



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:13 pm GMT

PDB ID : 5OQL
EMDB ID : EMD-3847
Title : Cryo-EM structure of the 90S pre-ribosome from *Chaetomium thermophilum*
Authors : Cheng, J.; Kellner, N.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2017-08-12
Resolution : 3.20 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:

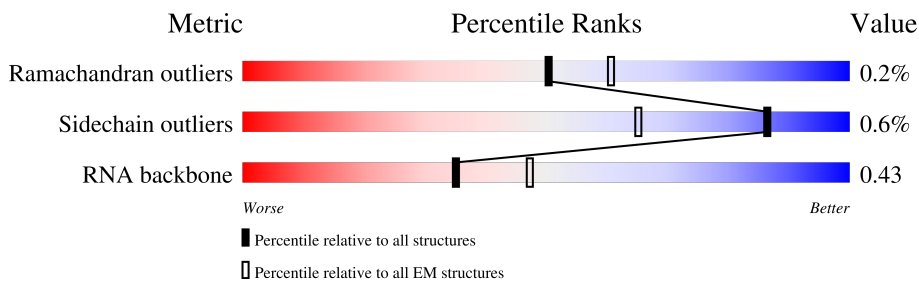
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.20 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.










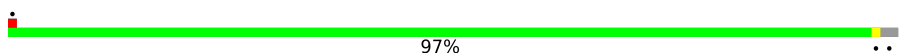




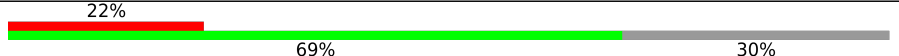
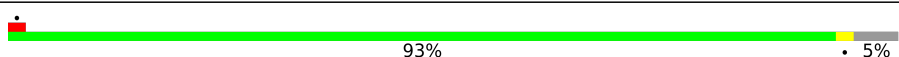
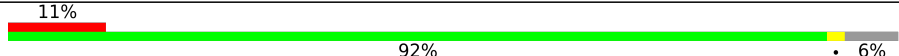

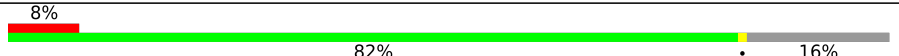
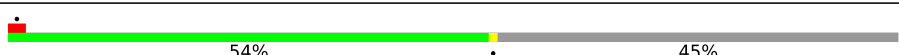
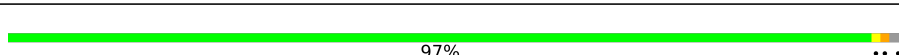
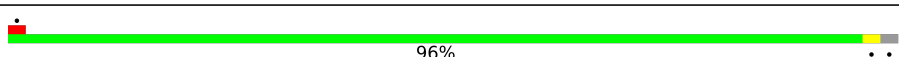

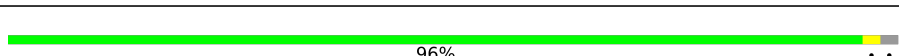


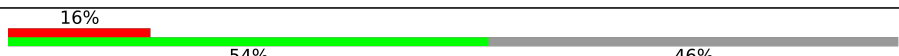
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	904	
2	B	907	
3	C	648	
4	D	884	
5	E	414	
6	F	558	
7	G	1802	
8	H	270	

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Mol	Chain	Length	Quality of chain
9	I	962	 16% 84%
10	J	912	 16% 83%
11	K	938	 16% 84%
12	L	557	 7% 49% 50%
13	M	960	 29% 70%
14	N	618	 71% 28%
15	O	1049	 81% 18%
16	P	194	 97%
17	Q	391	 13% 46% 53%
18	R	313	 76% 23%
18	S	313	 55% 74% 24%
19	T	523	 5% 73% 26%
20	U	582	 22% 69% 30%
21	V	127	 93% 5%
21	W	127	 11% 92% 6%
22	X	630	 5% 54% 45%
23	Y	411	 8% 82% 16%
24	Z	1163	 54% 45%
25	a	183	 97%
26	b	297	 96%
27	c	785	 22% 78%
28	d	446	 96%
29	e	252	 52% 83% 15%
29	f	252	 81% 83% 15%
30	g	322	 16% 54% 46%

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Mol	Chain	Length	Quality of chain
31	h	259	
32	i	1073	
32	j	1073	
33	k	203	
34	l	255	
35	m	264	
36	n	212	
37	o	239	
38	p	203	
39	q	202	
40	r	190	
41	s	151	
42	t	150	
43	u	143	
44	v	161	
45	w	130	
46	x	145	
47	y	136	
48	z	68	
49	0	311	
50	1	2568	
51	2	274	

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 135120 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	827	6242	4029	1114	1077	22	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	69	537	338	121	78	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	292	2170	1383	403	373	11	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	429	3282	2103	611	557	11	0	0

- Molecule 7 is a protein called Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	363	2772	1784	501	473	14	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	190	1456	915	306	230	5	0	0

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	155	1230	788	222	214	6	0	0

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	151	1201	765	214	222	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	147	1139	725	215	194	5	0	0

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	280	2070	1320	379	363	8	0	0

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	284	2134	1386	364	378	6	0	0

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	443	3435	2181	646	598	10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	864	6446	4152	1189	1079	26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	190	1460	928	281	241	10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	182	905	541	182	182	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	242	1778	1149	327	293	9	0	0
18	S	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Putative nucleolar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	405	3035	1954	539	532	10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	W	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	347	Total	C	N	O	S	0	0
			2686	1707	486	481	12		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	345	Total	C	N	O	S	0	0
			2594	1648	465	472	9		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	639	Total	C	N	O	S	0	0
			4848	3145	903	782	18		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	291	Total	C	N	O	S	0	0
			2279	1445	437	389	8		

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	175	Total	C	N	O	S	0	0
			1387	869	269	244	5		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d	439	3436	2158	663	600	15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	215	1683	1067	293	313	10	0	0
29	f	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	174	1393	890	250	244	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	167	1288	817	234	231	6	0	0

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	i	659	3254	1936	659	659	0	0
32	j	677	3342	1988	677	677	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	k	117	930	589	179	158	4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	l	214	1735	1105	322	303	5	0	0

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	m	258	2057	1305	386	359	7	0	0

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	n	192	1447	918	277	245	7	0	0

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	o	237	1911	1192	384	330	5	0	0

- Molecule 38 is a protein called 40S ribosomal protein S7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	p	159	1279	810	237	232		0	0

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	q	201	1622	1009	330	282	1	0	0

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	159	1242	801	255	184	2	0	0

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	49	416	270	82	64		0	0

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	115	Total	C	N	O	S	0	0
			791	492	154	141	4		

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	157	Total	C	N	O	S	0	0
			1286	825	248	208	5		

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	94	Total	C	N	O	S	0	0
			684	445	129	108	2		

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	93	Total	C	N	O	S	0	0
			752	481	140	129	2		

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	61	Total	C	N	O	0	0
			455	284	97	74		

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	0	92	Total	C	N	O	S	0	0
			694	426	144	120	4		

- Molecule 50 is a RNA chain called 35S rRNA.

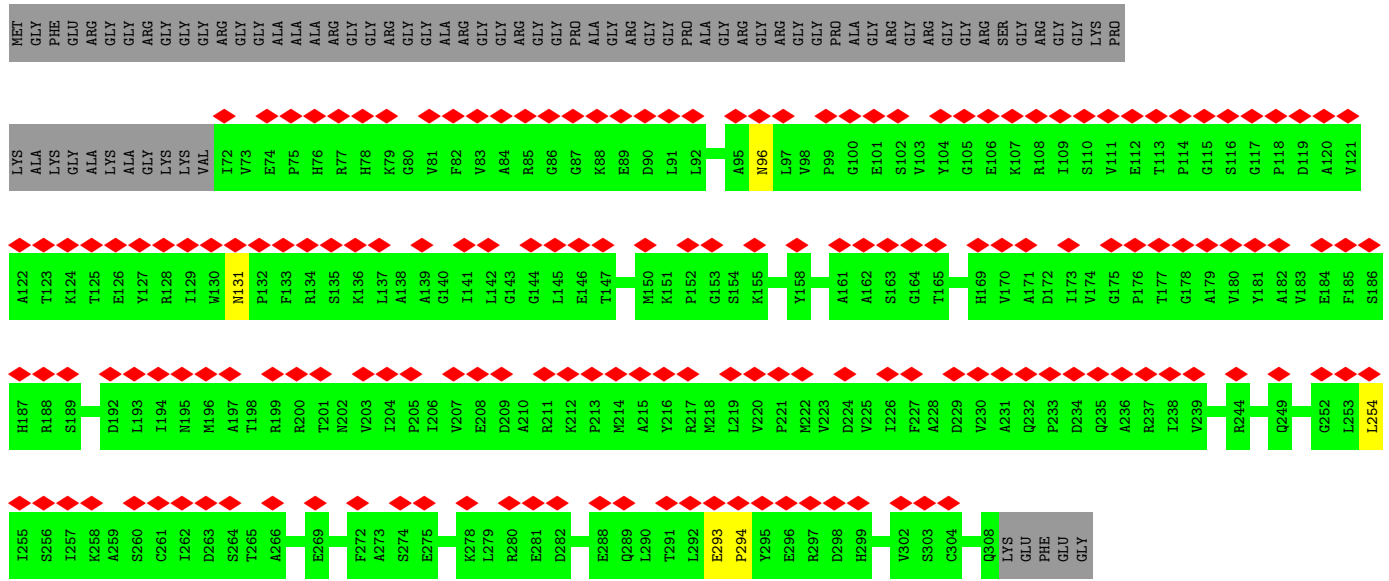
Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	1350	Total	C	N	O	P	0	0
			28796	12851	5157	9440	1348		

- Molecule 51 is a RNA chain called U3 snoRNA.

