wwPDB EM Validation Summary Report

Jul 5, 2025 – 07:58 am BST

PDB ID	:	9QEQ / pdb_00009qeq
EMDB ID	:	EMD-53087
Title	:	Structure of the transcribing Pol II-DSIF-SPT6-U1 snRNP complex
Authors	:	Zhang, S.
Deposited on	:	2025-03-10
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

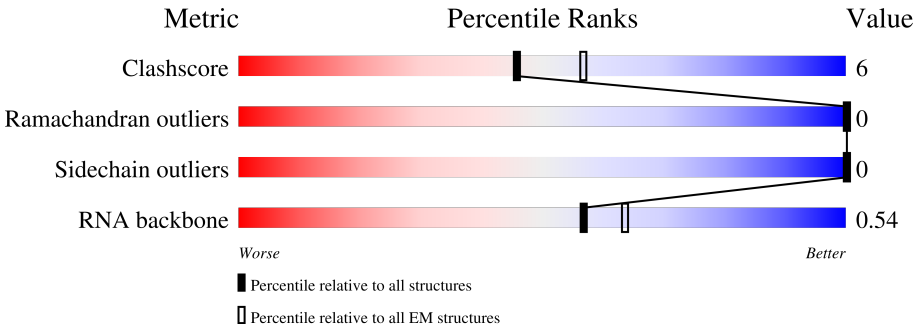
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	1970	64% 8% 28%
2	B	1174	85% 11% .
3	C	275	89% 5% 5%
4	D	142	70% 19% 11%
5	E	210	85% 14%
6	F	127	57% 7% 35%
7	G	172	85% 15% .

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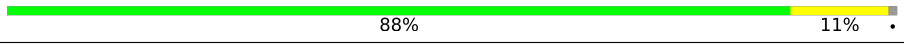
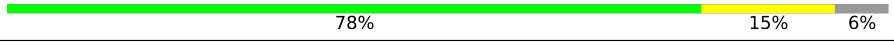
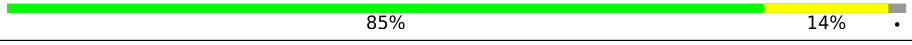
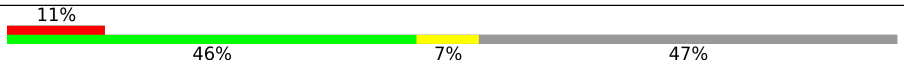
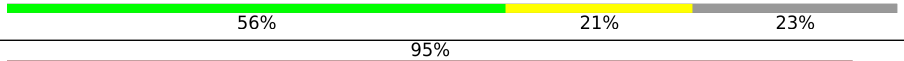
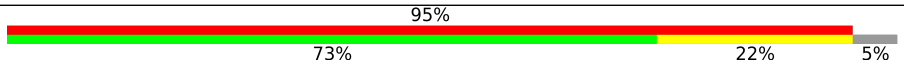
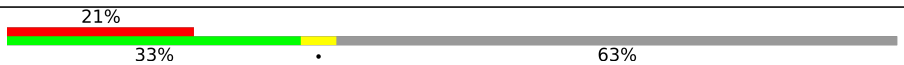
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1726	
14	N	48	
15	P	68	
16	T	48	
17	Y	121	
18	Z	1087	
19	a	164	
20	b	437	
21	c	282	
22	e	118	
23	f	86	
24	g	92	
25	h	76	
26	i	126	
27	j	231	
28	k	119	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 56145 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 protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1422	11266	7084	2018	2093	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9052	5727	1592	1669	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	260	2089	1309	359	415	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1030	642	175	209	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	922	Total	C	N	O	S	0	0
			7548	4769	1313	1431	35		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total 769	C 361	N 149	O 222	P 37	0	0

- Molecule 15 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	25	Total 539	C 241	N 103	O 170	P 25	0	0

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	37	Total 749	C 355	N 128	O 229	P 37	0	0

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	115	Total 906	C 567	N 158	O 172	S 9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	GLY	-	expression tag	UNP Q4R941
Y	2	PRO	-	expression tag	UNP Q4R941
Y	3	GLY	-	expression tag	UNP Q4R941
Y	4	SER	-	expression tag	UNP Q4R941

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	515	Total 4131	C 2626	N 731	O 756	S 18	0	0

- Molecule 19 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	164	Total 3485	C 1555	N 607	O 1159	P 164	0	0

- Molecule 20 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	186	Total	C	N	O	S	0	0
			1543	952	310	276	5		

- Molecule 21 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	98	Total	C	N	O	S	0	0
			796	513	136	143	4		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	95	Total	C	N	O	S	0	0
			777	486	141	144	6		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	77	Total	C	N	O	S	0	0
			638	405	113	115	5		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	h	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	81	Total	C	N	O	S	0	0
			637	400	112	119	6		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	86	Total 692	C 435	N 126	O 124	S 7	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	81	Total 641	C 408	N 112	O 118	S 3	0	0

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

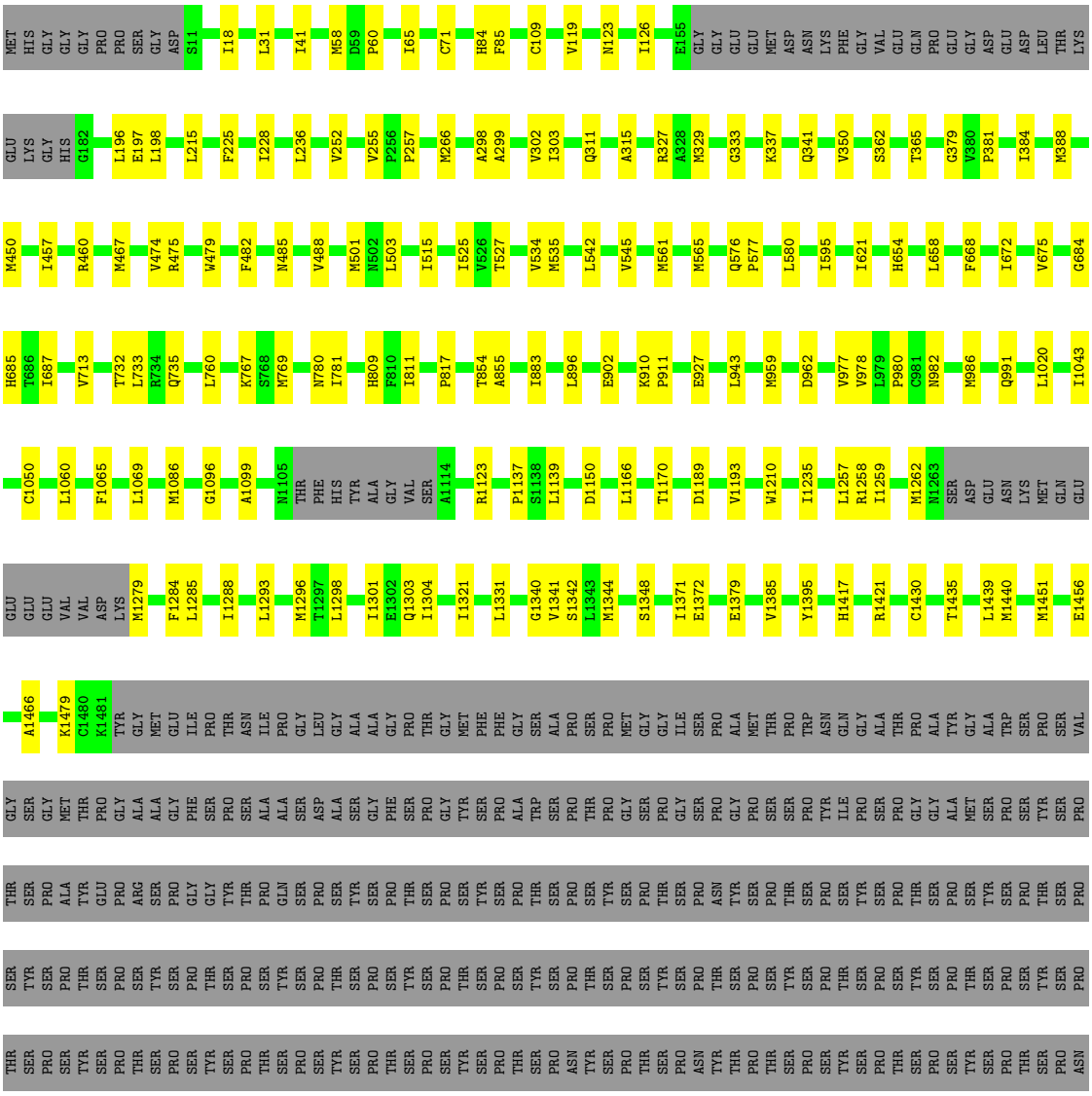
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total 1	Mg 1	0

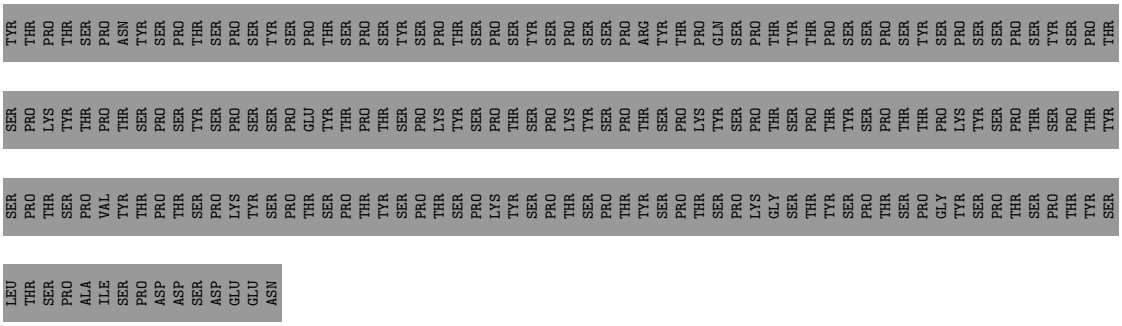
3 Residue-property plots (i)

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 subunit

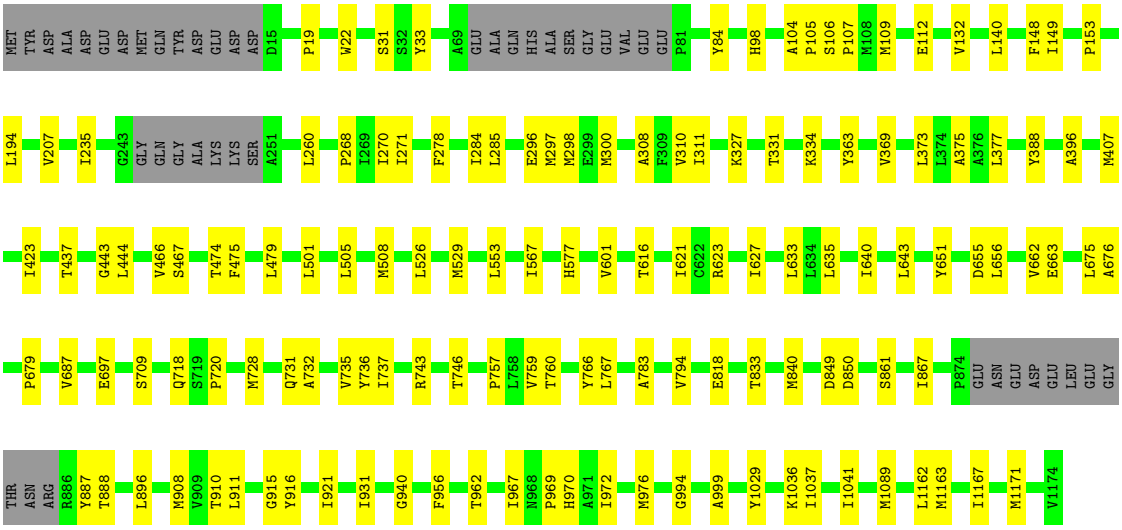
Chain A:





