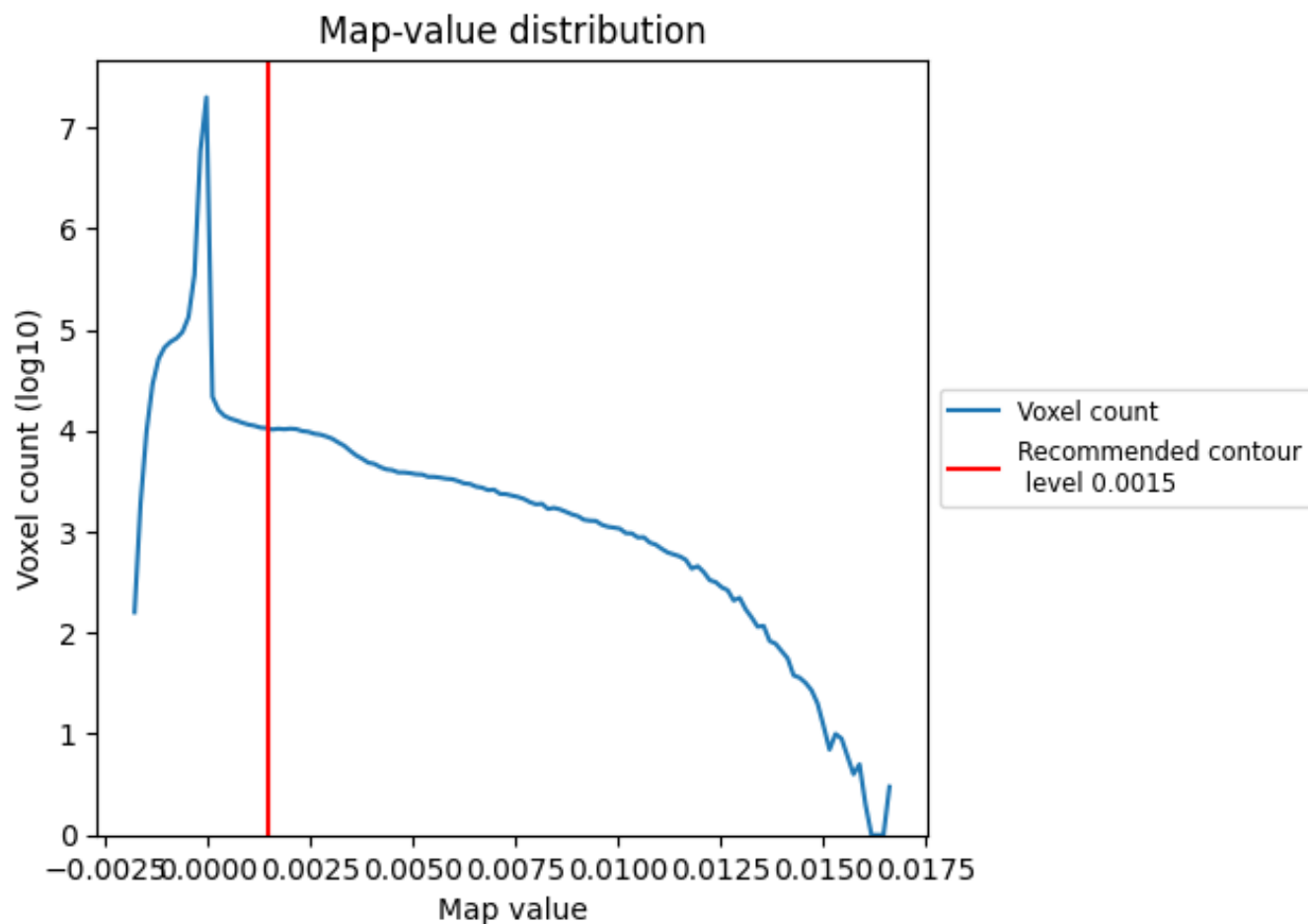
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

