



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:01 AM UTC

PDB ID : 6RXU / pdb_00006rxu
EMDB ID : EMD-10052
Title : Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from *Chaetomium thermophilum*, state B1
Authors : Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on : 2019-06-10
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 ⓘ symbol.

The types of validation reports are described at

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

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

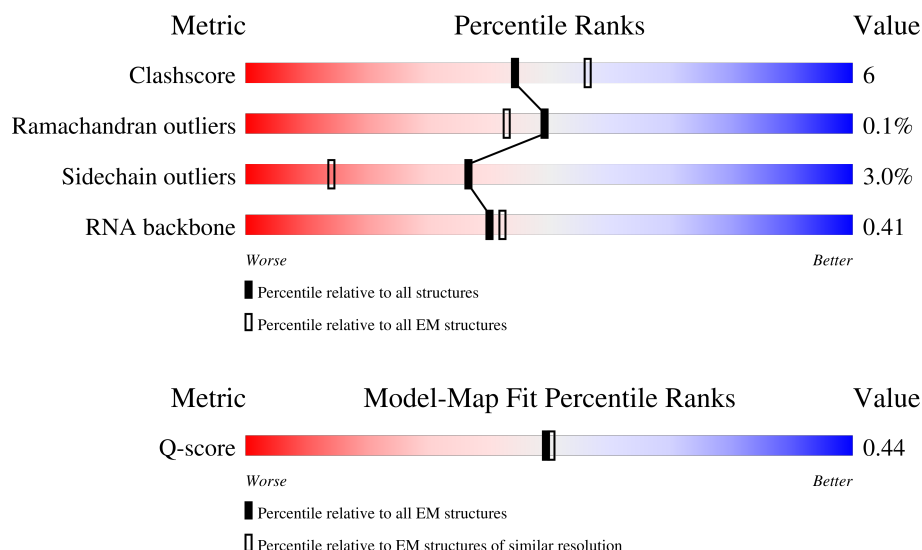
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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.



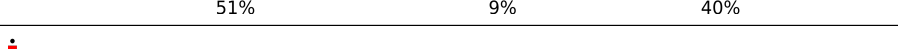
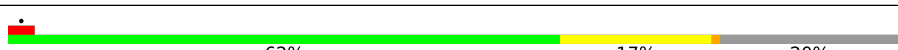
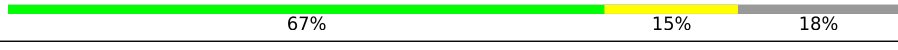
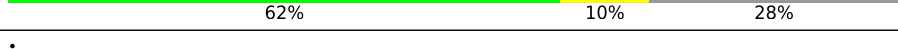
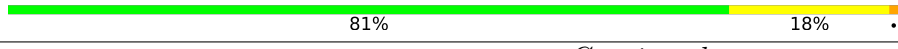
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	UA	904	
2	UB	907	
3	UC	648	

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Mol	Chain	Length	Quality of chain
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	938	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	
26	CK	297	

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Mol	Chain	Length	Quality of chain
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cb	264	
36	Cc	212	
37	Cd	239	
38	Ce	203	
39	Cf	202	
40	Cg	190	
41	Ch	151	
42	Ci	150	
43	Cj	143	
44	Ck	161	
45	Cm	130	
46	Cn	145	
47	Co	136	
48	Cp	68	
49	CU	311	

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Mol	Chain	Length	Quality of chain
50	C1	2352	
51	C2	230	
52	CW	668	
53	UT	2612	
54	UH	930	
55	UE	410	
55	UI	410	
56	US	549	
57	Cl	156	
58	CX	480	
59	CY	381	
60	CZ	609	
61	UP	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
63	GTP	CI	1201	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 211834 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
1	UA	839	Total	C	N	O	S	0	0
			6366	4101	1136	1105	24		

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	512	Total	C	N	O	S	0	0
			4079	2576	781	711	11		

- Molecule 3 is a protein called Utp3.

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

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	772	Total	C	N	O	S	0	0
			6071	3851	1093	1103	24		

- Molecule 5 is a protein called Utp6.

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

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	479	Total	C	N	O	S	0	0
			3717	2369	700	636	12		

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	1090	Total	C	N	O	S	0	0
			8416	5408	1452	1525	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1687	1062	351	269	5		

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	729	Total	C	N	O	S	0	0
			5643	3590	995	1045	13		

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	177	Total	C	N	O	S	0	0
			1401	892	263	239	7		

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	504	Total	C	N	O	S	0	0
			3819	2422	699	684	14		

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6008	3831	1037	1119	21		

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	S	0	0
			3491	2209	656	616	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	902	Total	C	N	O	S	0	0
			6734	4336	1236	1136	26		

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S	0	0
			1470	932	282	246	10		

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S	0	0
			1819	1186	331	299	3		

- Molecule 18 is a protein called Nop1.

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

- Molecule 19 is a protein called Nop56.

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

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	420	Total	C	N	O	S	0	0
			3150	2023	560	557	10		

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	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	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total	C	N	O	S	0	0
			6486	4169	1213	1077	27		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	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	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CM	445	Total	C	N	O	S	0	0
			3501	2195	672	619	15		

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CN	226	Total	C	N	O	S	0	0
			1762	1119	306	327	10		
29	CO	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CP	233	Total	C	N	O	S	0	0
			1893	1209	340	335	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	175	Total	C	N	O	S	0	0
			1361	862	250	242	7		

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		
32	CS	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CT	131	Total	C	N	O	S	0	0
			1035	656	197	178	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total	C	N	O	S	0	0
			1821	1160	341	315	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cb	232	Total	C	N	O	S	0	0
			1851	1179	340	325	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cc	192	Total	C	N	O	S	0	0
			1464	926	278	253	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cd	226	Total	C	N	O	S	0	0
			1819	1138	363	313	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Cf	174	Total	C	N	O	S	0	0
			1398	872	283	242	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ch	66	Total	C	N	O		0	0
			546	355	101	90			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Cj	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	Ck	140	Total	C	N	O	S	0	0
			1163	750	224	184	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cm	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	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Co	92	Total	C	N	O	S	0	0
			741	474	139	126	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Cp	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	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1575	Total	C	N	O	P	0	0
			33604	14992	6023	11014	1575		

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	C2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CW	382	Total	C	N	O	S	0	0
			2924	1857	530	524	13		

- Molecule 53 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	UT	2033	Total	C	N	O	S	0	0
			16053	10338	2819	2828	68		

- Molecule 54 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	UH	359	Total	C	N	O	S	0	0
			2809	1773	496	527	13		

- Molecule 55 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UE	125	Total	C	N	O	S	0	0
			972	608	183	175	6		
55	UI	125	Total	C	N	O	S	0	0
			972	608	183	175	6		

- Molecule 56 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 57 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 58 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CY	123	Total	C	N	O	S	0	0
			979	592	195	189	3		

- Molecule 60 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CZ	44	Total	C	N	O	S	0	0
			376	235	76	64	1		

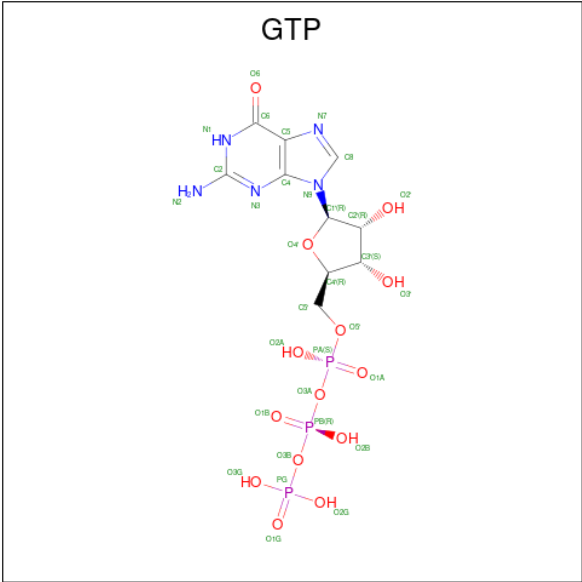
- Molecule 61 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UP	54	Total	C	N	O	0	0
			422	264	88	70		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	UX	1	Total	Zn	0
			1	1	

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
63	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

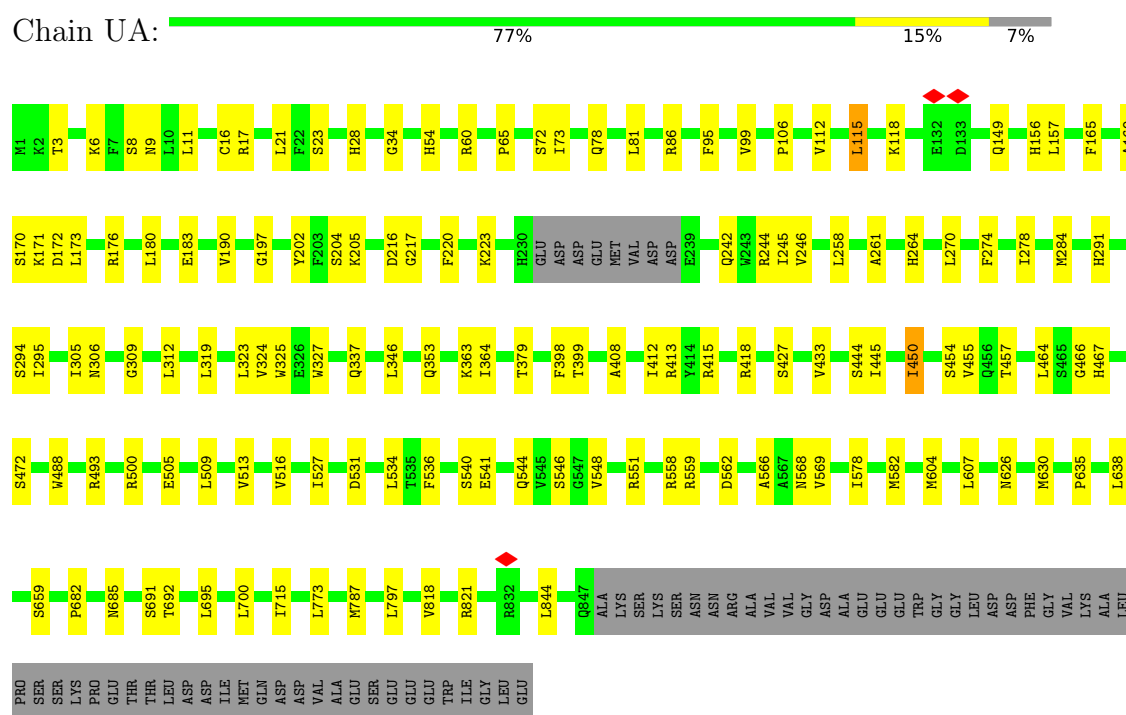
- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	CI	1	Total	Mg	0
			1	1	

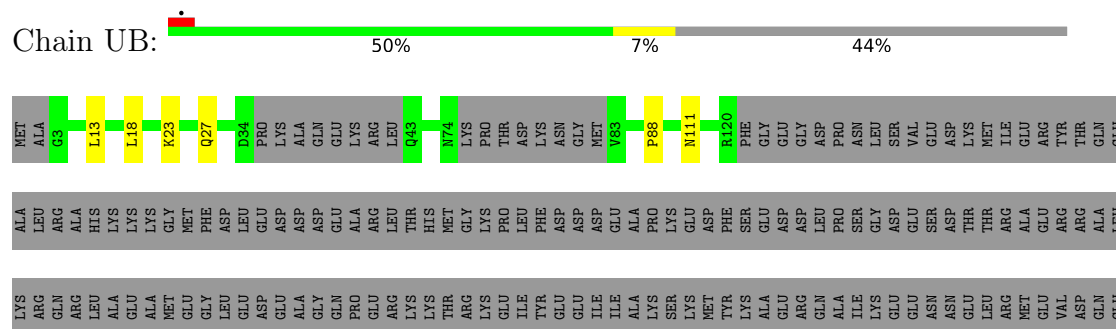
3 Residue-property plots

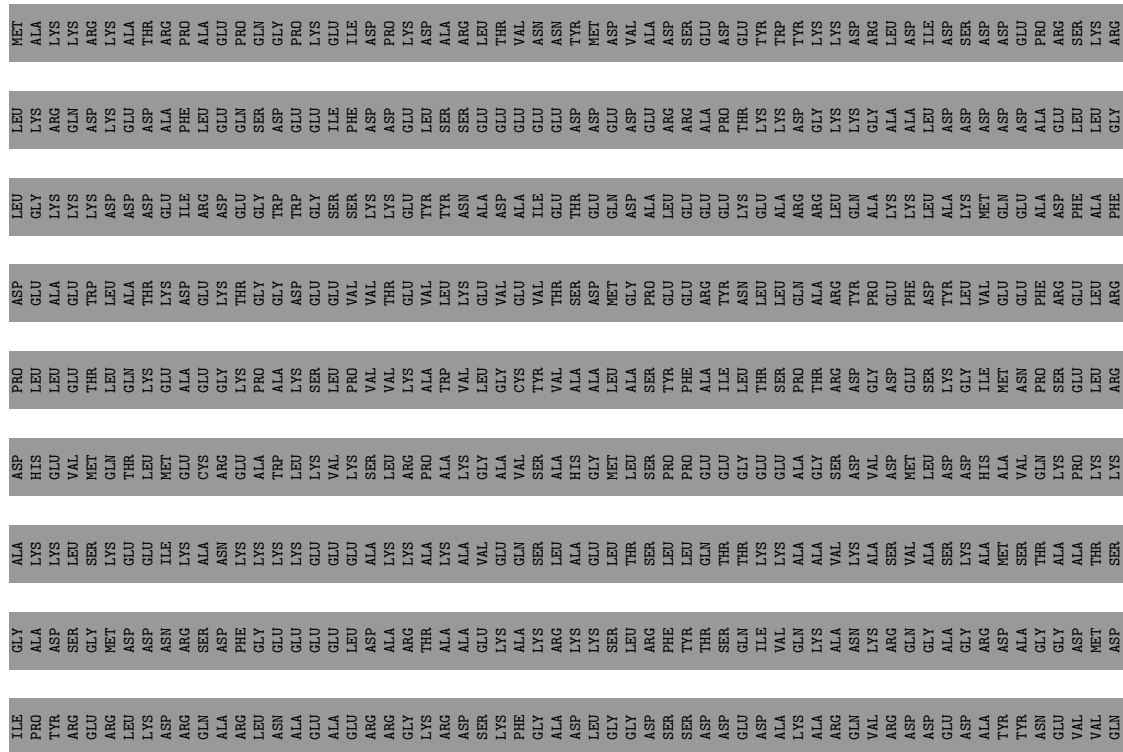
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Periodic tryptophan protein 2-like protein

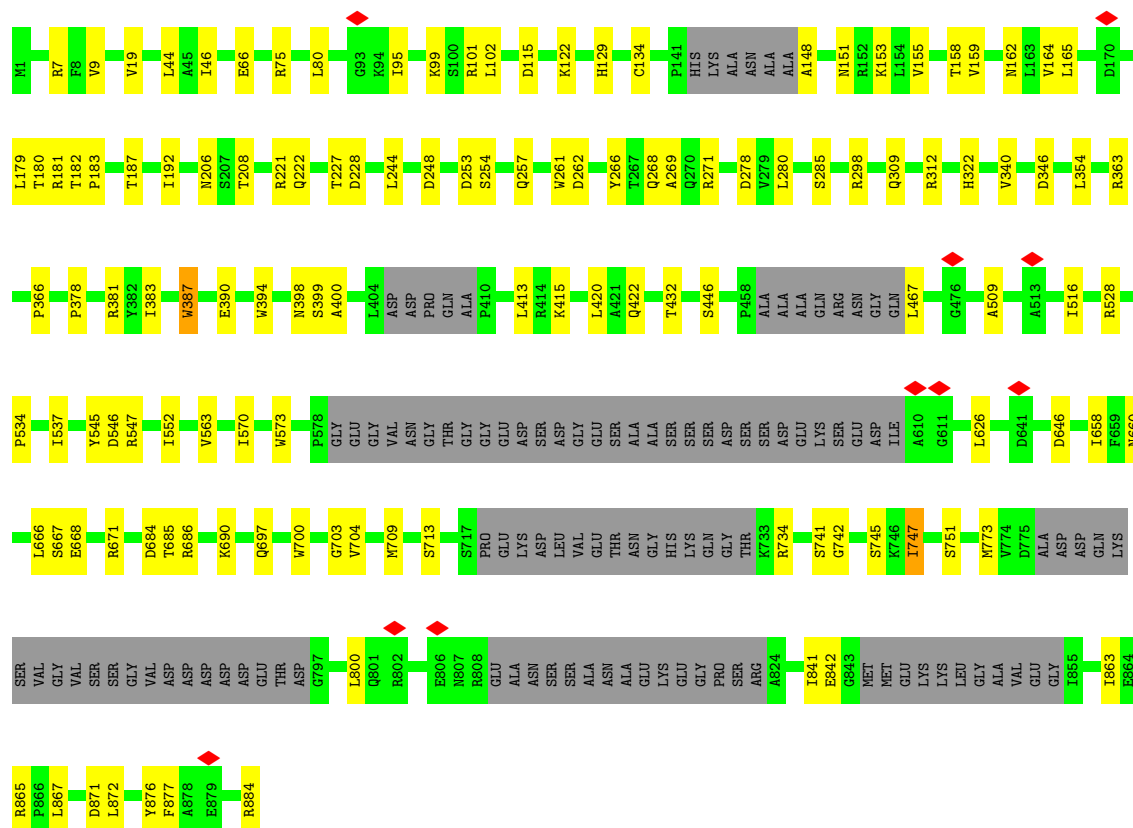
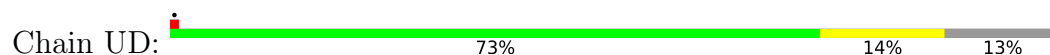


- Molecule 2: Utp2

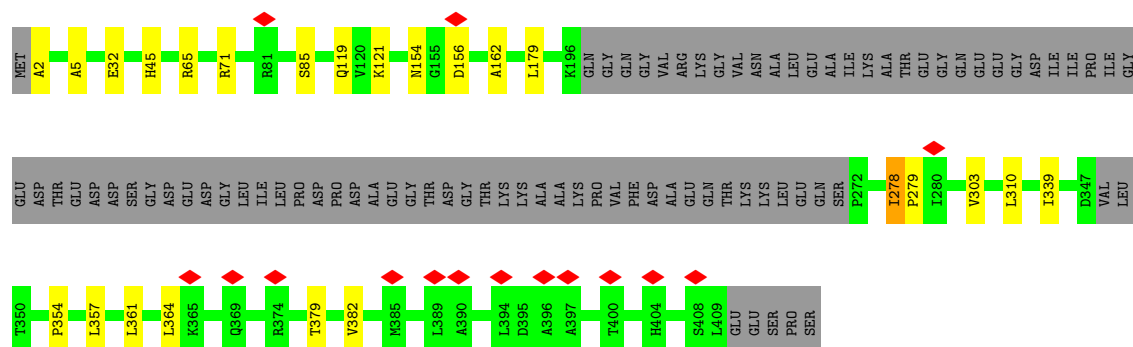
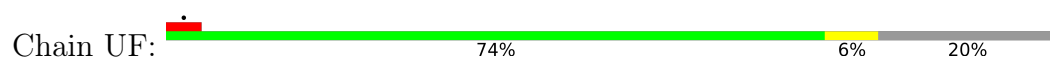