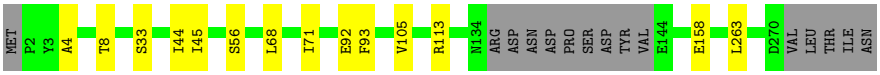
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



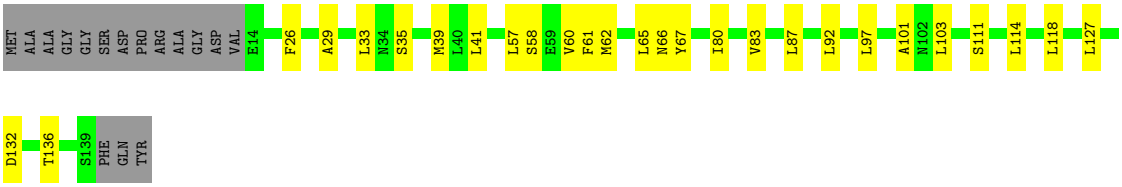
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



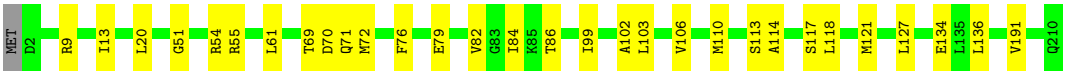
• Molecule 4: RNA polymerase II subunit D

Chain D:



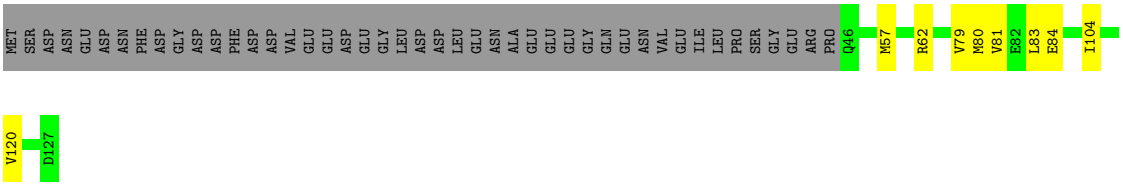
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



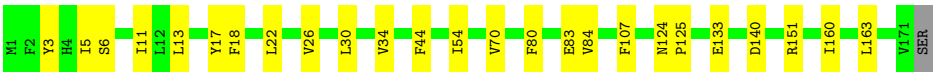
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



• Molecule 7: DNA-directed RNA polymerase subunit

Chain G:

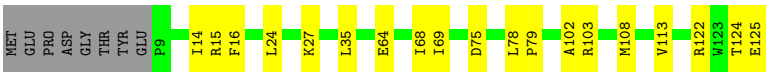


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

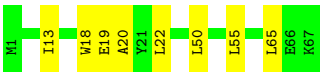
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



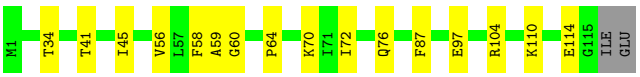
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



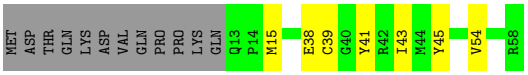
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



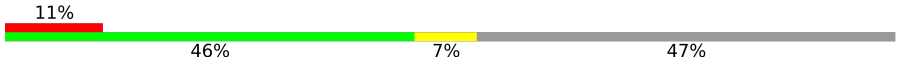
• Molecule 12: RNA polymerase II, I and III subunit K

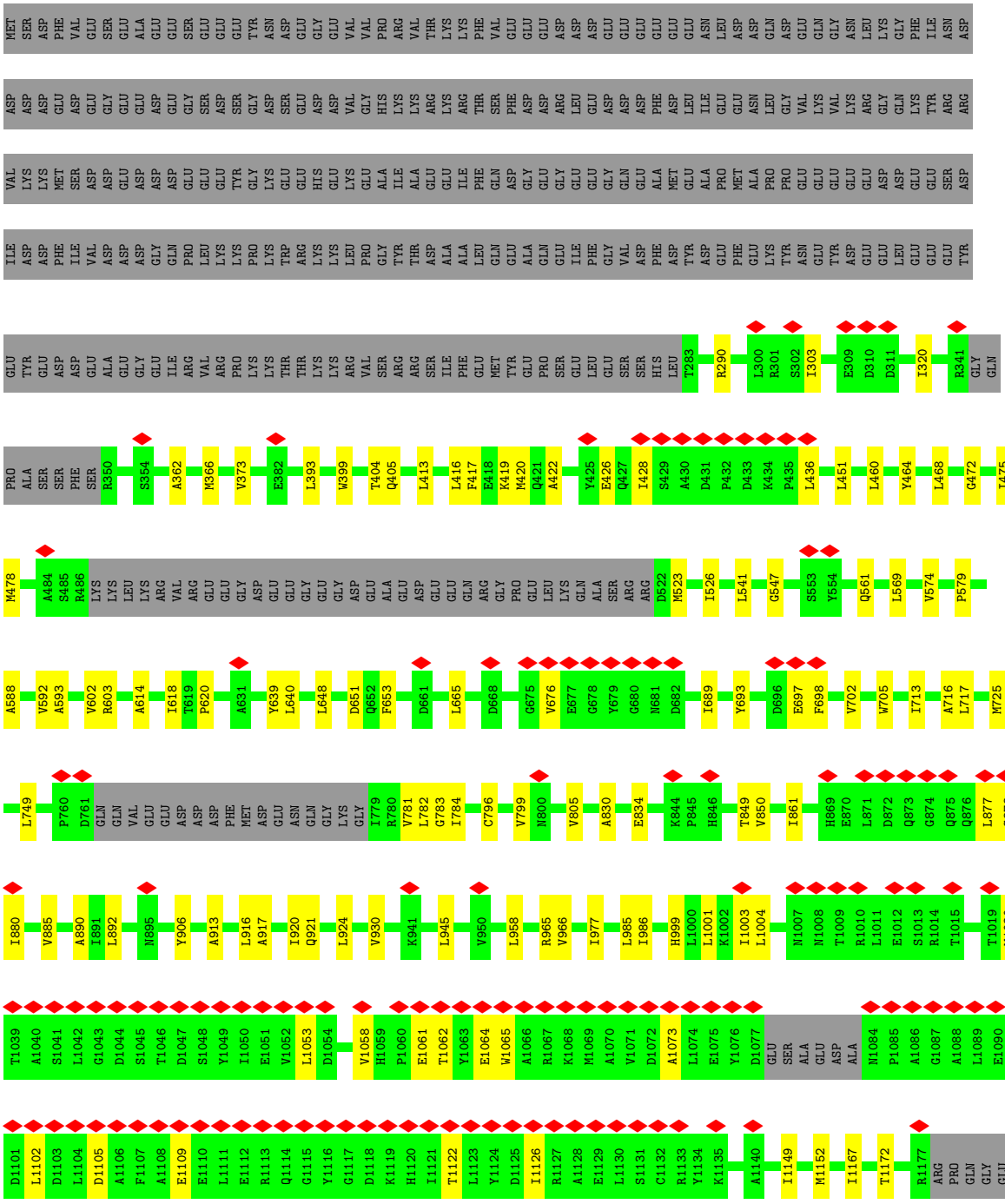
Chain L:

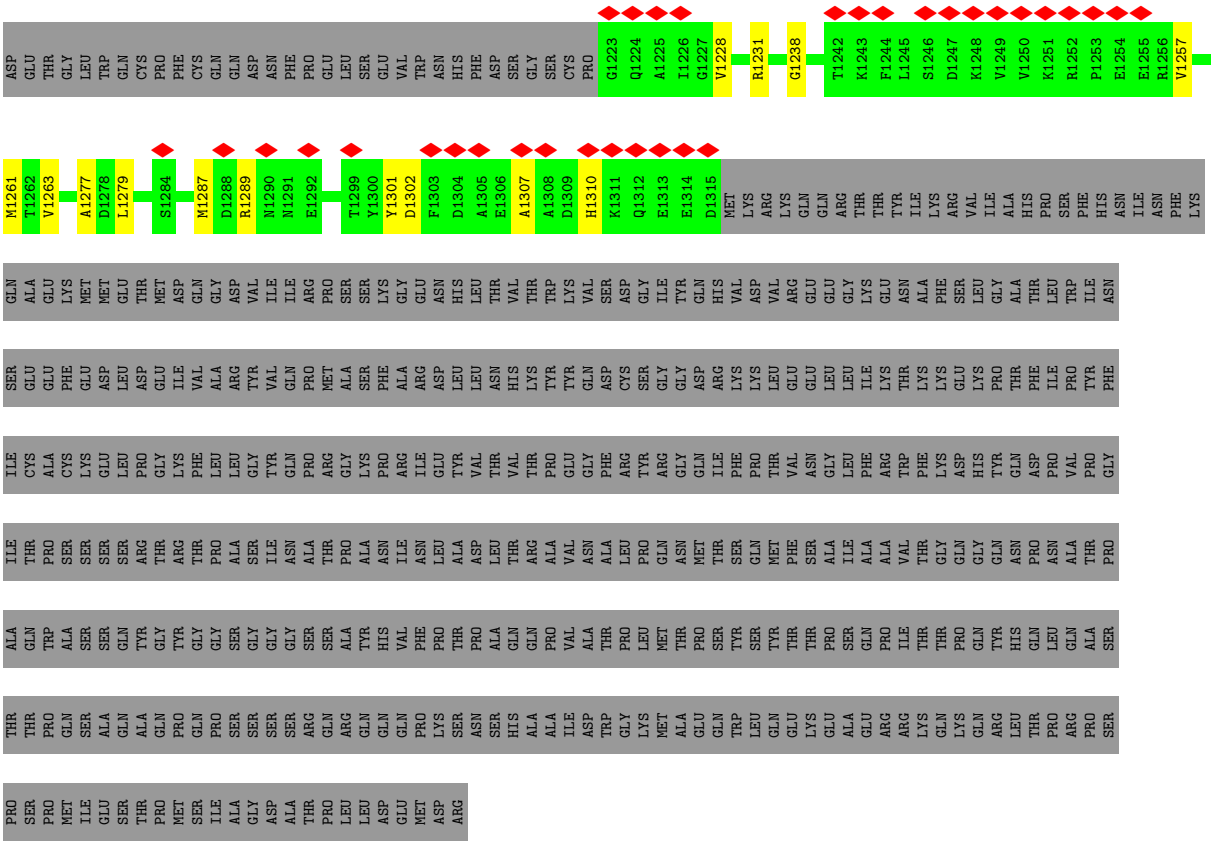


• Molecule 13: Transcription elongation factor SPT6

Chain M:

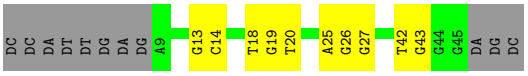






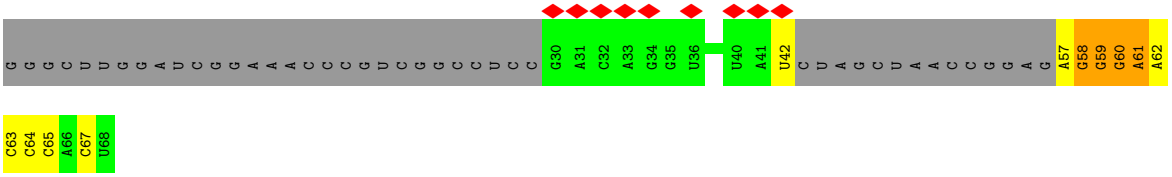
• Molecule 14: Non-template DNA

Chain N:



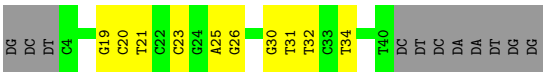
• Molecule 15: Pre-mRNA

Chain P:



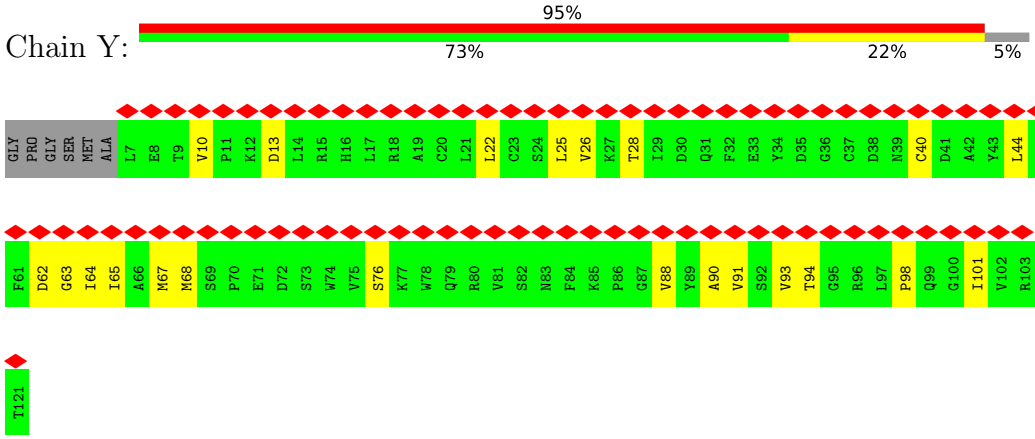
• Molecule 16: Template DNA

Chain T:



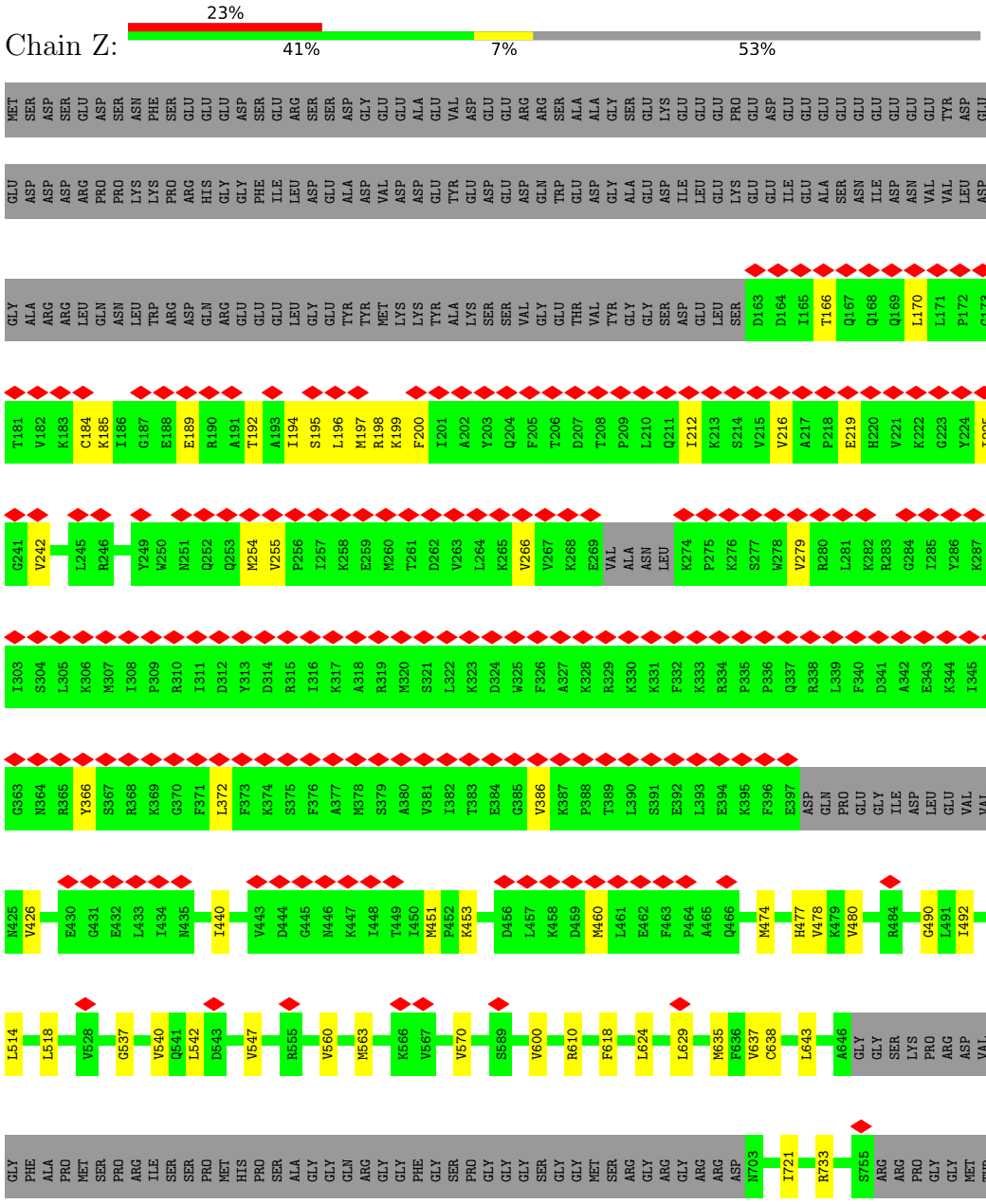
• Molecule 17: Transcription elongation factor SPT4

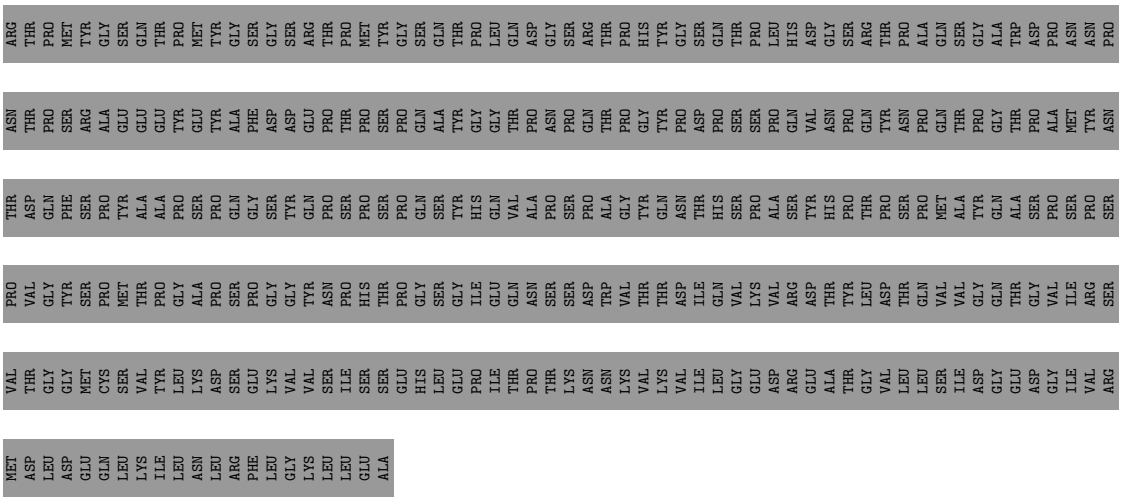
Chain Y:



• Molecule 18: Transcription elongation factor SPT5

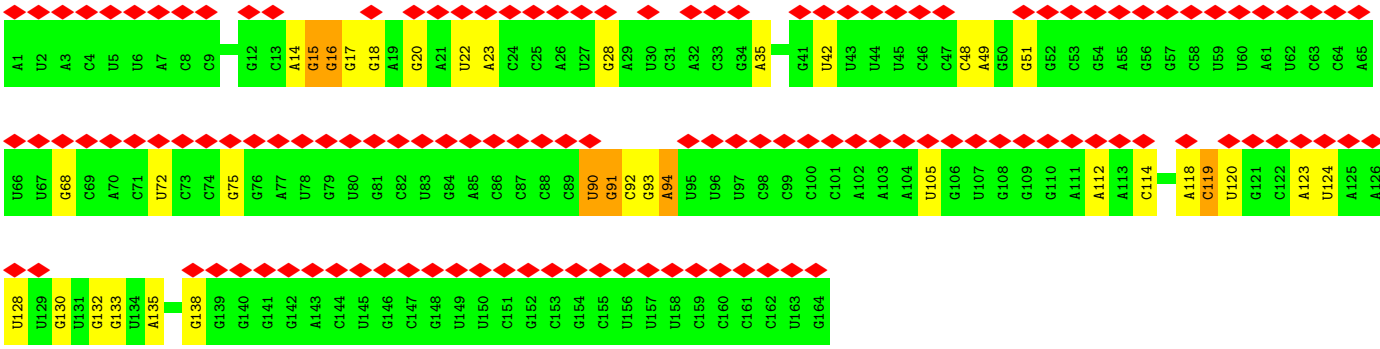
Chain Z:





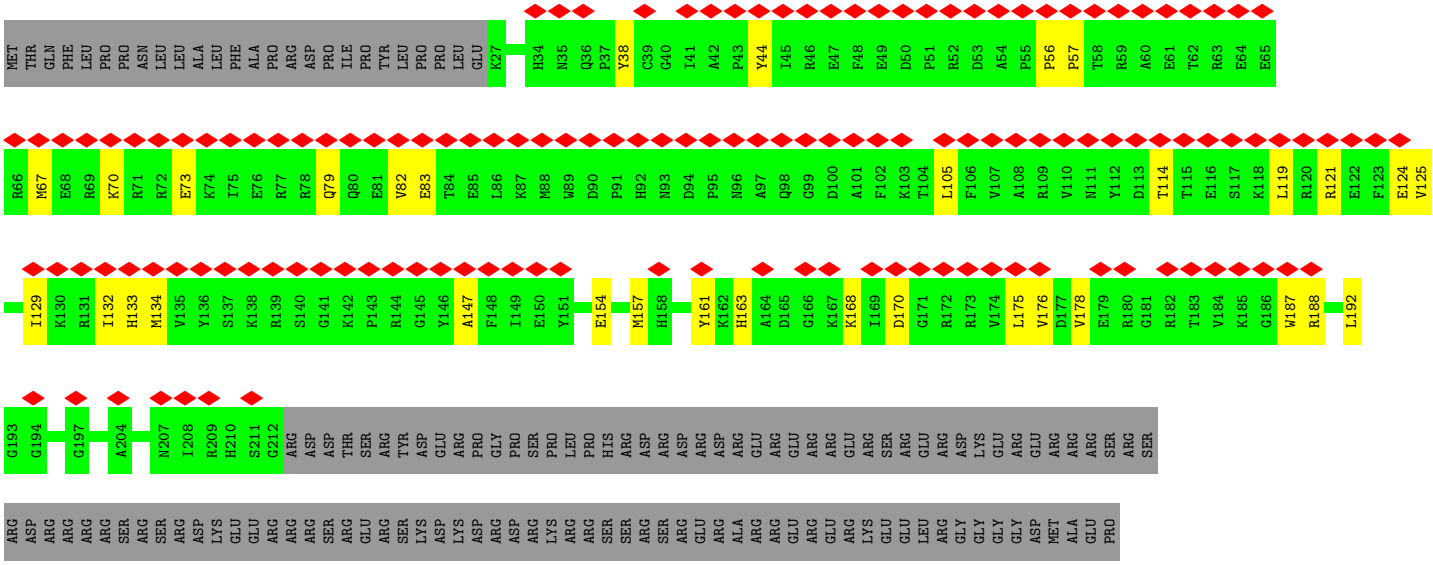
- Molecule 19: U1 snRNA

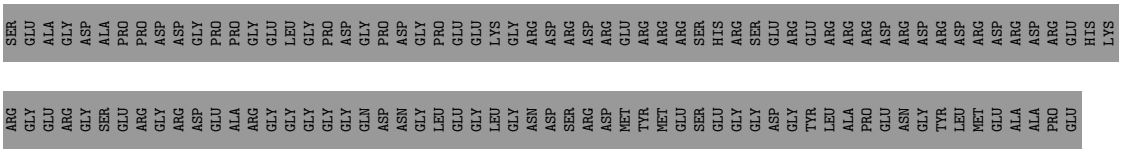
Chain a:



- Molecule 20: U1 small nuclear ribonucleoprotein 70 kDa

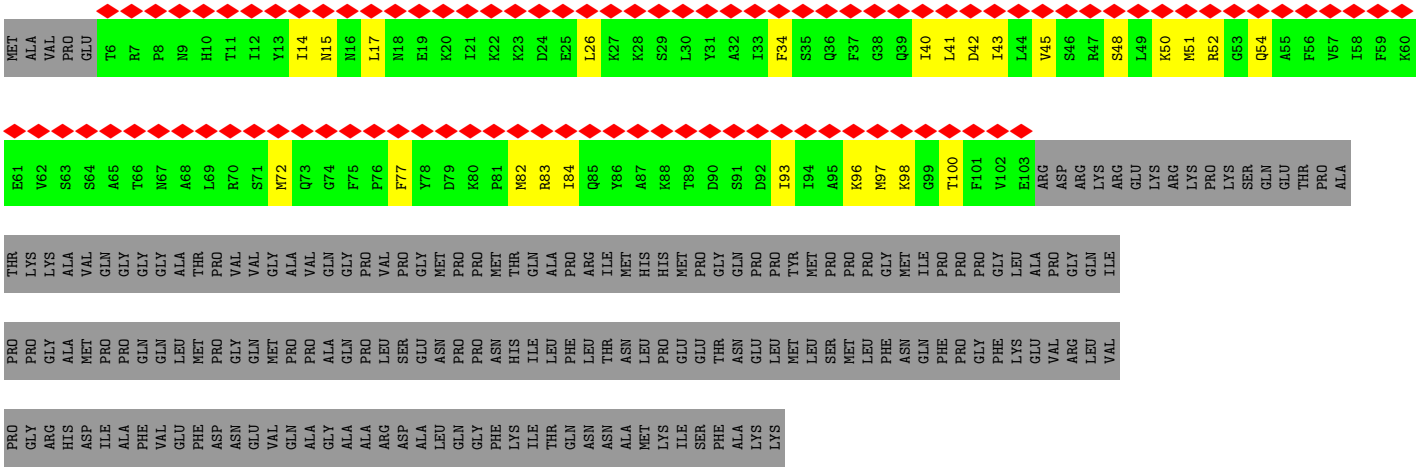
Chain b:





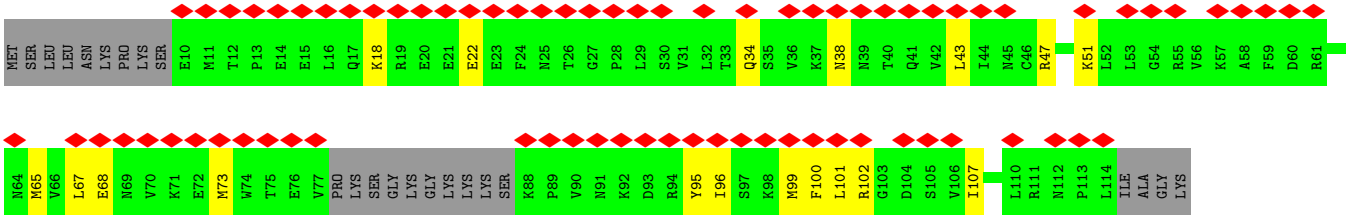
• Molecule 21: U1 small nuclear ribonucleoprotein A

Chain c:



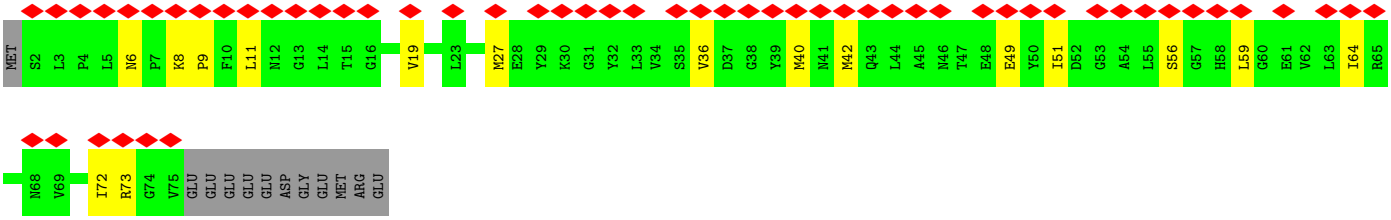
• Molecule 22: Small nuclear ribonucleoprotein Sm D2

Chain e:



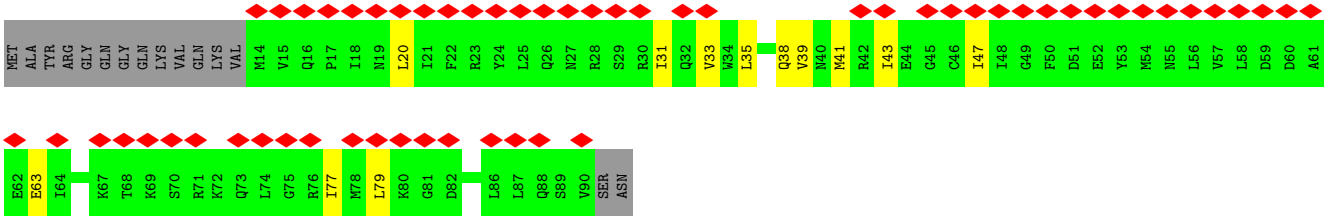
• Molecule 23: Small nuclear ribonucleoprotein F

Chain f:



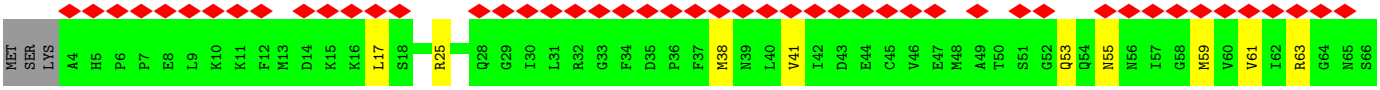
• Molecule 24: Small nuclear ribonucleoprotein E

Chain g:



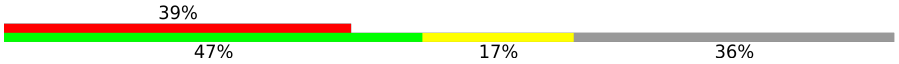
• Molecule 25: Small nuclear ribonucleoprotein G

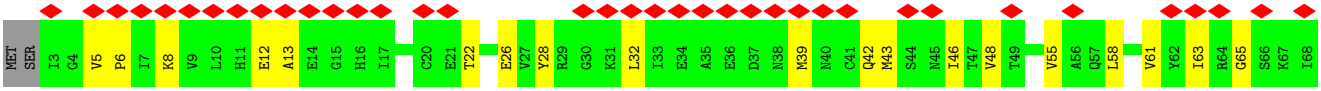
Chain h:

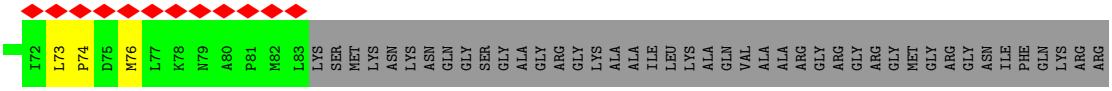


• Molecule 26: Small nuclear ribonucleoprotein Sm D3

Chain i:

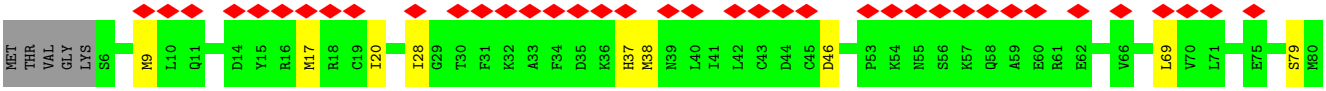


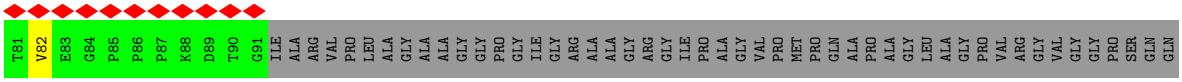


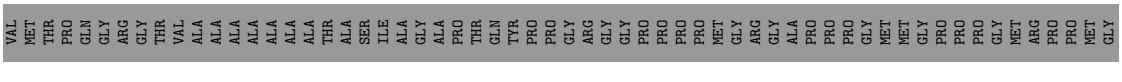


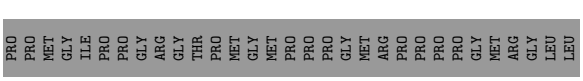
• Molecule 27: Small nuclear ribonucleoprotein-associated protein

Chain j:



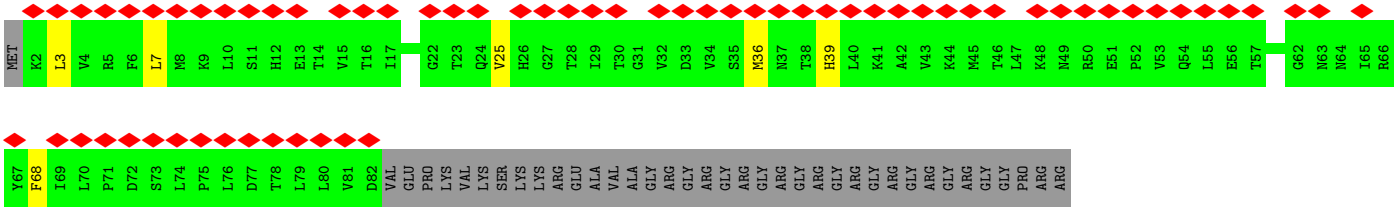






• Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain k:


MET K2 L3 V4 R5 F6 L7 M8 K9 L10 S11 H12 E13 T14 V15 T16 I17 G22 T23 Q24 V25 H26 G27 T28 I29 T30 G31 V32 D33 V34 S35 M36 N37 T38 H39 L40 K41 A42 V43 K44 M45 T46 L47 K48 N49 R50 E51 P52 V53 Q54 L55 E56 T57 G62 N63 N64 I65 R66
Y67 F68 I69 L70 P71 D72 S73 L74 P75 L76 D77 T78 L79 L80 V81 D82 VAL GLU PRO LYS VAL LYS SER LYS LYS ARG GLU ALA VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY PRO ARG ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52065	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	398.99997, 398.99997, 398.99997	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.22	0/11471	0.32	0/15487
2	B	0.23	0/9233	0.32	0/12463
3	C	0.22	0/2132	0.29	0/2896
4	D	0.12	0/1043	0.27	0/1400
5	E	0.21	0/1751	0.28	0/2366
6	F	0.22	0/667	0.32	0/901
7	G	0.15	0/1382	0.29	0/1874
8	H	0.21	0/1207	0.31	0/1628
9	I	0.15	0/972	0.28	0/1316
10	J	0.24	0/542	0.34	0/730
11	K	0.24	0/939	0.34	0/1271
12	L	0.20	0/394	0.35	0/524
13	M	0.12	0/7695	0.32	0/10382
14	N	0.20	0/864	0.39	0/1334
15	P	0.17	0/603	0.29	0/936
16	T	0.25	0/835	0.43	0/1285
17	Y	0.14	0/922	0.39	0/1243
18	Z	0.11	0/4205	0.33	0/5659
19	a	0.12	0/3891	0.34	0/6061
20	b	0.15	0/1580	0.38	0/2118
21	c	0.15	0/810	0.42	0/1084
22	e	0.13	0/786	0.37	0/1055
23	f	0.13	0/588	0.36	0/795
24	g	0.13	0/646	0.36	0/867
25	h	0.15	0/575	0.37	0/768
26	i	0.13	0/645	0.39	0/870
27	j	0.10	0/702	0.32	0/936
28	k	0.12	0/649	0.34	0/878
All	All	0.18	0/57729	0.33	0/79127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11266	0	11397	134	0
2	B	9052	0	9087	121	0
3	C	2089	0	2031	9	0
4	D	1030	0	1016	26	0
5	E	1720	0	1737	23	0
6	F	657	0	684	6	0
7	G	1351	0	1358	22	0
8	H	1186	0	1147	9	0
9	I	949	0	879	17	0
10	J	533	0	553	6	0
11	K	920	0	942	15	0
12	L	388	0	393	10	0
13	M	7548	0	7455	99	0
14	N	769	0	414	7	0
15	P	539	0	273	13	0
16	T	749	0	417	11	0
17	Y	906	0	900	22	0
18	Z	4131	0	4206	61	0
19	a	3485	0	1762	7	0
20	b	1543	0	1514	34	0
21	c	796	0	824	21	0
22	e	777	0	800	20	0
23	f	576	0	589	12	0
24	g	638	0	657	11	0
25	h	568	0	590	14	0
26	i	637	0	652	17	0
27	j	692	0	717	8	0
28	k	641	0	681	9	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
30	A	1	0	0	0	0
All	All	56145	0	53675	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 658 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:LEU:HD22	4:D:62:MET:HE3	1.55	0.88
4:D:57:LEU:HD21	4:D:61:PHE:HB2	1.62	0.82
7:G:30:LEU:O	7:G:34:VAL:HG22	1.82	0.80
2:B:104:ALA:HB2	20:b:163:HIS:CD2	2.16	0.79
18:Z:179:LEU:O	18:Z:255:VAL:HG22	1.87	0.75

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	1414/1970 (72%)	1342 (95%)	72 (5%)	0	100	100
2	B	1123/1174 (96%)	1051 (94%)	72 (6%)	0	100	100
3	C	256/275 (93%)	247 (96%)	9 (4%)	0	100	100
4	D	124/142 (87%)	124 (100%)	0	0	100	100
5	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	M	910/1726 (53%)	901 (99%)	9 (1%)	0	100	100
17	Y	113/121 (93%)	112 (99%)	1 (1%)	0	100	100
18	Z	507/1087 (47%)	497 (98%)	10 (2%)	0	100	100
20	b	184/437 (42%)	181 (98%)	3 (2%)	0	100	100
21	c	96/282 (34%)	93 (97%)	3 (3%)	0	100	100
22	e	91/118 (77%)	91 (100%)	0	0	100	100
23	f	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
24	g	75/92 (82%)	75 (100%)	0	0	100	100
25	h	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
26	i	79/126 (63%)	79 (100%)	0	0	100	100
27	j	84/231 (36%)	84 (100%)	0	0	100	100
28	k	79/119 (66%)	77 (98%)	2 (2%)	0	100	100
All	All	6217/9088 (68%)	5989 (96%)	228 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	1253/1749 (72%)	1253 (100%)	0	100	100
2	B	992/1027 (97%)	992 (100%)	0	100	100
3	C	237/252 (94%)	237 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	116/126 (92%)	116 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	817/1522 (54%)	817 (100%)	0	100	100
17	Y	102/105 (97%)	102 (100%)	0	100	100
18	Z	455/940 (48%)	455 (100%)	0	100	100
20	b	159/373 (43%)	159 (100%)	0	100	100
21	c	88/240 (37%)	88 (100%)	0	100	100
22	e	91/110 (83%)	91 (100%)	0	100	100
23	f	63/74 (85%)	63 (100%)	0	100	100
24	g	72/84 (86%)	72 (100%)	0	100	100
25	h	63/66 (96%)	63 (100%)	0	100	100
26	i	71/101 (70%)	71 (100%)	0	100	100
27	j	78/169 (46%)	78 (100%)	0	100	100
28	k	76/101 (75%)	76 (100%)	0	100	100
All	All	5584/7955 (70%)	5584 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	323	ASN
20	b	33	HIS
13	M	405	GLN
18	Z	364	ASN
20	b	80	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	23/68 (33%)	4 (17%)	2 (8%)
19	a	163/164 (99%)	32 (19%)	0
All	All	186/232 (80%)	36 (19%)	2 (1%)

5 of 36 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	42	U
15	P	58	G
15	P	59	G
15	P	61	A
19	a	14	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	58	G
15	P	60	G

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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.

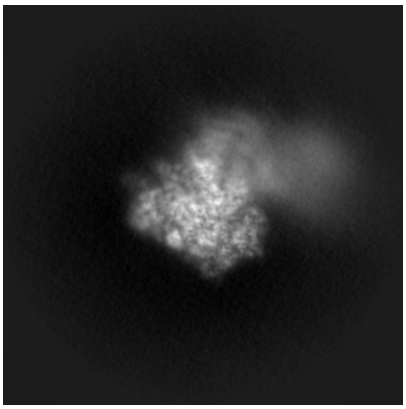
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53087. These allow visual inspection of the internal detail of the map and identification of artifacts.

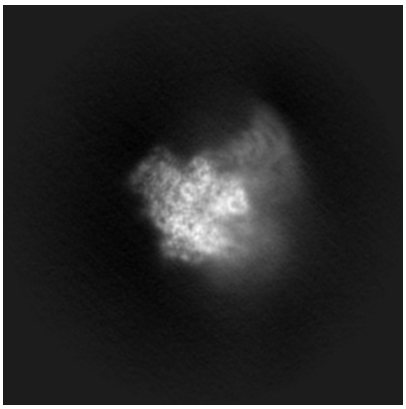
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

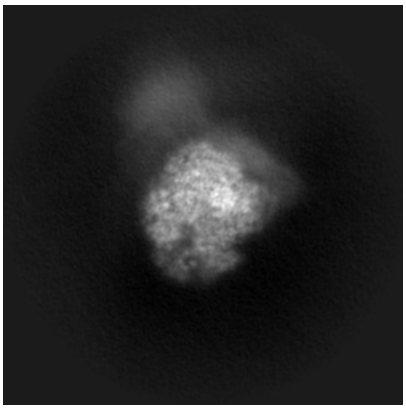
6.1.1 Primary map



X

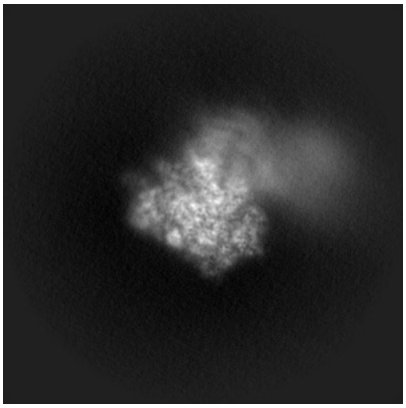


Y

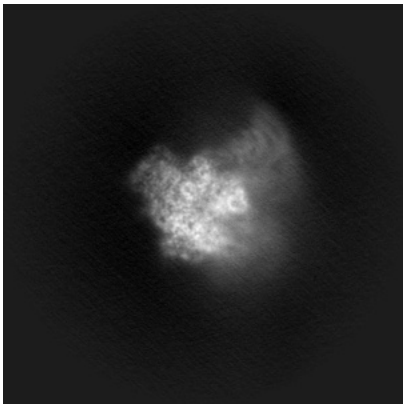


Z

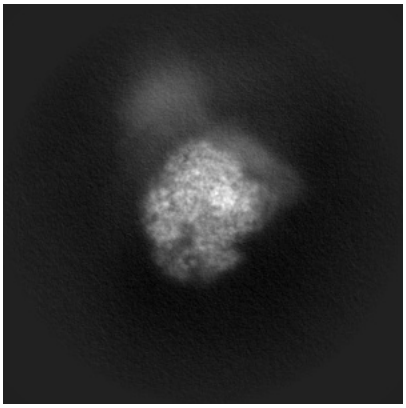
6.1.2 Raw map



X



Y

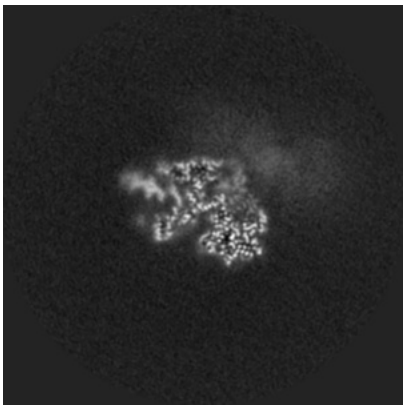


Z

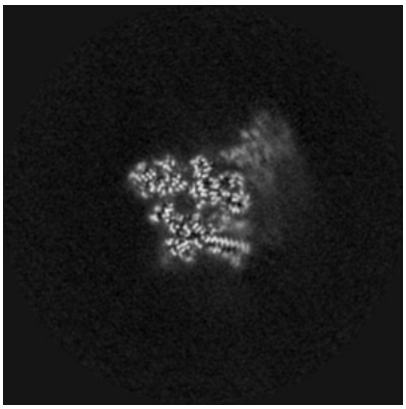
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

