



wwPDB EM Validation Summary Report ⓘ

Jul 10, 2026 – 06:58 AM JST

PDB ID : 9XAF / pdb_00009xaf
EMDB ID : EMD-66685
Title : Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 Mut) from *Chaetomium thermophilum*, state a
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.00 Å (reported)
Based on initial model : 6RXU

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

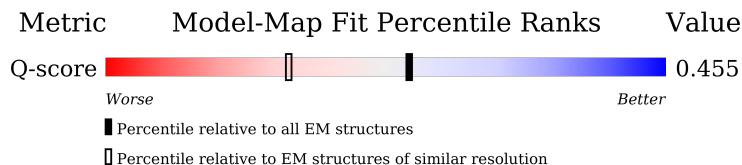
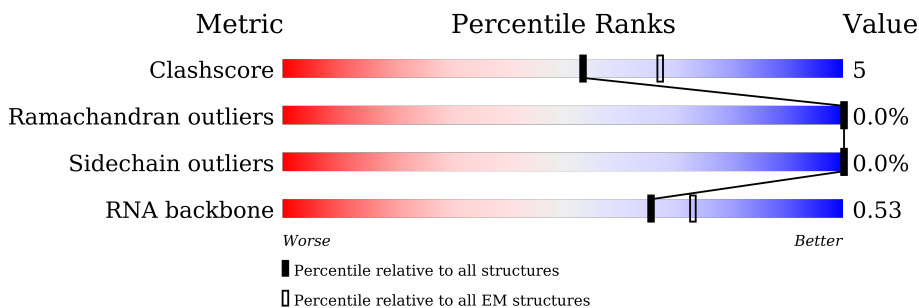
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 3.00 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.



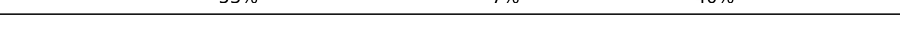
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	

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Mol	Chain	Length	Quality of chain
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	708	
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	

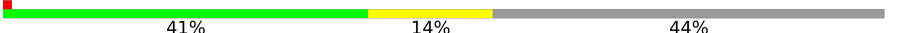
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Mol	Chain	Length	Quality of chain
26	CK	297	
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Cc	212	
35	Ce	203	
36	Cg	190	
37	Ci	150	
38	Cj	143	
39	Cm	130	
40	Cn	145	
41	Co	136	
42	Cp	68	
43	CU	311	
44	C1	2350	
45	C2	274	
46	UH	930	
47	UE	410	
47	UI	410	

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Mol	Chain	Length	Quality of chain
48	US	549	
49	Cl	156	
50	CX	480	
51	CY	381	
52	UP	364	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 177206 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	P	S	
			6411	4118	1136	1132	1	24	
								0	0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	566	Total	C	N	O	S		
			4506	2845	858	790	13		
								0	0

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	79	Total	C	N	O		
			630	396	125	109		
							0	0

- Molecule 4 is a protein called UTP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	777	Total	C	N	O	S		
			6108	3872	1099	1113	24		
								0	0

- Molecule 5 is a protein called U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UF	331	Total	C	N	O	S		
			2599	1678	504	403	14		
								0	0

- Molecule 6 is a protein called U three protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	479	Total	C	N	O	S		
			3765	2391	700	662	12		
								0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	449	Total	C	N	O	S	0	0
			3412	2192	610	596	14		

- 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
			1699	1068	351	275	5		

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

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 U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	843	Total	C	N	O	S	0	0
			6545	4139	1151	1241	14		

- 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 U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	503	Total	C	N	O	S	0	0
			3811	2417	698	683	13		

- Molecule 13 is a protein called UTP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6012	3834	1038	1119	21		

- Molecule 14 is a protein called UTP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	P	S	
			3498	2210	656	621	1	10	0
									0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	908	Total	C	N	O	S		
			6778	4361	1243	1148	26	0	0

- Molecule 16 is a protein called UTP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S		
			1480	938	286	246	10	0	0

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S		
			1815	1184	330	298	3	0	0

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 19 is a protein called Nucleolar protein 56.

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

- Molecule 20 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	446	Total	C	N	O	S		
			3355	2150	594	600	11	0	0

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

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 Ribosomal RNA-processing protein.

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-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	841	Total	C	N	O	S	0	0
			6666	4277	1246	1113	30		

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein 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 U3 small nucleolar ribonucleoprotein protein IMP4.

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 DDB1- and CUL4-associated factor 13.

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 Nucleolar essential protein 1.

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	201	Total	C	N	O	S	0	0
			1625	1047	286	283	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	180	Total	C	N	O	S	0	0
			1413	898	257	251	7		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	846	Total	C	N	O	S	0	0
			6677	4278	1137	1233	29		
32	CS	836	Total	C	N	O	S	0	0
			6591	4217	1118	1228	28		

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

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 s5-like protein.

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

- Molecule 35 is a protein called 40S ribosomal protein S7.

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

- Molecule 36 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cg	159	Total	C	N	O	S	0	0
			1248	804	258	184	2		

- Molecule 37 is a protein called 40S ribosomal protein S14-like protein.

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

- Molecule 38 is a protein called 40S ribosomal protein S16-like protein.

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

- Molecule 39 is a protein called 40S ribosomal protein S22-like protein.

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

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

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

- Molecule 41 is a protein called Small ribosomal subunit protein eS24.

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

- Molecule 42 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cp	61	Total	C	N	O	S	0	0
			458	286	97	74	1		

- Molecule 43 is a protein called faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CU	135	Total	C	N	O	S	0	0
			1035	637	210	182	6		

- Molecule 44 is a RNA chain called 35s rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C1	1189	Total	C	N	O	P	0	0
			25383	11319	4564	8311	1189		

- Molecule 45 is a RNA chain called u3 rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	C2	229	Total	C	N	O	P	0	0
			4869	2172	851	1617	229		

- Molecule 46 is a protein called utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	UH	799	Total	C	N	O	S	0	0
			6198	3903	1105	1171	19		

- Molecule 47 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	UE	178	Total	C	N	O	S	0	0
			1362	851	251	254	6		
47	UI	128	Total	C	N	O	S	0	0
			996	622	187	181	6		

- Molecule 48 is a protein called CCAAT-binding factor domain-containing protein.

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

- Molecule 49 is a protein called Putative ribosomal protein.

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

- Molecule 50 is a protein called Bystin-like protein.

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

- Molecule 51 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

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

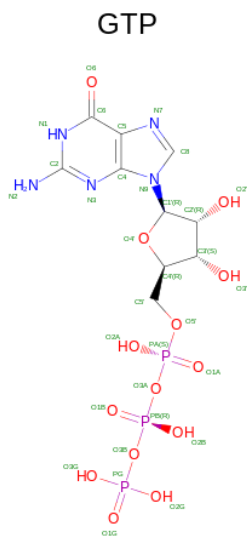
- Molecule 52 is a protein called utp16.