- Molecule 4: Utp4



- Molecule 5: Utp6



- Molecule 6: Utp7

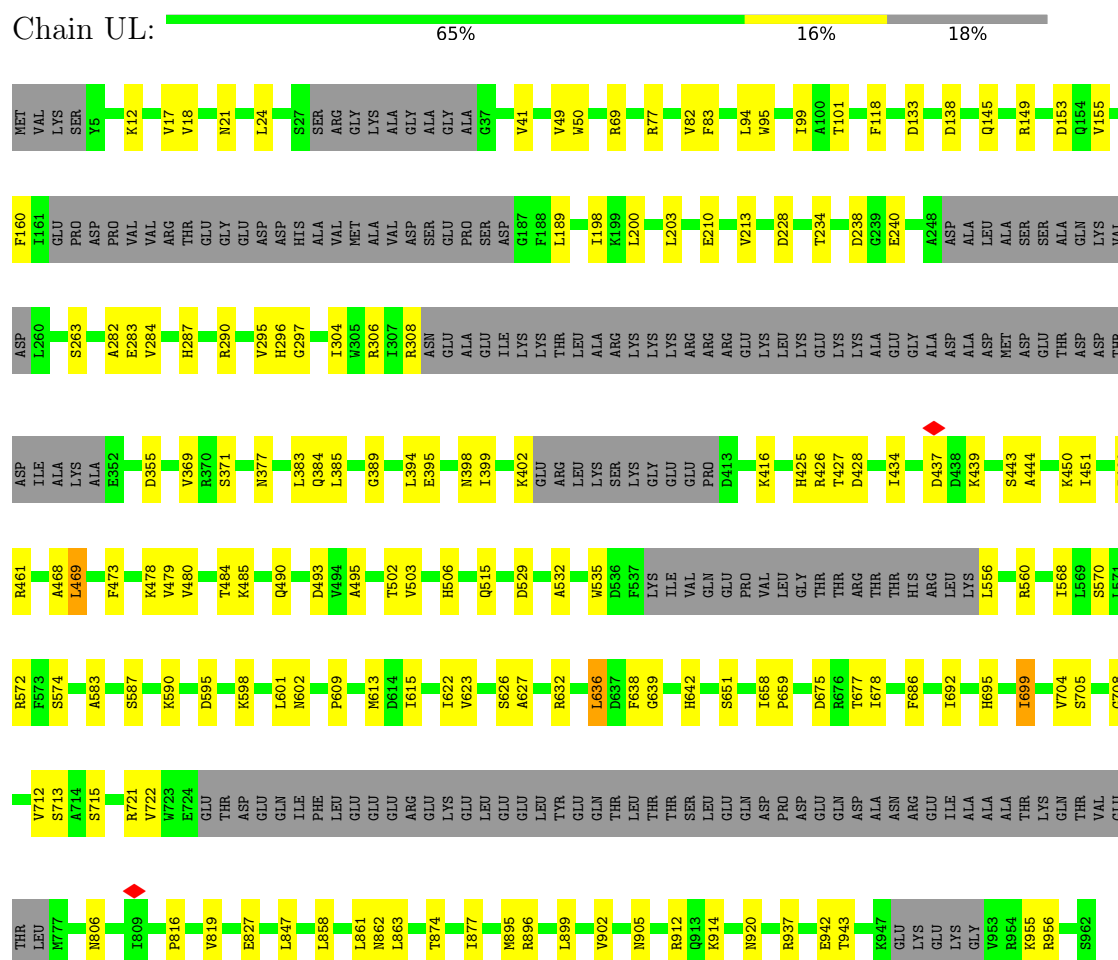
Response	Percentage
Yes, I have used a mobile app to book a flight	72%
No, I have not used a mobile app to book a flight	13%
I am unsure	14%



Response	Percentage
Good job	14%
Not a good job	51%
Don't know	9%
No answer	40%

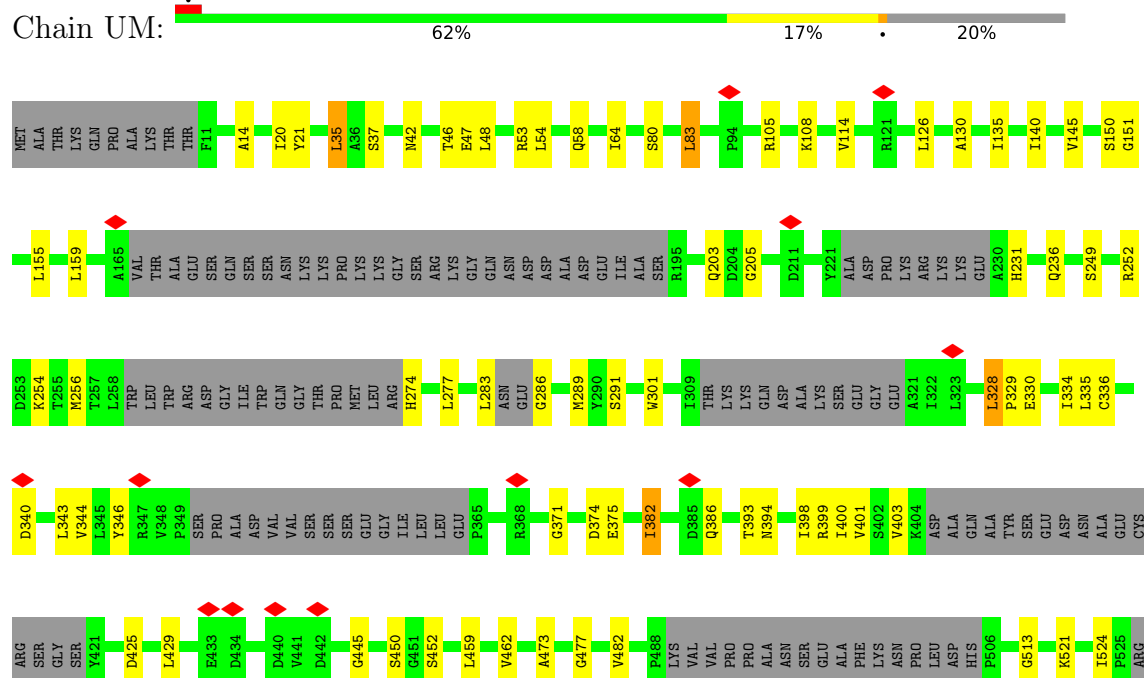


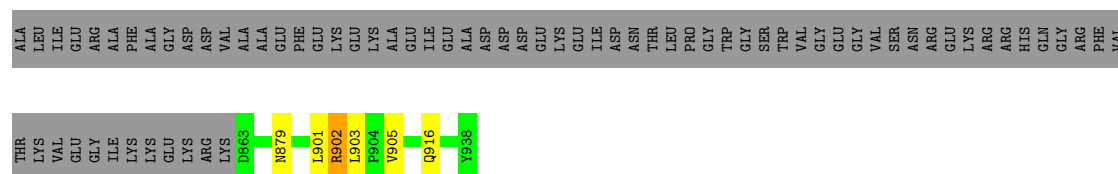
Chain UL:



• Molecule 10: Utp13

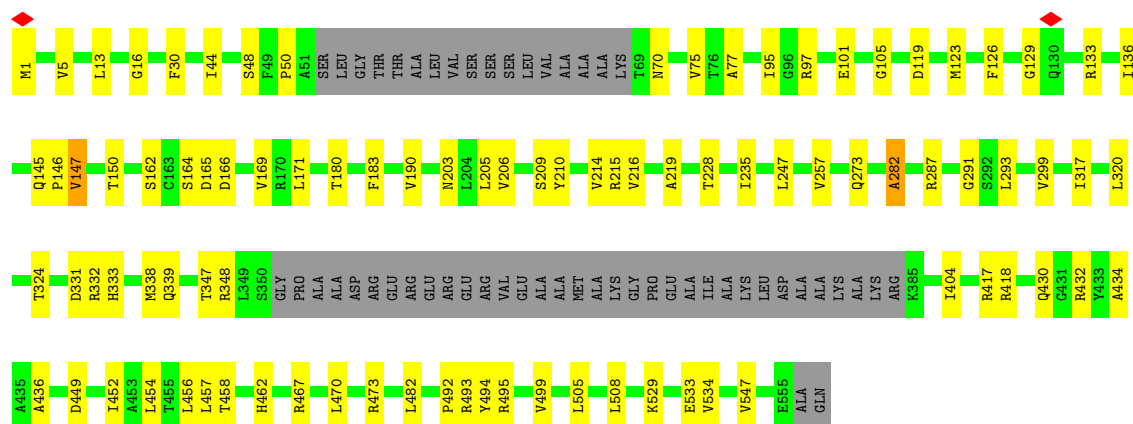
Chain UM:





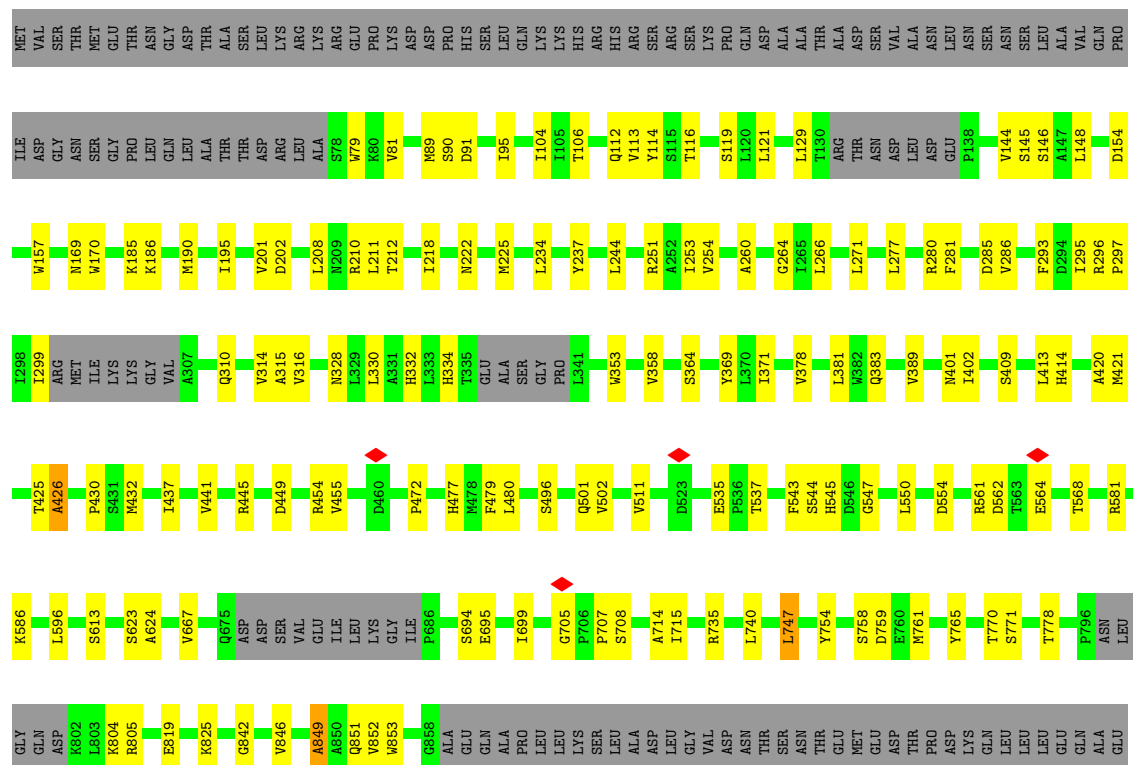
• Molecule 12: Utp15

Chain UO: 74% 16% 10%

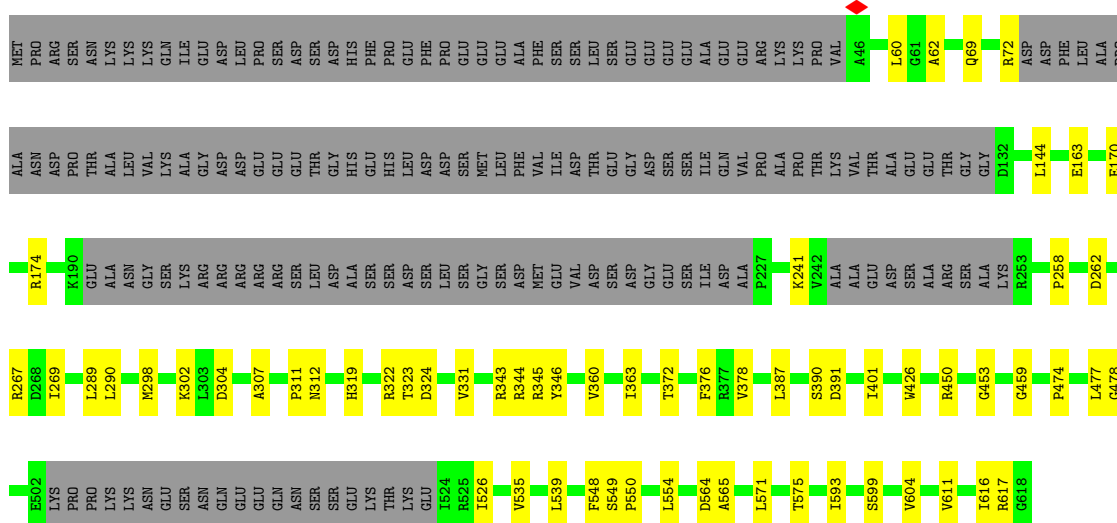


• Molecule 13: Utp17

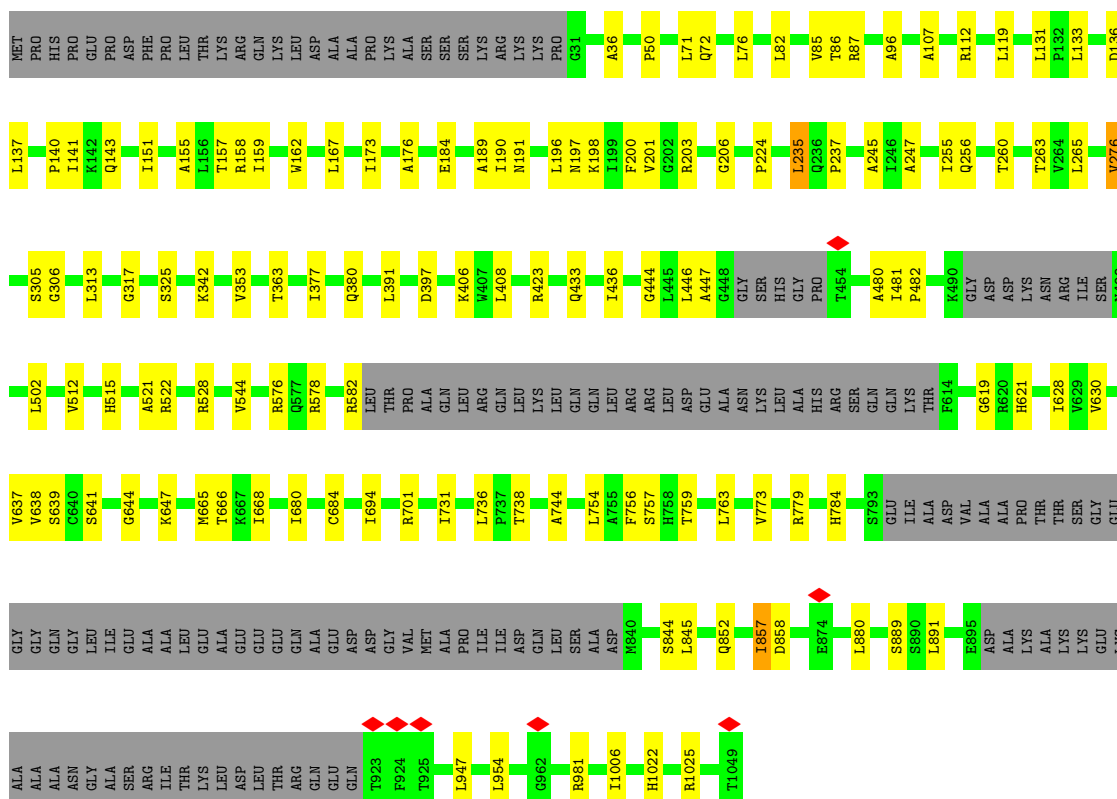
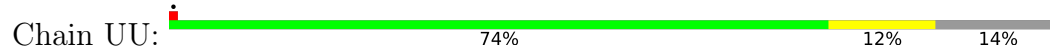
Chain UQ: 67% 15% 18%

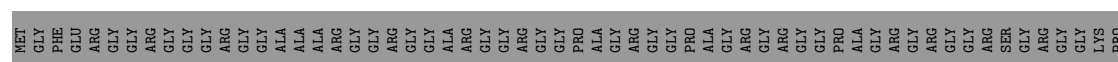


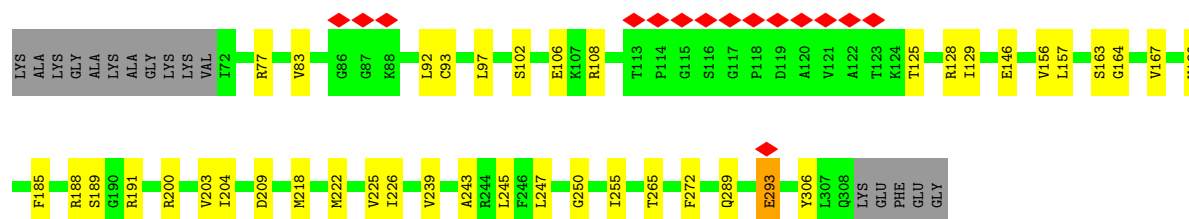
- Molecule 14: Utp18



- Molecule 15: Putative U3 snoRNP protein

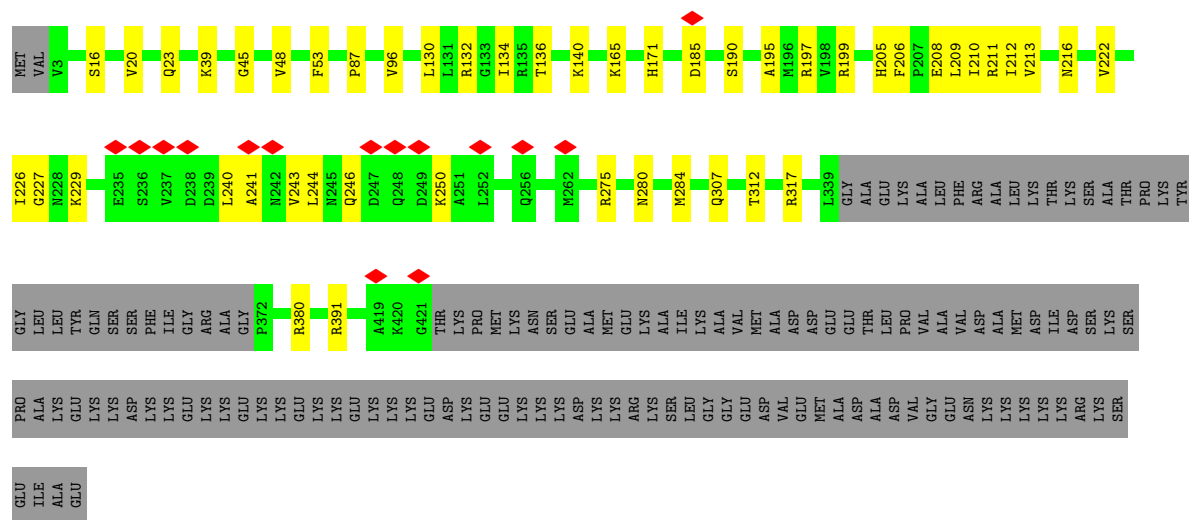






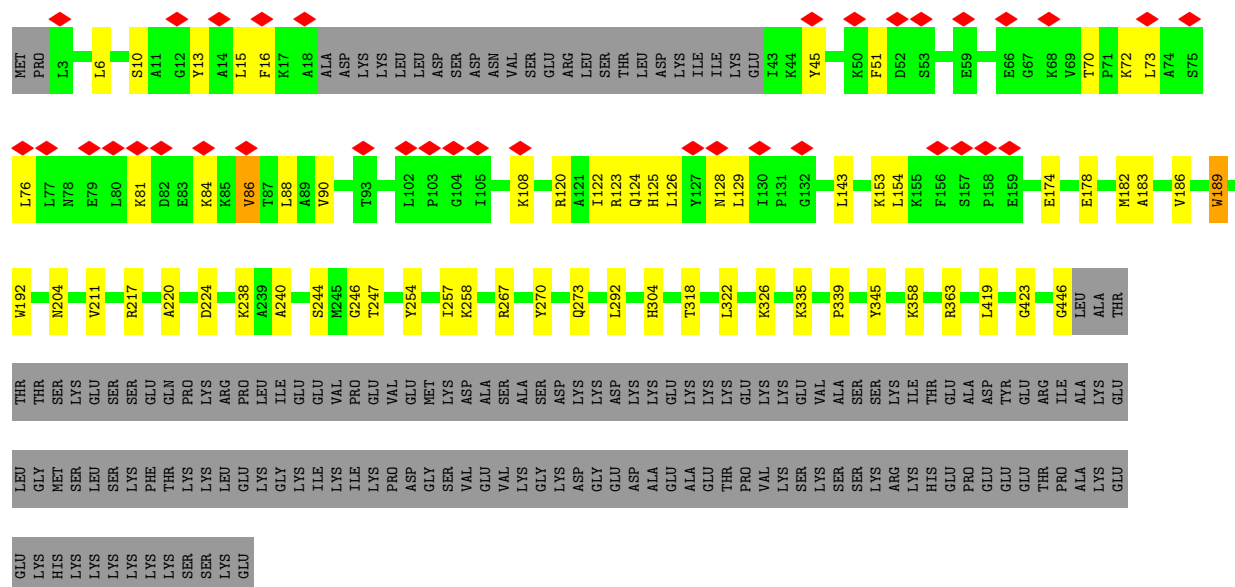
• Molecule 19: Nop56

Chain CC: 65% 9% 26%

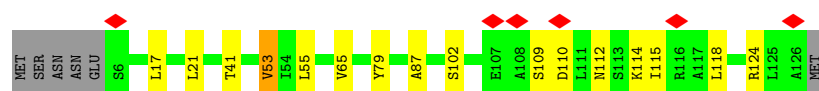
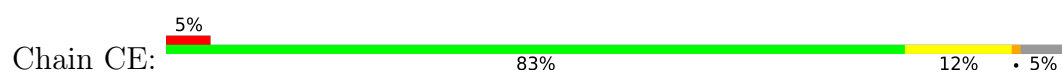