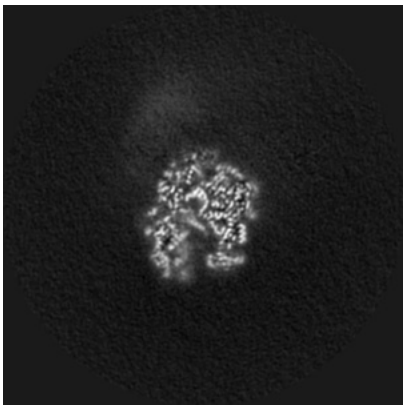
6.2.1 Primary map



X Index: 190

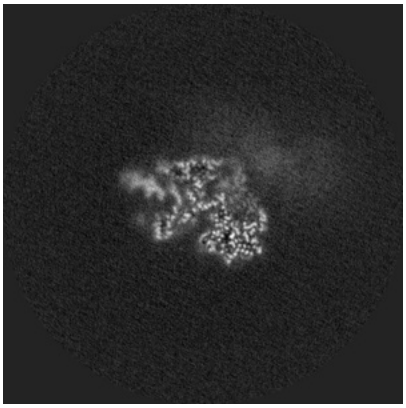


Y Index: 190

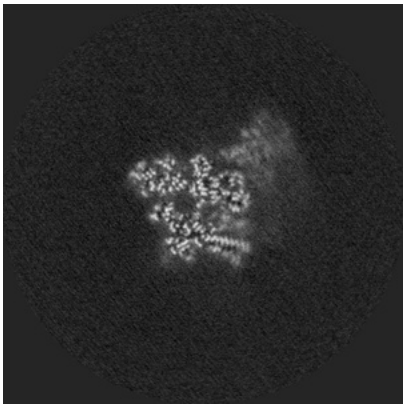


Z Index: 190

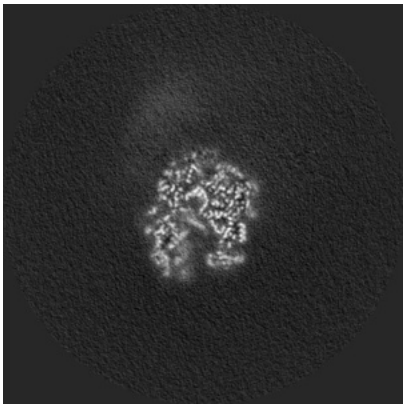
6.2.2 Raw map



X Index: 190



Y Index: 190

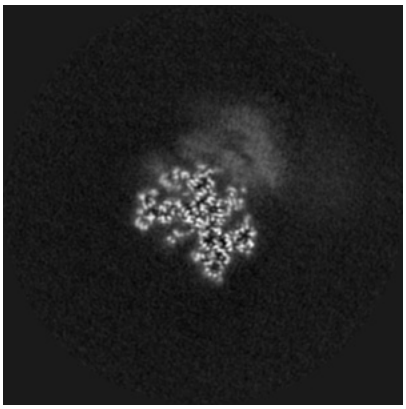


Z Index: 190

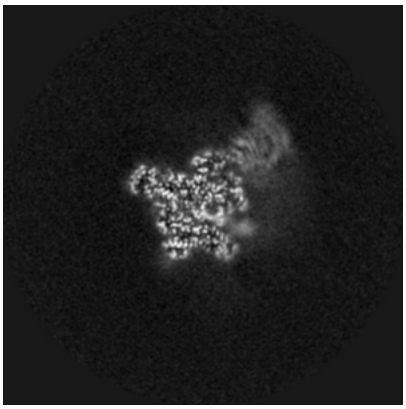
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

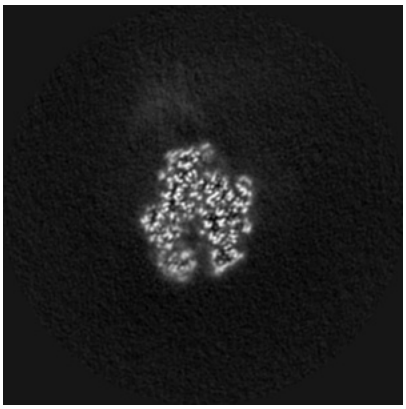
6.3.1 Primary map



X Index: 209

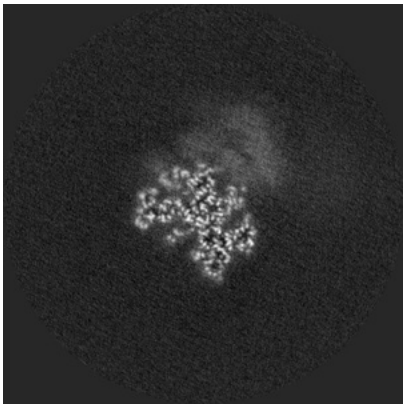


Y Index: 200

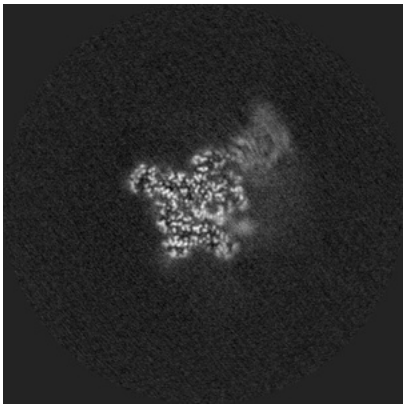


Z Index: 183

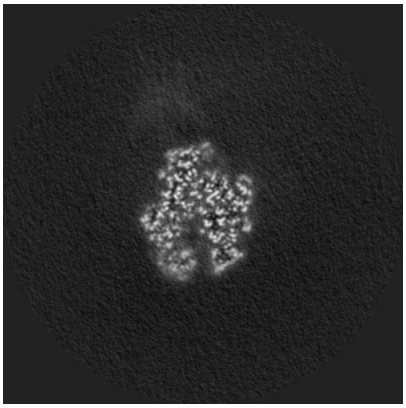
6.3.2 Raw map



X Index: 209



Y Index: 200

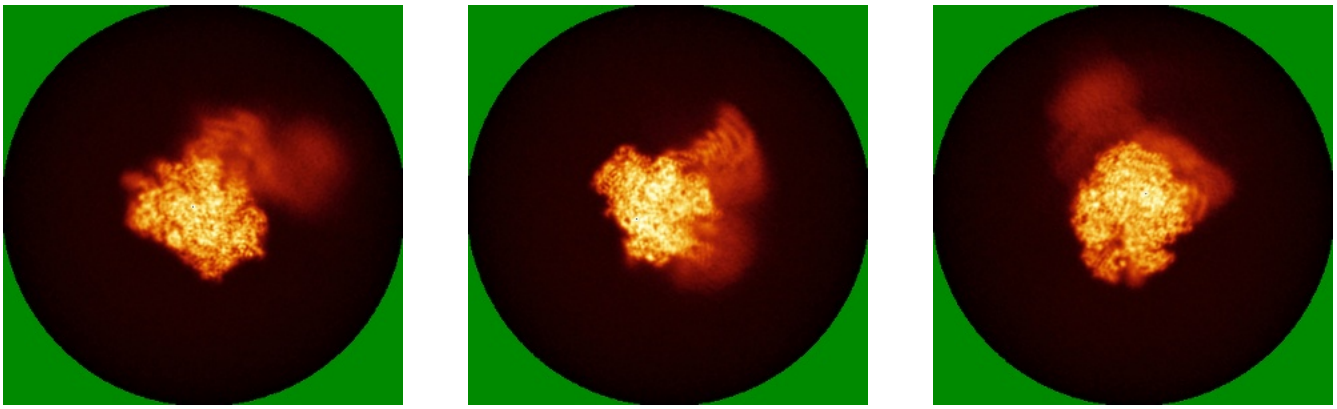


Z Index: 183

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

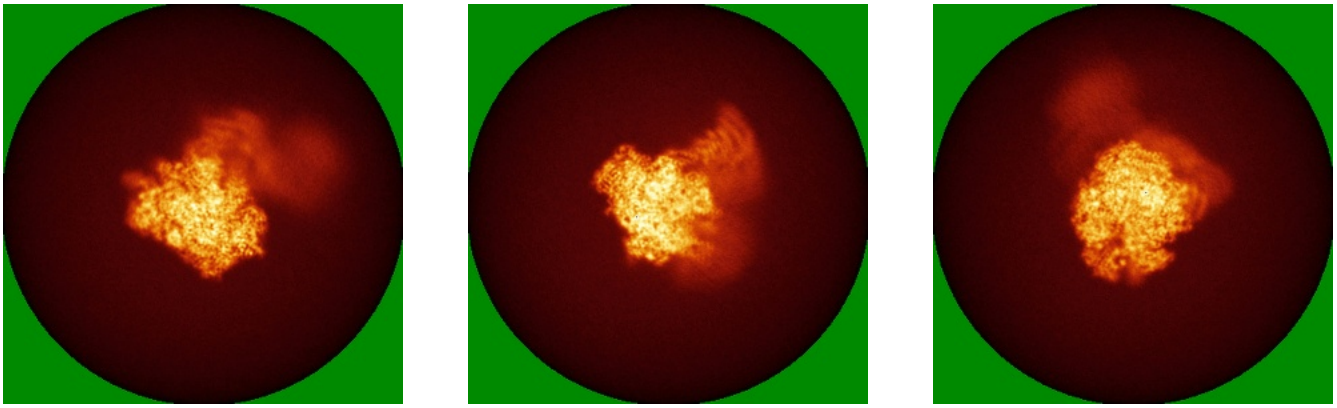
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

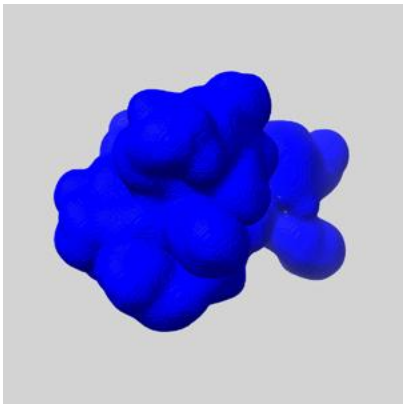
6.6 Mask visualisation (i)

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

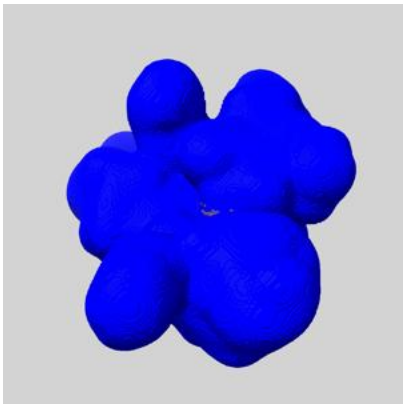
A mask typically either:

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

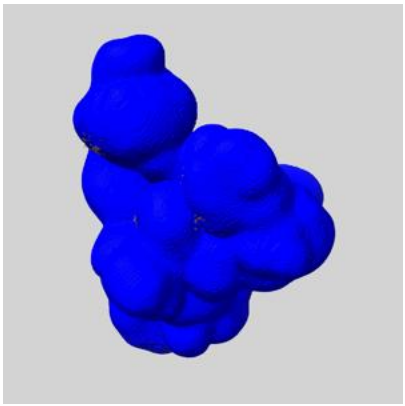
6.6.1 emd_53087_msk_1.map (i)