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

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

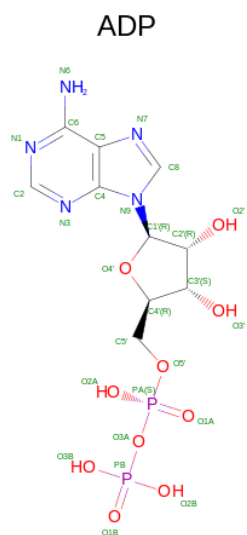


Mol	Chain	Residues	Atoms					AltConf
54	CI	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

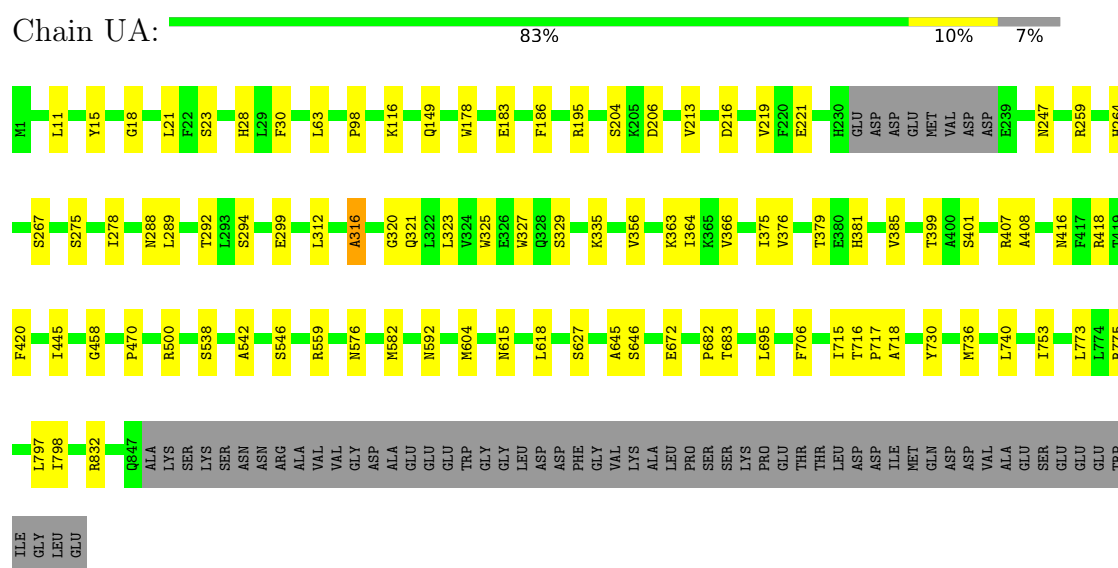


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	CS	1	27	10	5	10	2	0

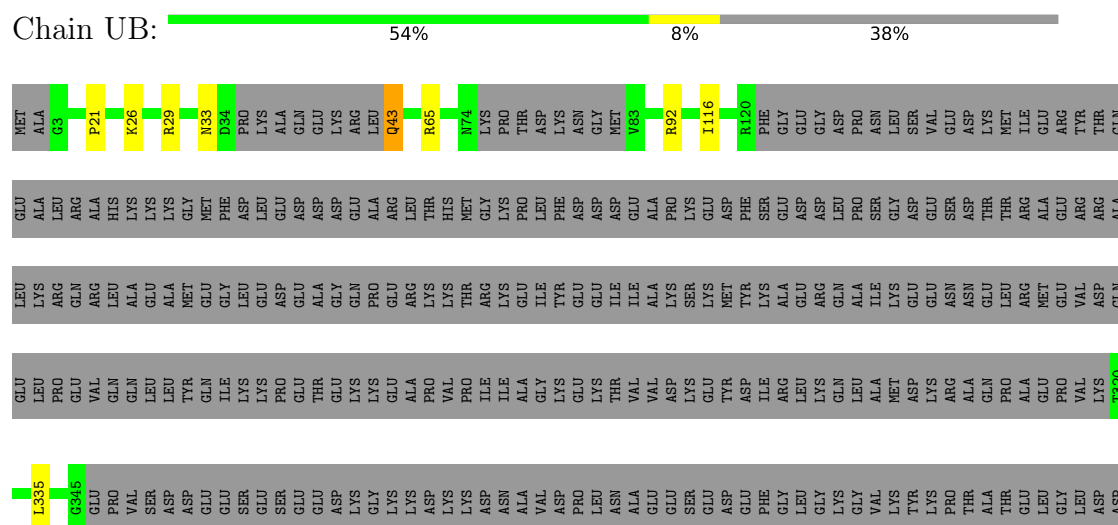
3 Residue-property plots

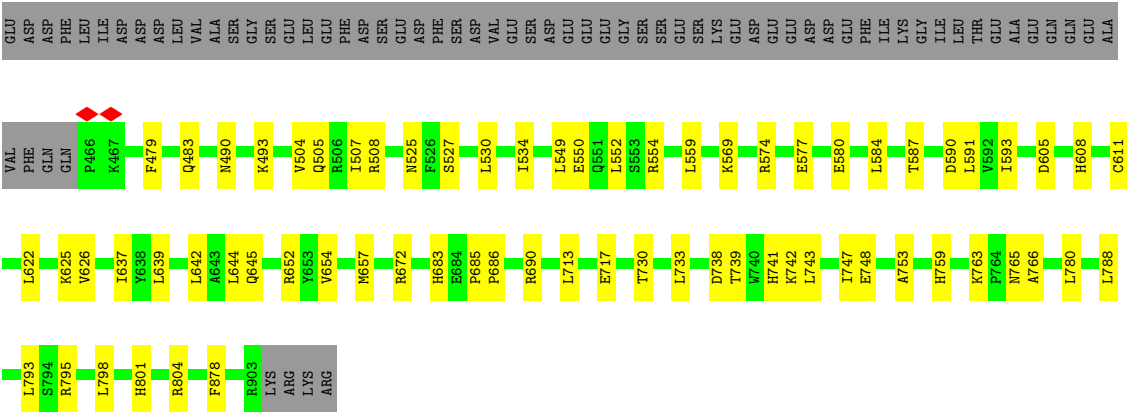
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Periodic tryptophan protein 2-like protein



• Molecule 2: Nucleolar complex protein 14





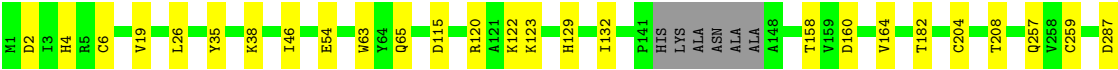
• Molecule 3: Sas10 C-terminal domain-containing protein