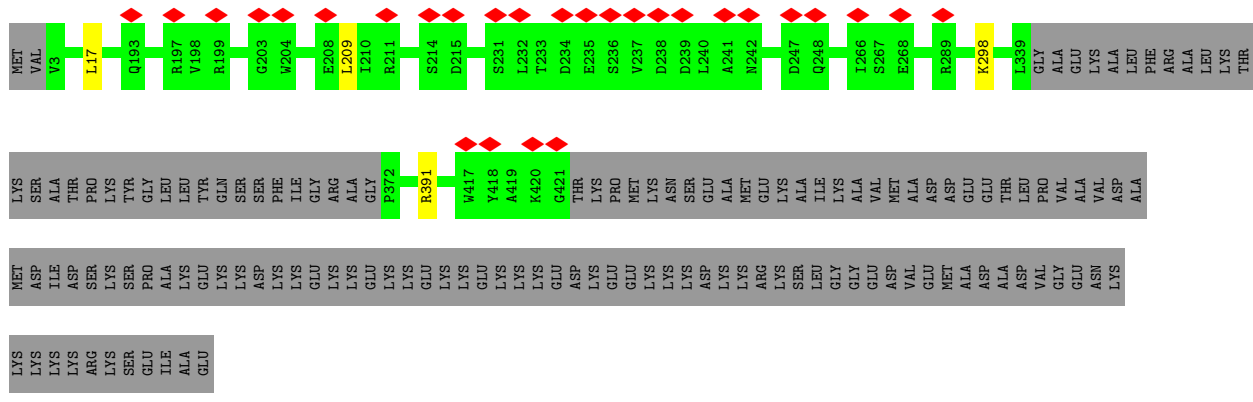
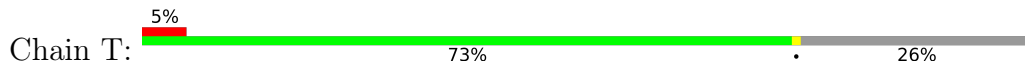
Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

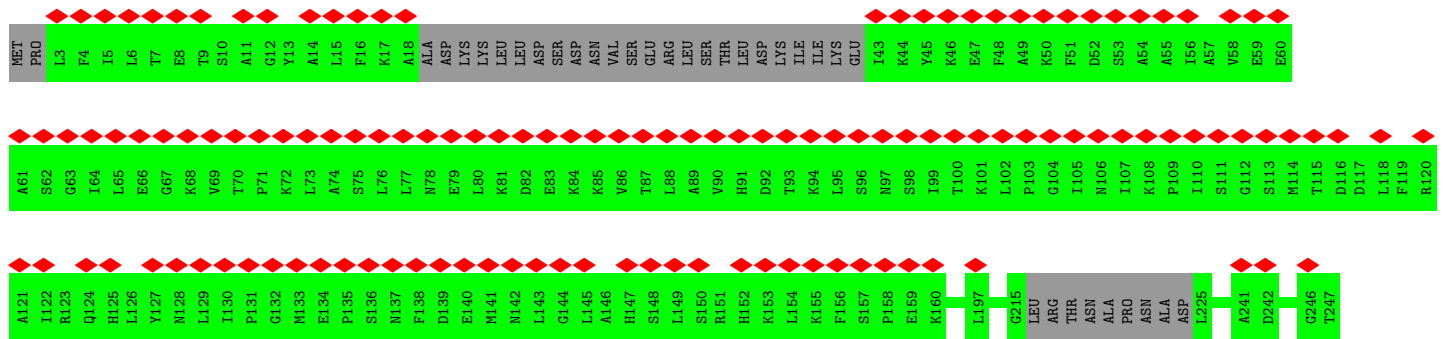
Mol	Chain	Residues	Atoms		AltConf
52	P	1	Total	Zn	0
			1	1	



• Molecule 19: Putative nucleolar protein

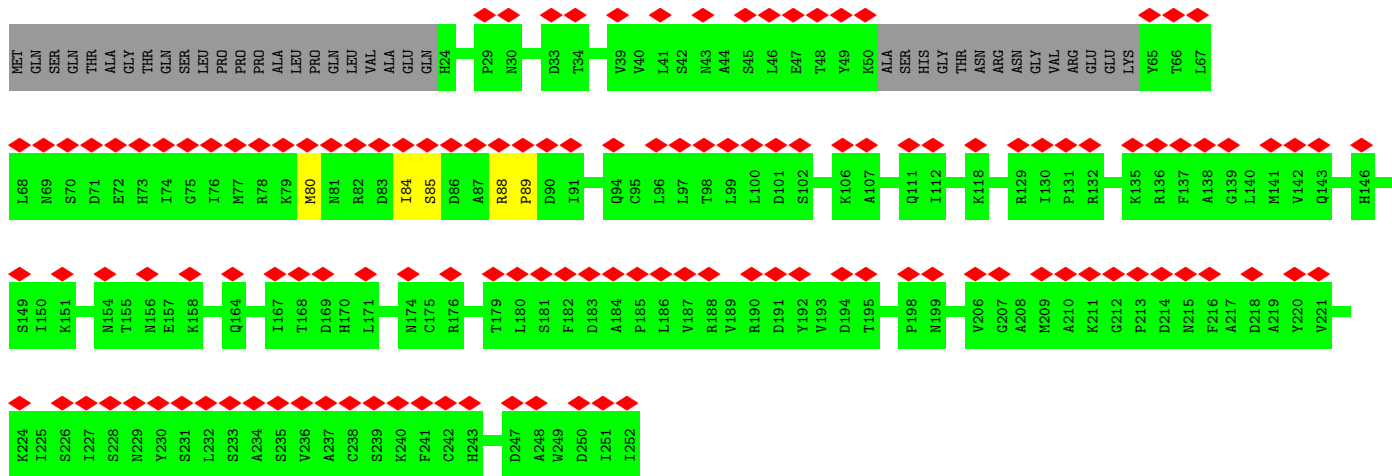
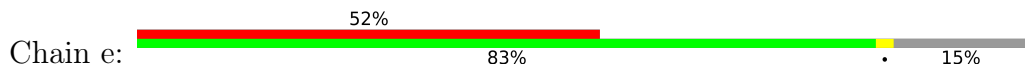


• Molecule 20: Nop58

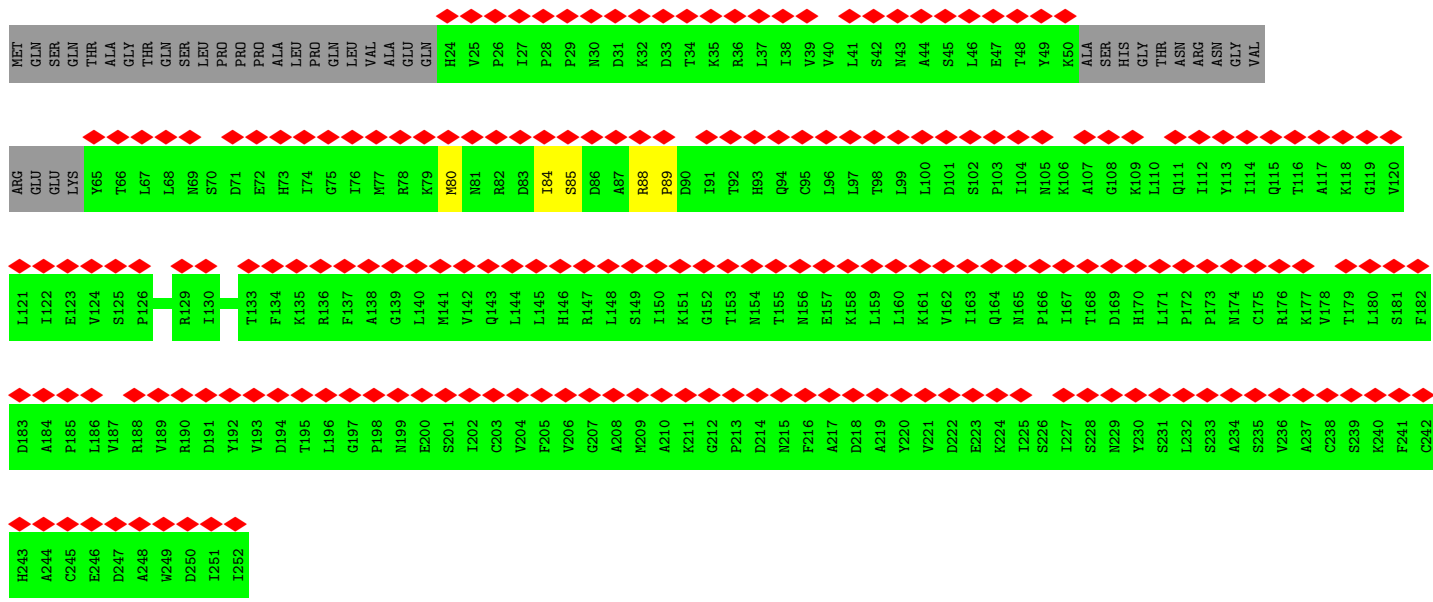
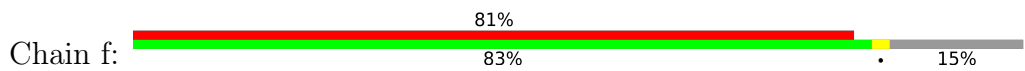




• Molecule 29: Emg1

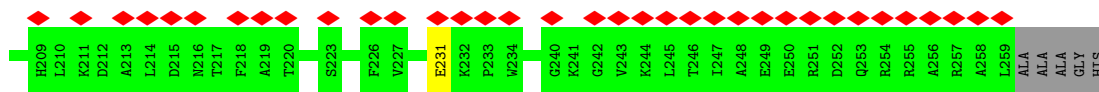


• Molecule 29: Emg1

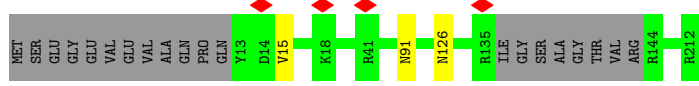
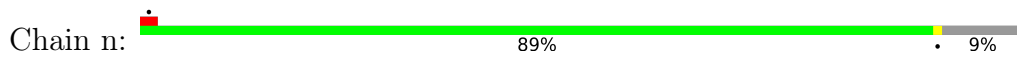