• Molecule 20: Nop58

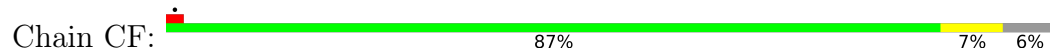
Chain CD: 6% 61% 11% 28%



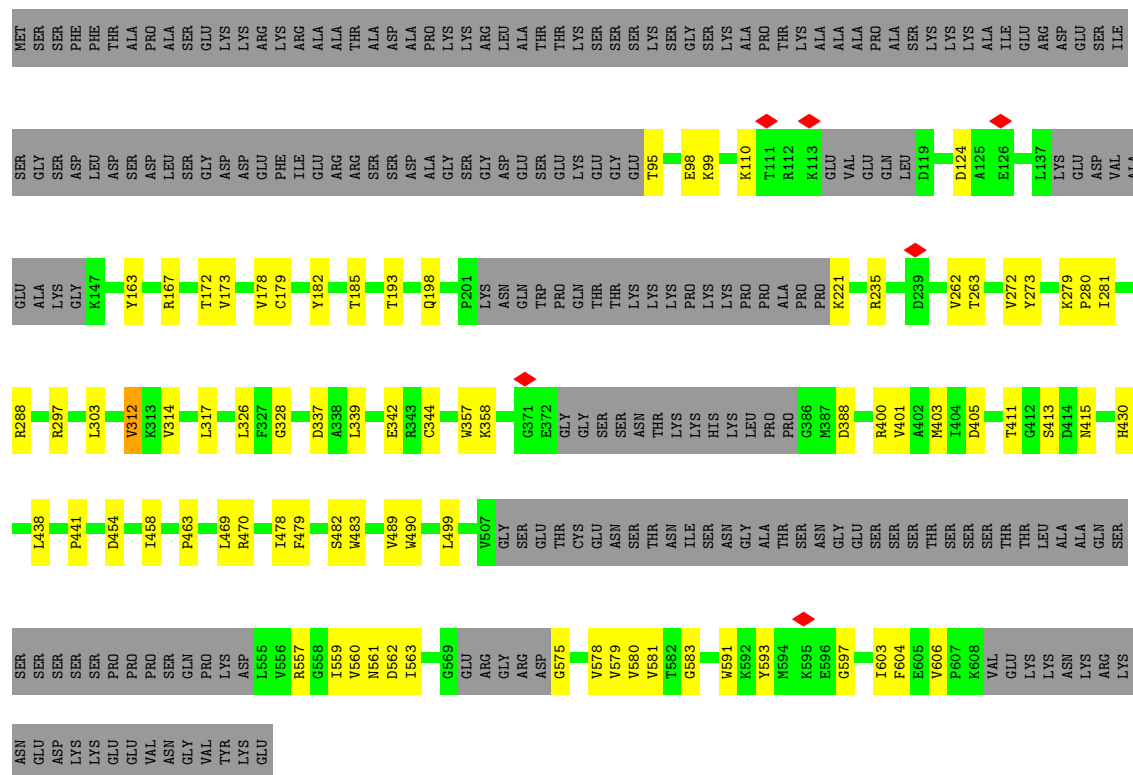
• Molecule 21: Snu13



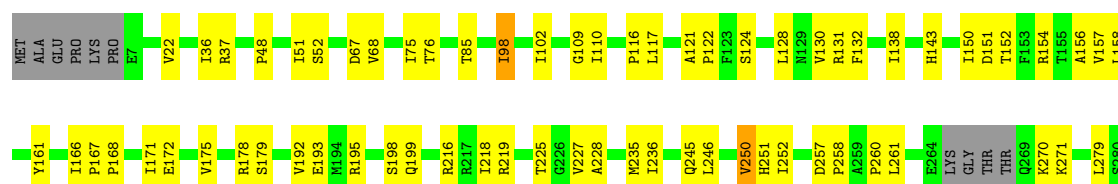
• Molecule 21: Snu13



• Molecule 22: Rrp9

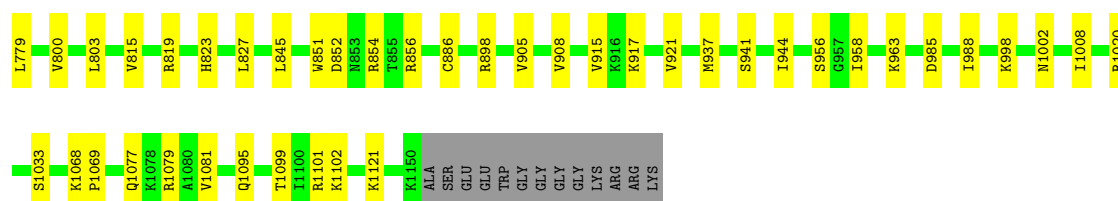
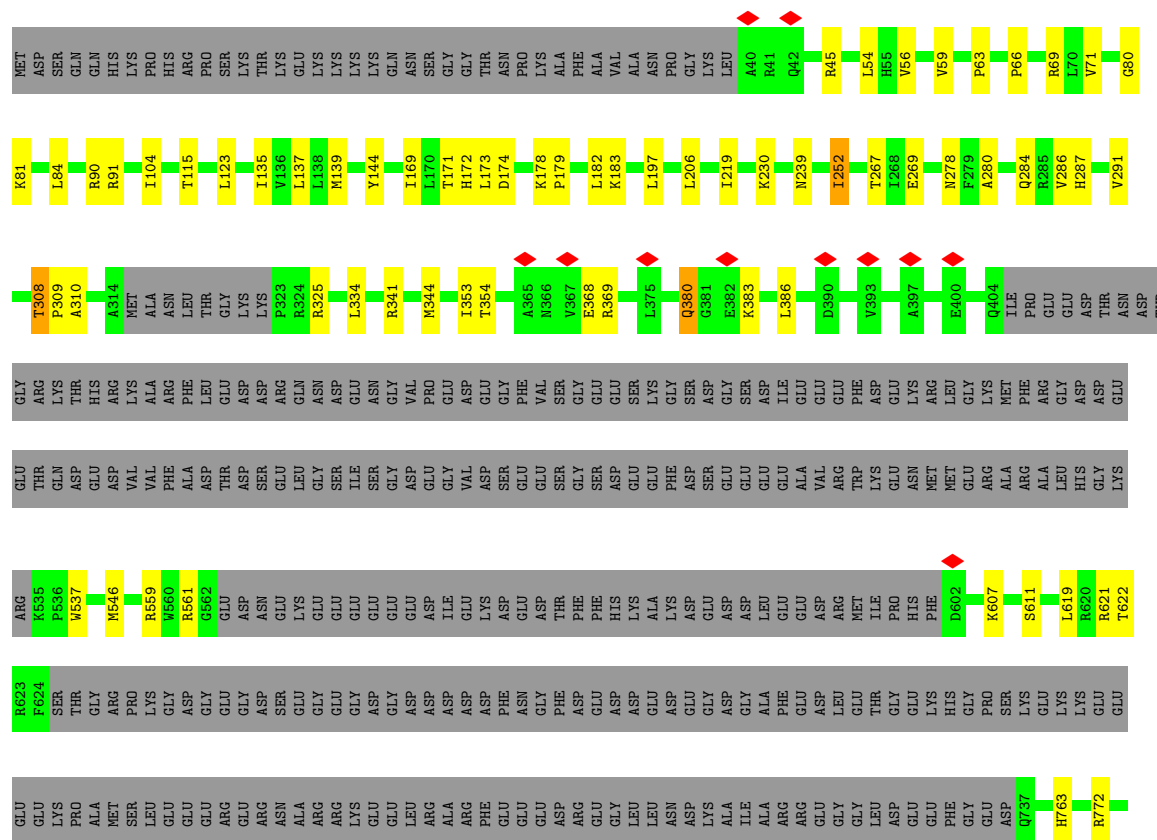


• Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

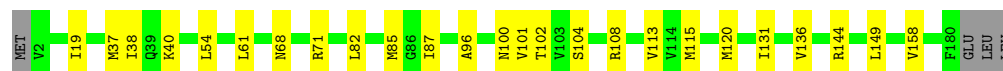
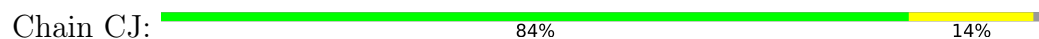




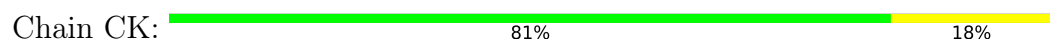
• Molecule 24: Bms1

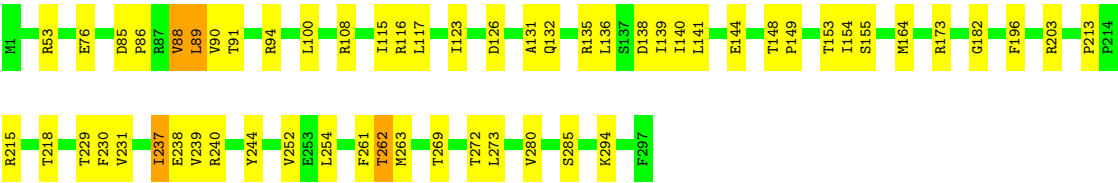


• Molecule 25: Imp3

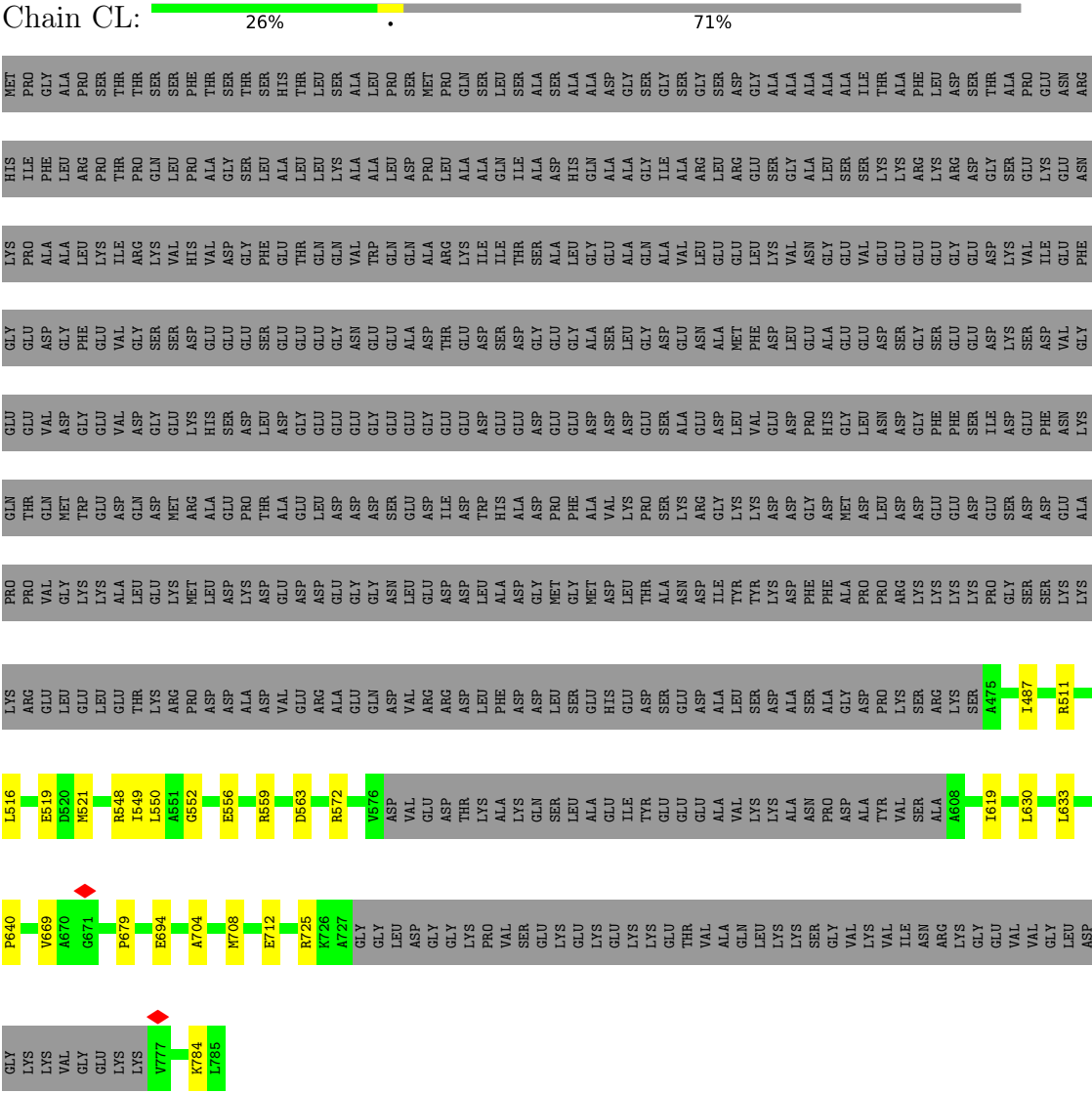


• Molecule 26: Putative U3 small nucleolar ribonucleoprotein

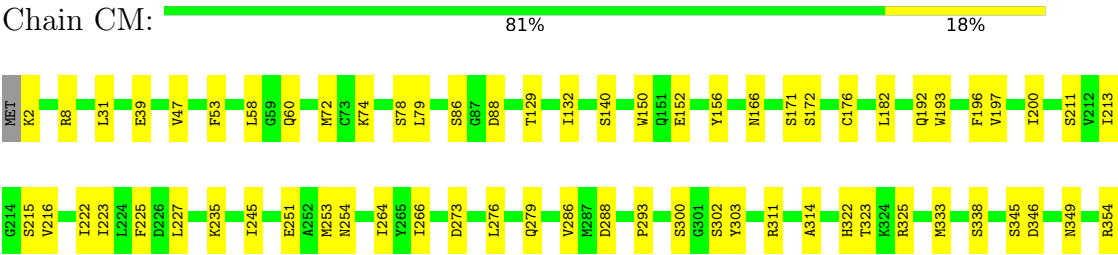




• Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein



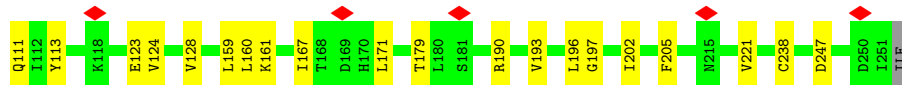
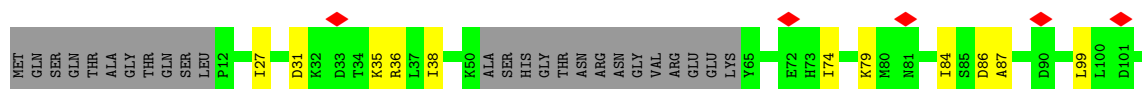
• Molecule 28: Sof1