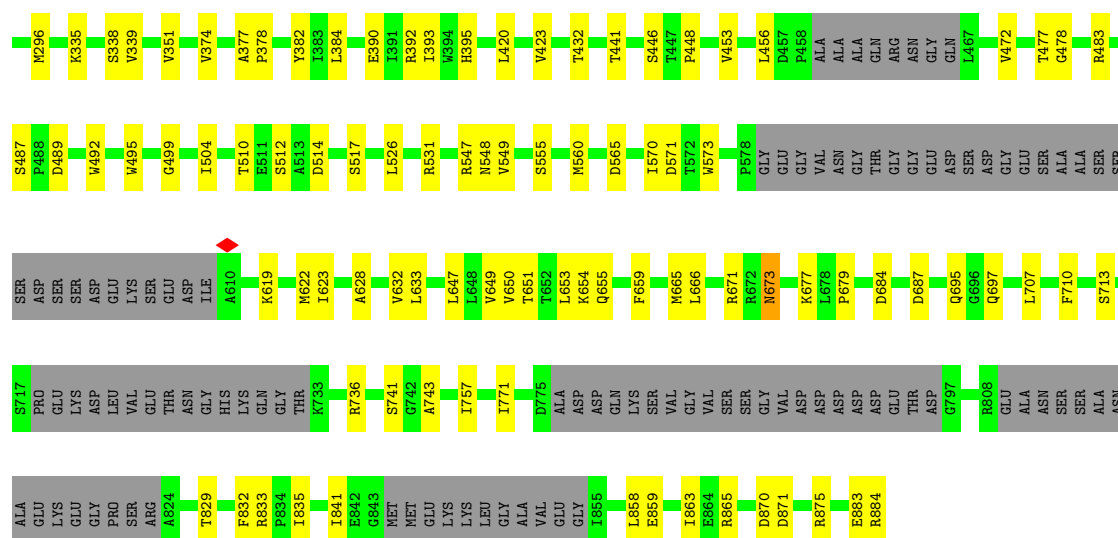
Chain UC: 11% 88%



• Molecule 4: UTP4

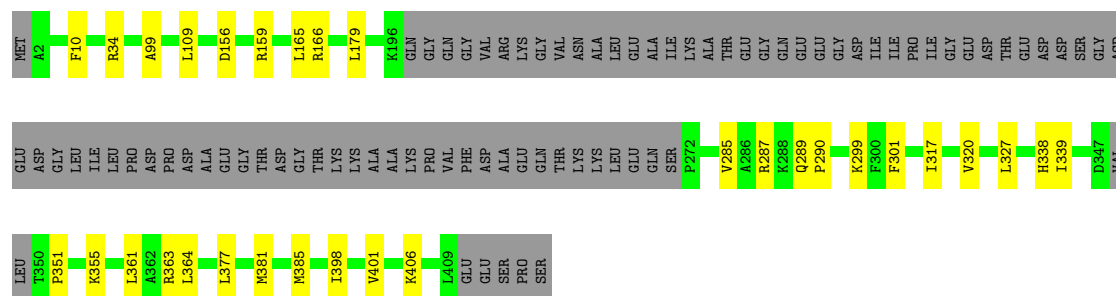
Chain UD: 74% 13% 12%





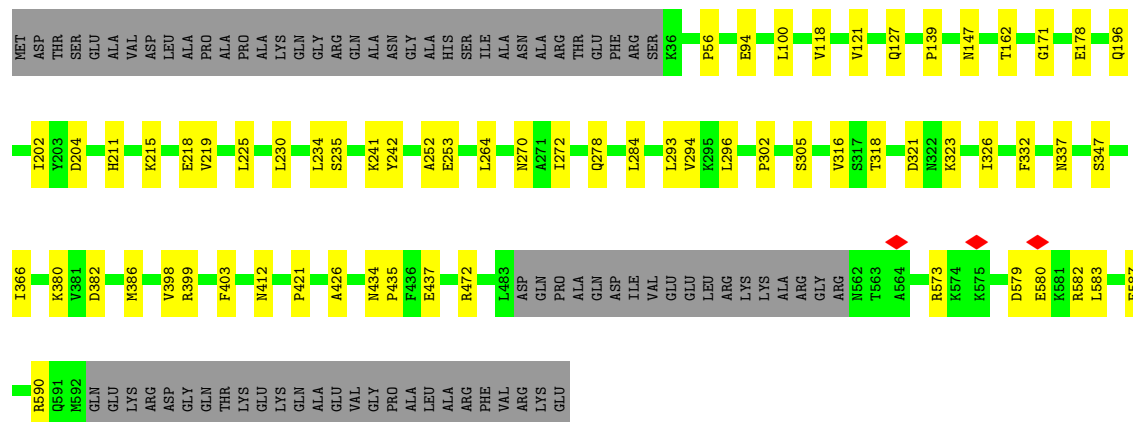
• Molecule 5: U3 snoRNP protein

Chain UF: 72% 7% 20%



• Molecule 6: U three protein 7

Chain UG: 74% 12% 14%



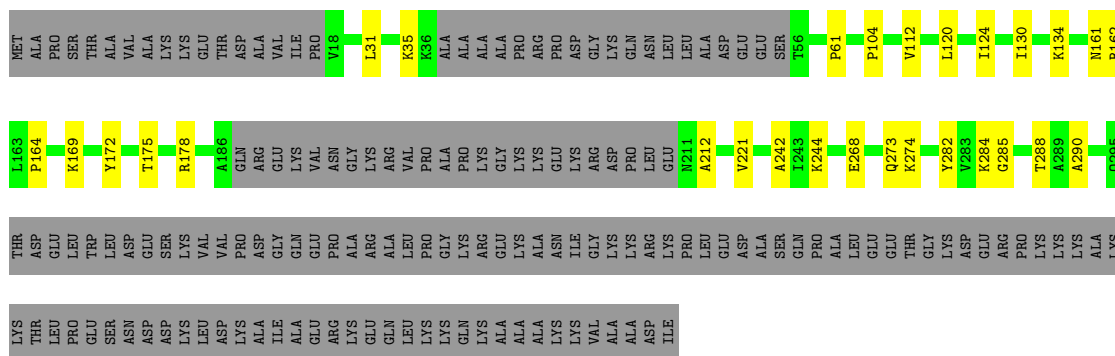
• Molecule 7: U3 small nucleolar RNA-associated protein 10

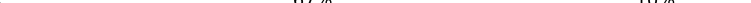
Chain UJ: 22% 75%

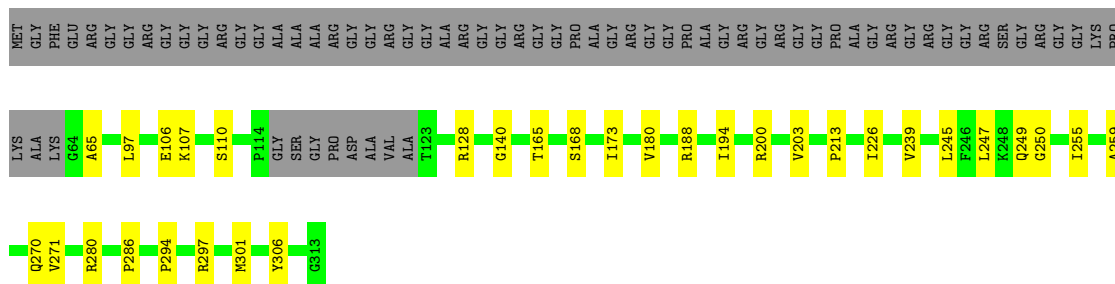


G-8	K-5	A1	R13	A16	V19	N57	N63	R67	M96	I112	A113	R114	R120	V135	Q139	R142	N149	D150	K154	I160	I165	V168	A181	PRO	ALA	SER
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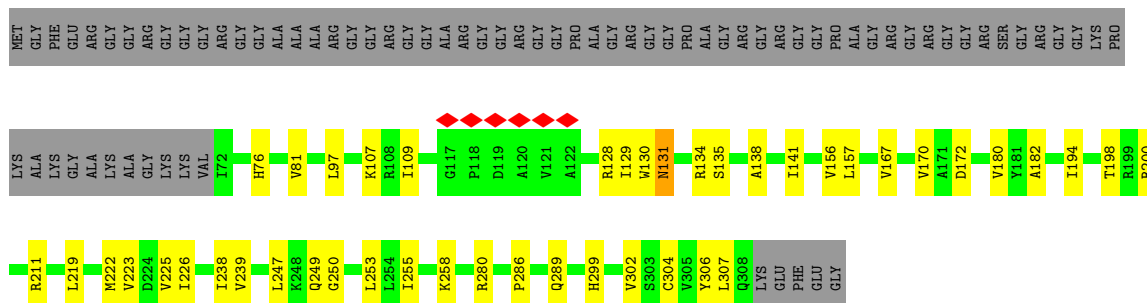
- Chain UZ:

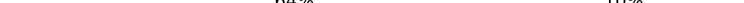


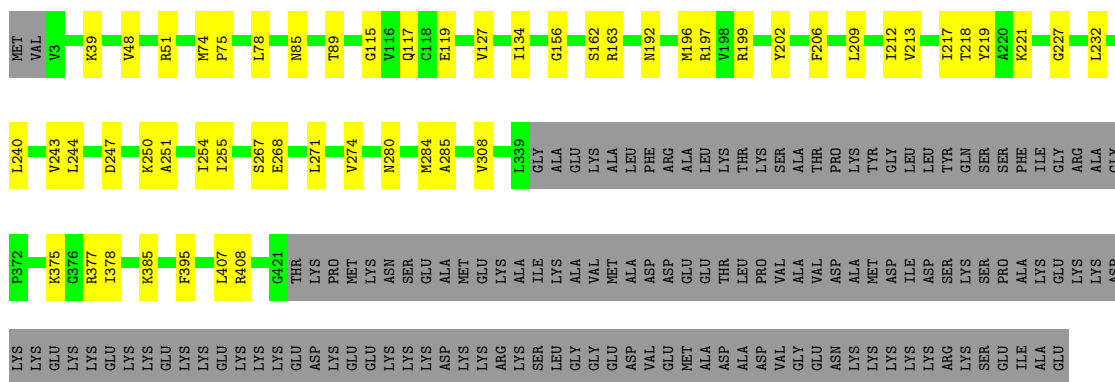
- Chain CA:  67% 10% 23%



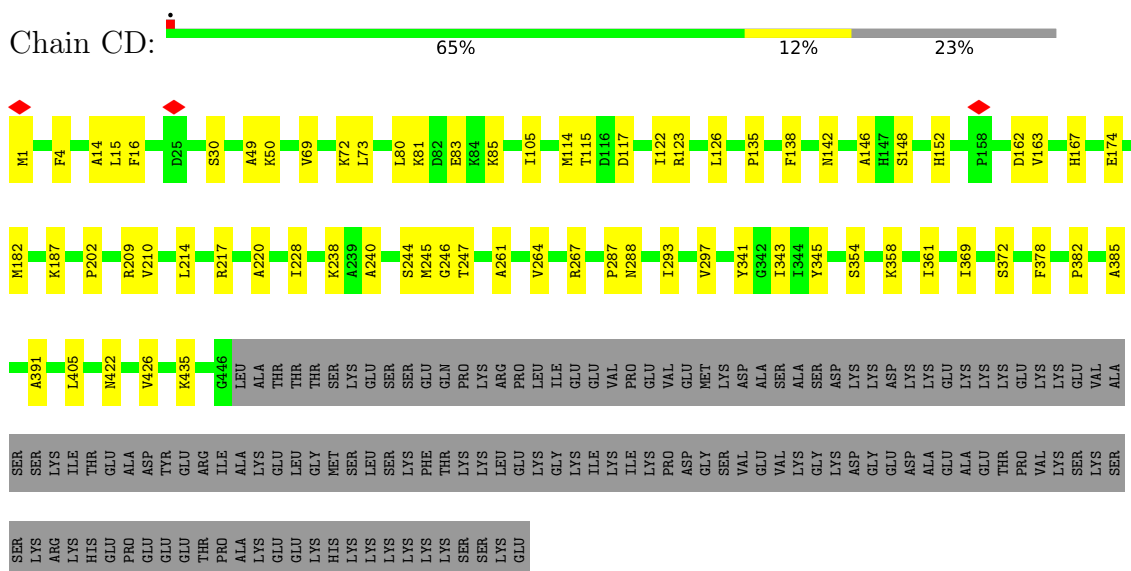
- Chain CB:



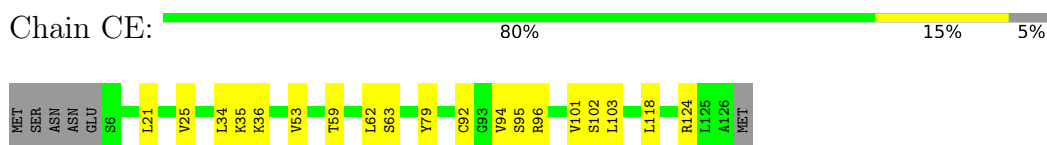
- Chain CC: 



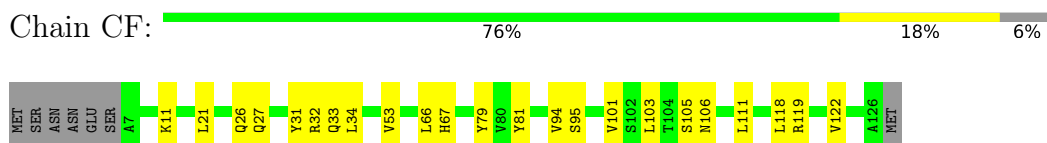
• Molecule 20: Nucleolar protein 58



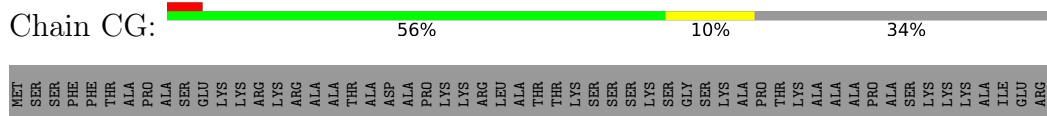
• Molecule 21: H/ACA ribonucleoprotein complex subunit 2

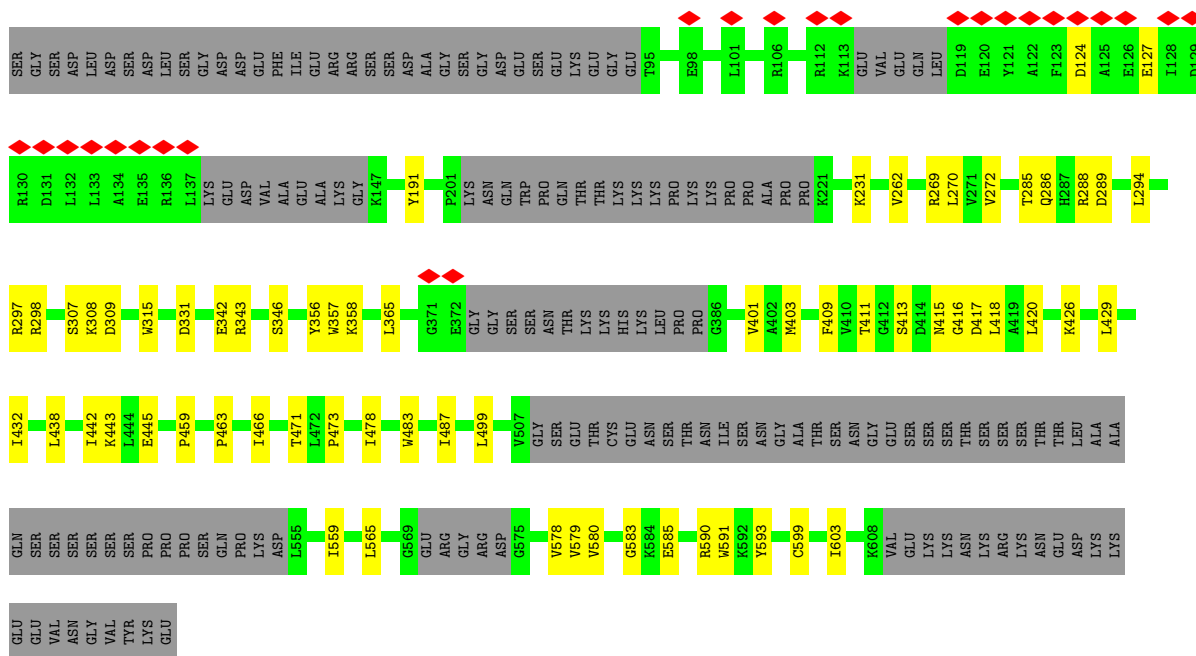


• Molecule 21: H/ACA ribonucleoprotein complex subunit 2

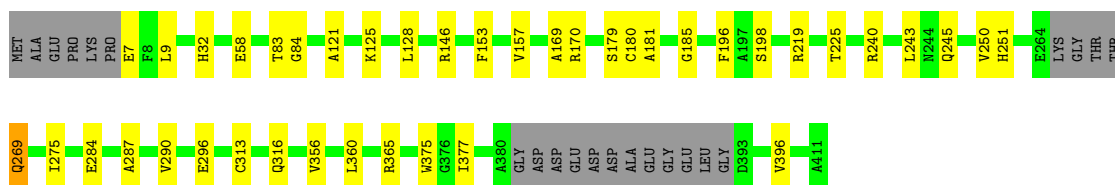
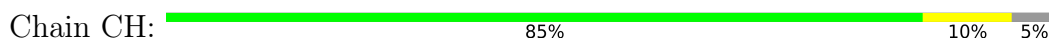