• Molecule 30: KRR1 small subunit processome component

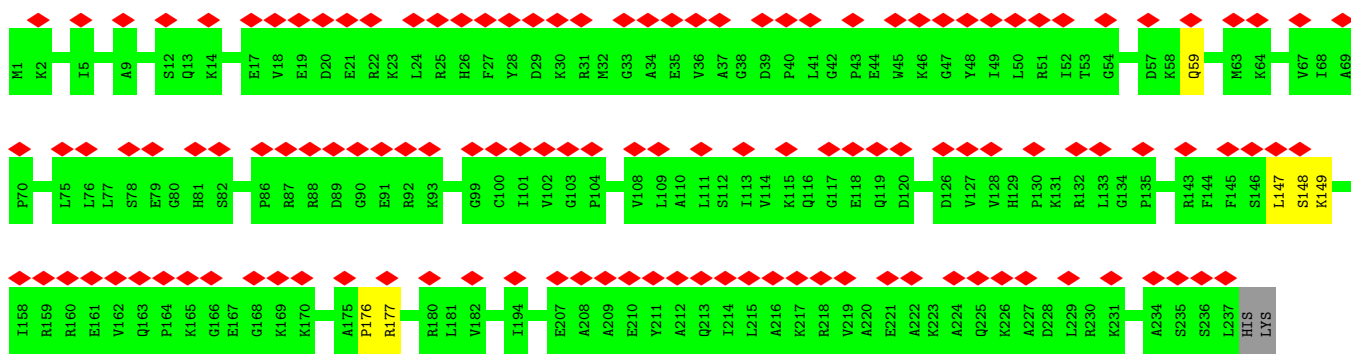




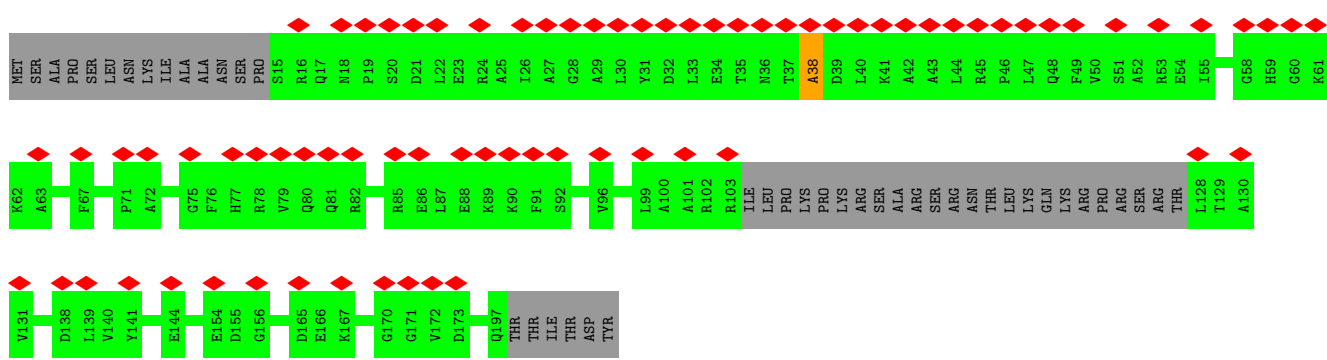
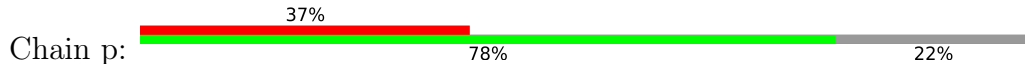
• Molecule 36: 40S ribosomal protein s5-like protein



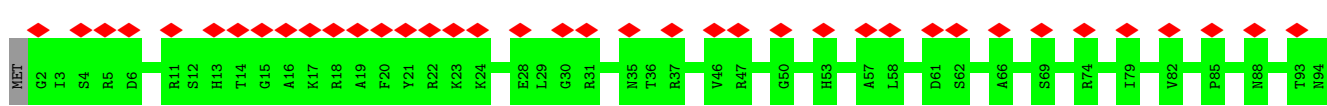
• Molecule 37: 40S ribosomal protein S6

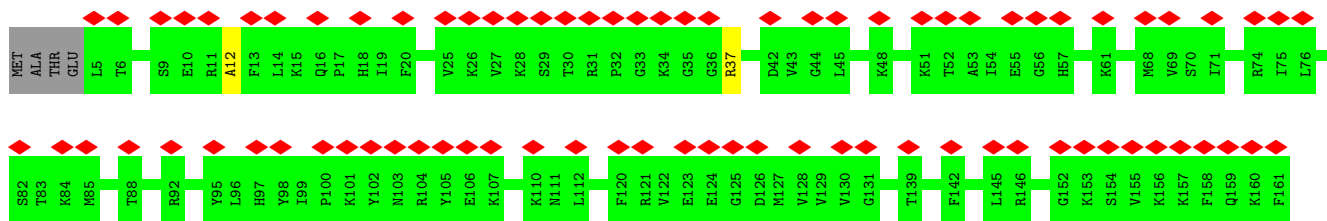


• Molecule 38: 40S ribosomal protein S7-like protein

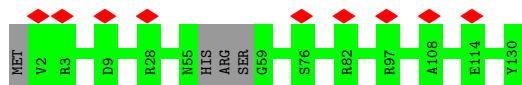


• Molecule 39: 40S ribosomal protein S8

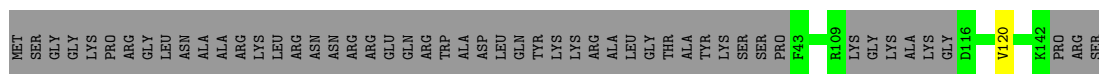




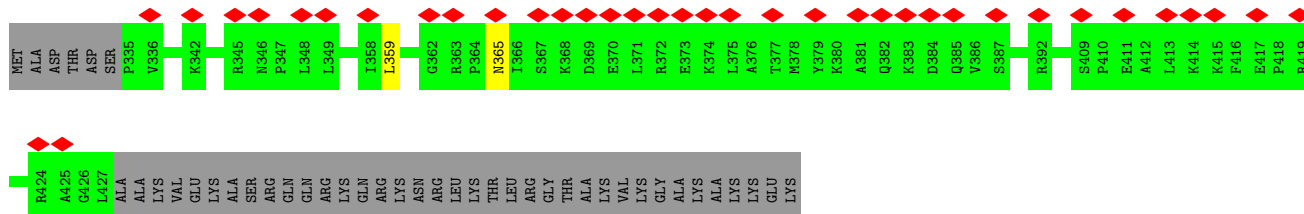
• Molecule 45: 40S ribosomal protein S22-like protein



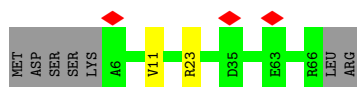
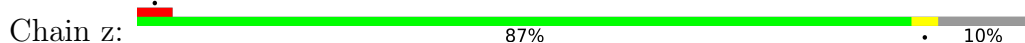
• Molecule 46: 40S ribosomal protein s23-like protein



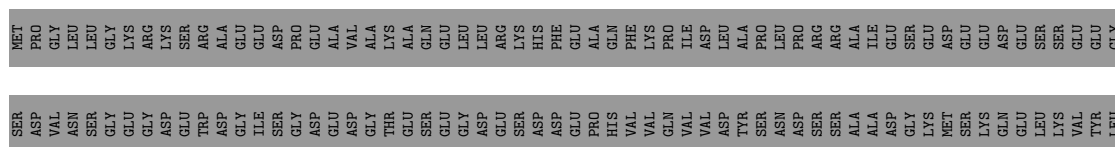
• Molecule 47: 40S ribosomal protein S24