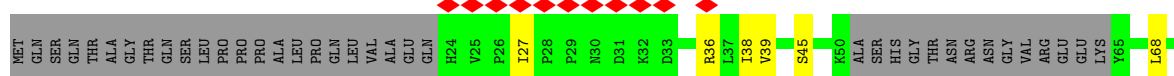
- Molecule 29: Emg1

Chain CN: 77% 12% 10%



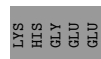
- Molecule 29: Emg1

Chain CO: 13% 75% 9% 15%



- Molecule 30: KRR1 small subunit processome component

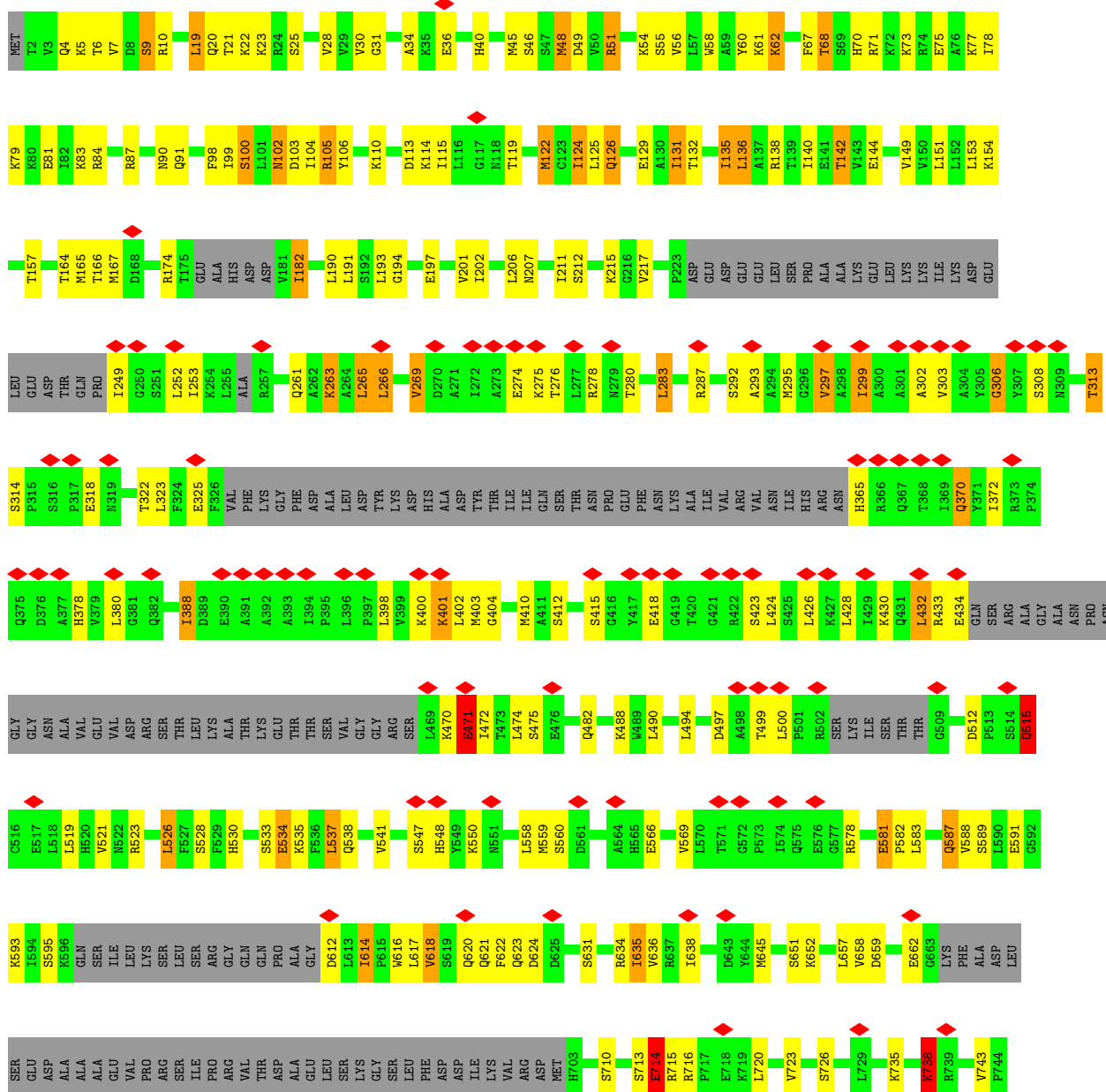
Chain CP: 58% 14% 28%

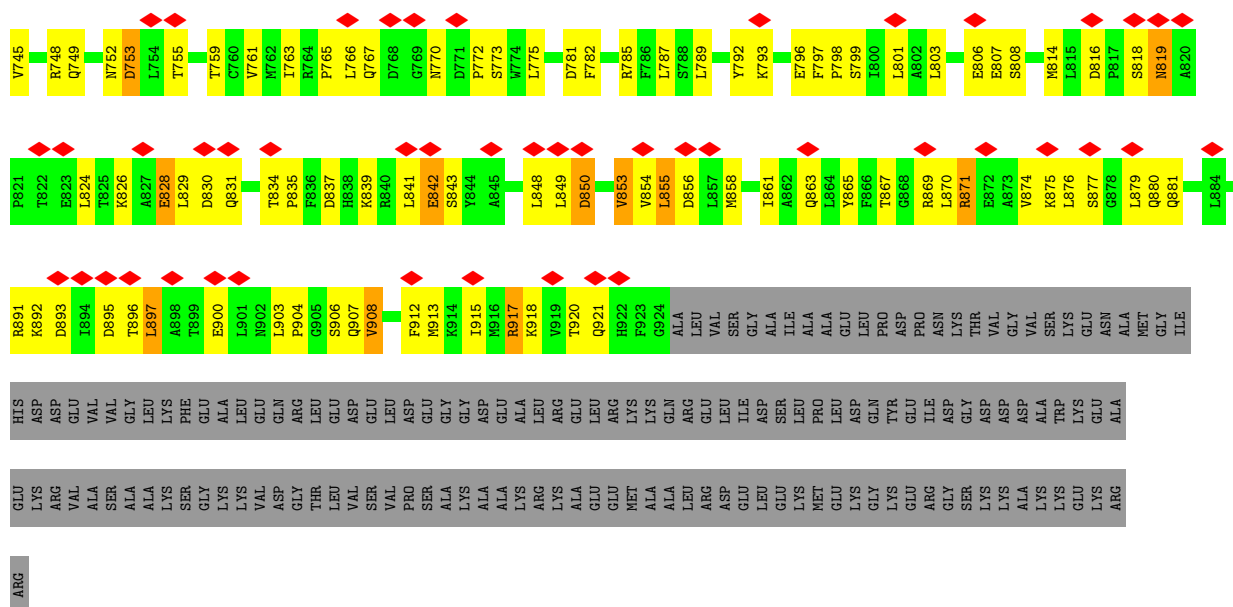


- Molecule 31: Pre-rRNA-processing protein PNO1

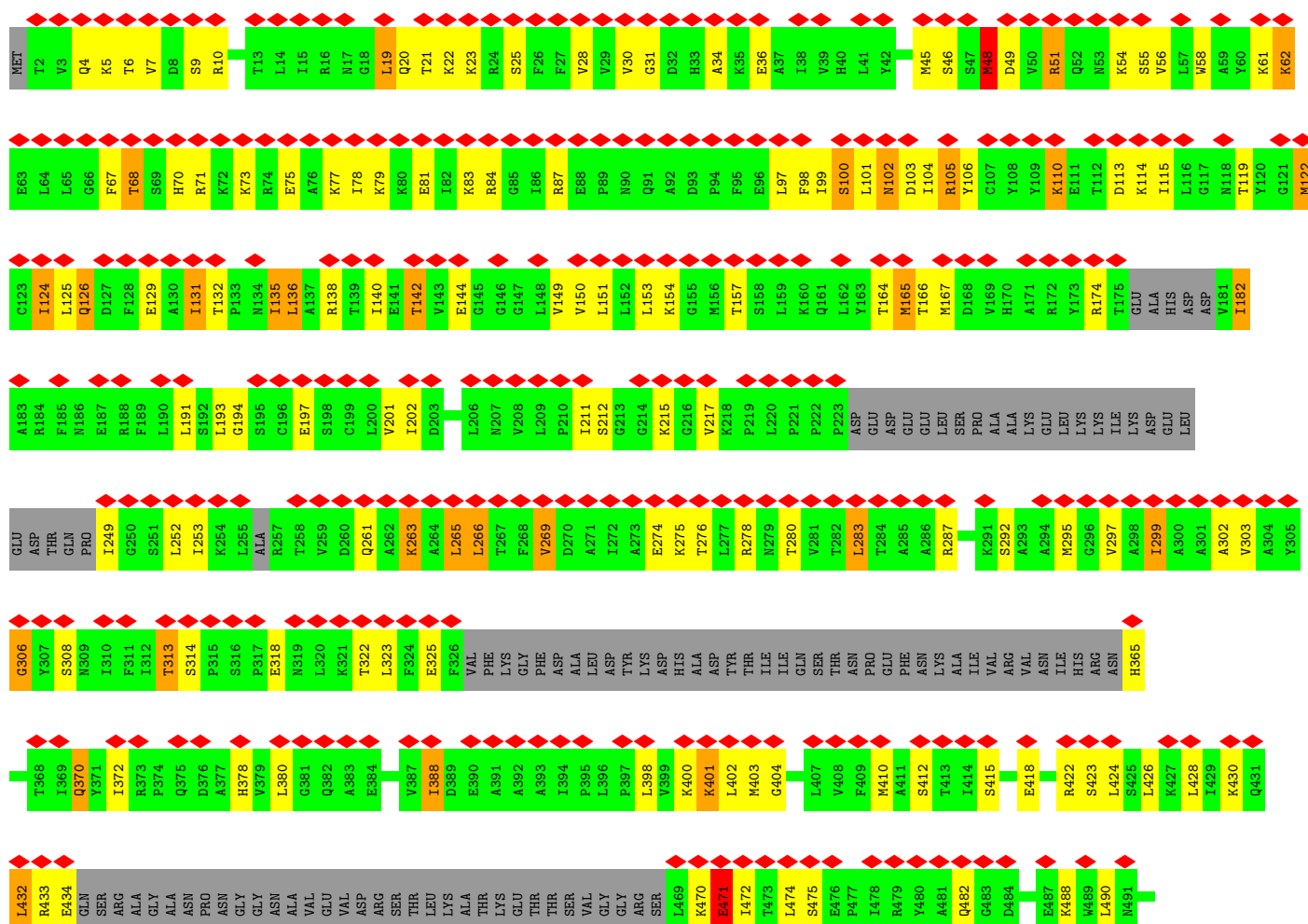
Chain CQ: 55% 13% 32%

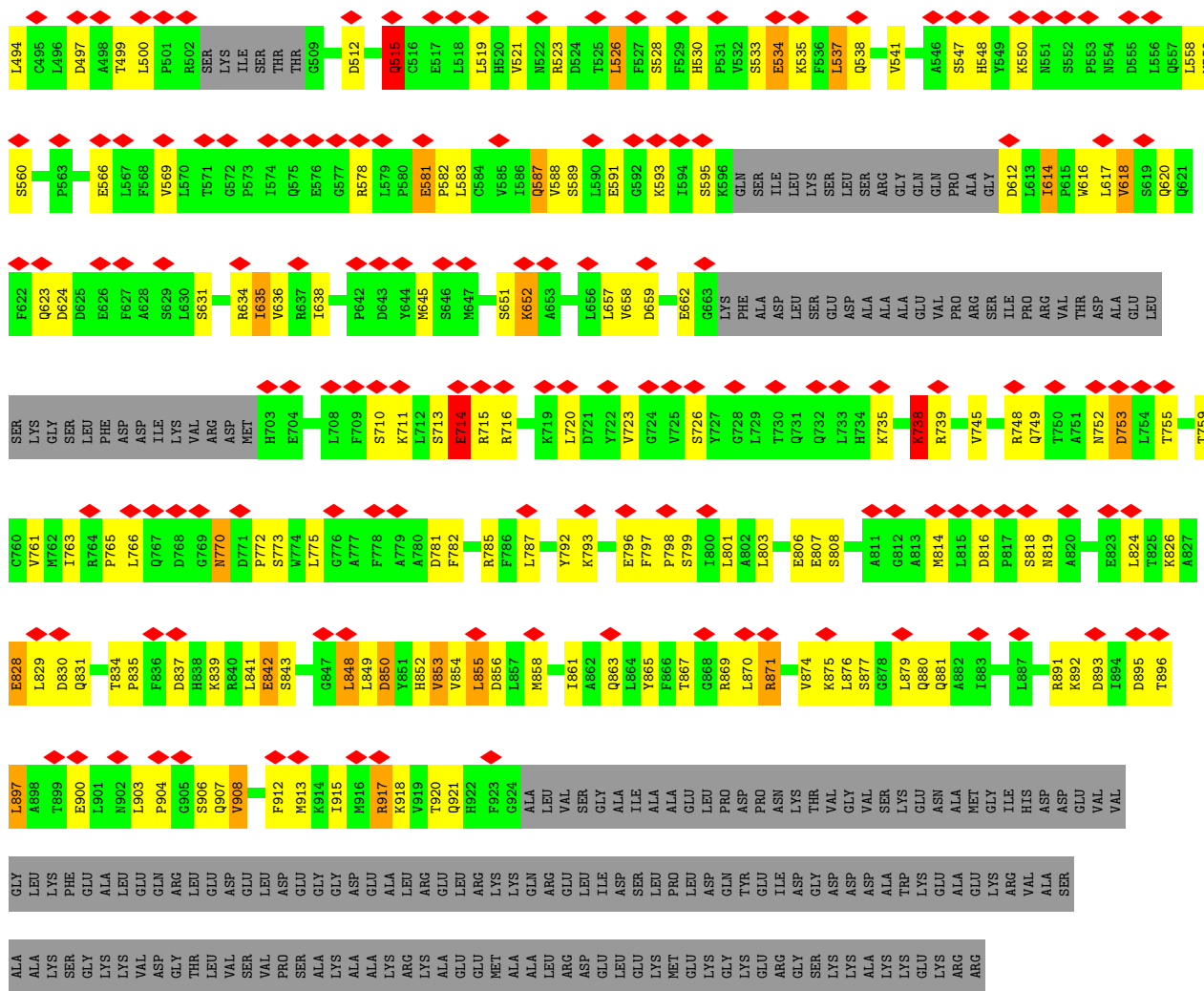
- Molecule 32: Kre33



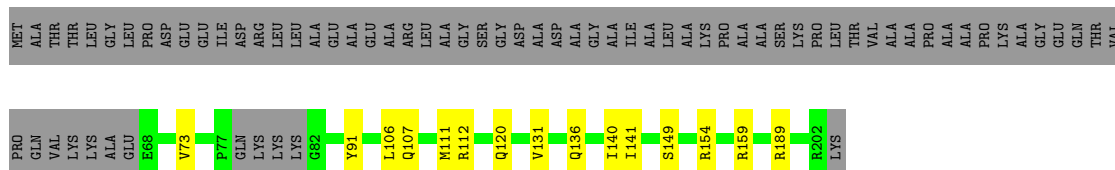


• Molecule 32: Kre33

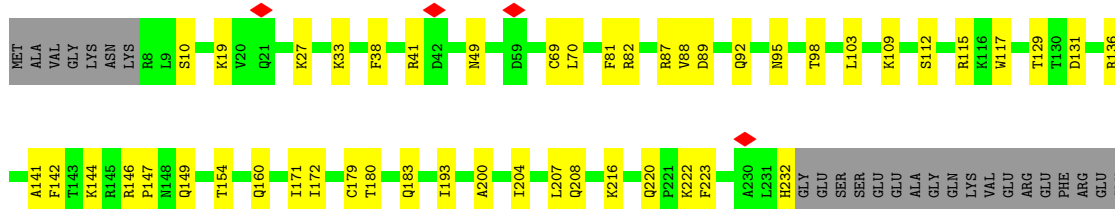


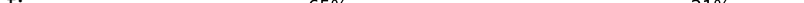


• Molecule 33: Fcf2

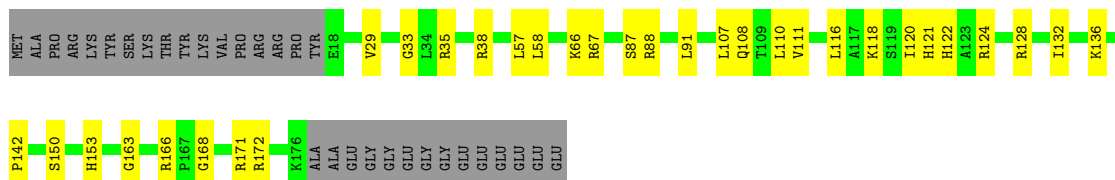


• Molecule 34: 40S ribosomal protein S1

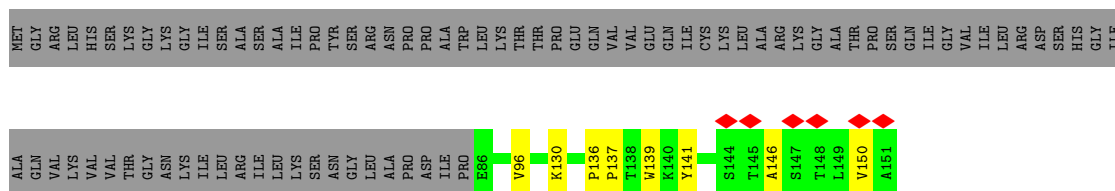
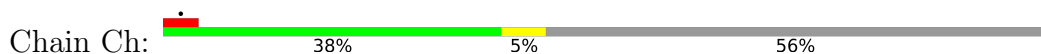


Chain Cf: 

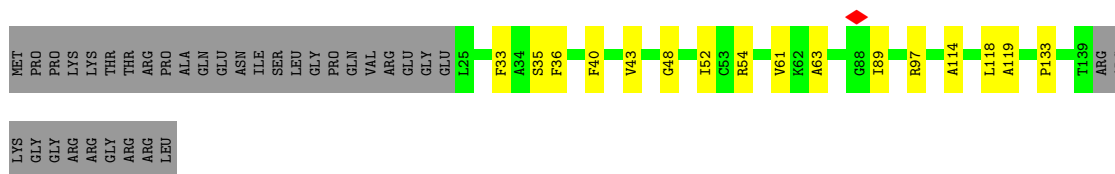
- Molecule 40: 40S ribosomal protein s9-like protein



- Molecule 41: 40S ribosomal protein S13-like protein



- Molecule 42: 40S ribosomal protein S14-like protein

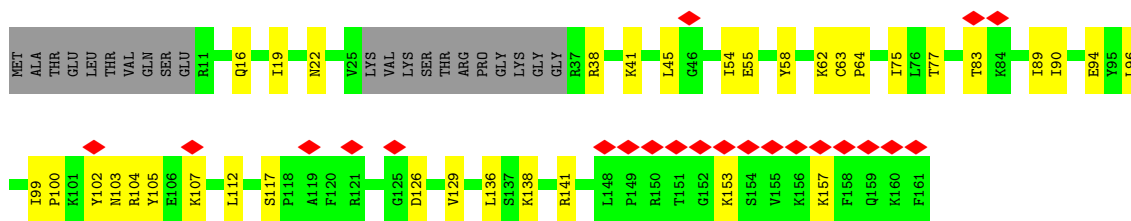


- Molecule 43: 40S ribosomal protein S16-like protein

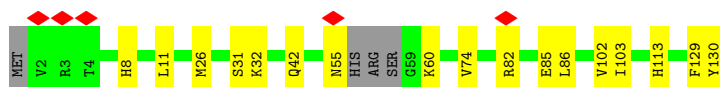
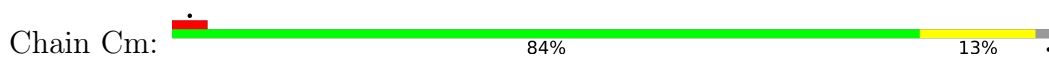


- Molecule 44: 40S ribosomal protein S11-like protein

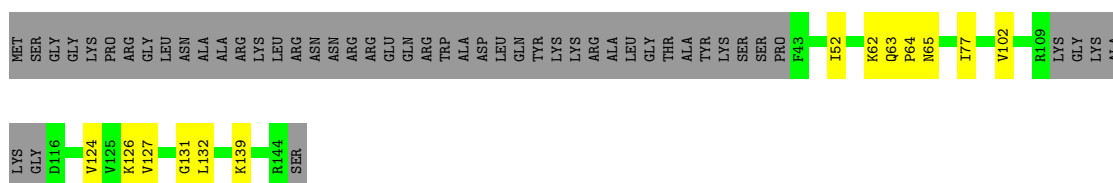




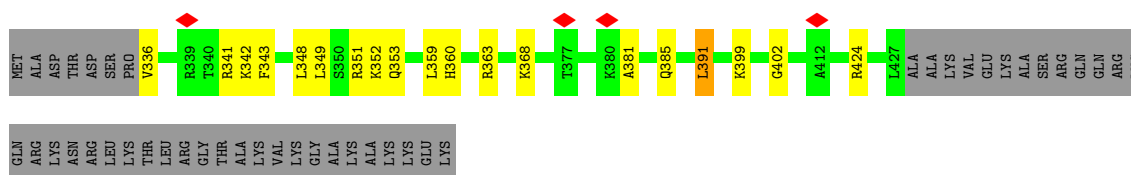
- Molecule 45: 40S ribosomal protein S22-like protein



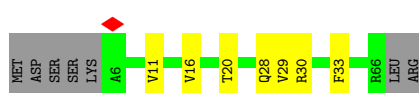
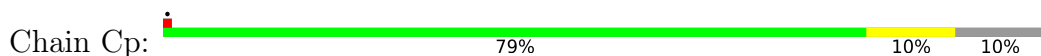
- Molecule 46: 40S ribosomal protein s23-like protein