• Molecule 22: Ribosomal RNA-processing protein

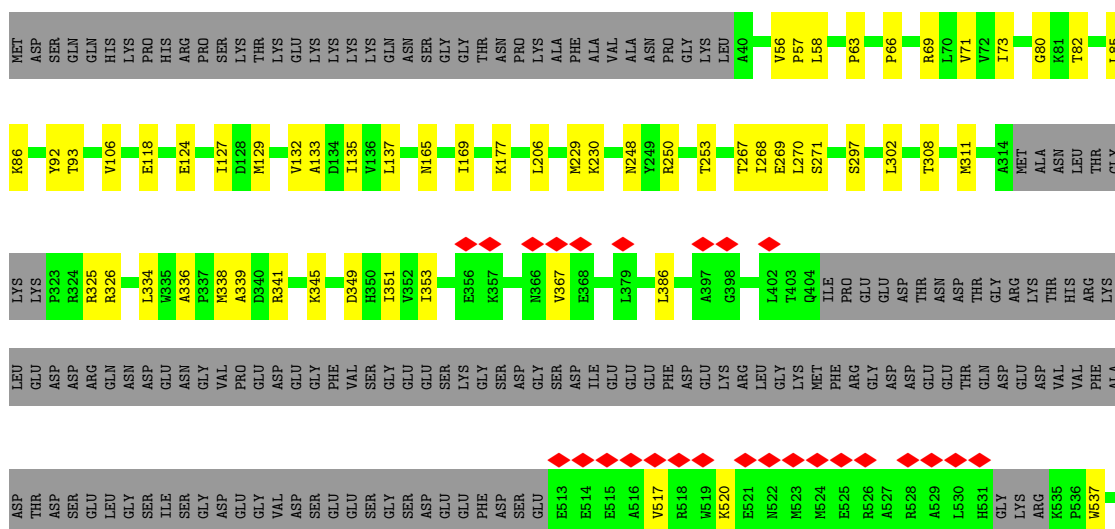


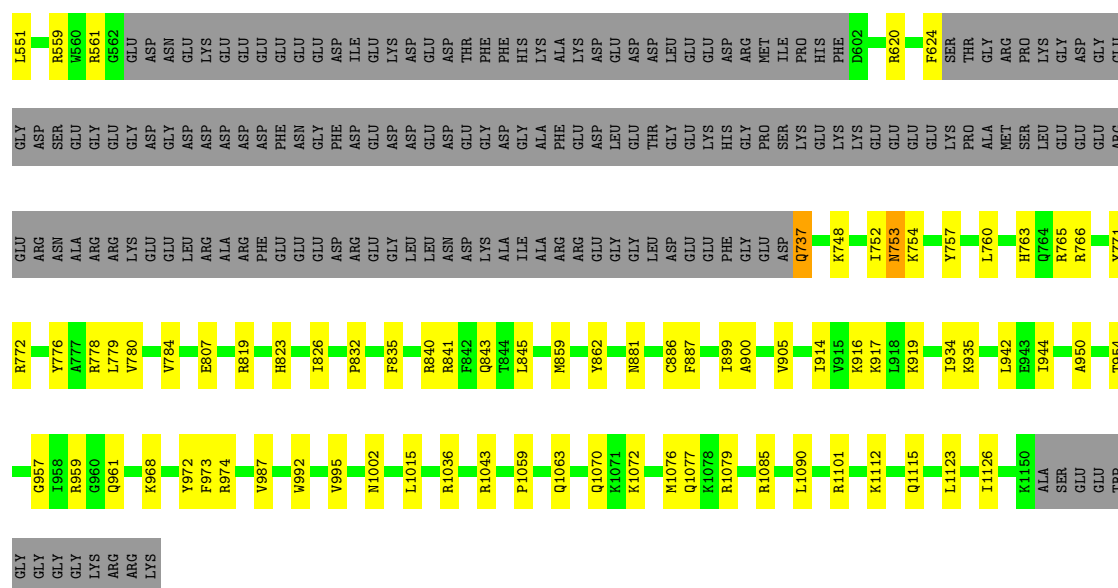


- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein.



- Molecule 24: Bms1-type G domain-containing protein





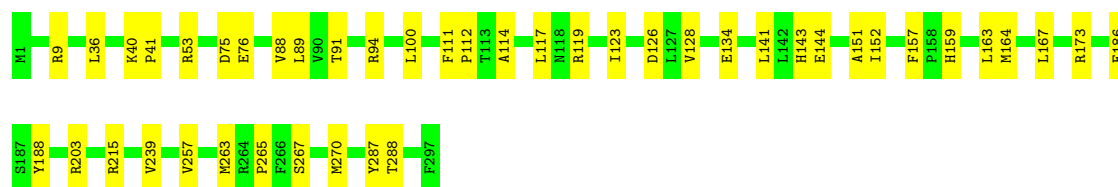
- Molecule 25: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CJ: 90% 8%



- Molecule 26: U3 small nucleolar ribonucleoprotein protein IMP4

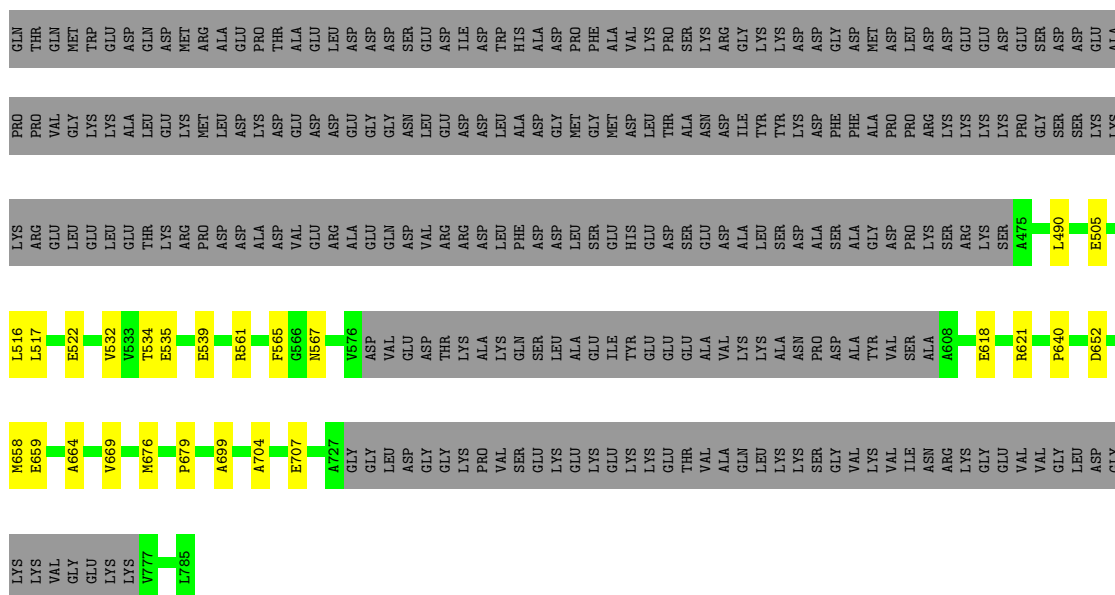
Chain CK: 85% 15%



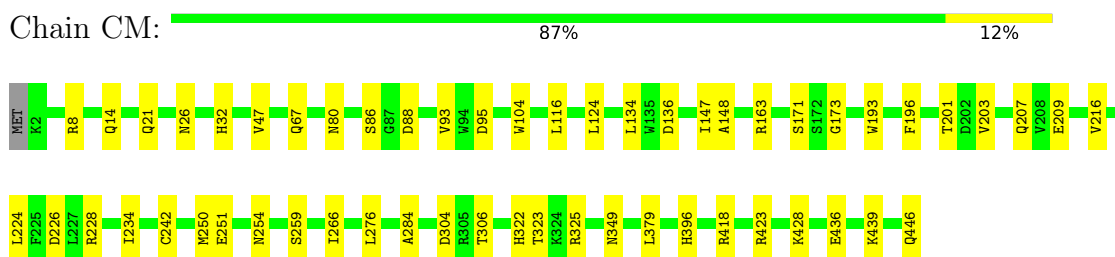
- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