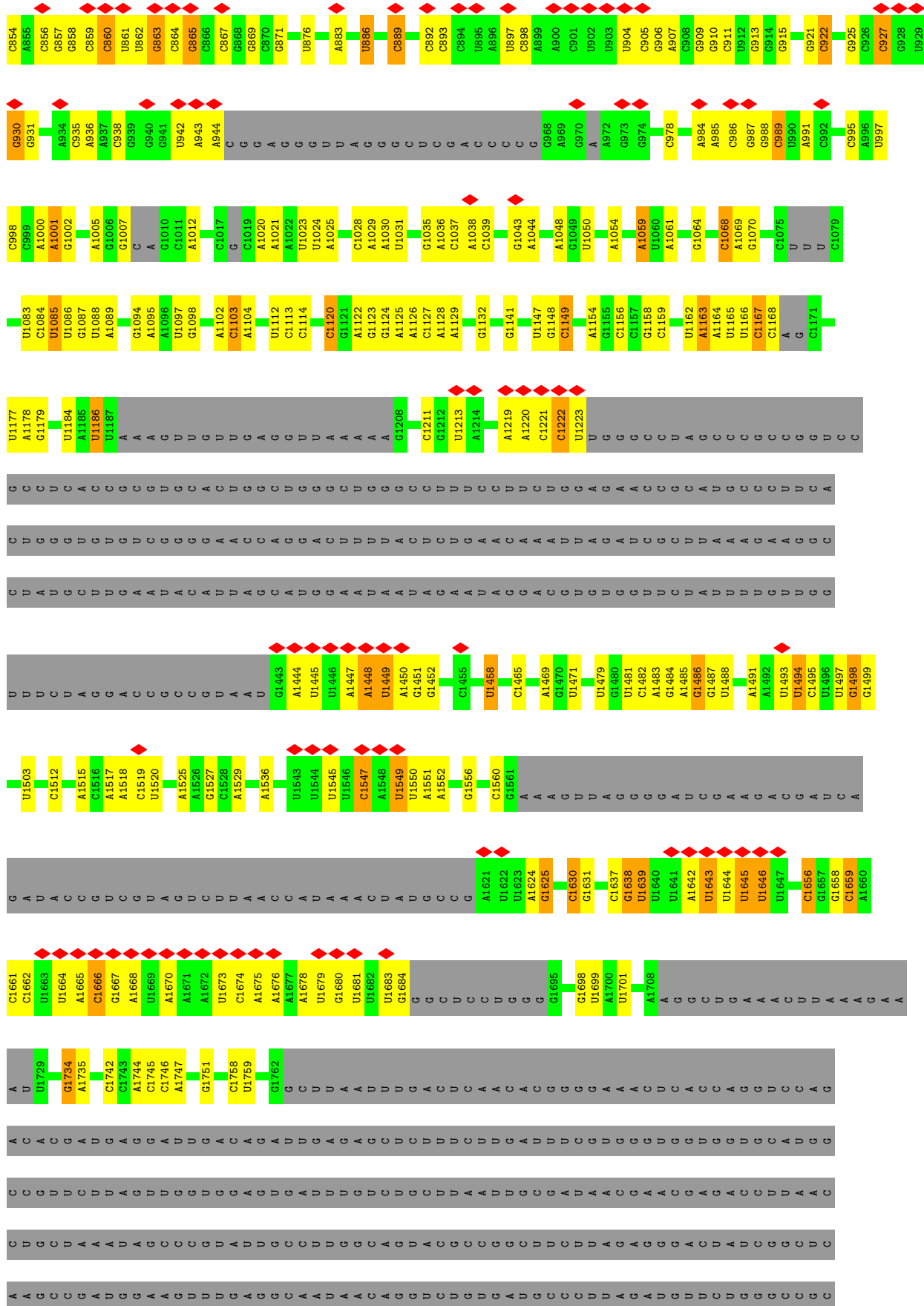


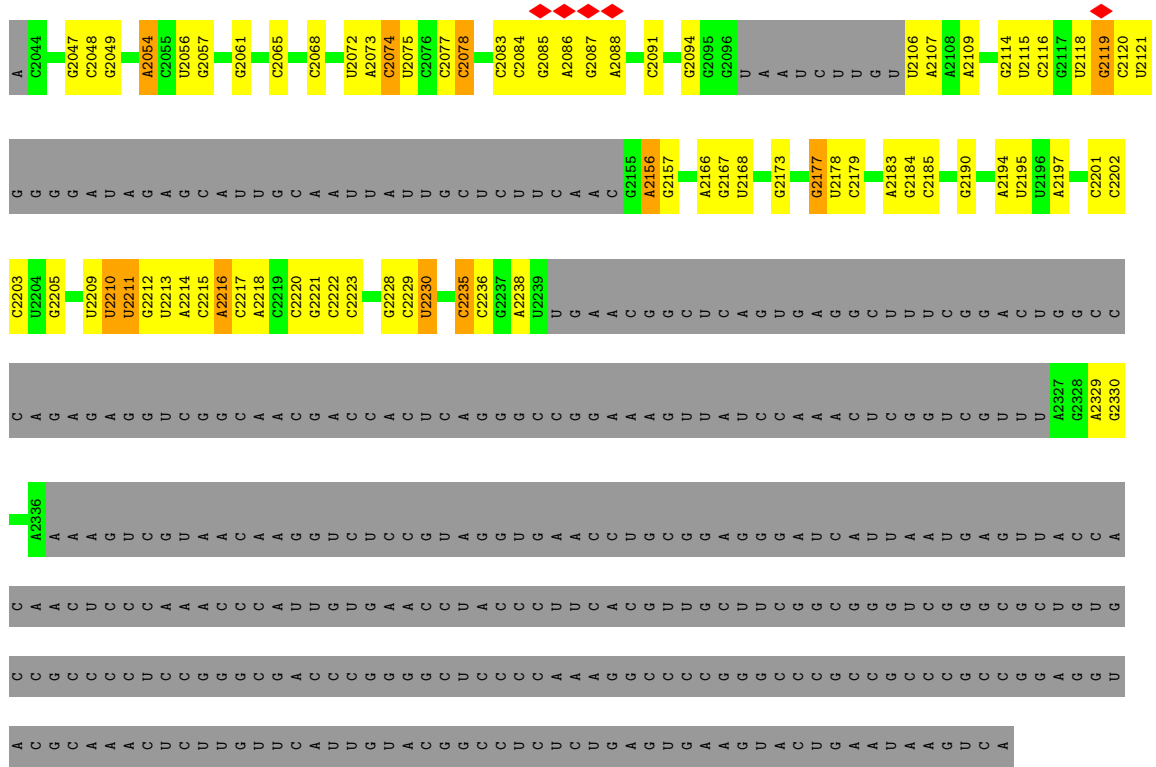
• Molecule 48: 40S ribosomal protein S28-like protein



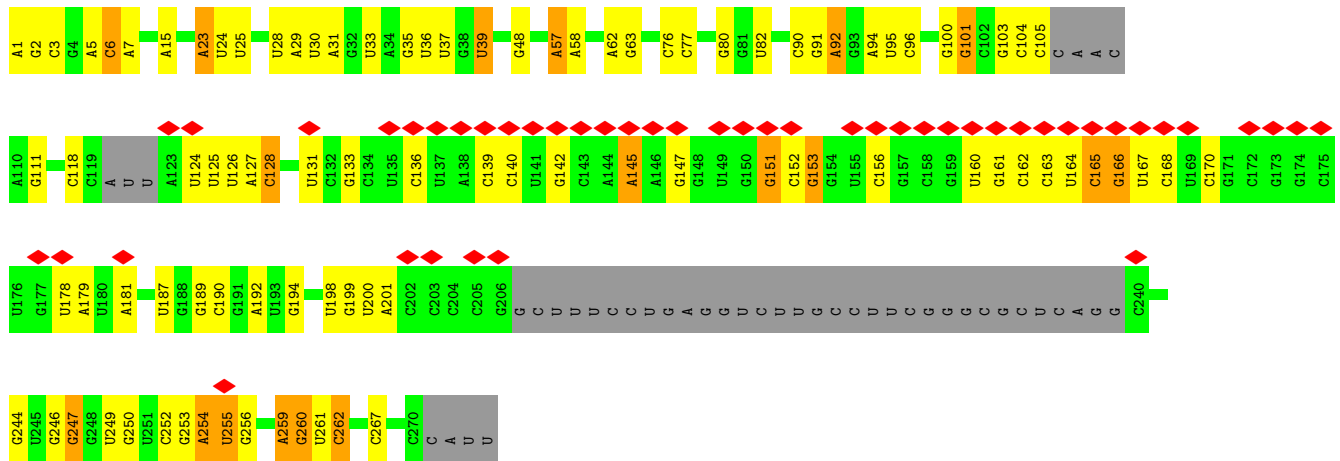
• Molecule 49: Faf1







● Molecule 51: U3 snoRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.596	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	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	A	0.50	0/6395	0.75	10/8703 (0.1%)
2	B	0.33	0/541	0.46	0/713
3	C	0.38	0/595	0.56	0/786
4	D	0.37	0/2209	0.66	0/2986
5	E	0.37	0/2657	0.55	1/3596 (0.0%)
6	F	0.51	0/3353	0.73	1/4544 (0.0%)
7	G	0.41	0/2828	0.65	1/3841 (0.0%)
8	H	0.42	0/1468	0.60	0/1946
9	I	0.34	0/1251	0.62	0/1696
10	J	0.38	0/1221	0.65	0/1662
11	K	0.39	0/1161	0.64	1/1570 (0.1%)
12	L	0.33	0/2117	0.69	3/2887 (0.1%)
13	M	0.37	0/2179	0.72	2/2972 (0.1%)
14	N	0.42	0/3508	0.64	2/4742 (0.0%)
15	O	0.45	0/6604	0.76	10/8981 (0.1%)
16	P	0.43	0/1483	0.70	0/1998
17	Q	0.25	0/900	0.49	0/1249
18	R	0.39	0/1814	0.59	0/2456
18	S	0.40	0/1853	0.59	0/2511
19	T	0.36	0/2911	0.66	1/3937 (0.0%)
20	U	0.35	0/3085	0.65	1/4169 (0.0%)
21	V	0.38	0/891	0.67	1/1214 (0.1%)
21	W	0.38	0/876	0.67	1/1195 (0.1%)
22	X	0.36	0/2739	0.69	1/3699 (0.0%)
23	Y	0.33	0/2638	0.63	1/3580 (0.0%)
24	Z	0.39	0/4960	0.66	4/6710 (0.1%)
25	a	0.49	0/1462	0.71	2/1967 (0.1%)
26	b	0.48	0/2324	0.73	4/3144 (0.1%)
27	c	0.36	0/1405	0.59	1/1879 (0.1%)
28	d	0.50	0/3506	0.72	3/4739 (0.1%)
29	e	0.28	0/1714	0.53	0/2325
29	f	0.28	0/1714	0.53	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	g	0.32	0/1412	0.61	0/1897
31	h	0.28	0/1304	0.61	0/1751
32	i	0.25	0/3246	0.45	0/4507
32	j	0.24	0/3335	0.45	0/4632
33	k	0.41	0/945	0.60	0/1264
34	l	0.31	0/1764	0.73	4/2377 (0.2%)
35	m	0.29	0/2097	0.63	1/2821 (0.0%)
36	n	0.41	0/1468	0.63	0/1987
37	o	0.32	0/1942	0.67	1/2595 (0.0%)
38	p	0.34	0/1298	0.69	1/1750 (0.1%)
39	q	0.28	0/1655	0.57	0/2213
40	r	0.38	0/1259	0.63	0/1687
41	s	0.26	0/422	0.48	0/561
42	t	0.31	0/801	0.62	1/1087 (0.1%)
43	u	0.48	0/958	0.70	0/1293
44	v	0.31	0/1315	0.59	0/1760
45	w	0.36	0/1001	0.63	0/1345
46	x	0.42	0/693	0.59	0/928
47	y	0.28	0/766	0.65	1/1027 (0.1%)
48	z	0.42	0/458	0.67	0/617
49	0	0.32	0/702	0.58	0/939
50	1	0.54	2/32166 (0.0%)	1.31	444/50073 (0.9%)
51	2	0.62	0/5459	1.45	76/8498 (0.9%)
All	All	0.44	2/140828 (0.0%)	0.91	580/198331 (0.3%)

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	4
4	D	0	1
6	F	0	3
12	L	0	1
13	M	0	4
14	N	0	1
15	O	0	5
17	Q	0	3
18	R	0	1
18	S	0	1
21	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	W	0	1
22	X	0	4
23	Y	0	2
24	Z	0	3
26	b	0	1
28	d	0	1
29	e	0	3
29	f	0	3
31	h	0	2
32	i	0	1
32	j	0	1
34	l	0	5
35	m	0	2
37	o	0	2
38	p	0	1
39	q	0	1
42	t	0	1
43	u	0	1
44	v	0	2
46	x	0	1
47	y	0	1
All	All	0	64

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	435	A	N9-C4	-5.50	1.34	1.37
50	1	2194	A	C2-N3	-5.21	1.28	1.33