- Molecule 47: 40S ribosomal protein S24

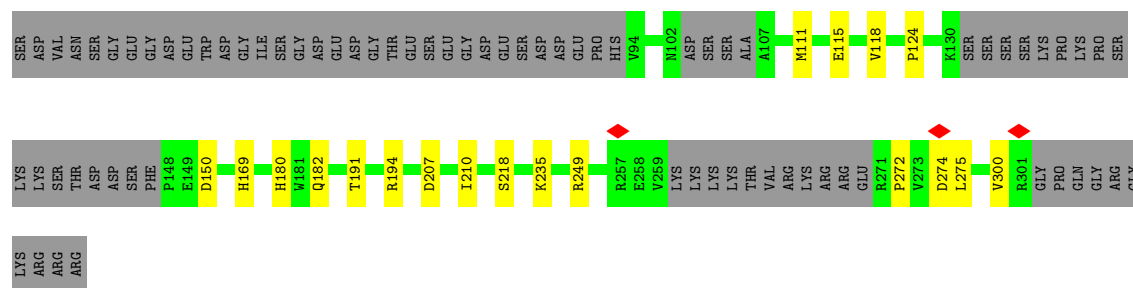


- Molecule 48: 40S ribosomal protein S28-like protein

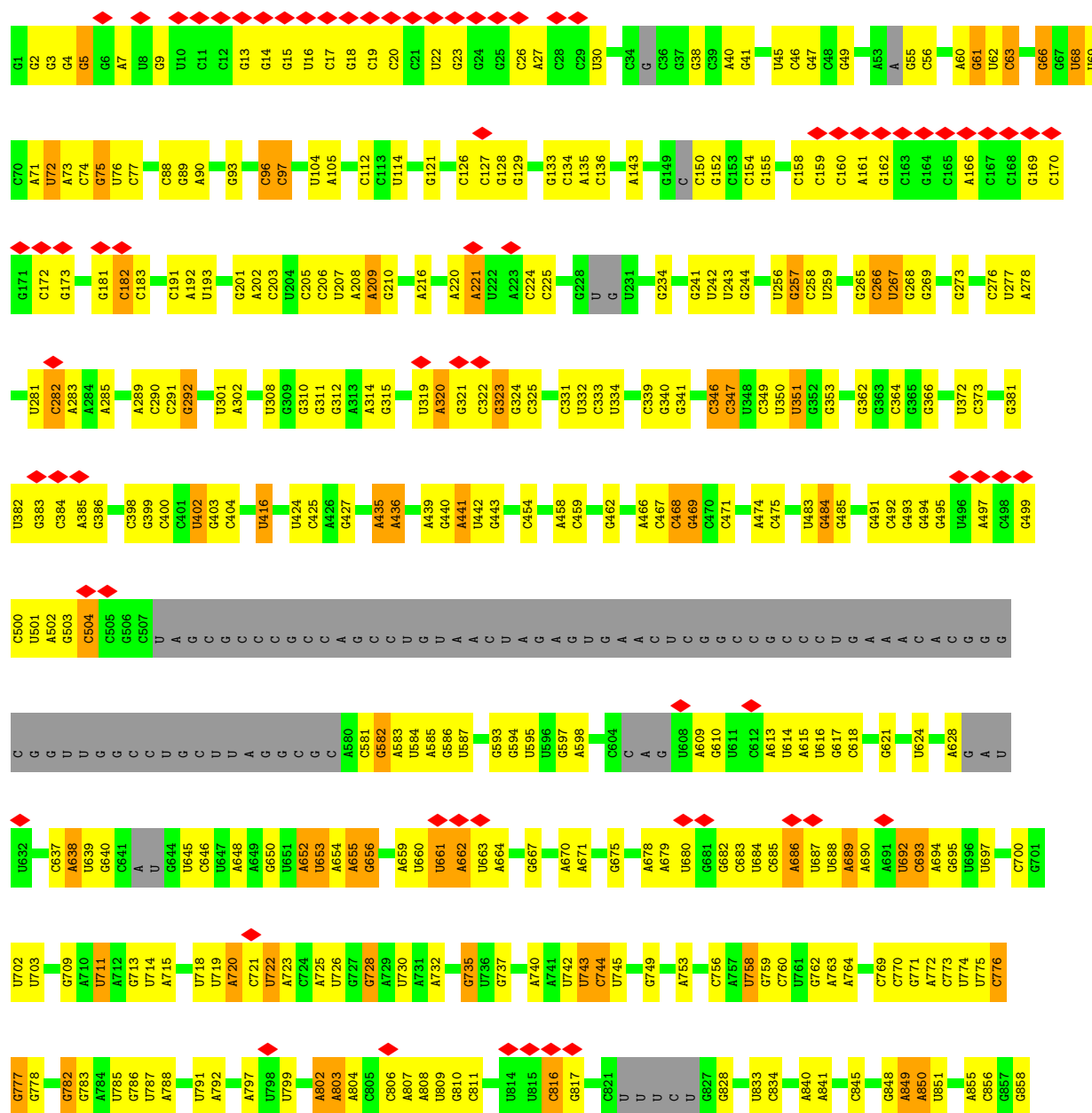


- Molecule 49: Faf1

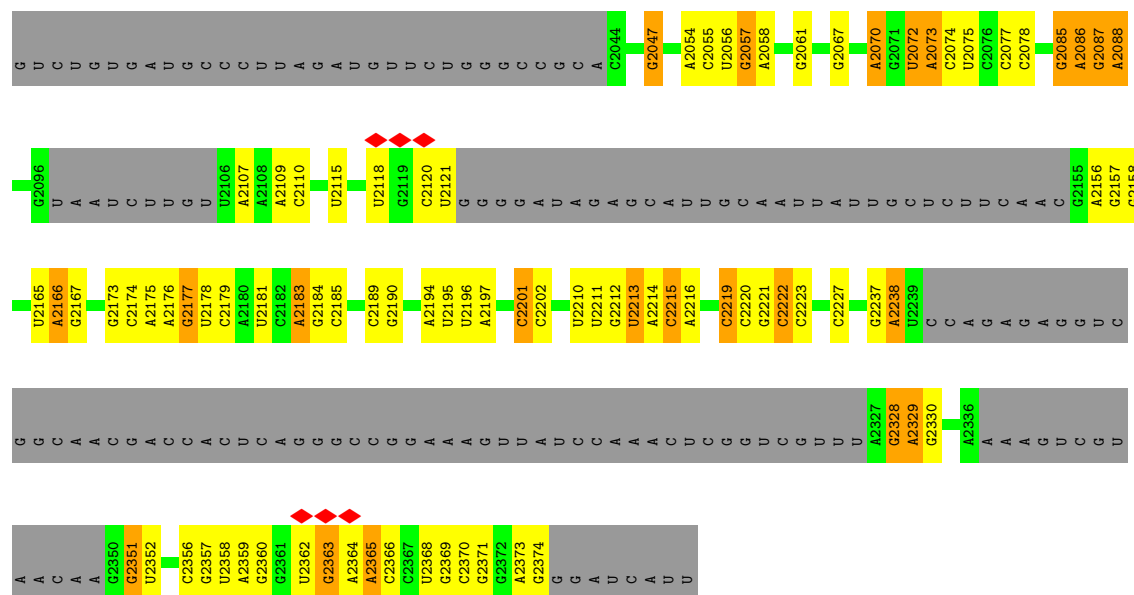




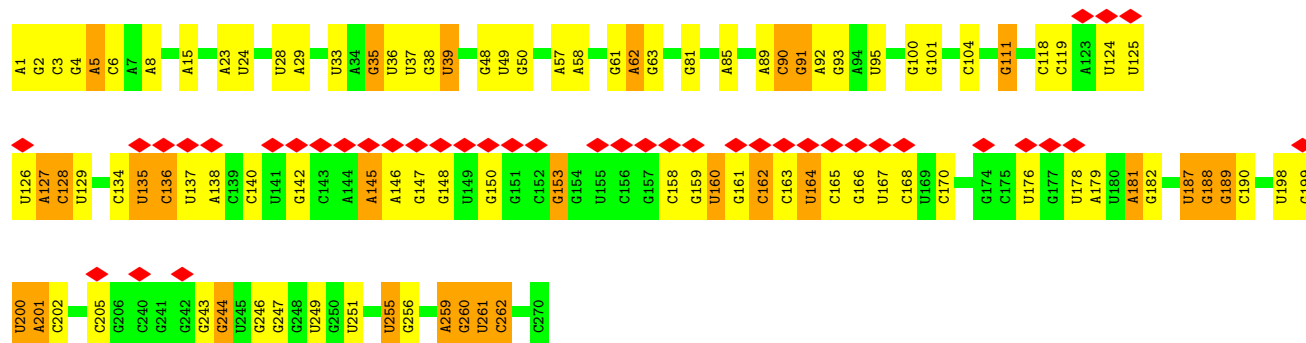
Molecule 50: 35S rRNA



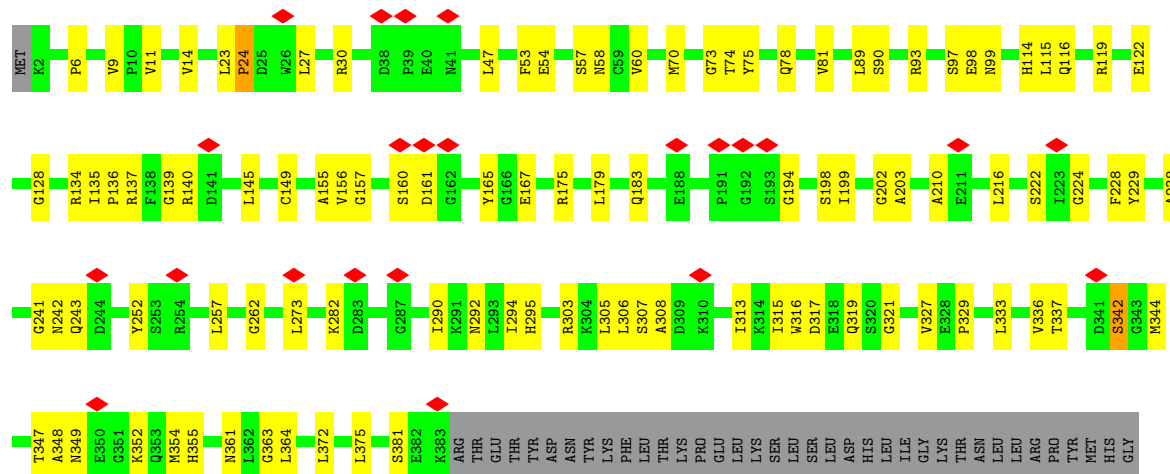




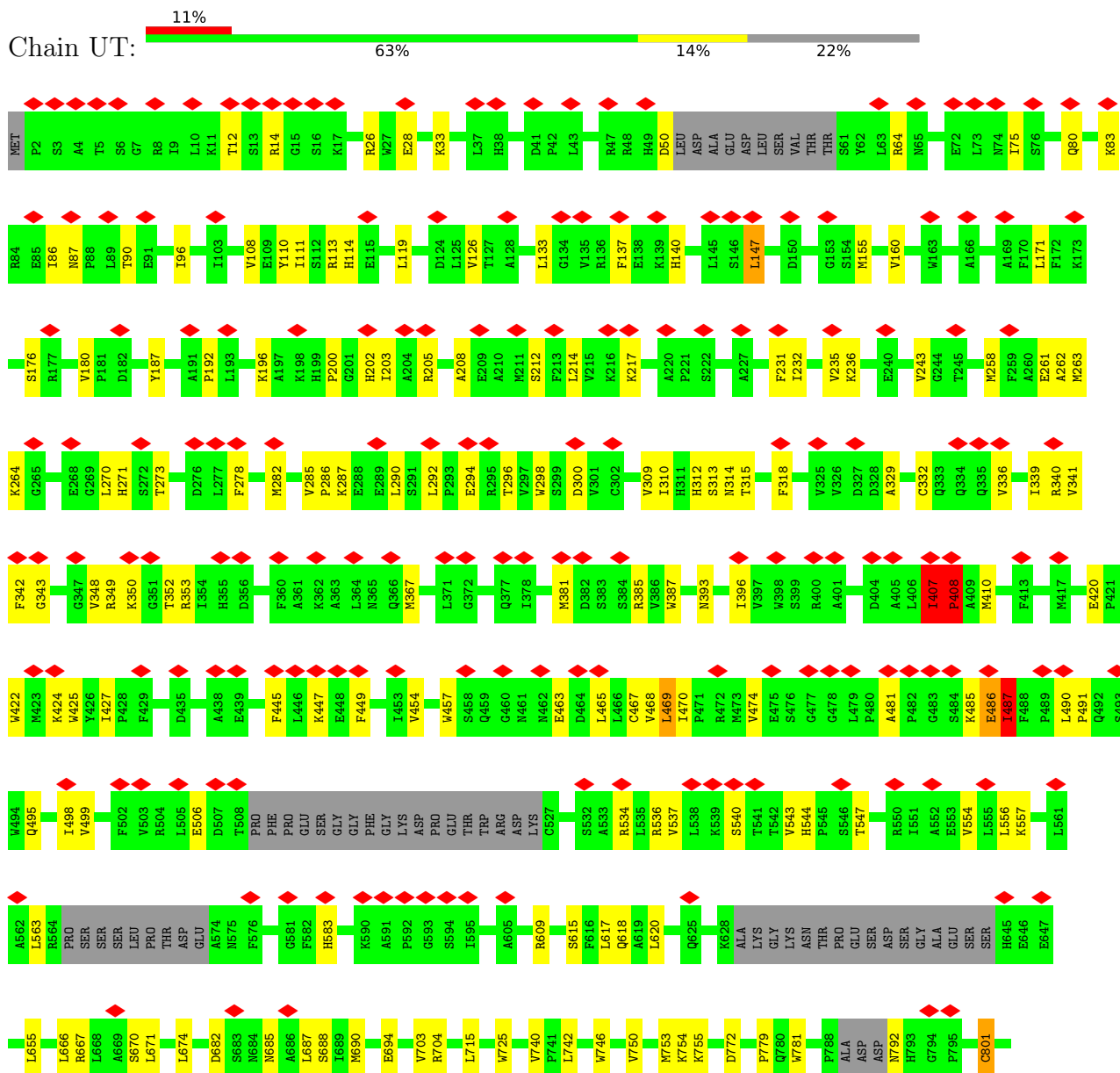
• Molecule 51: U3 snoRNA



• Molecule 52: Ribosome biogenesis protein ENP2



- Molecule 53: Utp20

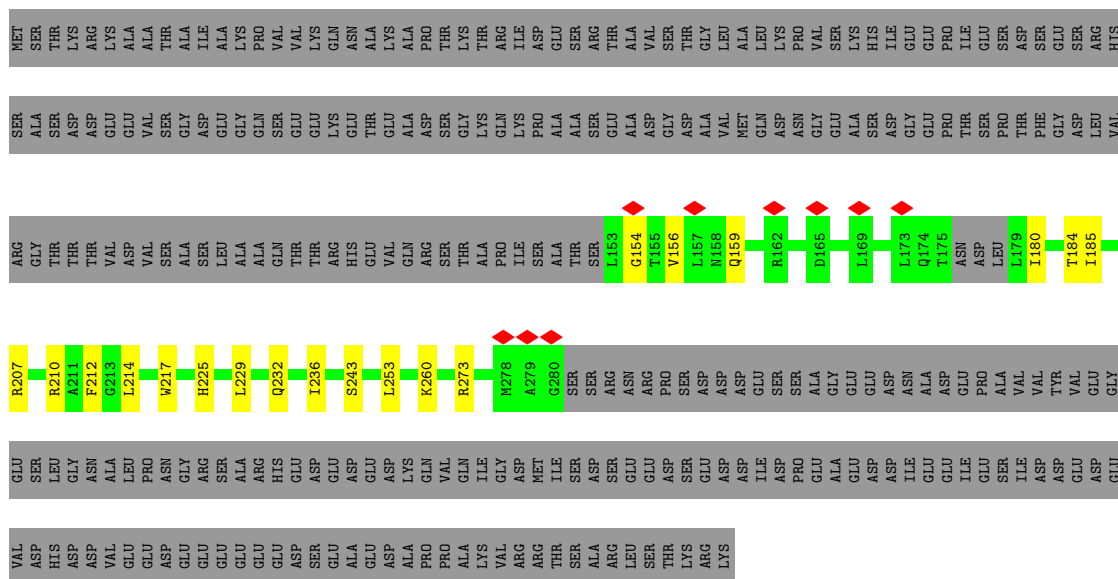




- Molecule 55: Utp5

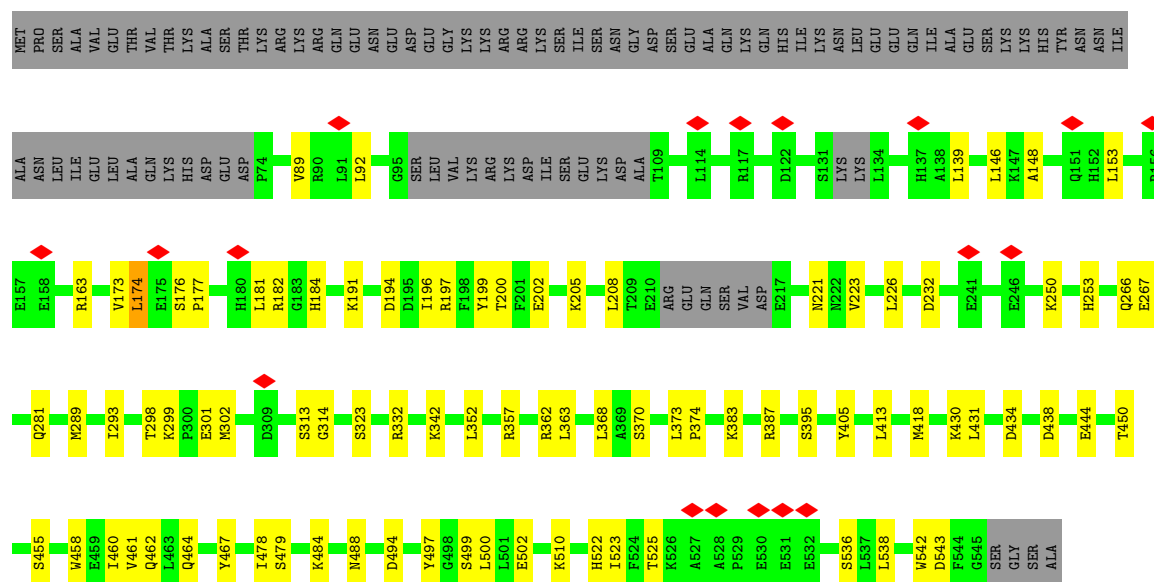


- Molecule 55: Utp5



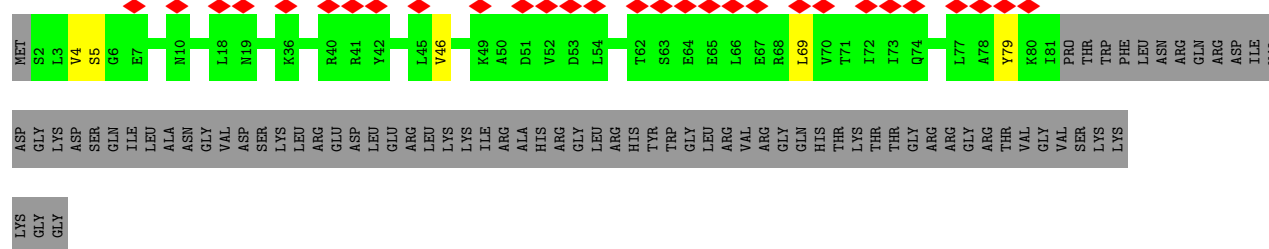
- Molecule 56: Noc4

Chain US: 

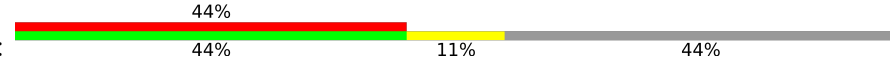


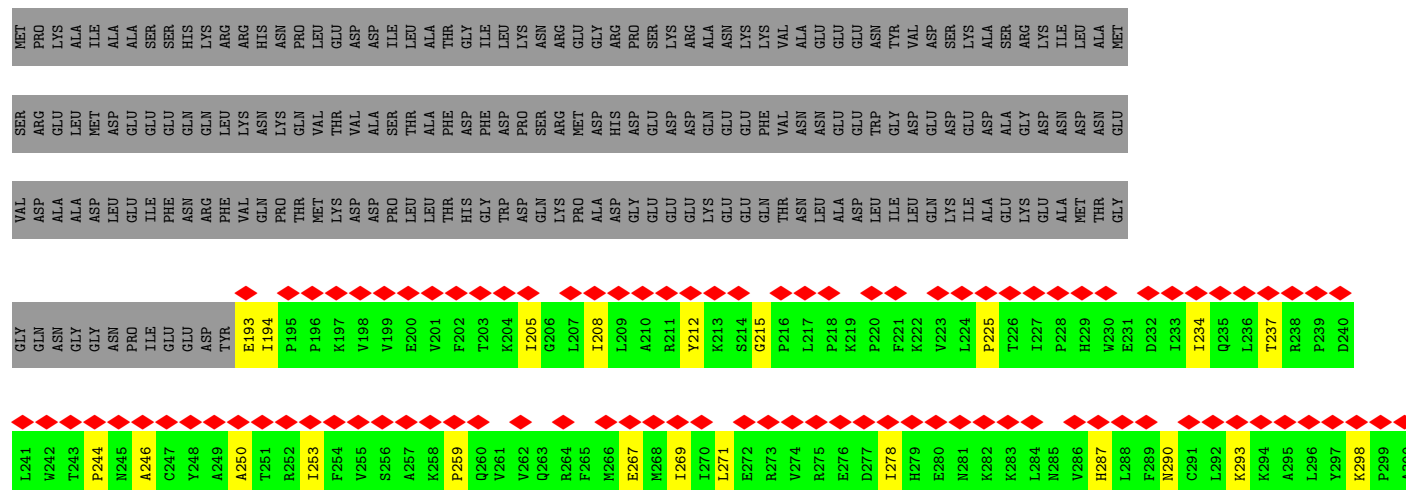
• Molecule 57: Putative ribosomal protein

Chain Cl: 