X



Y

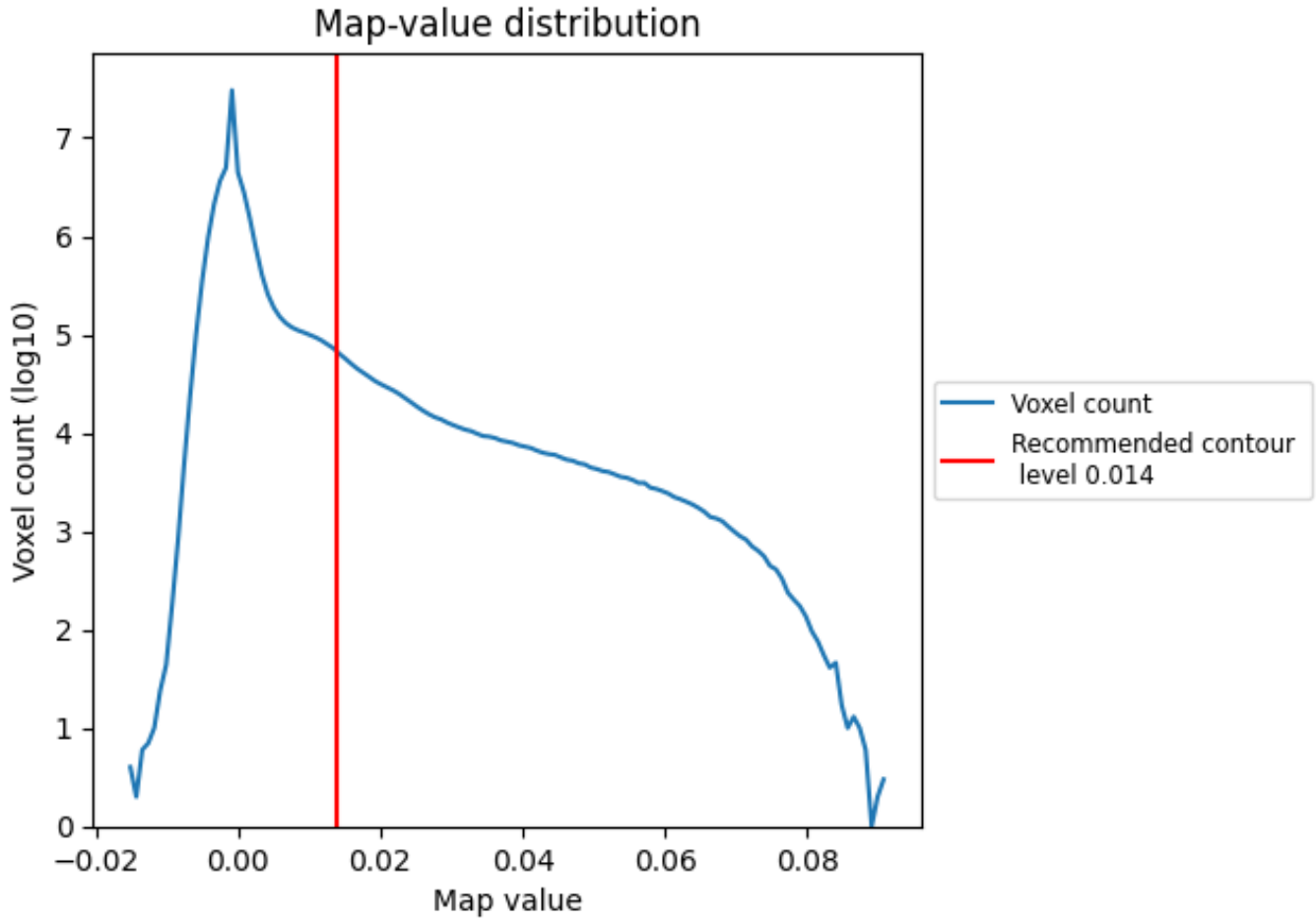


Z

7 Map analysis

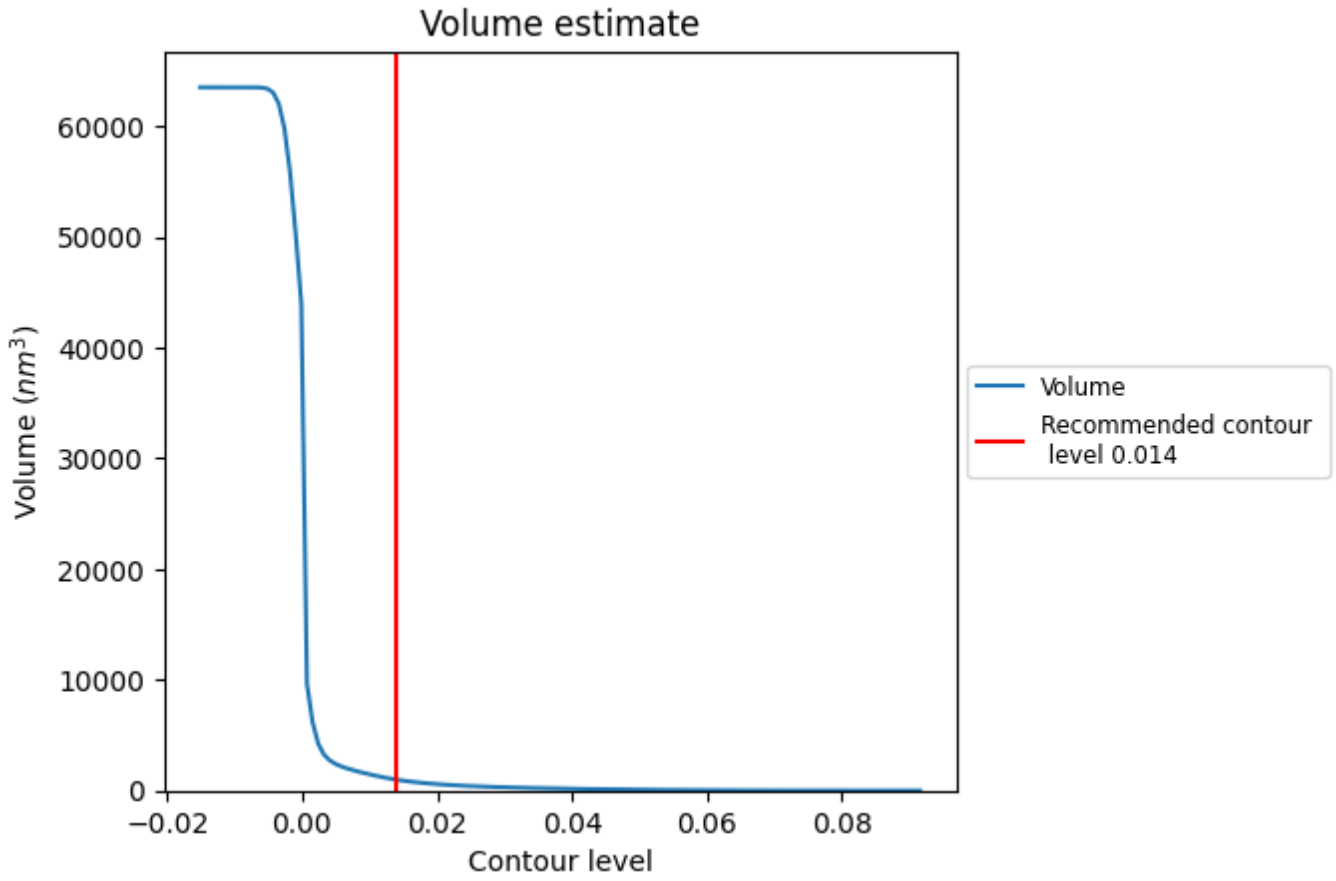
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

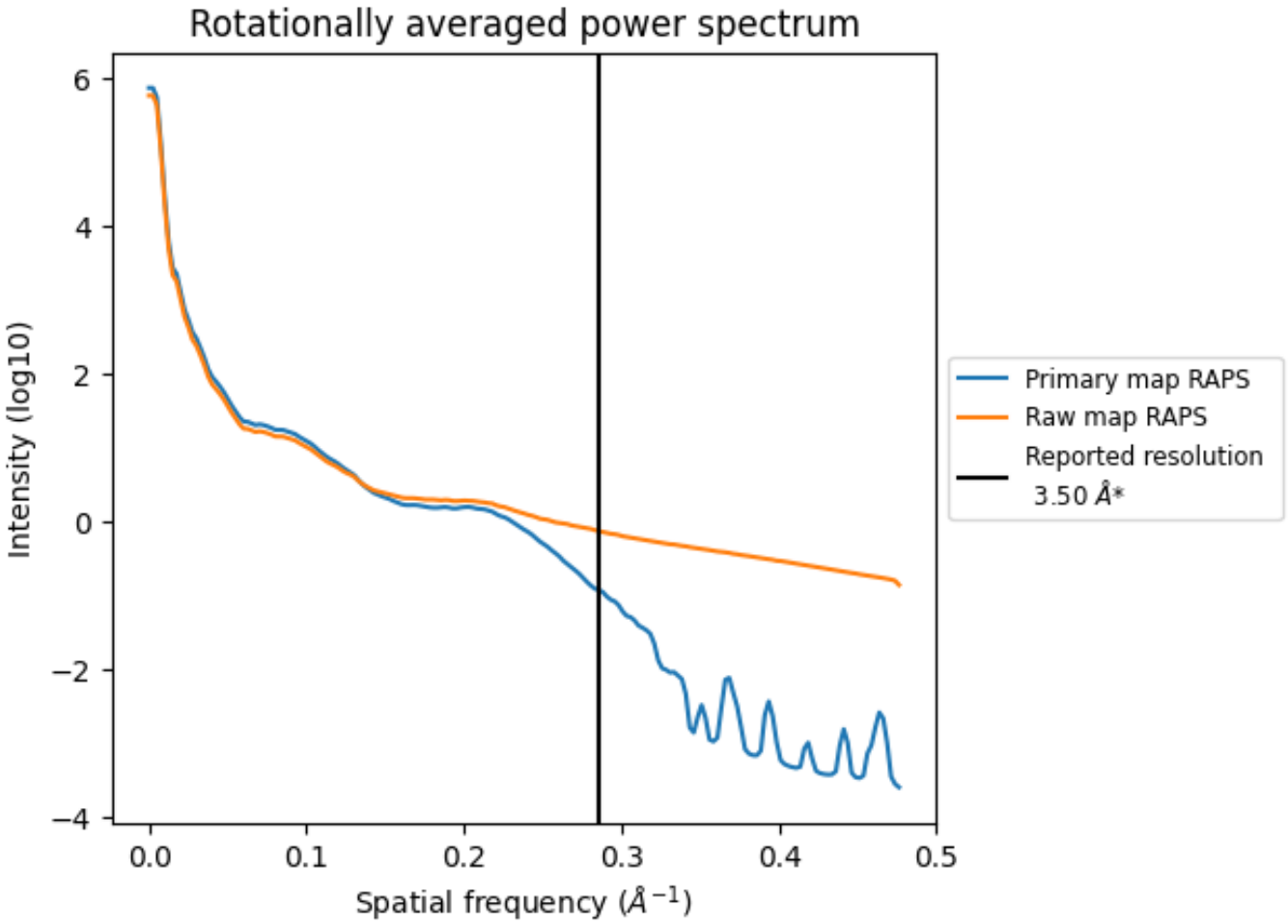
7.2 Volume estimate



The volume at the recommended contour level is 980 nm^3; this corresponds to an approximate mass of 885 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)