The worst 5 of 580 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	2	G	O5'-P-OP1	-32.85	71.28	110.70
51	2	2	G	OP1-P-OP2	-26.67	79.59	119.60
50	1	18	G	N1-C6-O6	-19.83	108.00	119.90
51	2	2	G	O5'-P-OP2	19.02	133.53	110.70
50	1	18	G	C5-C6-O6	16.50	138.50	128.60

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	SER	Peptide
1	A	284	MET	Peptide
1	A	556	GLY	Peptide
1	A	686	SER	Peptide
4	D	169	GLU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	823/904 (91%)	739 (90%)	83 (10%)	1 (0%)	51	83
2	B	67/907 (7%)	66 (98%)	1 (2%)	0	100	100
3	C	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	D	280/884 (32%)	256 (91%)	23 (8%)	1 (0%)	34	69
5	E	325/414 (78%)	312 (96%)	13 (4%)	0	100	100
6	F	425/558 (76%)	390 (92%)	34 (8%)	1 (0%)	47	79
7	G	361/1802 (20%)	340 (94%)	21 (6%)	0	100	100
8	H	186/270 (69%)	178 (96%)	8 (4%)	0	100	100
9	I	153/962 (16%)	141 (92%)	12 (8%)	0	100	100
10	J	147/912 (16%)	139 (95%)	8 (5%)	0	100	100
11	K	143/938 (15%)	130 (91%)	13 (9%)	0	100	100
12	L	272/557 (49%)	237 (87%)	35 (13%)	0	100	100
13	M	266/960 (28%)	222 (84%)	43 (16%)	1 (0%)	34	69
14	N	433/618 (70%)	404 (93%)	29 (7%)	0	100	100
15	O	850/1049 (81%)	768 (90%)	82 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	188/194 (97%)	173 (92%)	15 (8%)	0	100	100
17	Q	172/391 (44%)	146 (85%)	23 (13%)	3 (2%)	9	42
18	R	238/313 (76%)	222 (93%)	15 (6%)	1 (0%)	34	69
18	S	235/313 (75%)	221 (94%)	13 (6%)	1 (0%)	34	69
19	T	383/523 (73%)	352 (92%)	31 (8%)	0	100	100
20	U	397/582 (68%)	375 (94%)	22 (6%)	0	100	100
21	V	119/127 (94%)	105 (88%)	13 (11%)	1 (1%)	19	58
21	W	118/127 (93%)	104 (88%)	13 (11%)	1 (1%)	19	58
22	X	337/630 (54%)	294 (87%)	42 (12%)	1 (0%)	41	74
23	Y	333/411 (81%)	300 (90%)	30 (9%)	3 (1%)	17	56
24	Z	627/1163 (54%)	582 (93%)	44 (7%)	1 (0%)	47	79
25	a	177/183 (97%)	162 (92%)	15 (8%)	0	100	100
26	b	287/297 (97%)	263 (92%)	24 (8%)	0	100	100
27	c	169/785 (22%)	160 (95%)	9 (5%)	0	100	100
28	d	435/446 (98%)	390 (90%)	45 (10%)	0	100	100
29	e	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	17	56
29	f	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	17	56
30	g	172/322 (53%)	164 (95%)	8 (5%)	0	100	100
31	h	163/259 (63%)	154 (94%)	9 (6%)	0	100	100
32	i	643/1073 (60%)	569 (88%)	74 (12%)	0	100	100
32	j	663/1073 (62%)	588 (89%)	75 (11%)	0	100	100
33	k	115/203 (57%)	101 (88%)	14 (12%)	0	100	100
34	l	212/255 (83%)	184 (87%)	27 (13%)	1 (0%)	29	67
35	m	256/264 (97%)	219 (86%)	37 (14%)	0	100	100
36	n	188/212 (89%)	170 (90%)	17 (9%)	1 (0%)	29	67
37	o	235/239 (98%)	202 (86%)	31 (13%)	2 (1%)	17	56
38	p	155/203 (76%)	137 (88%)	18 (12%)	0	100	100
39	q	199/202 (98%)	187 (94%)	12 (6%)	0	100	100
40	r	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	s	47/151 (31%)	45 (96%)	2 (4%)	0	100	100
42	t	113/150 (75%)	95 (84%)	16 (14%)	2 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	u	124/143 (87%)	113 (91%)	11 (9%)	0	100	100
44	v	155/161 (96%)	134 (86%)	21 (14%)	0	100	100
45	w	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
46	x	90/145 (62%)	79 (88%)	11 (12%)	0	100	100
47	y	91/136 (67%)	82 (90%)	9 (10%)	0	100	100
48	z	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
49	0	90/311 (29%)	82 (91%)	8 (9%)	0	100	100
All	All	13489/25262 (53%)	12254 (91%)	1209 (9%)	26 (0%)	50	79

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	e	85	SER
29	f	85	SER
34	l	62	LYS
23	Y	105	THR
36	n	91	ASN

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	633/775 (82%)	628 (99%)	5 (1%)	81	93
2	B	43/788 (6%)	43 (100%)	0	100	100
3	C	61/536 (11%)	60 (98%)	1 (2%)	62	84
4	D	222/738 (30%)	222 (100%)	0	100	100
5	E	248/341 (73%)	248 (100%)	0	100	100
6	F	326/474 (69%)	322 (99%)	4 (1%)	71	88
7	G	289/1526 (19%)	289 (100%)	0	100	100
8	H	135/227 (60%)	134 (99%)	1 (1%)	84	94
9	I	134/821 (16%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	129/770 (17%)	127 (98%)	2 (2%)	62	84
11	K	115/765 (15%)	115 (100%)	0	100	100
12	L	218/456 (48%)	217 (100%)	1 (0%)	88	95
13	M	219/817 (27%)	217 (99%)	2 (1%)	78	91
14	N	351/524 (67%)	349 (99%)	2 (1%)	86	94
15	O	638/863 (74%)	633 (99%)	5 (1%)	81	93
16	P	147/168 (88%)	146 (99%)	1 (1%)	84	94
18	R	175/228 (77%)	172 (98%)	3 (2%)	60	83
18	S	195/228 (86%)	192 (98%)	3 (2%)	65	85
19	T	287/435 (66%)	284 (99%)	3 (1%)	76	90
20	U	307/489 (63%)	307 (100%)	0	100	100
21	V	91/108 (84%)	91 (100%)	0	100	100
21	W	88/108 (82%)	88 (100%)	0	100	100
22	X	273/525 (52%)	273 (100%)	0	100	100
23	Y	275/320 (86%)	274 (100%)	1 (0%)	91	95
24	Z	466/1009 (46%)	461 (99%)	5 (1%)	73	88
25	a	147/169 (87%)	146 (99%)	1 (1%)	84	94
26	b	238/266 (90%)	237 (100%)	1 (0%)	91	95
27	c	138/642 (22%)	138 (100%)	0	100	100
28	d	354/383 (92%)	348 (98%)	6 (2%)	60	83
29	e	193/223 (86%)	193 (100%)	0	100	100
29	f	193/223 (86%)	193 (100%)	0	100	100
30	g	153/287 (53%)	153 (100%)	0	100	100
31	h	138/215 (64%)	138 (100%)	0	100	100
33	k	95/167 (57%)	95 (100%)	0	100	100
34	l	189/223 (85%)	188 (100%)	1 (0%)	88	95
35	m	219/221 (99%)	219 (100%)	0	100	100
36	n	144/178 (81%)	142 (99%)	2 (1%)	67	86
37	o	202/204 (99%)	201 (100%)	1 (0%)	88	95
38	p	137/177 (77%)	137 (100%)	0	100	100
39	q	163/164 (99%)	162 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	r	122/162 (75%)	121 (99%)	1 (1%)	81	93
41	s	43/130 (33%)	43 (100%)	0	100	100
42	t	74/117 (63%)	74 (100%)	0	100	100
43	u	92/115 (80%)	92 (100%)	0	100	100
44	v	140/143 (98%)	140 (100%)	0	100	100
45	w	103/113 (91%)	103 (100%)	0	100	100
46	x	68/116 (59%)	68 (100%)	0	100	100
47	y	81/115 (70%)	81 (100%)	0	100	100
48	z	46/61 (75%)	44 (96%)	2 (4%)	29	64
49	0	68/260 (26%)	68 (100%)	0	100	100
All	All	9605/19113 (50%)	9550 (99%)	55 (1%)	86	94

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	131	ASN
24	Z	841	ARG
48	z	23	ARG
36	n	126	ASN
18	S	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	299	HIS
43	u	15	ASN
23	Y	316	GLN
39	q	179	GLN
46	x	89	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	1	1319/2568 (51%)	478 (36%)	27 (2%)
51	2	226/274 (82%)	76 (33%)	5 (2%)
All	All	1545/2842 (54%)	554 (35%)	32 (2%)

5 of 554 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	1	3	G
50	1	5	G
50	1	6	G
50	1	7	A
50	1	8	U

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	2	23	A
51	2	35	G
50	1	612	C
50	1	593	G
51	2	246	G

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

There are no chain breaks in this entry.

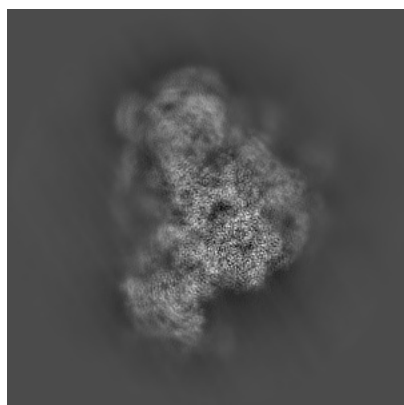
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3847. These allow visual inspection of the internal detail of the map and identification of artifacts.