Chain CL: 26% 71%

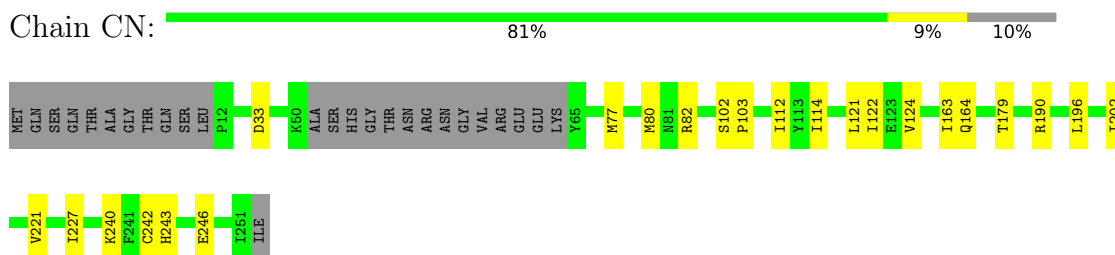




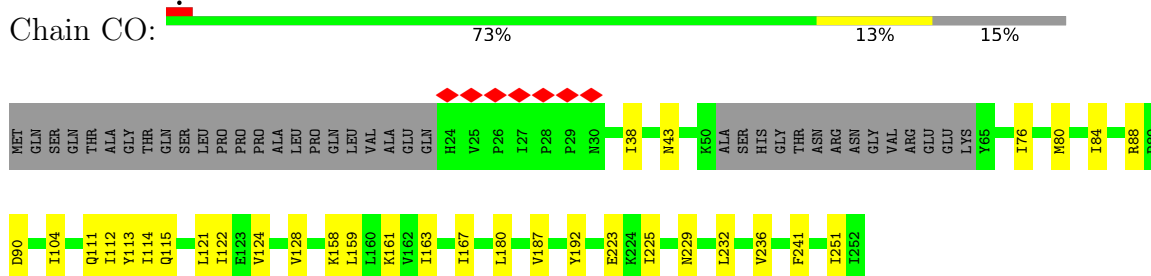
- Molecule 28: DDB1- and CUL4-associated factor 13



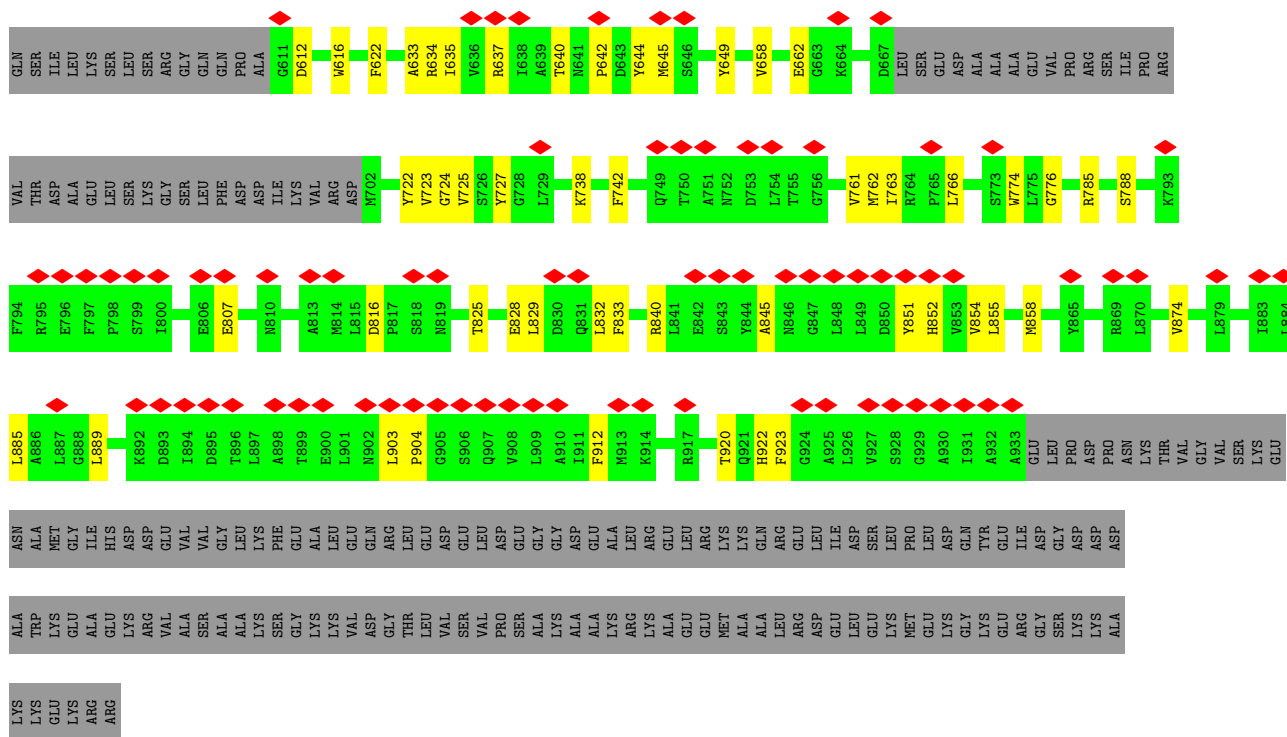
- Molecule 29: Nucleolar essential protein 1