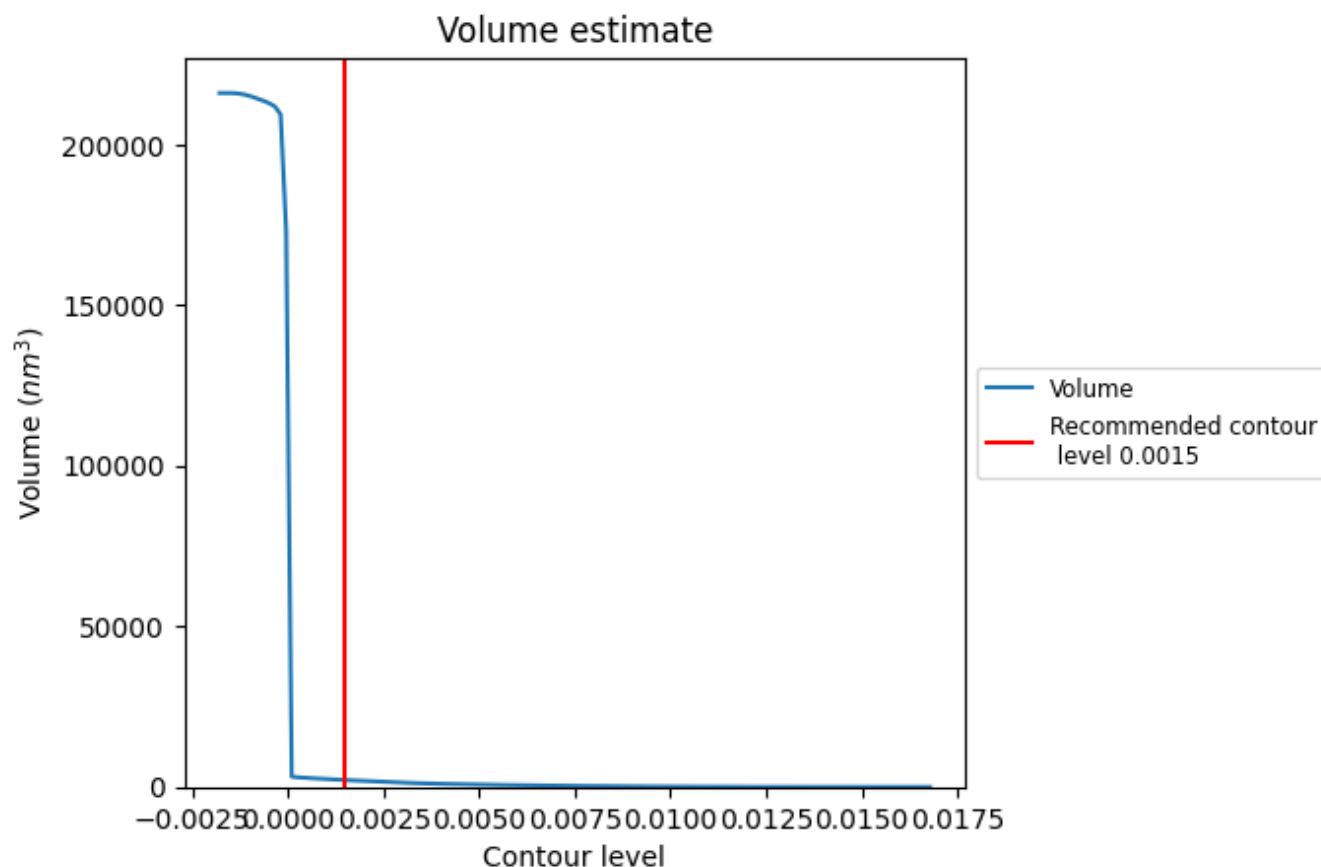
This section contains the results of statistical analysis of the map.

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.