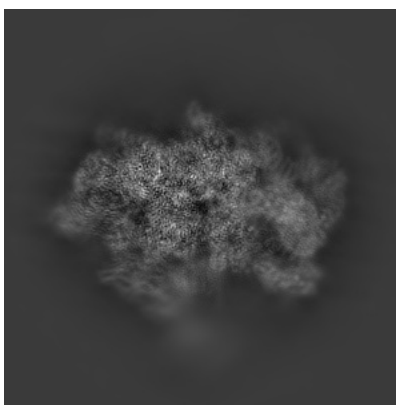
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

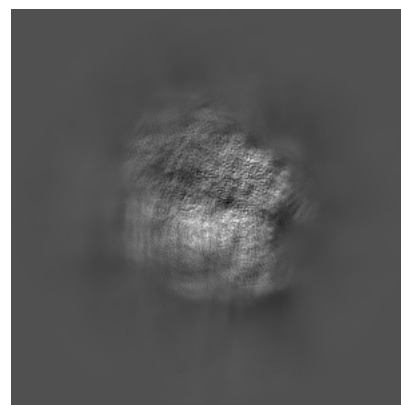
6.1.1 Primary map



X



Y

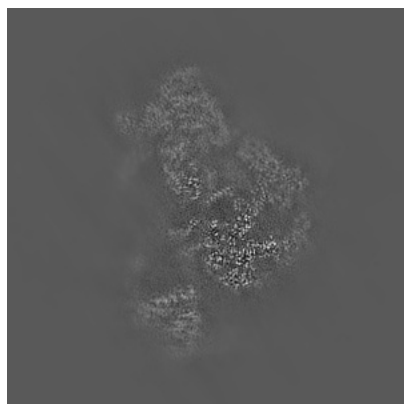


Z

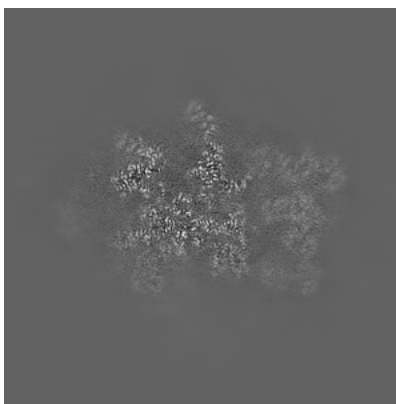
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

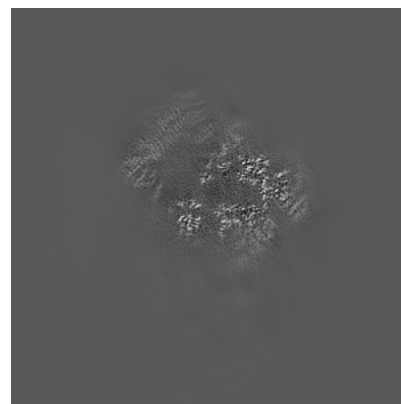
6.2.1 Primary map



X Index: 240



Y Index: 240

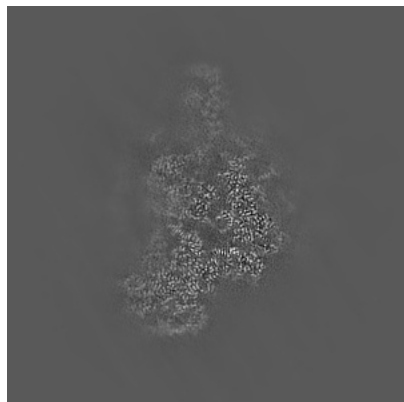


Z Index: 240

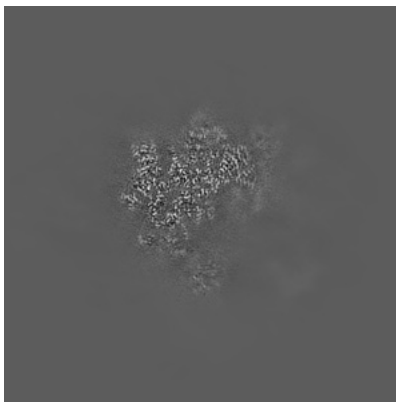
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 279



Y Index: 281



Z Index: 183

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

6.4 Orthogonal surface views [i](#)

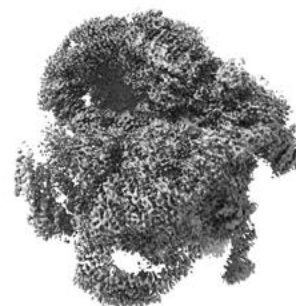
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

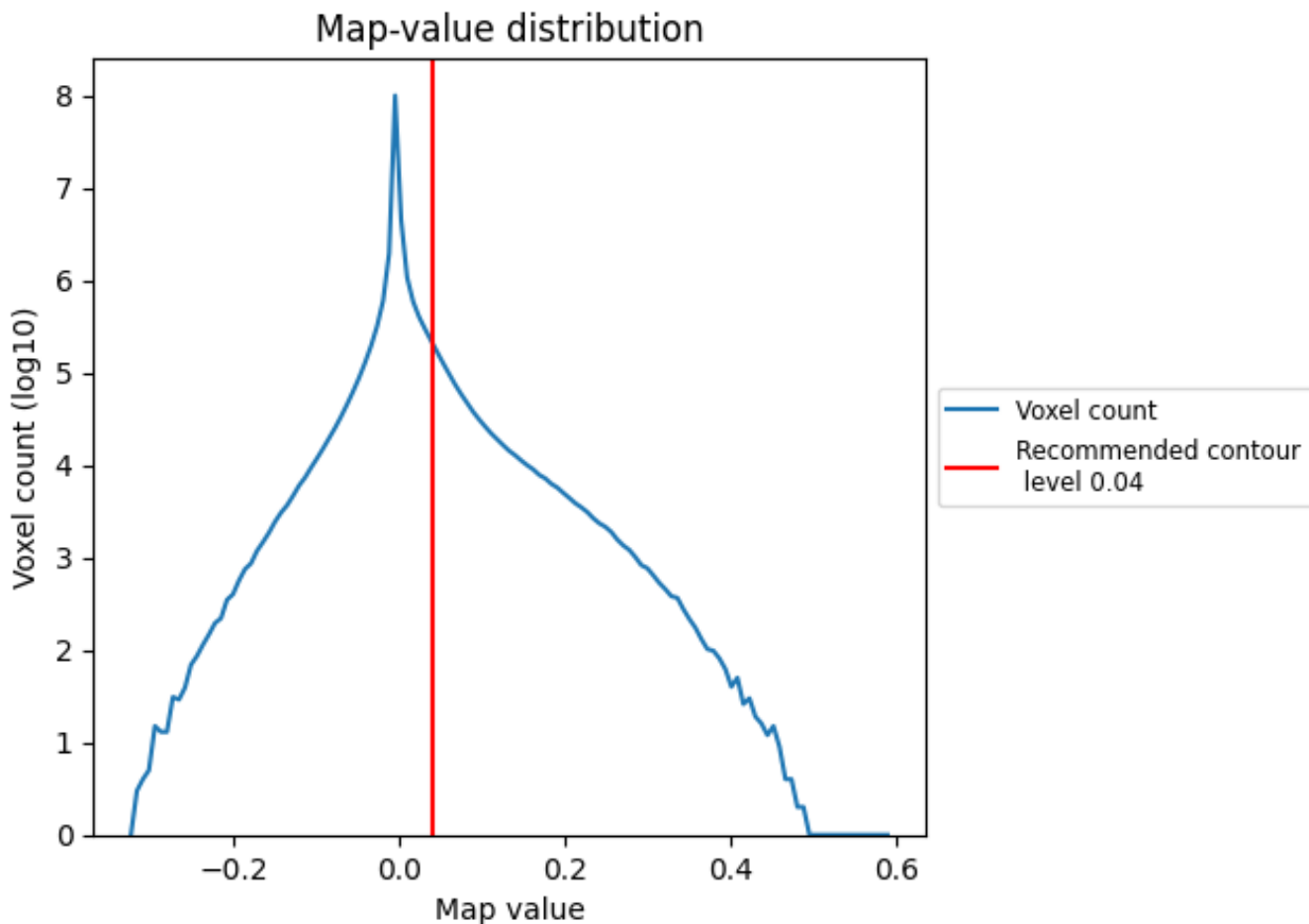
6.5 Mask visualisation

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

7 Map analysis [i](#)

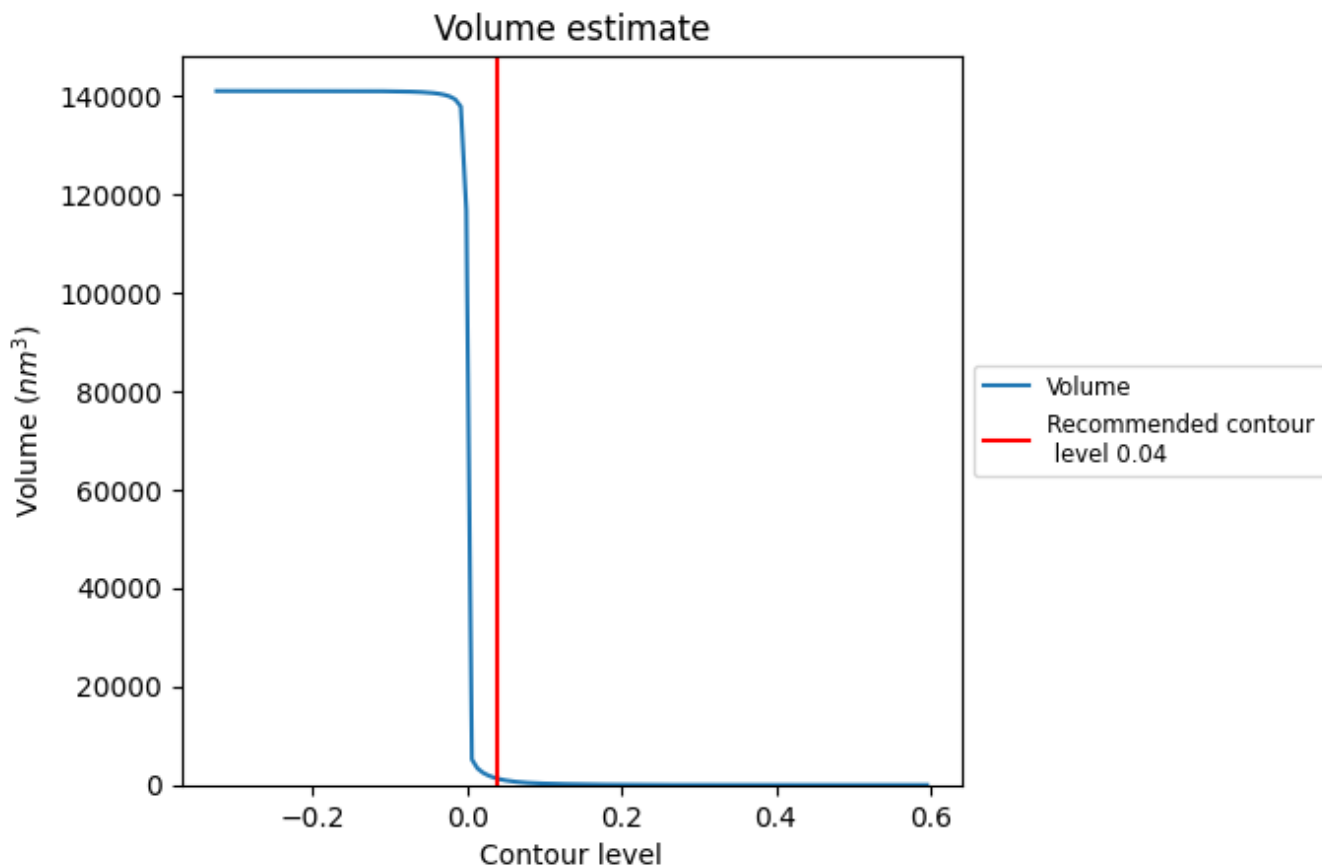
This section contains the results of statistical analysis of the map.