• Molecule 58: Enp1

Chain CX: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	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	0.359	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	UA	0.42	0/6521	0.66	1/8867 (0.0%)
2	UB	0.28	0/4154	0.58	0/5583
3	UC	0.35	0/595	0.57	0/786
4	UD	0.32	0/6211	0.55	0/8408
5	UF	0.31	0/2657	0.57	0/3596
6	UG	0.42	0/3790	0.66	2/5120 (0.0%)
7	UJ	0.31	0/8567	0.64	3/11619 (0.0%)
8	UK	0.35	0/1701	0.51	0/2251
9	UL	0.33	0/6299	0.70	4/8531 (0.0%)
10	UM	0.29	0/5755	0.68	2/7827 (0.0%)
11	UN	0.35	0/1425	0.58	0/1913
12	UO	0.35	0/3903	0.63	0/5312
13	UQ	0.34	0/6136	0.64	5/8348 (0.1%)
14	UR	0.39	0/3564	0.60	0/4816
15	UU	0.40	0/6903	0.63	0/9392
16	UX	0.38	0/1493	0.63	1/2011 (0.0%)
17	UZ	0.31	0/1861	0.66	0/2531
18	CA	0.39	0/1814	0.60	2/2456 (0.1%)
18	CB	0.27	0/1853	0.54	0/2511
19	CC	0.33	0/2911	0.59	0/3937
20	CD	0.32	0/3205	0.66	3/4338 (0.1%)
21	CE	0.40	0/891	0.65	0/1214
21	CF	0.36	0/876	0.67	0/1195
22	CG	0.30	0/3307	0.61	2/4462 (0.0%)
23	CH	0.32	0/2939	0.59	0/3988
24	CI	0.37	0/6631	0.61	0/8943
25	CJ	0.43	0/1462	0.62	0/1967
26	CK	0.41	0/2376	0.64	1/3214 (0.0%)
27	CL	0.32	0/1812	0.54	0/2437
28	CM	0.42	0/3573	0.62	0/4829
29	CN	0.30	0/1797	0.59	0/2443
29	CO	0.25	0/1714	0.60	2/2325 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.30	0/1923	0.55	0/2577
31	CQ	0.26	0/1379	0.60	0/1850
32	CR	0.37	1/6108 (0.0%)	0.92	15/8266 (0.2%)
32	CS	0.37	1/6108 (0.0%)	0.92	15/8266 (0.2%)
33	CT	0.34	0/1053	0.64	0/1413
34	Ca	0.32	0/1850	0.64	0/2486
35	Cb	0.27	0/1890	0.62	0/2548
36	Cc	0.35	0/1485	0.56	0/2008
37	Cd	0.30	0/1850	0.61	0/2474
38	Ce	0.30	0/1298	0.76	2/1750 (0.1%)
39	Cf	0.28	0/1429	0.60	0/1915
40	Cg	0.36	0/1259	0.58	0/1687
41	Ch	0.24	0/557	0.54	0/749
42	Ci	0.30	0/819	0.59	2/1107 (0.2%)
43	Cj	0.41	0/958	0.63	0/1293
44	Ck	0.24	0/1190	0.57	0/1592
45	Cm	0.33	0/1001	0.57	0/1345
46	Cn	0.37	0/712	0.55	0/954
47	Co	0.27	0/754	0.68	0/1011
48	Cp	0.35	0/458	0.57	0/617
49	CU	0.28	0/1350	0.60	0/1810
50	C1	0.30	0/37546	0.47	7/58475 (0.0%)
51	C2	0.32	0/5459	0.56	6/8498 (0.1%)
52	CW	0.27	0/2996	0.70	4/4075 (0.1%)
53	UT	0.30	0/16371	0.74	7/22154 (0.0%)
54	UH	0.27	0/2852	0.59	0/3846
55	UE	0.31	0/980	0.64	0/1316
55	UI	0.22	0/980	0.56	0/1316
56	US	0.28	0/3765	0.61	0/5100
57	Cl	0.24	0/638	0.70	0/857
58	CX	0.27	1/2180 (0.0%)	0.62	0/2956
59	CY	0.39	0/986	0.74	0/1303
60	CZ	0.45	0/384	0.76	0/511
61	UP	0.30	0/428	0.66	0/570
All	All	0.33	3/219692 (0.0%)	0.63	86/305865 (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
1	UA	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	UD	0	1
7	UJ	0	2
9	UL	0	2
10	UM	0	4
12	UO	0	1
13	UQ	0	4
14	UR	0	1
15	UU	0	3
17	UZ	0	3
18	CB	0	1
21	CF	0	1
22	CG	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cb	0	1
36	Cc	0	1
37	Cd	0	1
38	Ce	0	1
52	CW	0	2
53	UT	0	10
55	UE	0	1
56	US	0	1
57	Cl	0	1
59	CY	0	1
All	All	0	59

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CX	402	ALA	C-N	5.50	1.38	1.33
32	CR	714	GLU	CA-CB	5.29	1.59	1.52
32	CS	714	GLU	CA-CB	5.27	1.59	1.52

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C2	2	G	OP1-P-OP2	-13.63	78.70	119.60
51	C2	2	G	O5'-P-OP1	-11.30	74.11	108.00
51	C2	1	A	OP2-P-O3'	-10.57	76.29	108.00
50	C1	55	G	OP1-P-O3'	-9.88	78.35	108.00
50	C1	45	U	OP1-P-O3'	-9.29	80.14	108.00

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
7	UJ	1661	ASP	Peptide
7	UJ	1662	GLN	Peptide
9	UL	153	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	6366	0	6273	89	0
2	UB	4079	0	4201	42	0
3	UC	588	0	647	12	0
4	UD	6071	0	6080	87	0
5	UF	2591	0	2642	15	0
6	UG	3717	0	3756	48	0
7	UJ	8416	0	8591	103	0
8	UK	1687	0	1820	6	0
9	UL	6175	0	6188	96	0
10	UM	5643	0	5643	97	0
11	UN	1401	0	1455	14	0
12	UO	3819	0	3873	58	0
13	UQ	6008	0	6033	88	0
14	UR	3491	0	3507	44	0
15	UU	6734	0	6745	78	0
16	UX	1470	0	1533	20	0
17	UZ	1819	0	1902	36	0
18	CA	1778	0	1830	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CB	1816	0	1847	28	0
19	CC	2866	0	2960	30	0
20	CD	3150	0	3262	47	0
21	CE	879	0	918	11	0
21	CF	864	0	900	4	0
22	CG	3245	0	3262	48	0
23	CH	2888	0	2979	55	0
24	CI	6486	0	6649	85	0
25	CJ	1434	0	1482	18	0
26	CK	2329	0	2373	35	0
27	CL	1786	0	1826	22	0
28	CM	3501	0	3498	55	0
29	CN	1762	0	1807	18	0
29	CO	1683	0	1726	14	0
30	CP	1893	0	1993	36	0
31	CQ	1361	0	1431	22	0
32	CR	5989	0	6130	112	0
32	CS	5989	0	6130	109	0
33	CT	1035	0	1063	15	0
34	Ca	1821	0	1936	38	0
35	Cb	1851	0	1905	38	0
36	Cc	1464	0	1504	10	0
37	Cd	1819	0	1920	38	0
38	Ce	1279	0	1322	18	0
39	Cf	1398	0	1401	30	0
40	Cg	1242	0	1354	26	0
41	Ch	546	0	580	6	0
42	Ci	808	0	831	10	0
43	Cj	943	0	1002	15	0
44	Ck	1163	0	1230	20	0
45	Cm	985	0	1021	12	0
46	Cn	702	0	750	12	0
47	Co	741	0	785	11	0
48	Cp	455	0	482	5	0
49	CU	1337	0	1376	15	0
50	C1	33604	0	17014	328	0
51	C2	4891	0	2476	40	0
52	CW	2924	0	2854	83	0
53	UT	16053	0	16457	232	0
54	UH	2809	0	2843	55	0
55	UE	972	0	1032	12	0
55	UI	972	0	1032	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	US	3672	0	3679	65	0
57	CI	633	0	676	3	0
58	CX	2130	0	2219	29	0
59	CY	979	0	995	39	0
60	CZ	376	0	371	17	0
61	UP	422	0	457	10	0
62	UX	1	0	0	0	0
63	CI	32	0	12	11	0
64	CI	1	0	0	0	0
All	All	211834	0	196471	2575	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 2575 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)
54:UH:557:GLU:O	54:UH:565:GLY:HA2	1.36	1.25
54:UH:555:GLY:O	54:UH:567:LEU:HA	1.37	1.20
24:CI:80:GLY:HA2	63:CI:1201:GTP:O2A	1.01	1.15
24:CI:80:GLY:CA	63:CI:1201:GTP:O2A	1.95	1.14
17:UZ:280:ASN:HB2	17:UZ:282:TYR:CE2	1.81	1.14

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	UA	835/904 (92%)	768 (92%)	67 (8%)	0	100	100
2	UB	502/907 (55%)	470 (94%)	32 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	UC	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	UD	754/884 (85%)	722 (96%)	32 (4%)	0	100	100
5	UF	325/414 (78%)	310 (95%)	14 (4%)	1 (0%)	36	67
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	30	62
7	UJ	1062/1802 (59%)	1010 (95%)	52 (5%)	0	100	100
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	711 (93%)	56 (7%)	0	100	100
10	UM	705/912 (77%)	656 (93%)	48 (7%)	1 (0%)	48	79
11	UN	171/938 (18%)	167 (98%)	3 (2%)	1 (1%)	21	54
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	36	67
14	UR	437/618 (71%)	416 (95%)	21 (5%)	0	100	100
15	UU	890/1049 (85%)	832 (94%)	58 (6%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	212 (93%)	16 (7%)	1 (0%)	30	62
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	220 (94%)	15 (6%)	0	100	100
19	CC	383/523 (73%)	367 (96%)	16 (4%)	0	100	100
20	CD	416/582 (72%)	393 (94%)	23 (6%)	0	100	100
21	CE	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	16	49
22	CG	402/630 (64%)	375 (93%)	27 (7%)	0	100	100
23	CH	383/411 (93%)	344 (90%)	38 (10%)	1 (0%)	36	67
24	CI	812/1163 (70%)	761 (94%)	49 (6%)	2 (0%)	43	74
25	CJ	177/183 (97%)	166 (94%)	11 (6%)	0	100	100
26	CK	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
27	CL	225/785 (29%)	212 (94%)	12 (5%)	1 (0%)	30	62
28	CM	443/446 (99%)	417 (94%)	26 (6%)	0	100	100
29	CN	222/252 (88%)	210 (95%)	12 (5%)	0	100	100
29	CO	211/252 (84%)	197 (93%)	12 (6%)	2 (1%)	14	47
30	CP	227/322 (70%)	221 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	24	57
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	24	57
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	211 (95%)	12 (5%)	0	100	100
35	Cb	230/264 (87%)	204 (89%)	26 (11%)	0	100	100
36	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
37	Cd	224/239 (94%)	211 (94%)	13 (6%)	0	100	100
38	Ce	155/203 (76%)	140 (90%)	15 (10%)	0	100	100
39	Cf	170/202 (84%)	164 (96%)	6 (4%)	0	100	100
40	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
42	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
43	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
44	Ck	136/161 (84%)	129 (95%)	7 (5%)	0	100	100
45	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
46	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
47	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
48	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
49	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100
52	CW	380/668 (57%)	349 (92%)	31 (8%)	0	100	100
53	UT	1987/2612 (76%)	1871 (94%)	110 (6%)	6 (0%)	36	67
54	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100	100
55	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100	100
55	UI	121/410 (30%)	121 (100%)	0	0	100	100
56	US	443/549 (81%)	415 (94%)	28 (6%)	0	100	100
57	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
58	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100	100
59	CY	119/381 (31%)	109 (92%)	10 (8%)	0	100	100
60	CZ	42/609 (7%)	34 (81%)	8 (19%)	0	100	100
61	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	21864/32830 (67%)	20513 (94%)	1321 (6%)	30 (0%)	49 79

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
53	UT	487	ILE
6	UG	580	GLU
13	UQ	708	SER
17	UZ	293	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	UA	651/775 (84%)	649 (100%)	2 (0%)	86 83
2	UB	425/788 (54%)	425 (100%)	0	100 100
3	UC	61/536 (11%)	61 (100%)	0	100 100
4	UD	653/738 (88%)	649 (99%)	4 (1%)	78 79
5	UF	248/341 (73%)	247 (100%)	1 (0%)	84 81
6	UG	373/474 (79%)	370 (99%)	3 (1%)	73 77
7	UJ	898/1526 (59%)	893 (99%)	5 (1%)	78 79
8	UK	159/227 (70%)	159 (100%)	0	100 100
9	UL	667/821 (81%)	662 (99%)	5 (1%)	76 78
10	UM	606/770 (79%)	598 (99%)	8 (1%)	61 72
11	UN	146/765 (19%)	146 (100%)	0	100 100
12	UO	404/456 (89%)	396 (98%)	8 (2%)	48 67
13	UQ	650/817 (80%)	646 (99%)	4 (1%)	78 79
14	UR	360/524 (69%)	358 (99%)	2 (1%)	78 79
15	UU	672/863 (78%)	666 (99%)	6 (1%)	70 76
16	UX	150/167 (90%)	147 (98%)	3 (2%)	48 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	UZ	187/329 (57%)	183 (98%)	4 (2%)	47	66
18	CA	175/228 (77%)	172 (98%)	3 (2%)	53	70
18	CB	195/228 (86%)	193 (99%)	2 (1%)	68	75
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	319/489 (65%)	318 (100%)	1 (0%)	86	83
21	CE	91/108 (84%)	90 (99%)	1 (1%)	65	74
21	CF	88/108 (82%)	87 (99%)	1 (1%)	65	74
22	CG	331/525 (63%)	326 (98%)	5 (2%)	57	71
23	CH	303/320 (95%)	299 (99%)	4 (1%)	61	72
24	CI	661/1009 (66%)	653 (99%)	8 (1%)	63	73
25	CJ	147/169 (87%)	146 (99%)	1 (1%)	76	78
26	CK	245/266 (92%)	238 (97%)	7 (3%)	37	60
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	363 (100%)	1 (0%)	86	83
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	192 (100%)	1 (0%)	81	80
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	145/215 (67%)	145 (100%)	0	100	100
32	CR	654/916 (71%)	446 (68%)	208 (32%)	0	2
32	CS	654/916 (71%)	446 (68%)	208 (32%)	0	2
33	CT	108/167 (65%)	107 (99%)	1 (1%)	70	76
34	Ca	198/223 (89%)	197 (100%)	1 (0%)	81	80
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	149 (100%)	0	100	100
37	Cd	192/204 (94%)	190 (99%)	2 (1%)	68	75
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	122/162 (75%)	122 (100%)	0	100	100
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	Ck	126/143 (88%)	126 (100%)	0	100	100
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	77 (98%)	2 (2%)	42	63
48	Cp	46/61 (75%)	46 (100%)	0	100	100
49	CU	137/260 (53%)	137 (100%)	0	100	100
52	CW	309/587 (53%)	308 (100%)	1 (0%)	86	83
53	UT	1732/2276 (76%)	1717 (99%)	15 (1%)	70	76
54	UH	301/788 (38%)	298 (99%)	3 (1%)	68	75
55	UE	105/346 (30%)	105 (100%)	0	100	100
55	UI	105/346 (30%)	105 (100%)	0	100	100
56	US	404/493 (82%)	403 (100%)	1 (0%)	87	85
57	Cl	71/135 (53%)	71 (100%)	0	100	100
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	100/322 (31%)	92 (92%)	8 (8%)	11	35
60	CZ	38/519 (7%)	37 (97%)	1 (3%)	40	62
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	18216/27810 (66%)	17675 (97%)	541 (3%)	37	60

5 of 541 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	CS	781	ASP
32	CS	831	GLN
32	CS	773	SER
53	UT	1341	LEU
32	CR	488	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

Mol	Chain	Res	Type
44	Ck	103	ASN
56	US	151	GLN
47	Co	382	GLN
53	UT	575	ASN

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Mol	Chain	Res	Type
55	UI	232	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1550/2352 (65%)	483 (31%)	33 (2%)
51	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1776/2582 (68%)	551 (31%)	37 (2%)

5 of 551 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	5	G
50	C1	7	A
50	C1	13	G
50	C1	14	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	2054	A
51	C2	91	G
50	C1	2077	C
50	C1	2219	C
50	C1	684	U

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
63	GTP	CI	1201	-	33,34,34	1.10	3 (9%)	50,54,54	1.81	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GTP	CI	1201	-	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	CI	1201	GTP	C6-N1	-2.81	1.33	1.38
63	CI	1201	GTP	C5-C4	2.77	1.46	1.38
63	CI	1201	GTP	C5-N7	-2.31	1.34	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	CI	1201	GTP	C5-C4-N3	-6.31	118.35	128.39
63	CI	1201	GTP	C2-N3-C4	5.14	121.15	112.30
63	CI	1201	GTP	N9-C4-N3	4.70	135.35	125.95
63	CI	1201	GTP	C6-C5-N7	3.34	136.38	130.29
63	CI	1201	GTP	C4-C5-N7	-2.57	106.59	110.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

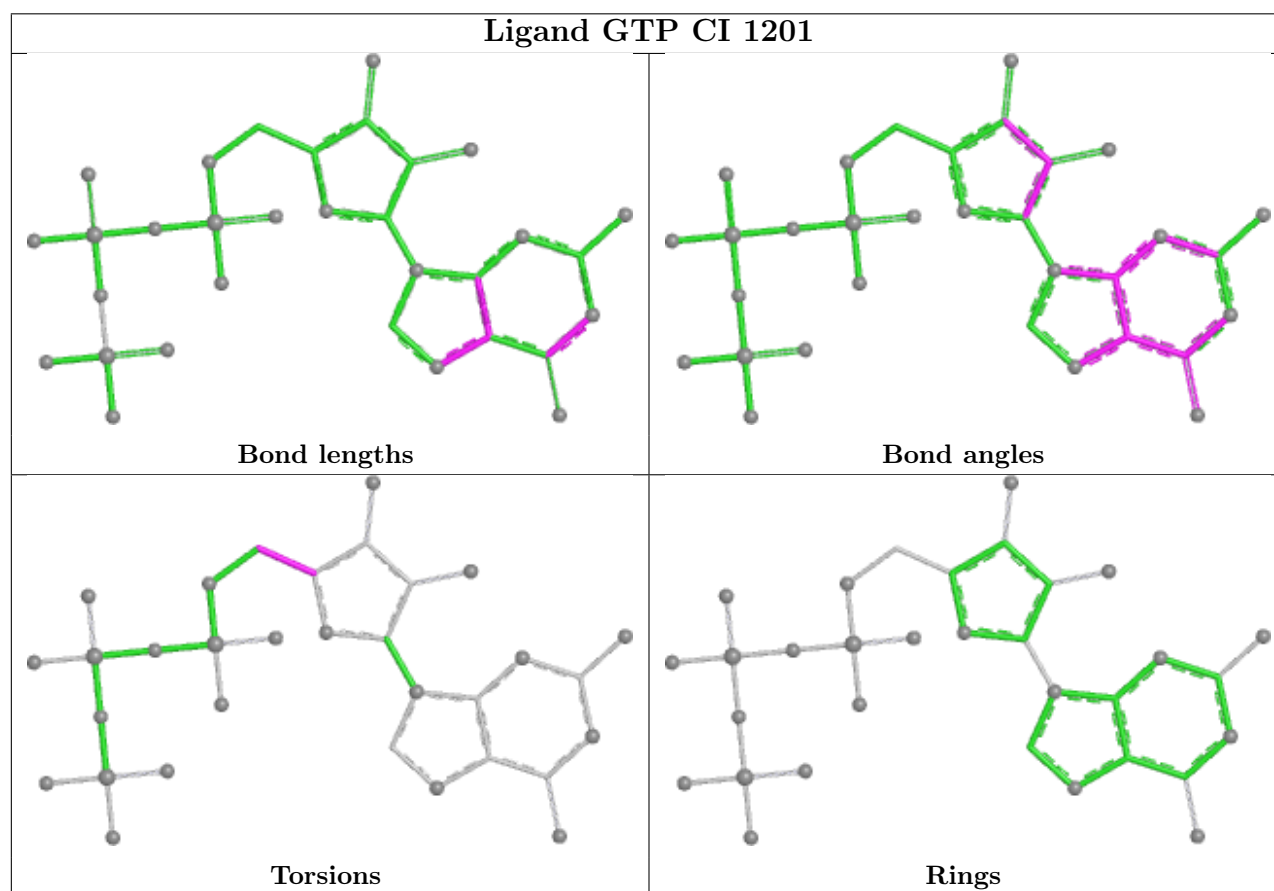
Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	O4'-C4'-C5'-O5'
63	CI	1201	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	CI	1201	GTP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.77
1	C2	105:C	O3'	110:A	P	16.05
1	C2	119:C	O3'	123:A	P	11.95

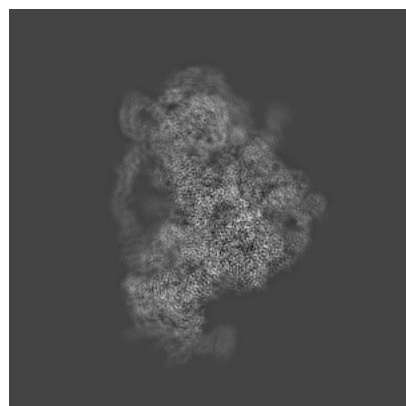
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10052. These allow visual inspection of the internal detail of the map and identification of artifacts.