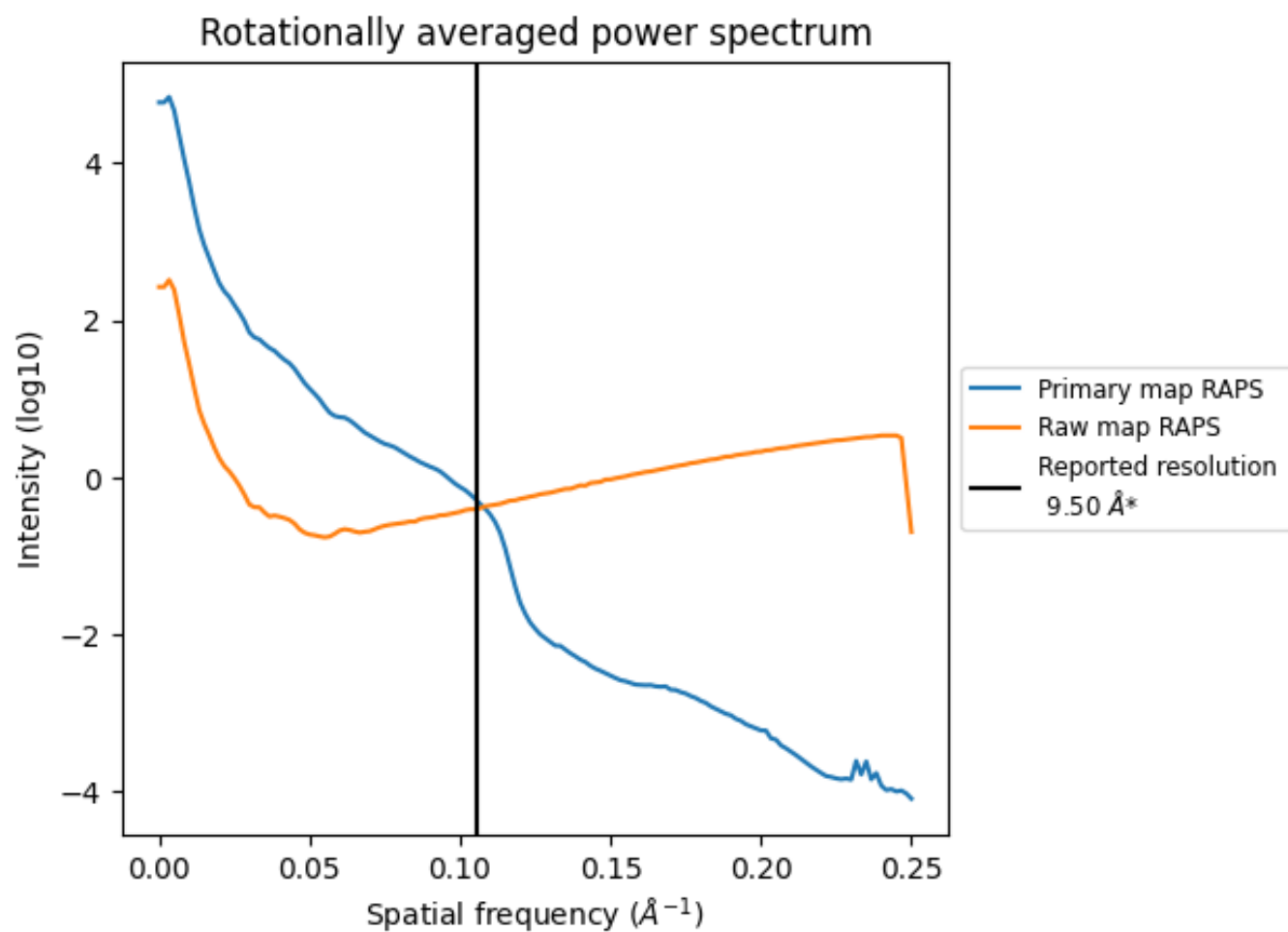
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2157 nm^3 ; this corresponds to an approximate mass of 1949 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 ⓘ