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.

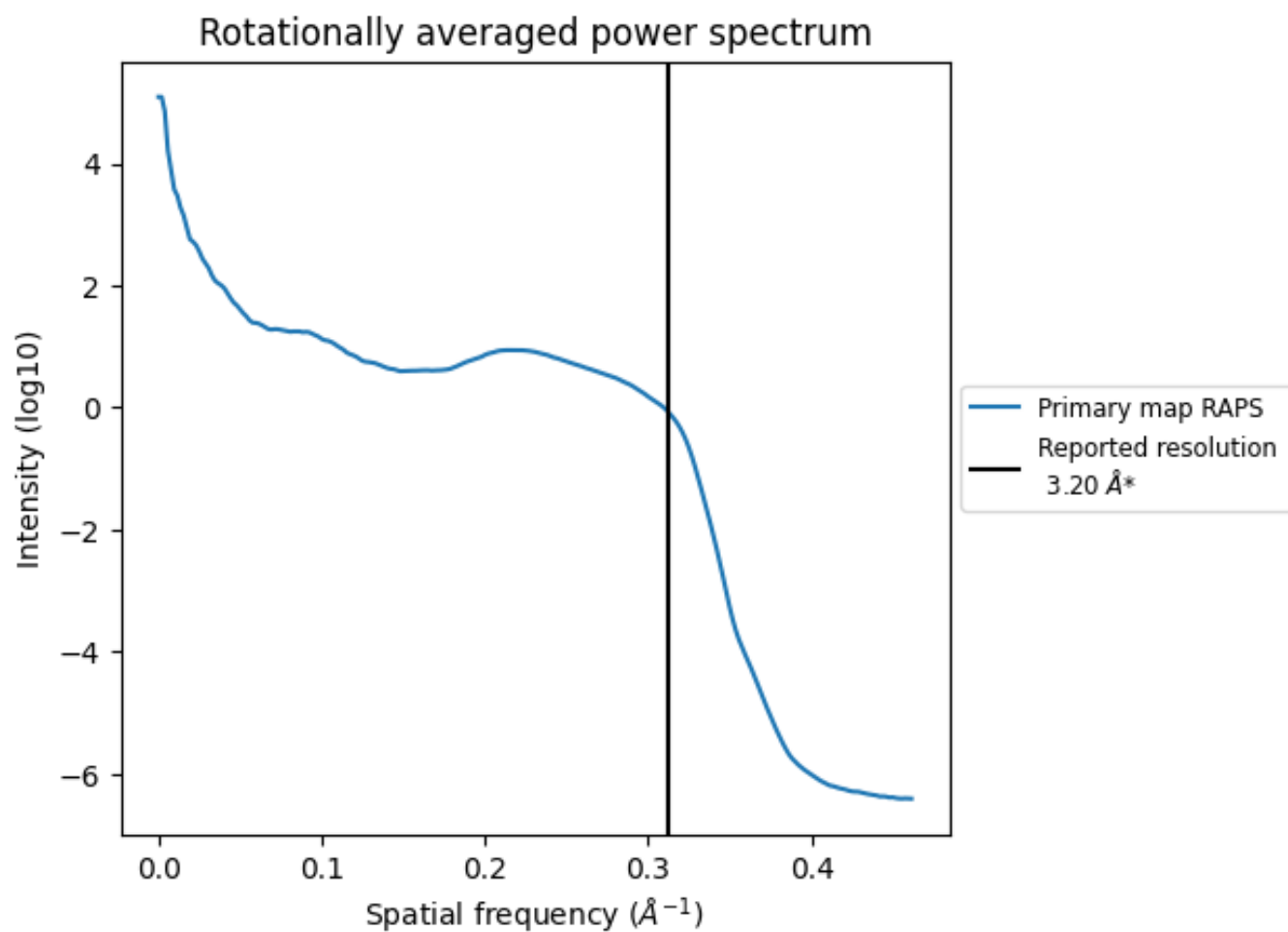
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1269 nm^3 ; this corresponds to an approximate mass of 1146 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](#)

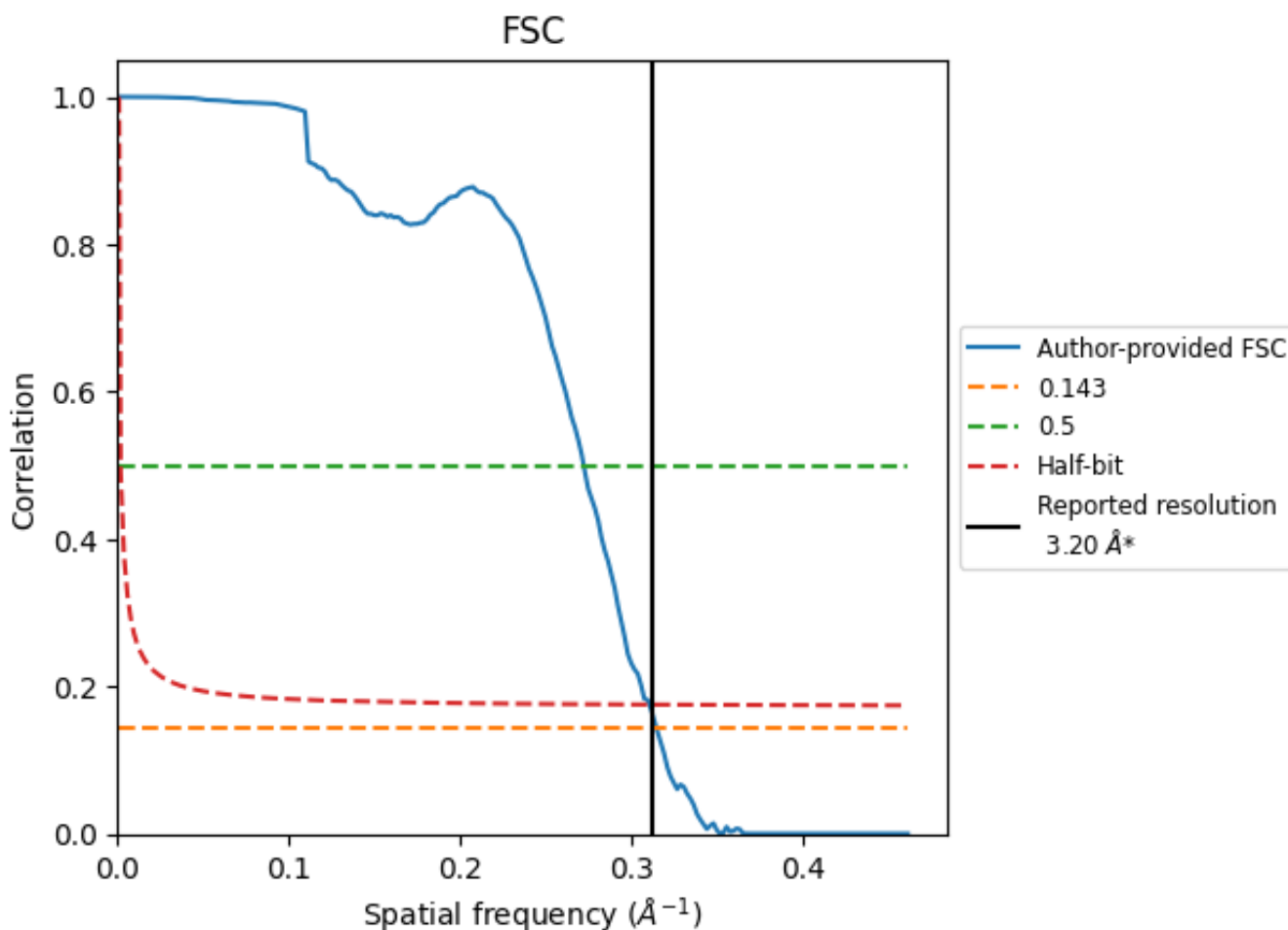


*Reported resolution corresponds to spatial frequency of 0.312\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

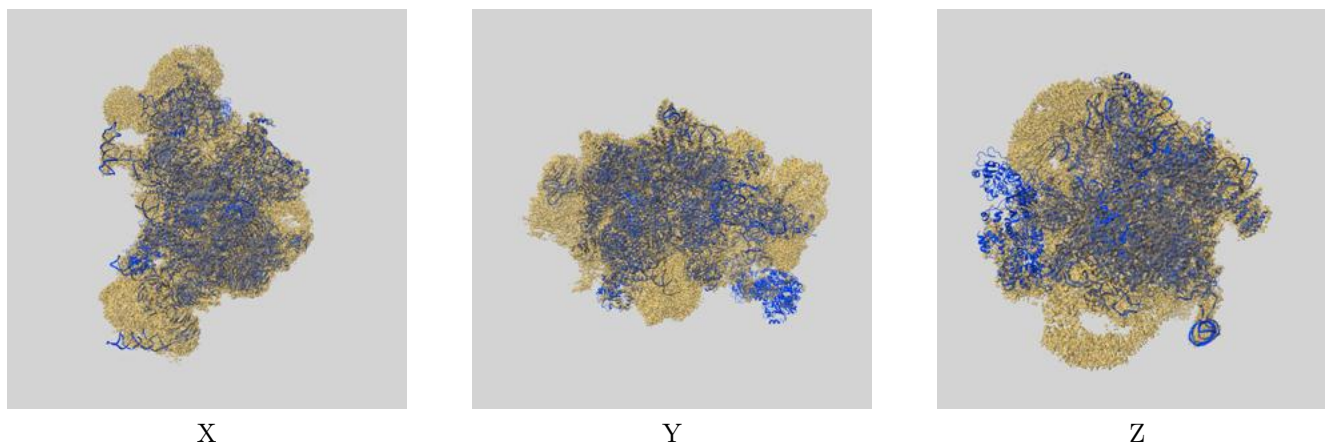
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.68	3.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