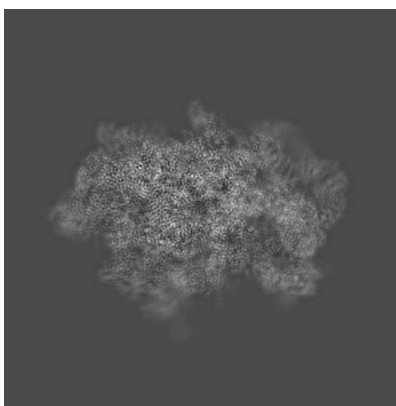
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

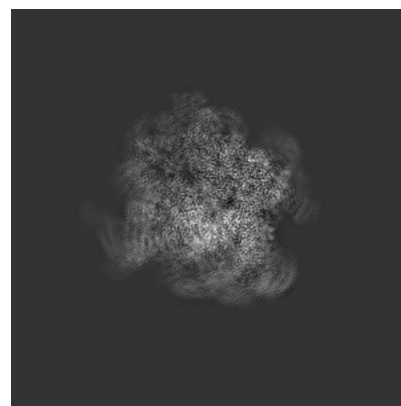
6.1.1 Primary map



X

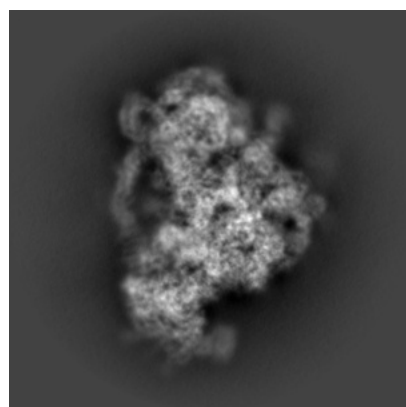


Y

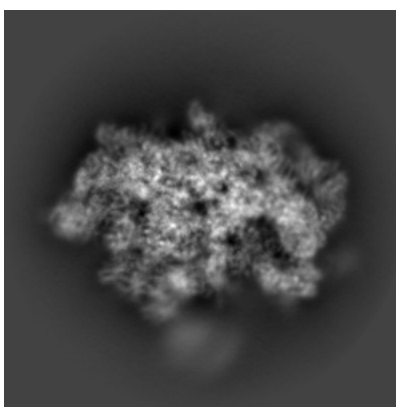


Z

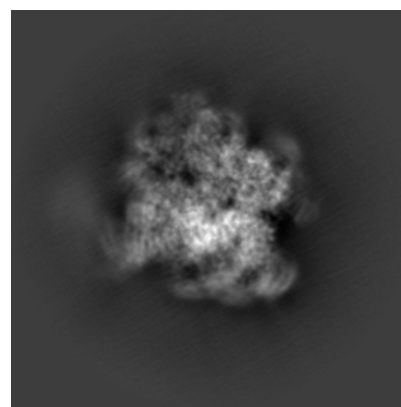
6.1.2 Raw map



X



Y

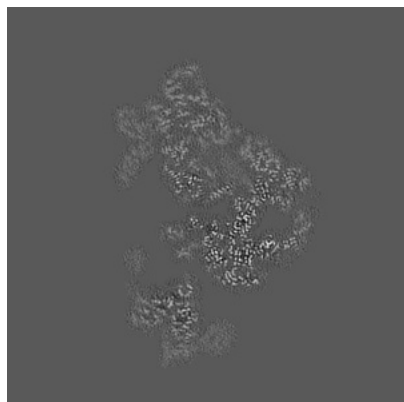


Z

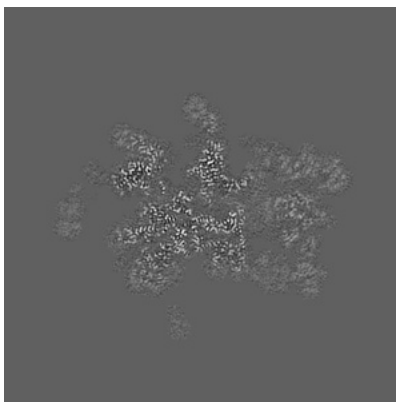
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

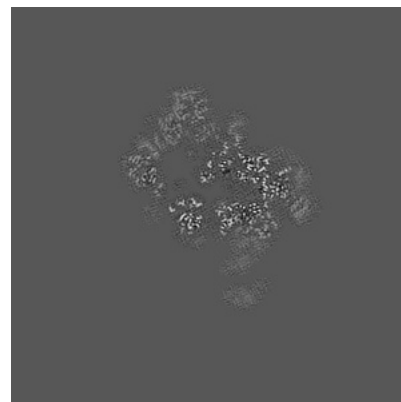
6.2.1 Primary map



X Index: 240

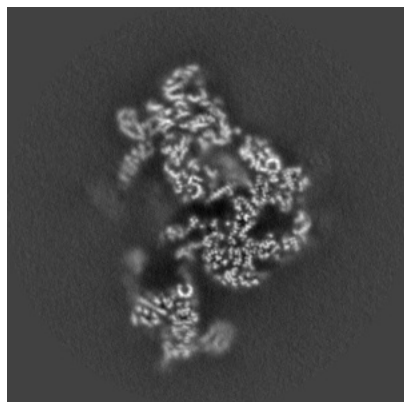


Y Index: 240

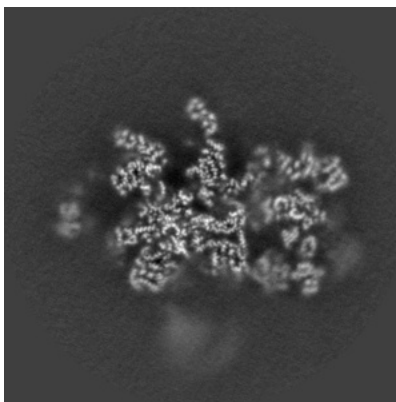


Z Index: 240

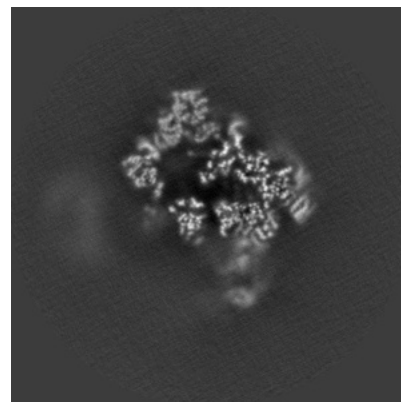
6.2.2 Raw map



X Index: 240



Y Index: 240

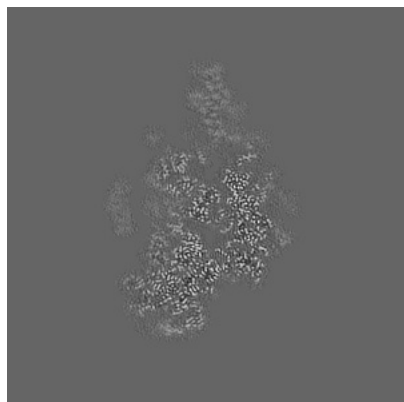


Z Index: 240

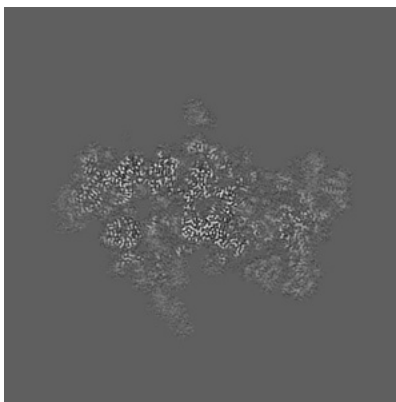
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

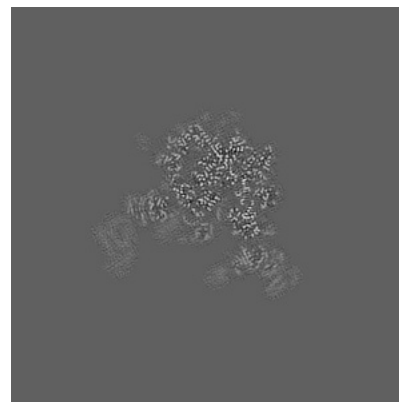
6.3.1 Primary map



X Index: 282

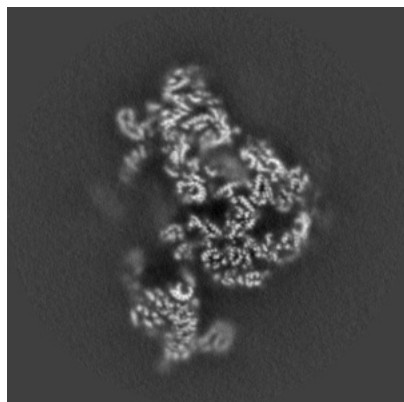


Y Index: 224

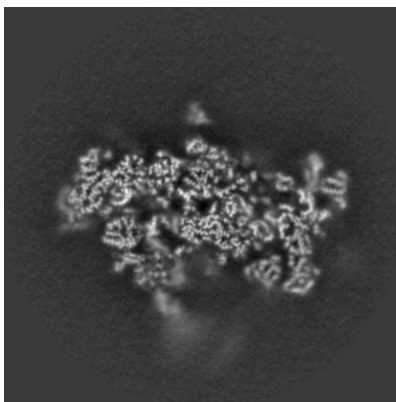


Z Index: 183

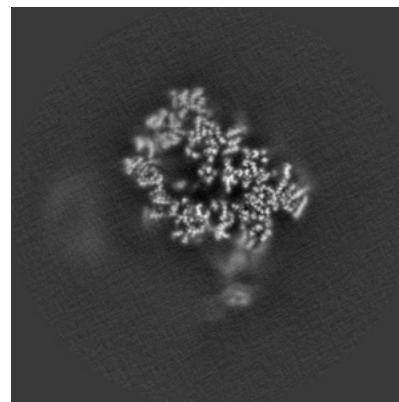
6.3.2 Raw map



X Index: 237



Y Index: 224

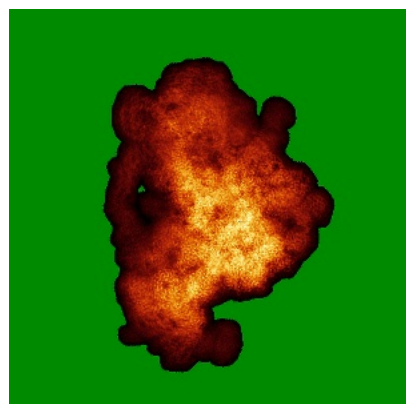


Z Index: 247

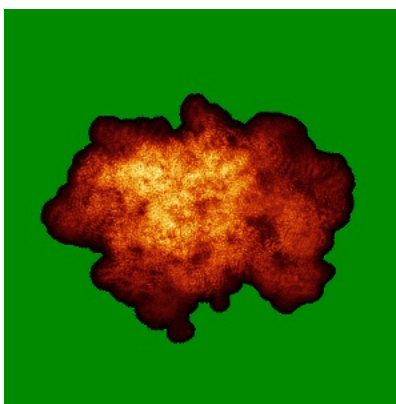
The images above show the largest variance slices of the map in three orthogonal directions.

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

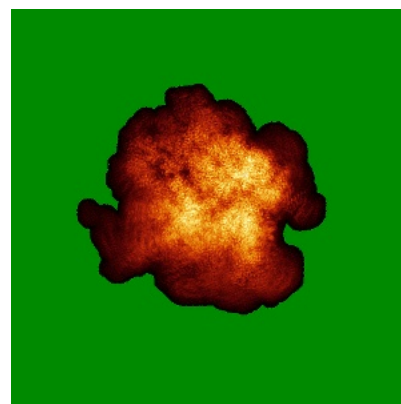
6.4.1 Primary map



X

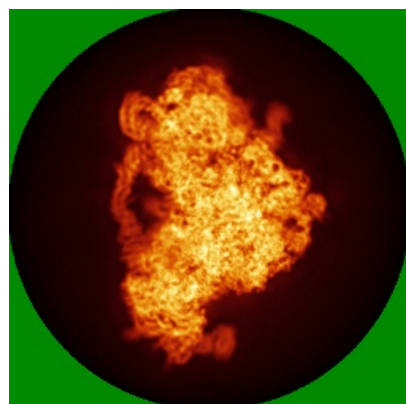


Y

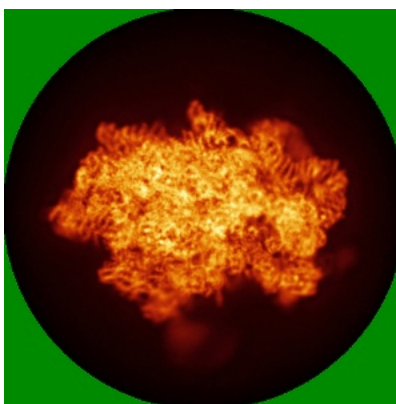


Z

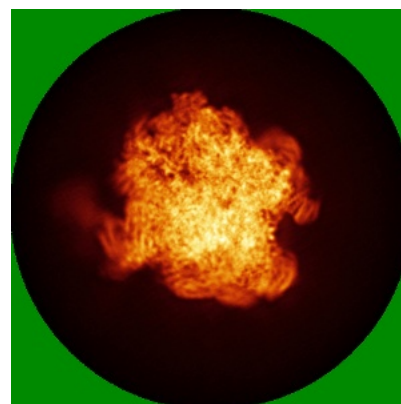
6.4.2 Raw map



X



Y

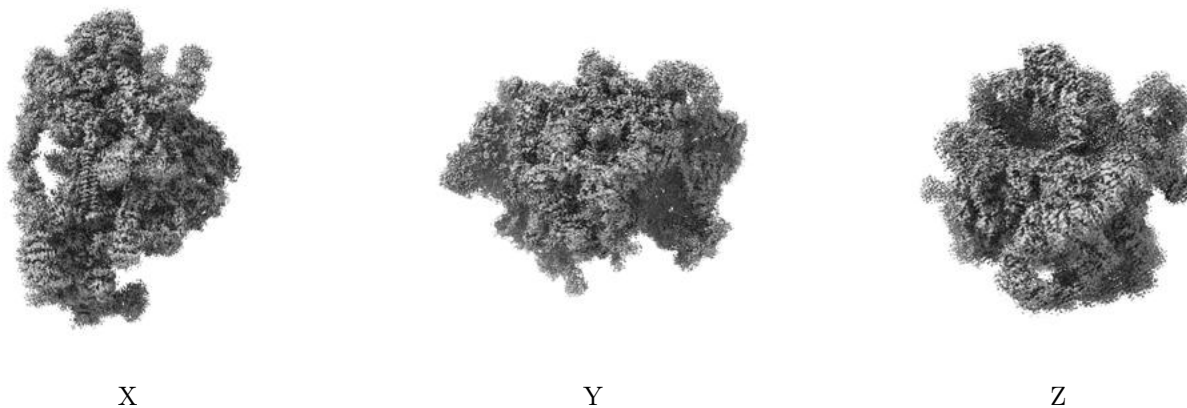


Z

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 0.03. 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.

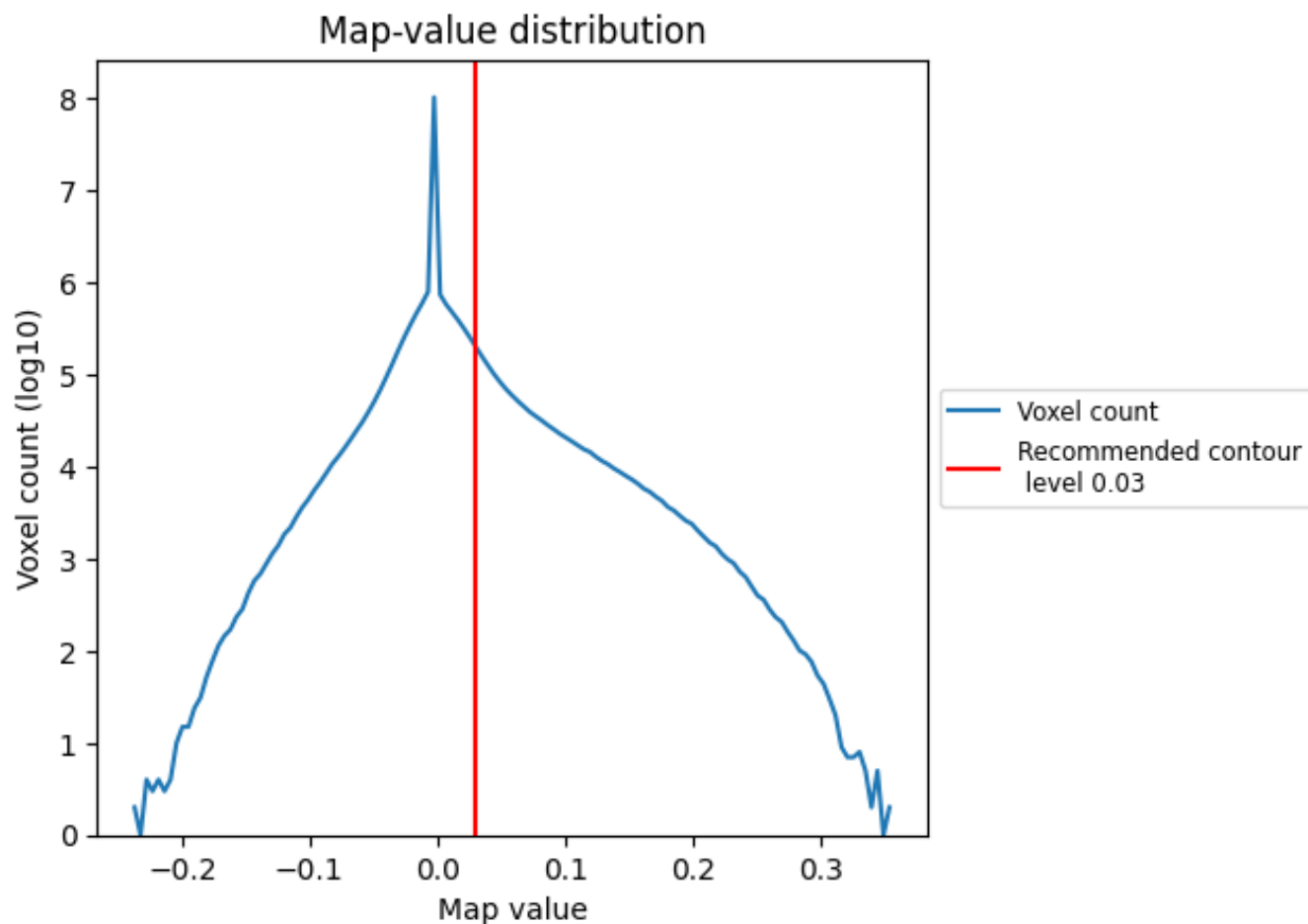
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

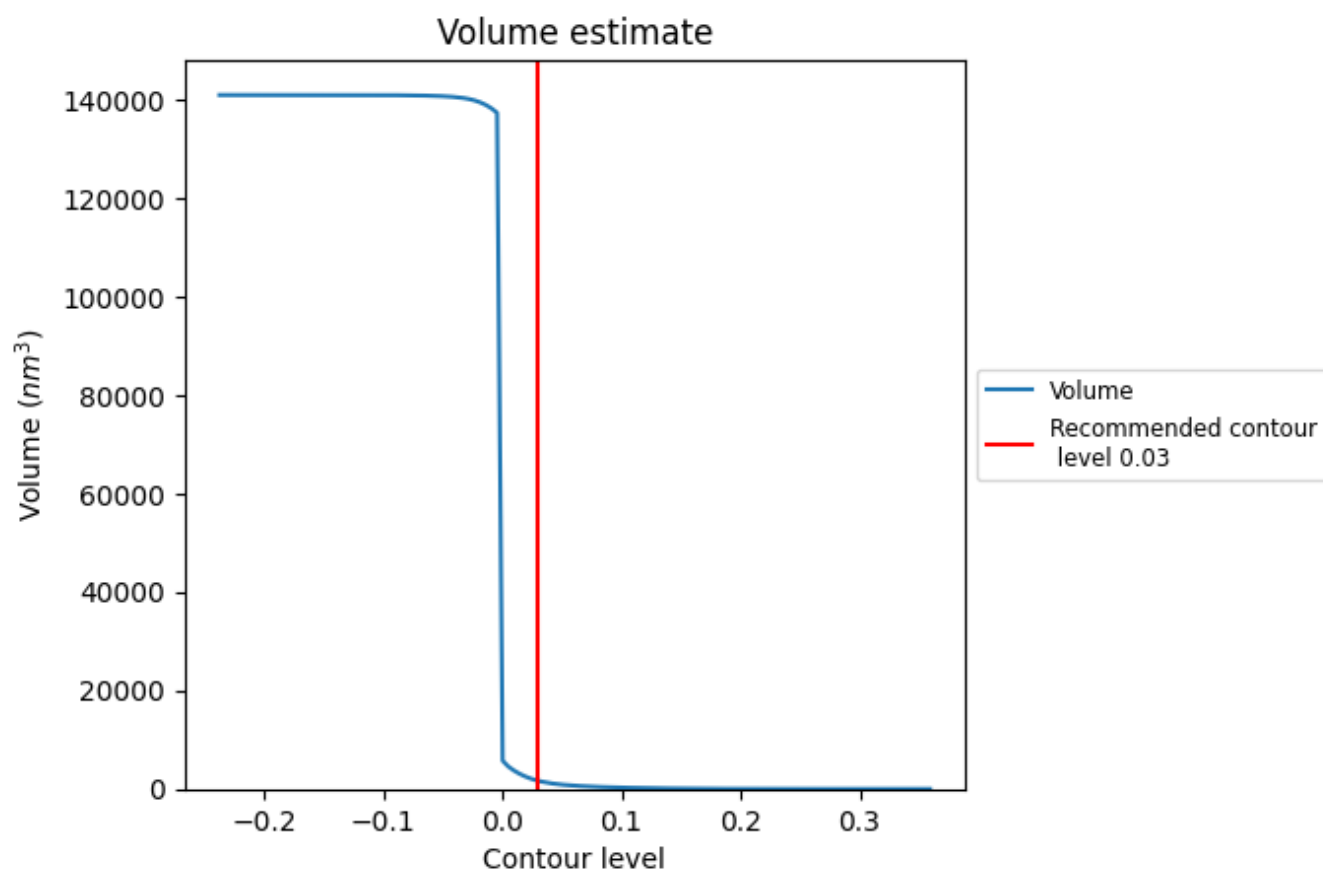
This section contains the results of statistical analysis of the map.