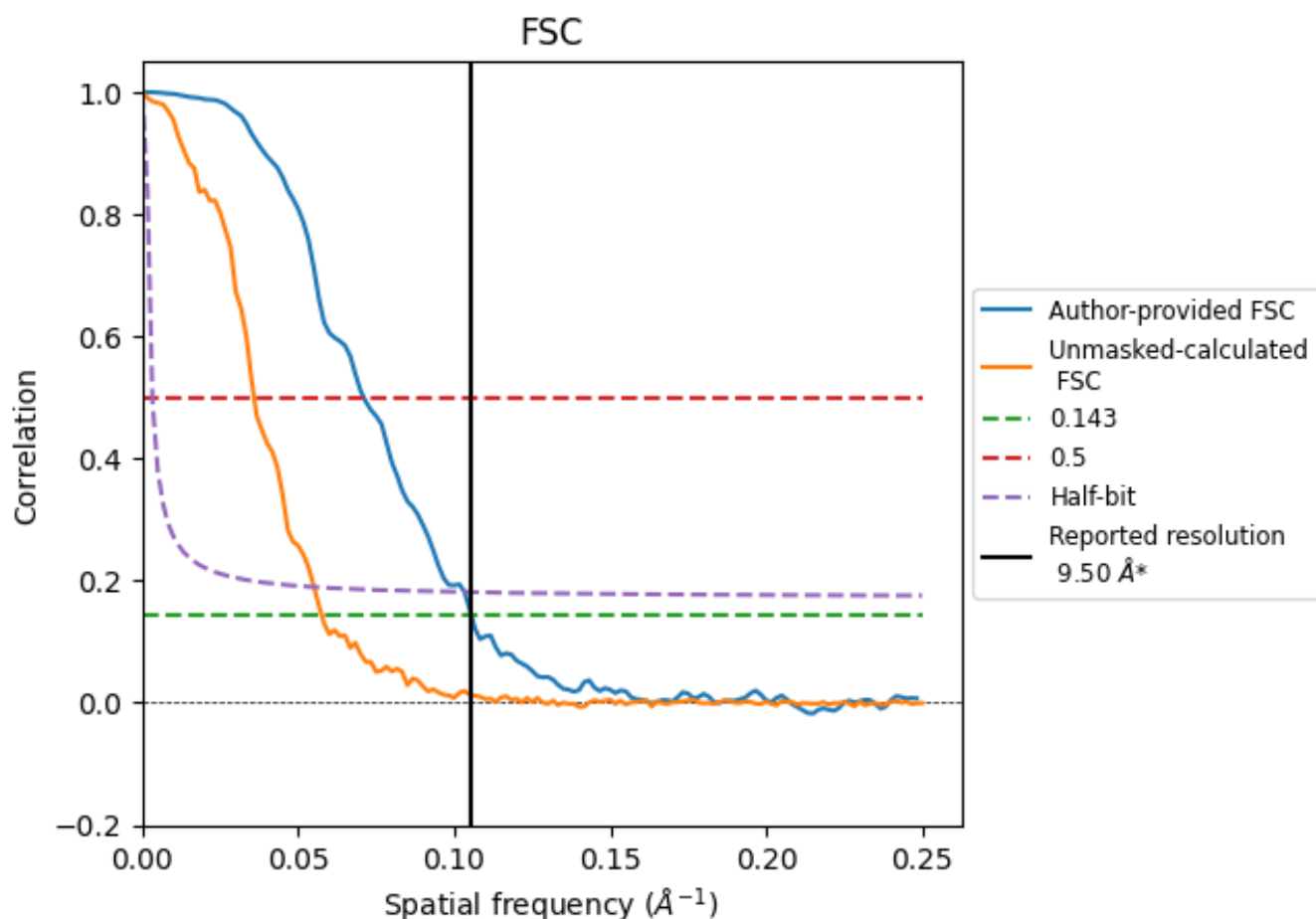


*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

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 0.105 Å⁻¹

8.2 Resolution estimates [i](#)

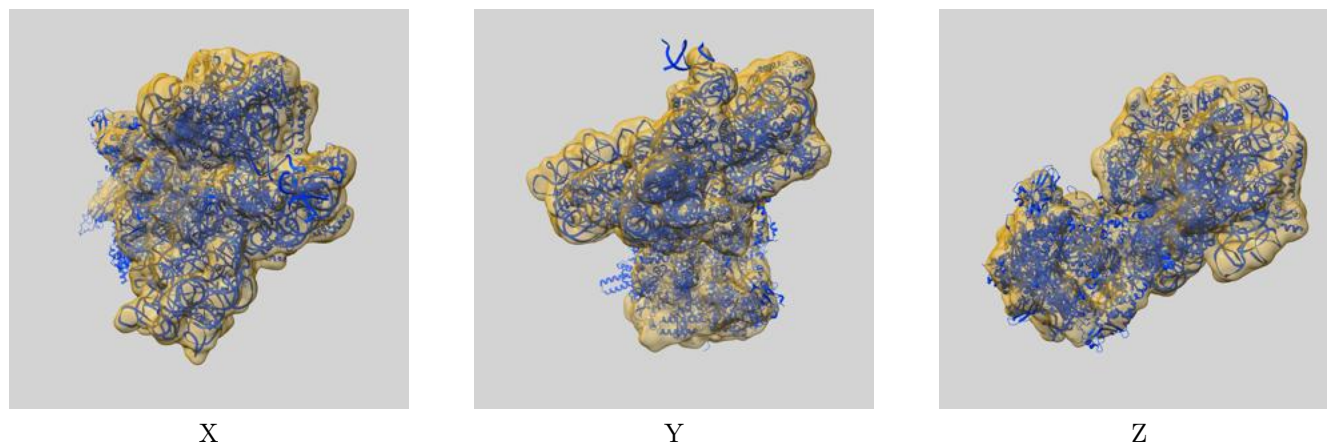
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.50	-	-
Author-provided FSC curve	9.48	14.08	9.67
Unmasked-calculated*	17.39	27.93	18.15