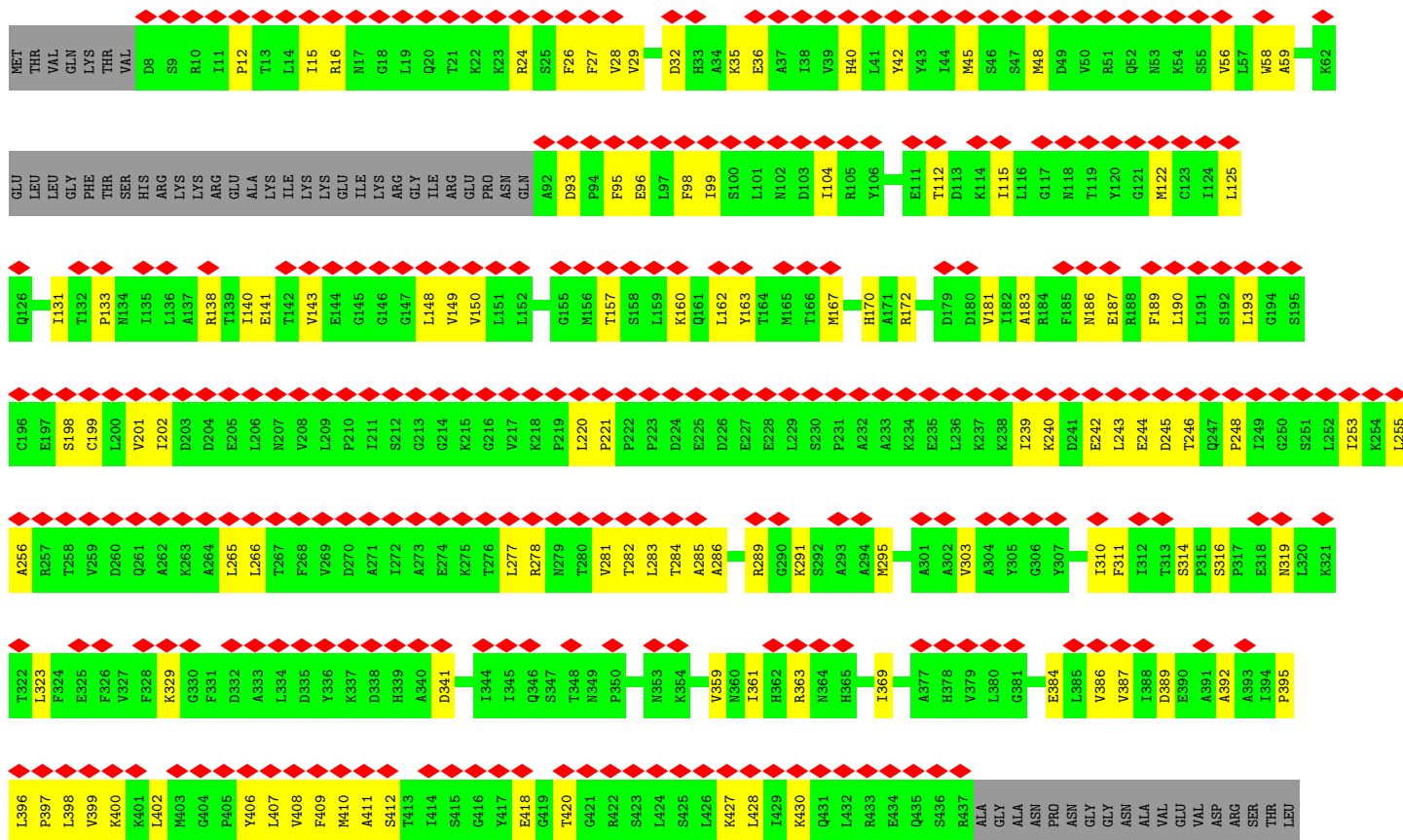
- Molecule 29: Nucleolar essential protein 1

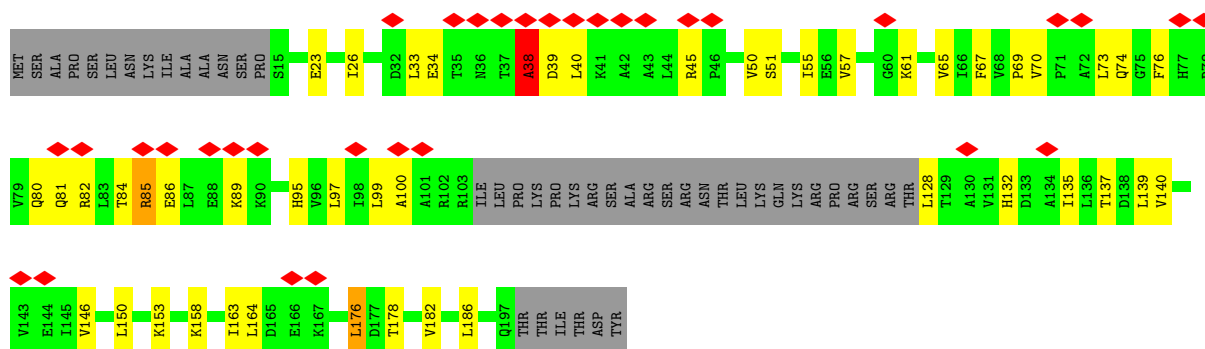


- Molecule 30: KRR1 small subunit processome component



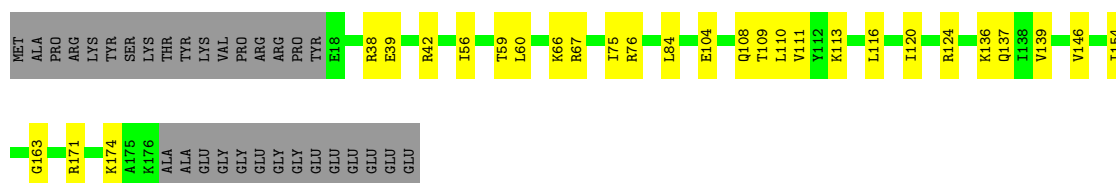
- Molecule 32: RNA cytidine acetyltransferase





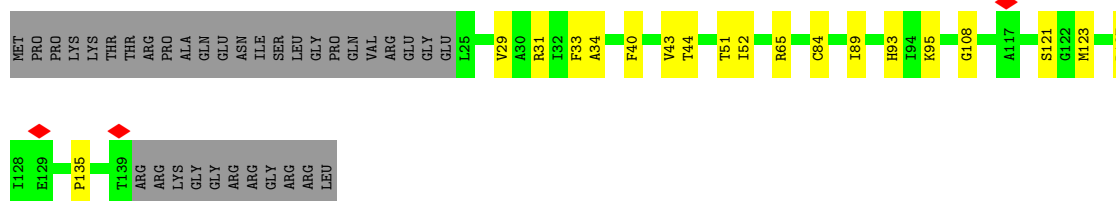
- Molecule 36: 40S ribosomal protein s9-like protein

Chain Cg: 69% 15% 16%



- Molecule 37: 40S ribosomal protein S14-like protein

Chain Ci: 64% 13% 23%



- Molecule 38: 40S ribosomal protein S16-like protein

Chain Cj: 81% 7% 12%



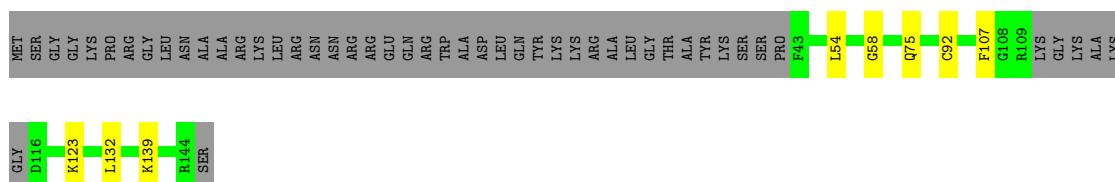
- Molecule 39: 40S ribosomal protein S22-like protein