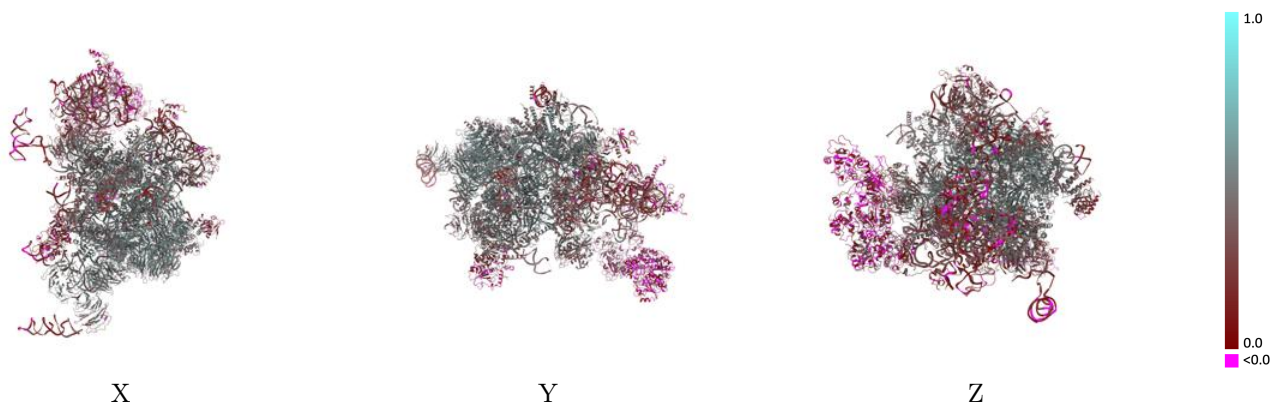
This section contains information regarding the fit between EMDB map EMD-3847 and PDB model 5OQL. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



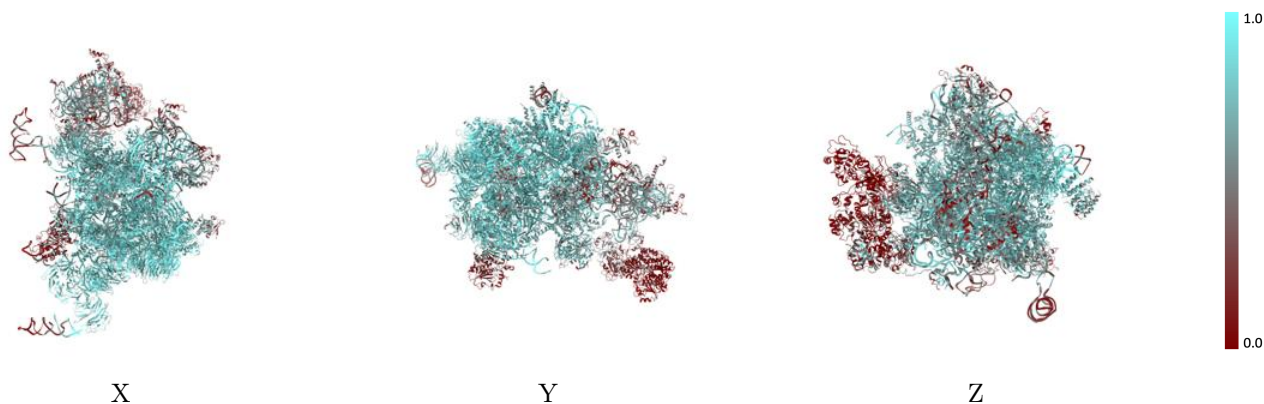
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



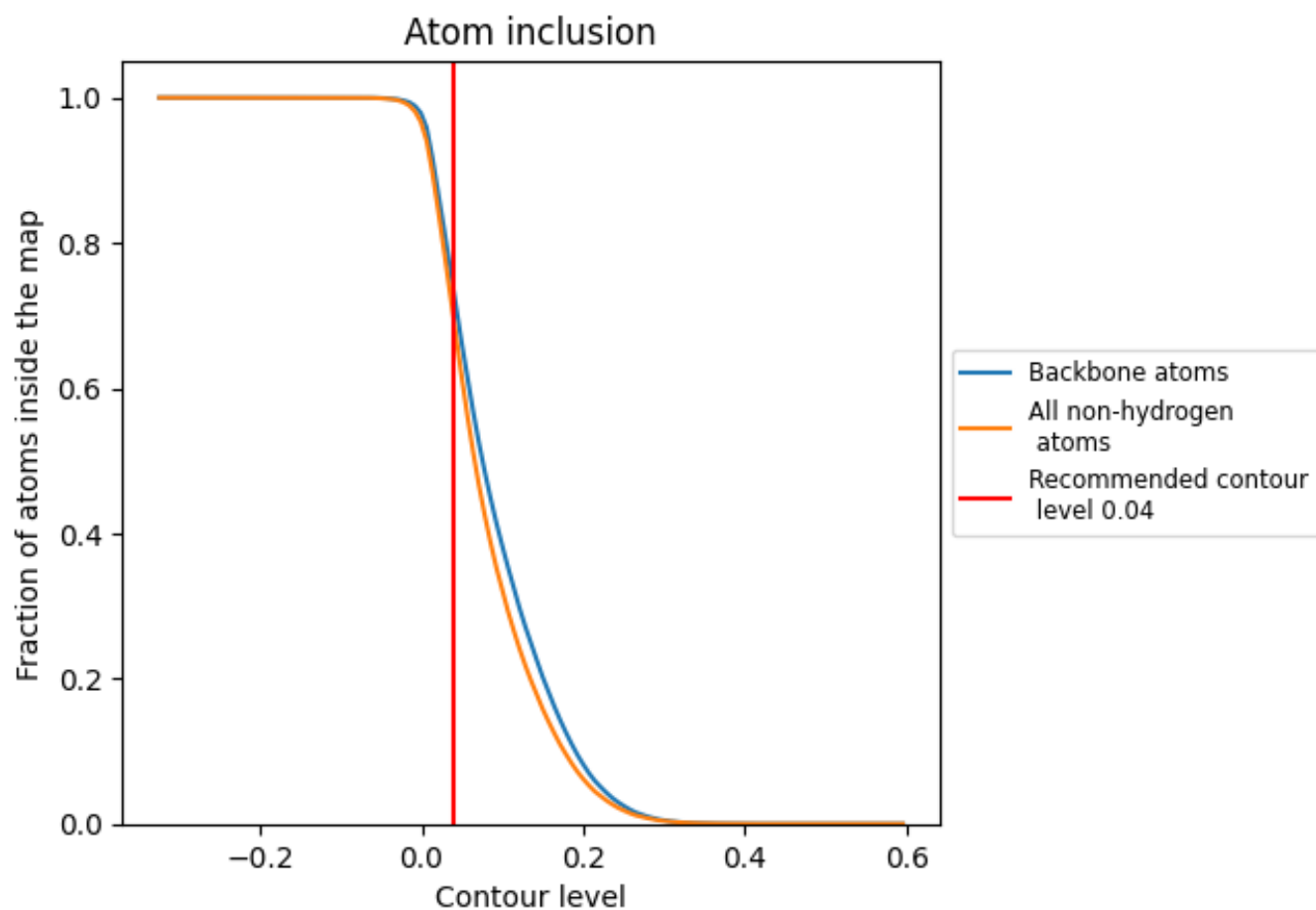
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6914	 0.3820
0	 0.7120	 0.4640
1	 0.7329	 0.3550
2	 0.7236	 0.3600
A	 0.8650	 0.4950
B	 0.7524	 0.4400
C	 0.8252	 0.4940
D	 0.8141	 0.4580
E	 0.7666	 0.3920
F	 0.8921	 0.5210
G	 0.8691	 0.4970
H	 0.8379	 0.4990
I	 0.6944	 0.3900
J	 0.7809	 0.4010
K	 0.8401	 0.4800
L	 0.6571	 0.3730
M	 0.8073	 0.4230
N	 0.8741	 0.5100
O	 0.8819	 0.5000
P	 0.8121	 0.4790
Q	 0.6088	 0.3400
R	 0.8712	 0.5060
S	 0.2729	 0.2150
T	 0.7630	 0.4080
U	 0.5738	 0.3530
V	 0.8014	 0.4560
W	 0.6851	 0.3740
X	 0.6945	 0.3800
Y	 0.6758	 0.3870
Z	 0.8123	 0.4610
a	 0.8957	 0.5260
b	 0.8093	 0.4820
c	 0.7776	 0.4460
d	 0.8735	 0.5080
e	 0.3277	 0.2480



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Chain	Atom inclusion	Q-score
f	 0.0895	 0.0800
g	 0.5353	 0.3700
h	 0.4822	 0.2610
i	 0.2136	 0.1550
j	 0.0386	 0.0820
k	 0.8276	 0.4800
l	 0.4555	 0.2900
m	 0.4329	 0.2260
n	 0.8196	 0.4630
o	 0.4029	 0.1770
p	 0.4306	 0.2430
q	 0.3828	 0.1720
r	 0.8208	 0.4630
s	 0.4436	 0.2070
t	 0.5712	 0.3280
u	 0.8698	 0.5000
v	 0.3863	 0.1660
w	 0.7536	 0.4290
x	 0.8430	 0.4850
y	 0.4615	 0.2300
z	 0.7816	 0.4430