*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 17.39 differs from the reported value 9.5 by more than 10 %

9 Map-model fit [i](#)

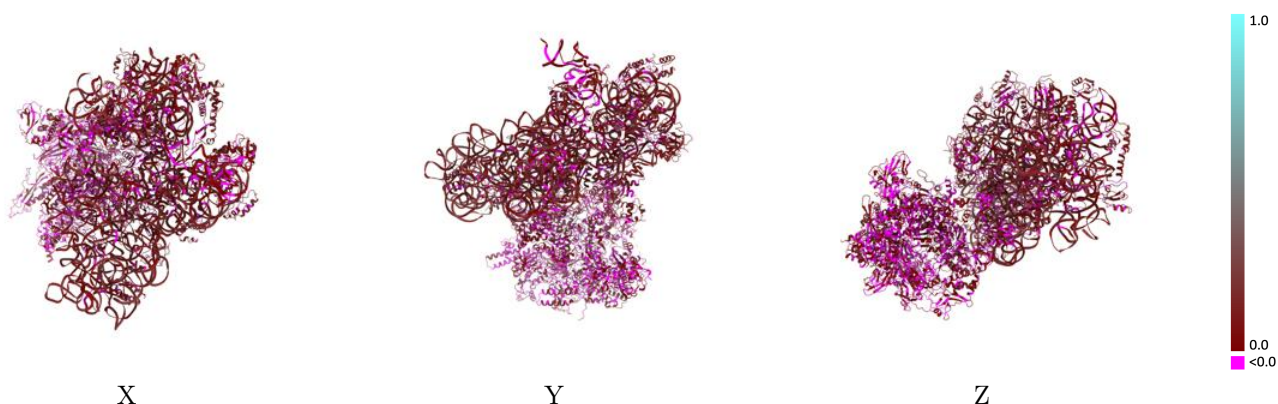
This section contains information regarding the fit between EMDB map EMD-53761 and PDB model 9SKC. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



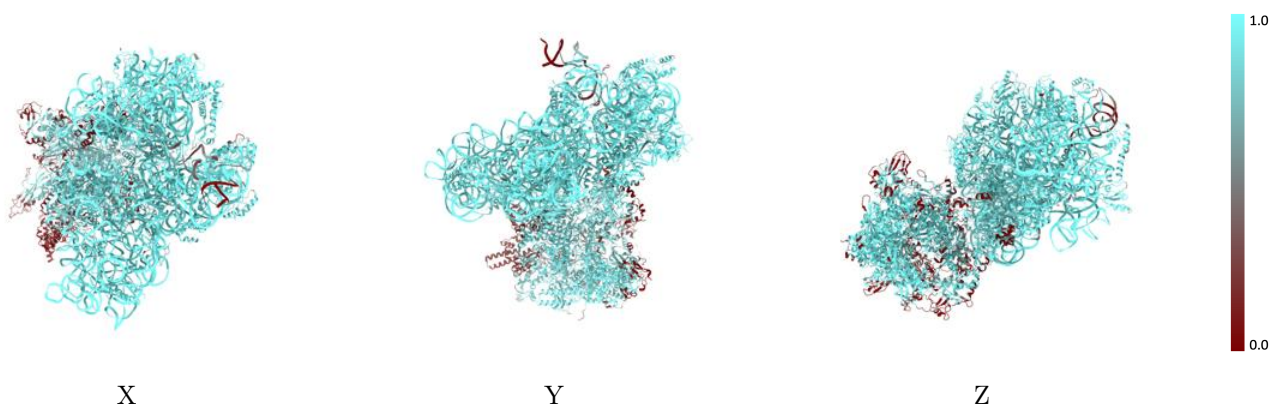
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