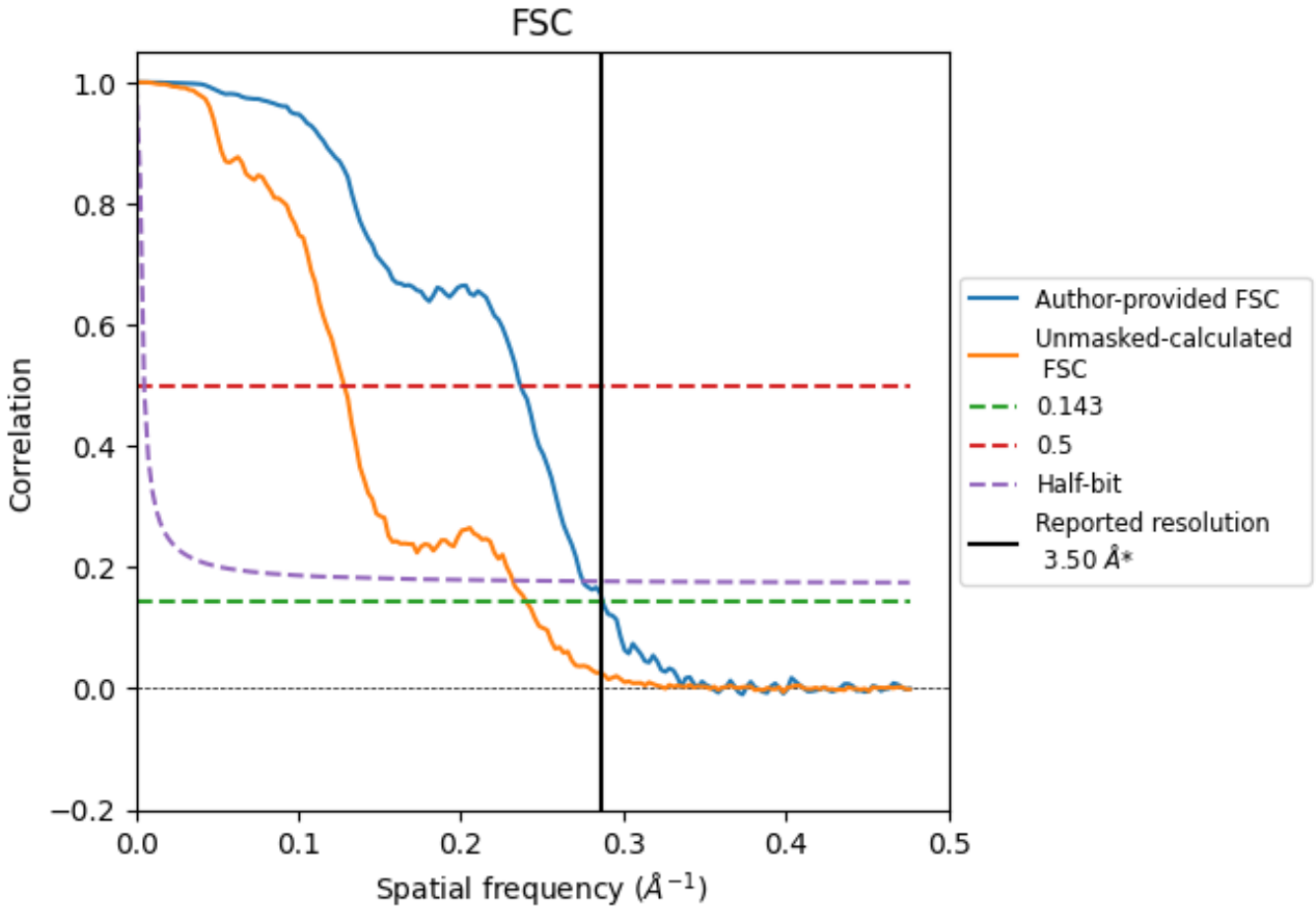


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

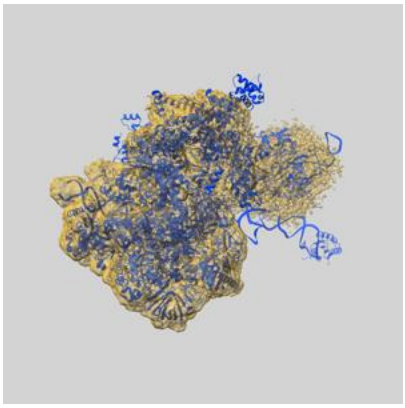
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.23	3.64
Unmasked-calculated*	4.16	7.81	4.31

*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 4.16 differs from the reported value 3.5 by more than 10 %

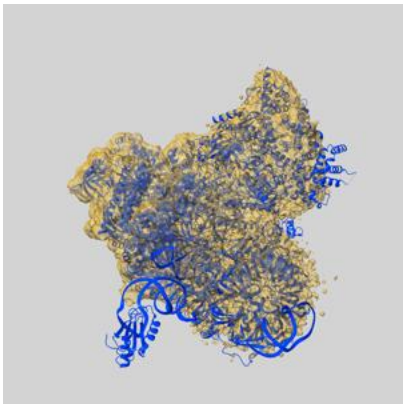
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53087 and PDB model 9QEQ. Per-residue inclusion information can be found in section 3 on page 9.

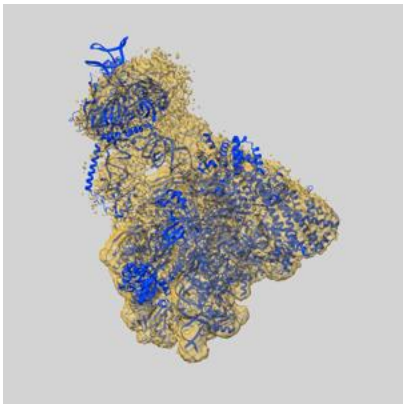
9.1 Map-model overlay



X



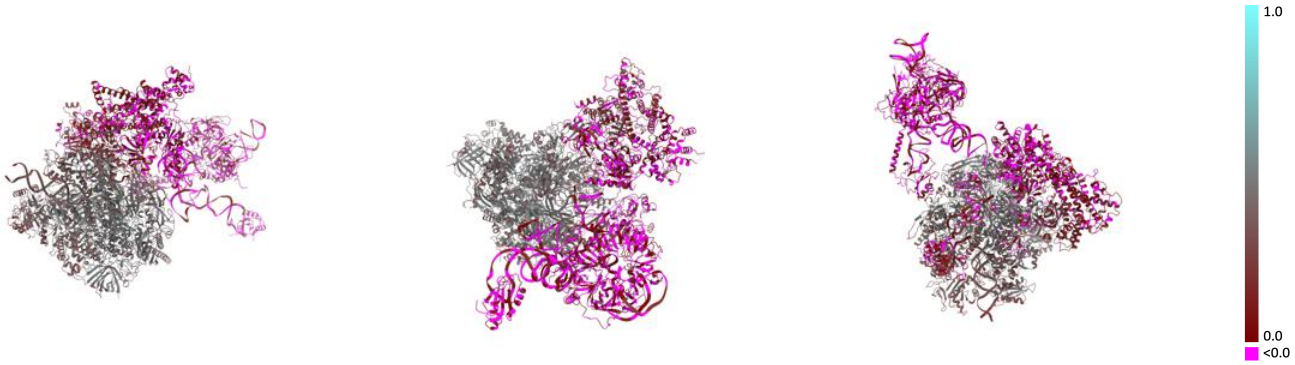
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

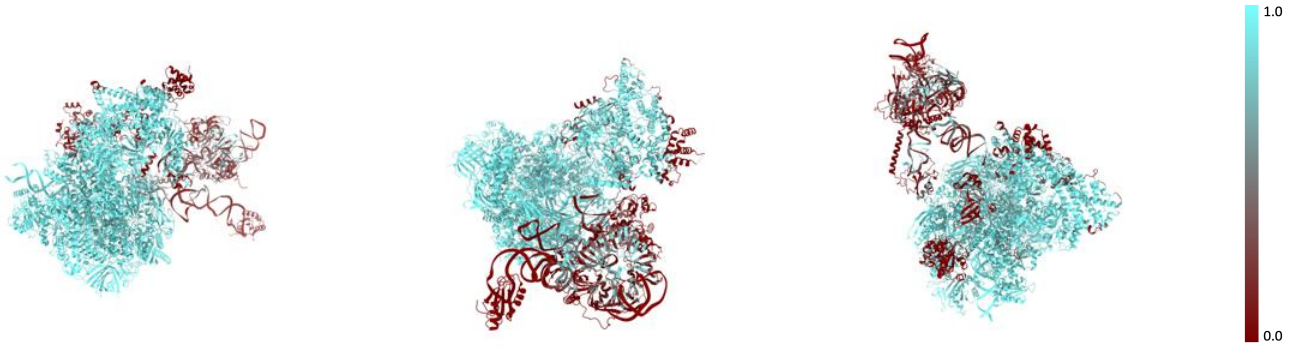
9.2 Q-score mapped to coordinate model



X Y Z

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.

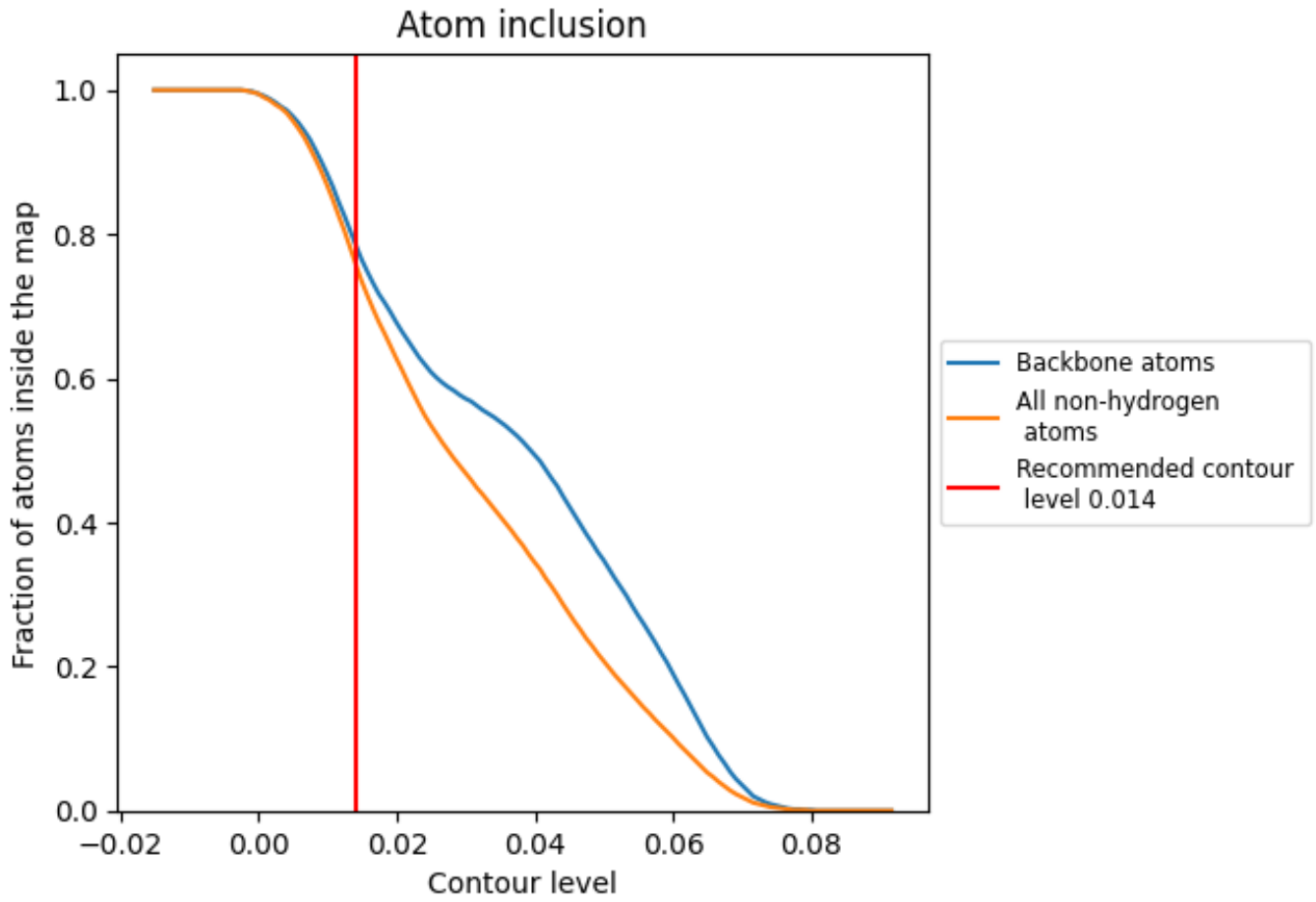
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 76% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.2550
A	0.9960	0.4200
B	0.9960	0.4300
C	0.9930	0.4500
D	0.9720	0.2150
E	0.9950	0.4080
F	1.0000	0.4360
G	0.9860	0.2820
H	0.9970	0.4460
I	0.9990	0.3650
J	0.9890	0.4420
K	0.9950	0.4430
L	0.9890	0.3950
M	0.7610	0.0510
N	0.9950	0.2490
P	0.6290	0.1680
T	1.0000	0.3570
Y	0.0010	0.0760
Z	0.4590	0.0910
a	0.1850	0.0090
b	0.2270	0.0280
c	0.0000	-0.0230
e	0.1840	0.0150
f	0.2860	-0.0160
g	0.2330	-0.0050
h	0.2360	0.0180
i	0.3770	0.0310
j	0.3520	0.0140
k	0.1790	-0.0100