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.

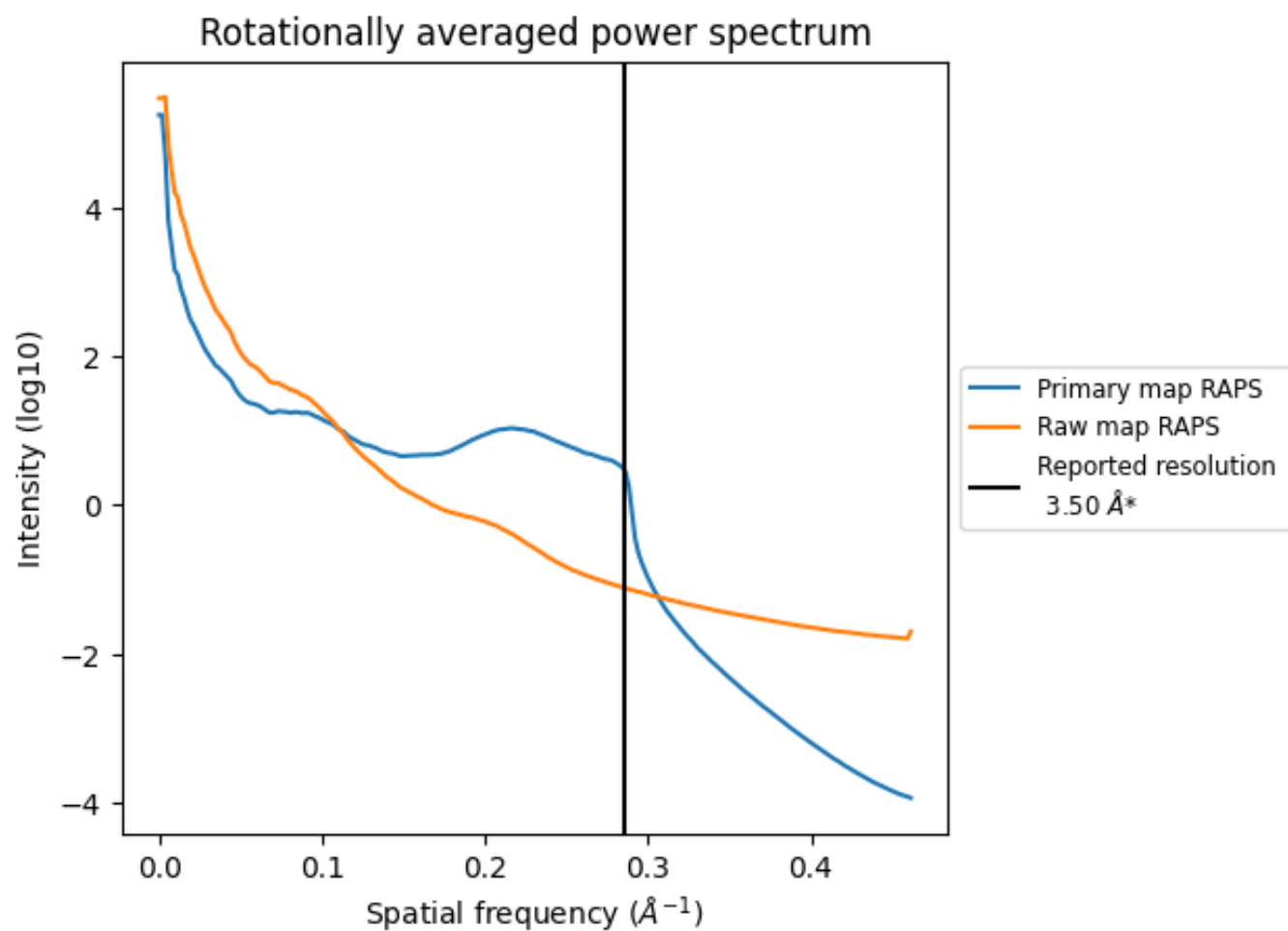
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1676 nm^3 ; this corresponds to an approximate mass of 1514 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 ⓘ

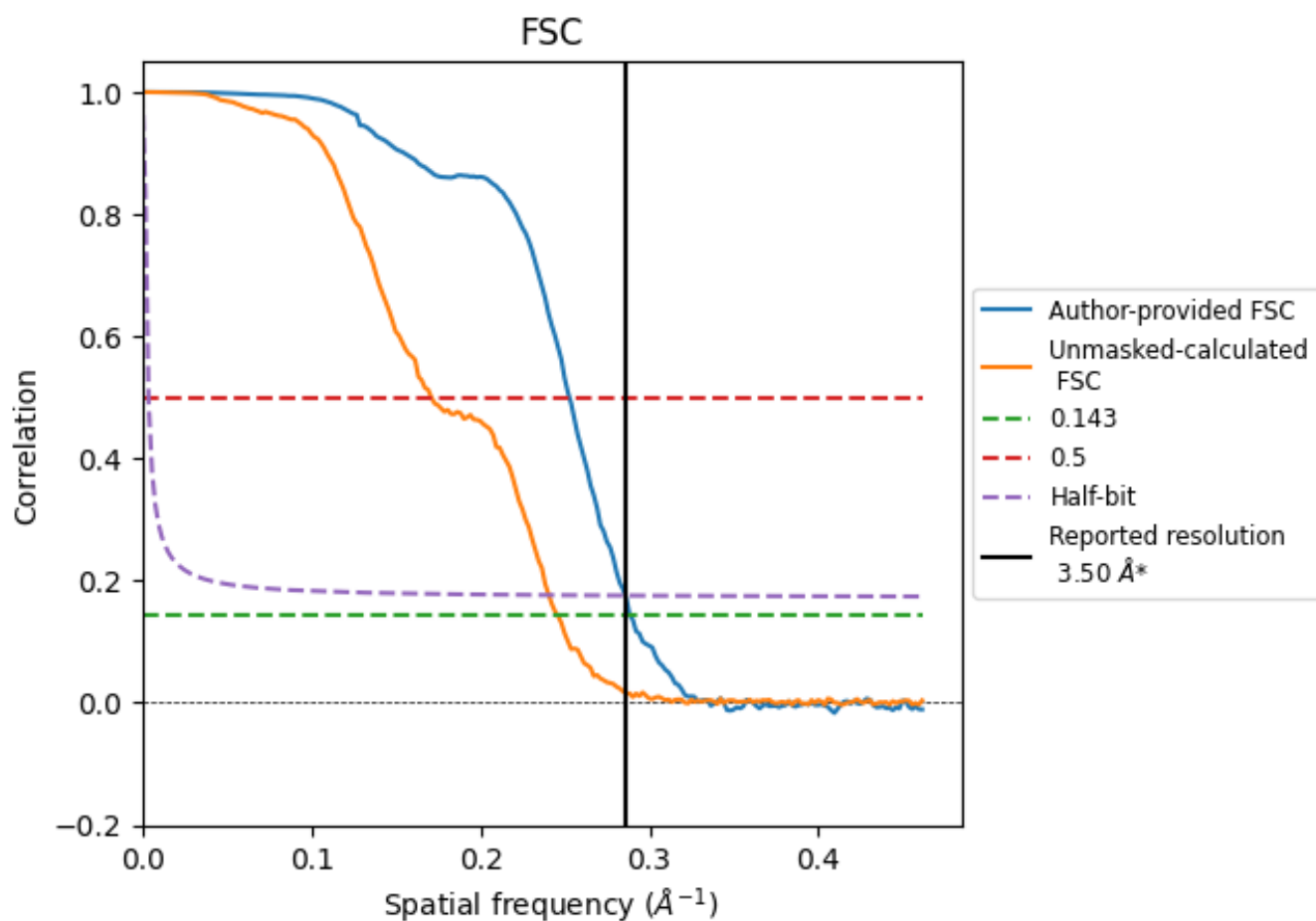


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

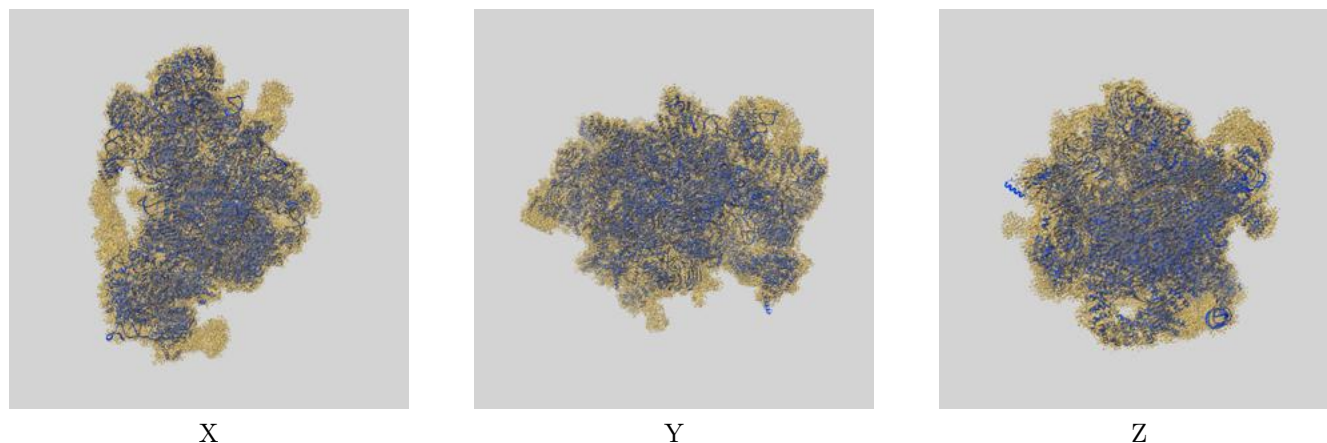
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.96	3.50
Unmasked-calculated*	4.07	5.85	4.16

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

9 Map-model fit [i](#)

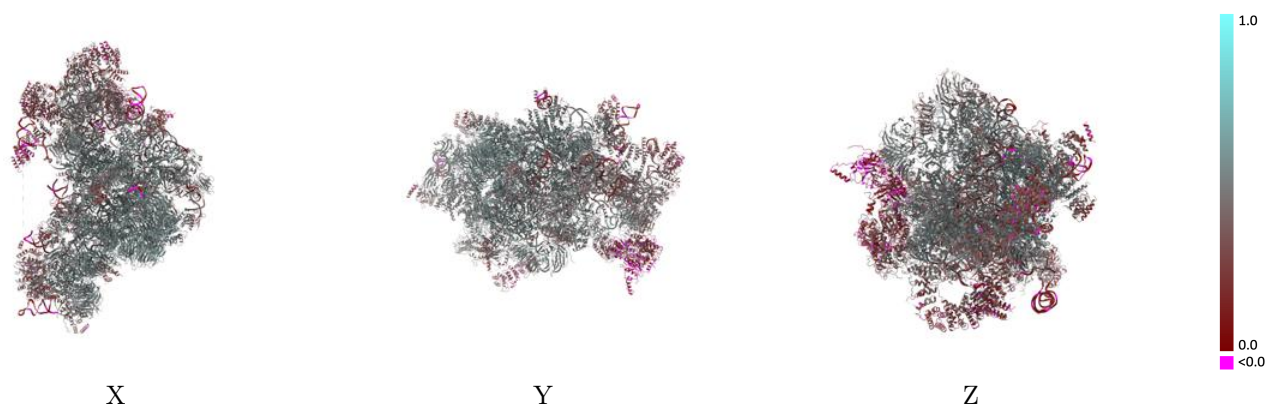
This section contains information regarding the fit between EMDB map EMD-10052 and PDB model 6RXU. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



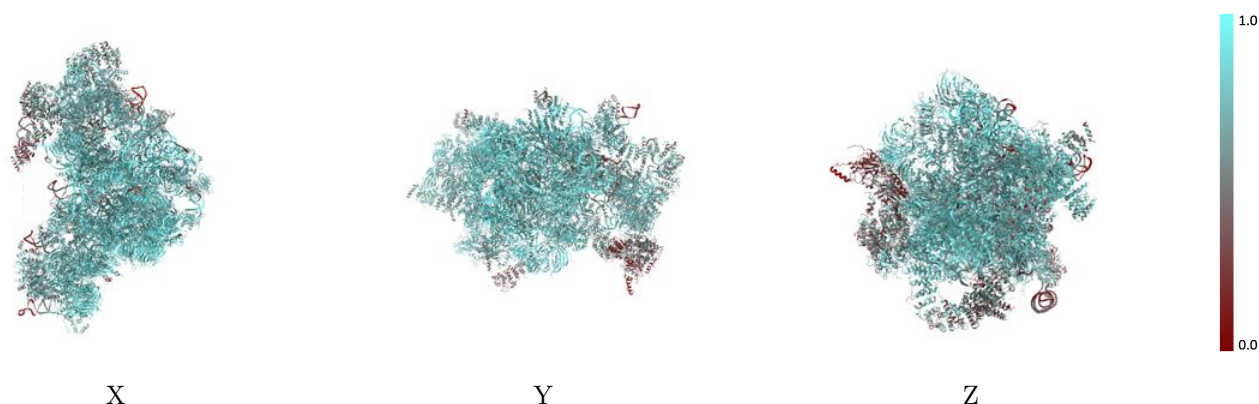
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



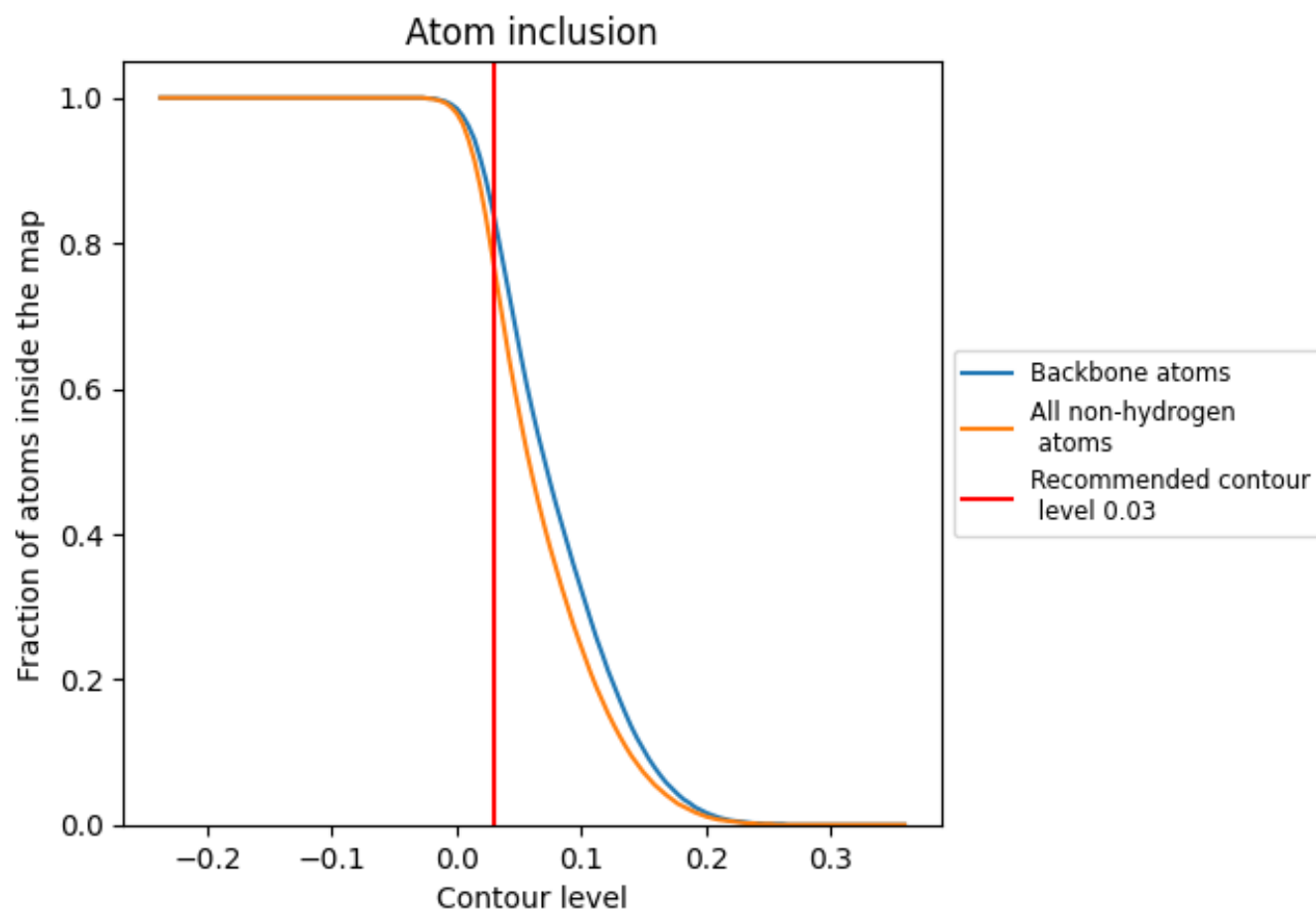
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.4400
C1	 0.8230	 0.4110
C2	 0.7410	 0.3660
CA	 0.8780	 0.5410
CB	 0.7490	 0.4650
CC	 0.8020	 0.4770
CD	 0.7540	 0.4500
CE	 0.8580	 0.5240
CF	 0.8360	 0.5030
CG	 0.8050	 0.4810
CH	 0.8440	 0.5140
CI	 0.8510	 0.5170
CJ	 0.9060	 0.5520
CK	 0.8580	 0.5350
CL	 0.8260	 0.5230
CM	 0.8810	 0.5460
CN	 0.7700	 0.4780
CO	 0.6590	 0.3720
CP	 0.7880	 0.4850
CQ	 0.7440	 0.4110
CR	 0.6340	 0.3440
CS	 0.3500	 0.1330
CT	 0.8400	 0.5180
CU	 0.8020	 0.5020
CW	 0.7410	 0.4390
CX	 0.2710	 0.1710
CY	 0.7170	 0.4500
CZ	 0.6420	 0.3770
Ca	 0.7970	 0.4700
Cb	 0.7350	 0.4470
Cc	 0.8540	 0.5260
Cd	 0.7650	 0.4640
Ce	 0.6970	 0.4030
Cf	 0.7560	 0.4560
Cg	 0.8620	 0.5290



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Chain	Atom inclusion	Q-score
Ch	 0.7610	 0.4240
Ci	 0.8520	 0.5120
Cj	 0.8820	 0.5460
Ck	 0.6570	 0.3810
Cl	 0.4600	 0.3680
Cm	 0.8000	 0.5000
Cn	 0.8900	 0.5390
Co	 0.7340	 0.4210
Cp	 0.8690	 0.5350
UA	 0.8930	 0.5450
UB	 0.7550	 0.4400
UC	 0.8710	 0.5420
UD	 0.8450	 0.5090
UE	 0.7720	 0.4560
UF	 0.8190	 0.4510
UG	 0.8820	 0.5360
UH	 0.7240	 0.4060
UI	 0.7210	 0.4200
UJ	 0.6230	 0.3650
UK	 0.8550	 0.5260
UL	 0.8300	 0.4840
UM	 0.7500	 0.4370
UN	 0.8300	 0.5090
UO	 0.8540	 0.5150
UP	 0.7690	 0.4730
UQ	 0.8440	 0.5040
UR	 0.8880	 0.5400
US	 0.7580	 0.4300
UT	 0.6450	 0.3360
UU	 0.8960	 0.5390
UX	 0.8600	 0.5340
UZ	 0.7620	 0.4480