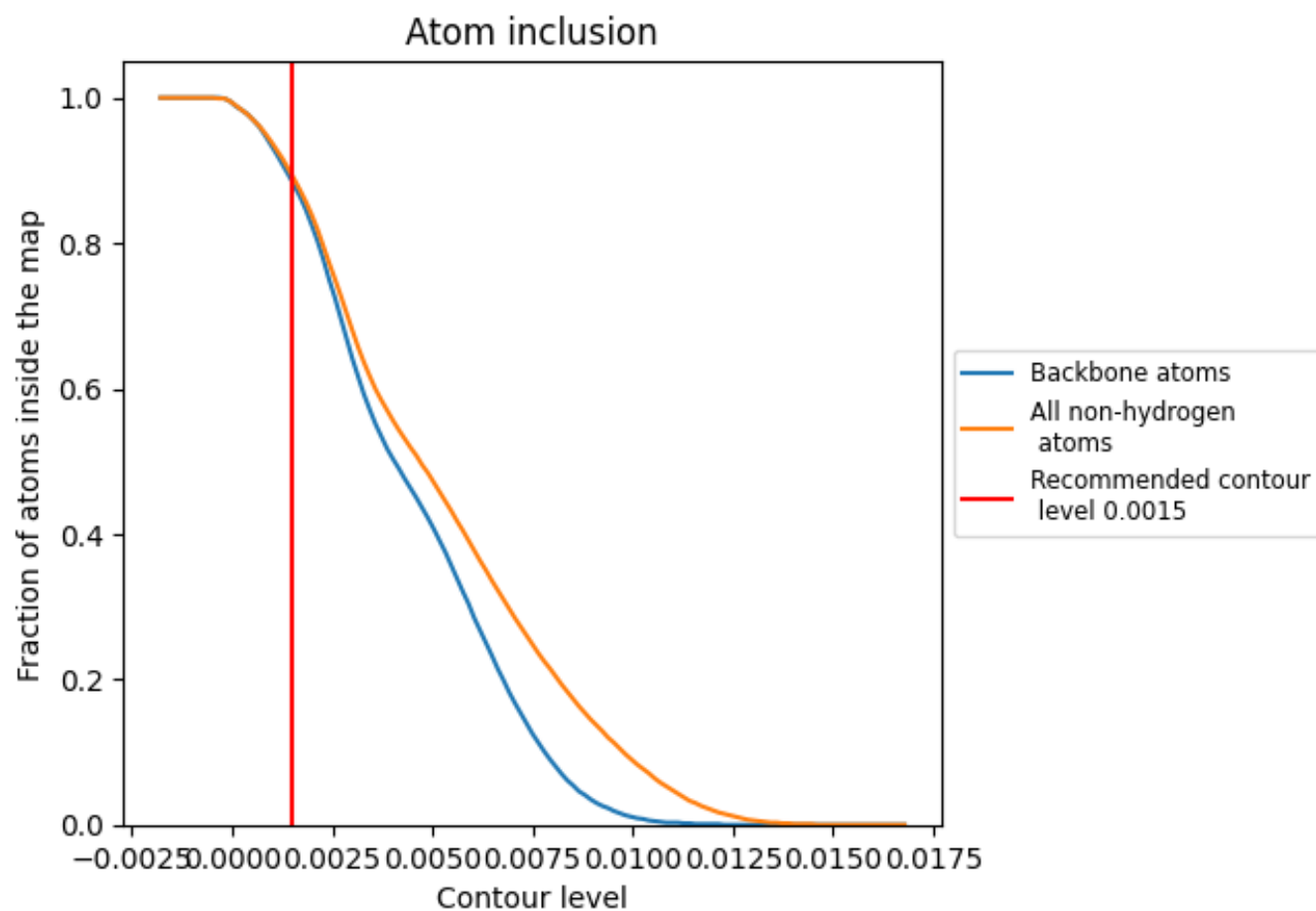
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.0830
5	 0.9970	 0.1360
6	 0.5450	 0.0150
A	 0.9690	 0.0940
B	 0.9940	 0.0960
C	 0.9940	 0.0830
D	 0.9960	 0.0980
E	 0.9620	 0.1250
F	 0.9860	 0.1030
G	 0.9880	 0.0920
H	 0.9930	 0.0910
I	 0.9850	 0.0750
J	 0.9670	 0.0500
K	 0.9880	 0.0740
L	 0.9660	 0.0700
M	 1.0000	 0.0480
N	 0.9740	 0.1160
O	 0.9960	 0.0860
P	 0.9740	 0.1000
Q	 0.9900	 0.0780
R	 0.9740	 0.0680
S	 0.9980	 0.1120
T	 0.9690	 0.1190
U	 0.7240	 0.0350
V	 0.9540	 0.1140
W	 0.8010	 0.0350
X	 0.7510	 0.0380
Y	 0.7450	 0.0120
Z	 0.6850	 0.0310
a	 0.6240	 0.0270
b	 0.6120	 0.0280