Chain Cm: 80% 17% 3%

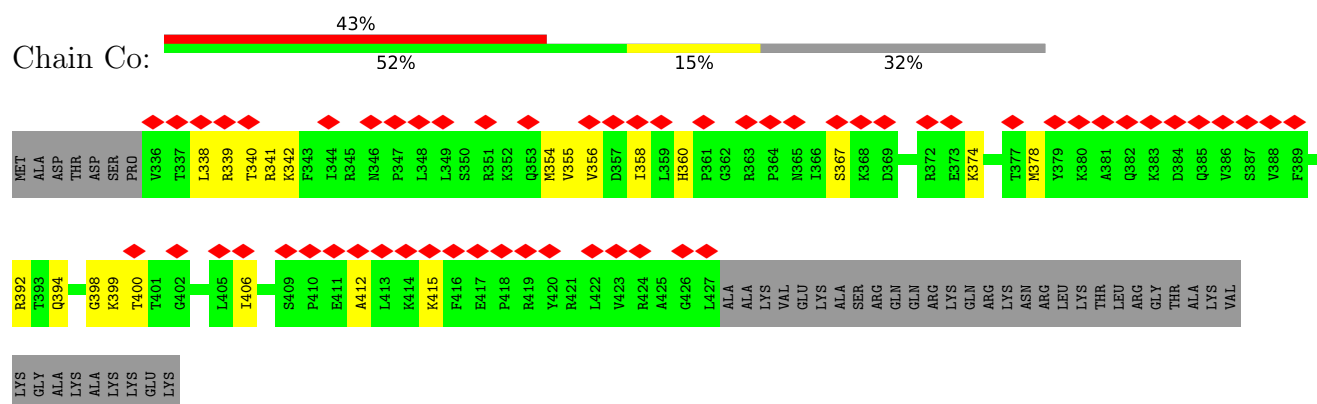


- Molecule 40: 40S ribosomal protein s23-like protein

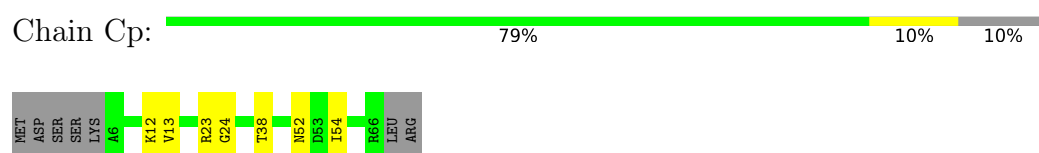
Chain Cn: 61% 6% 34%



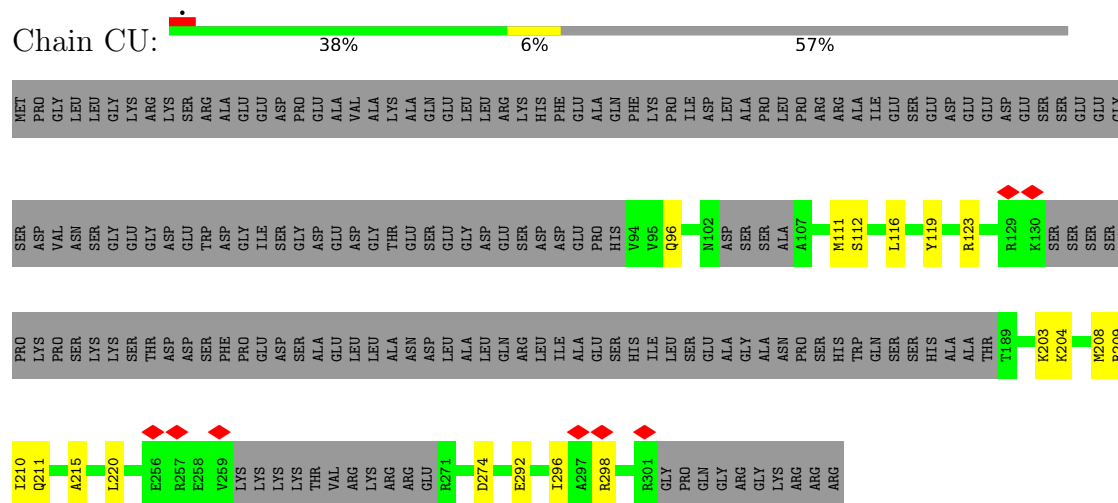
- Molecule 41: Small ribosomal subunit protein eS24



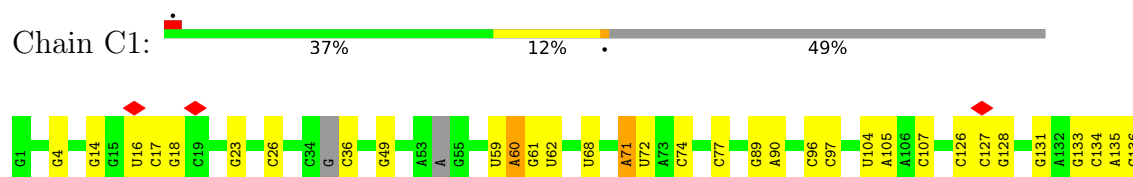
- Molecule 42: 40S ribosomal protein S28-like protein

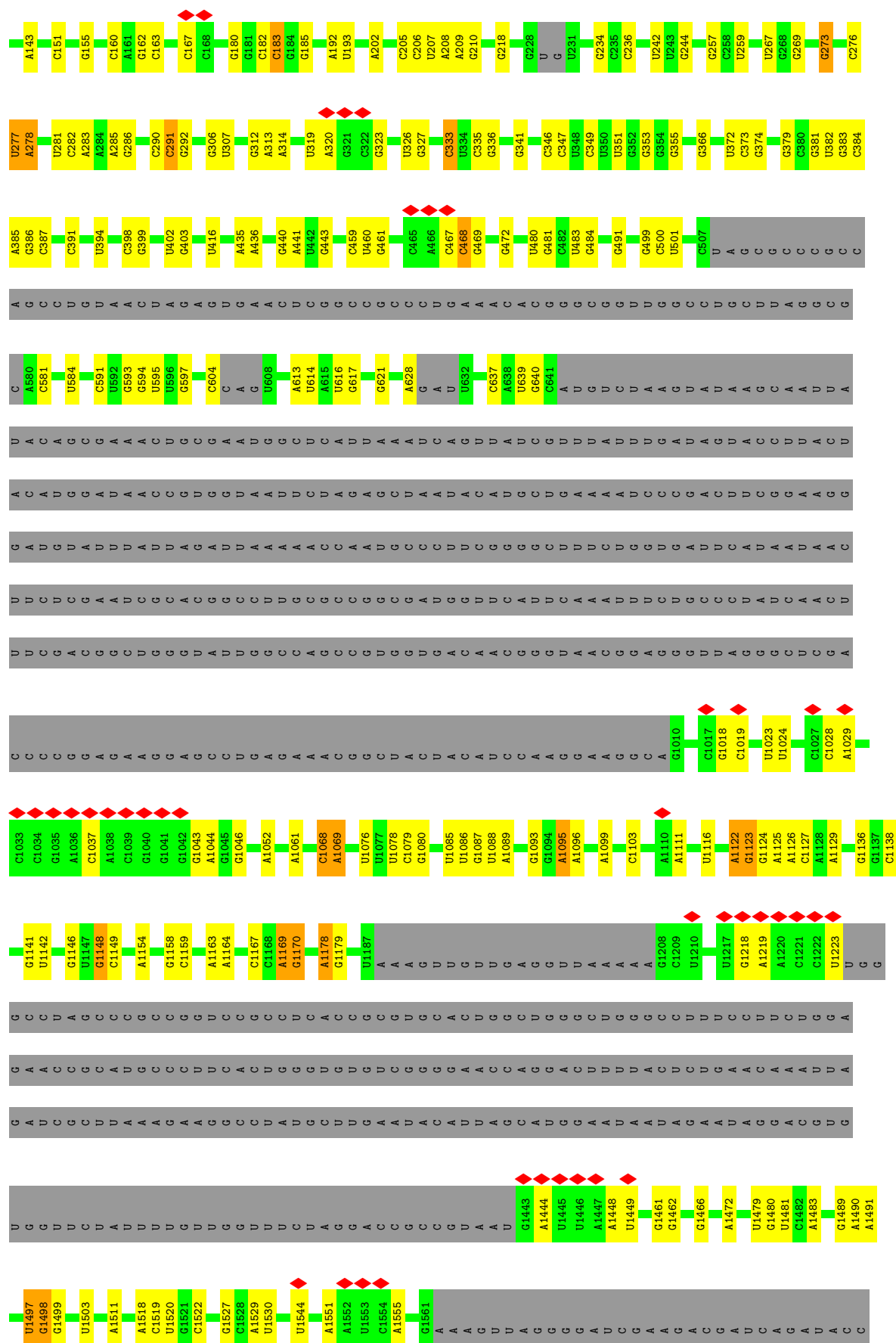


- Molecule 43: faf1

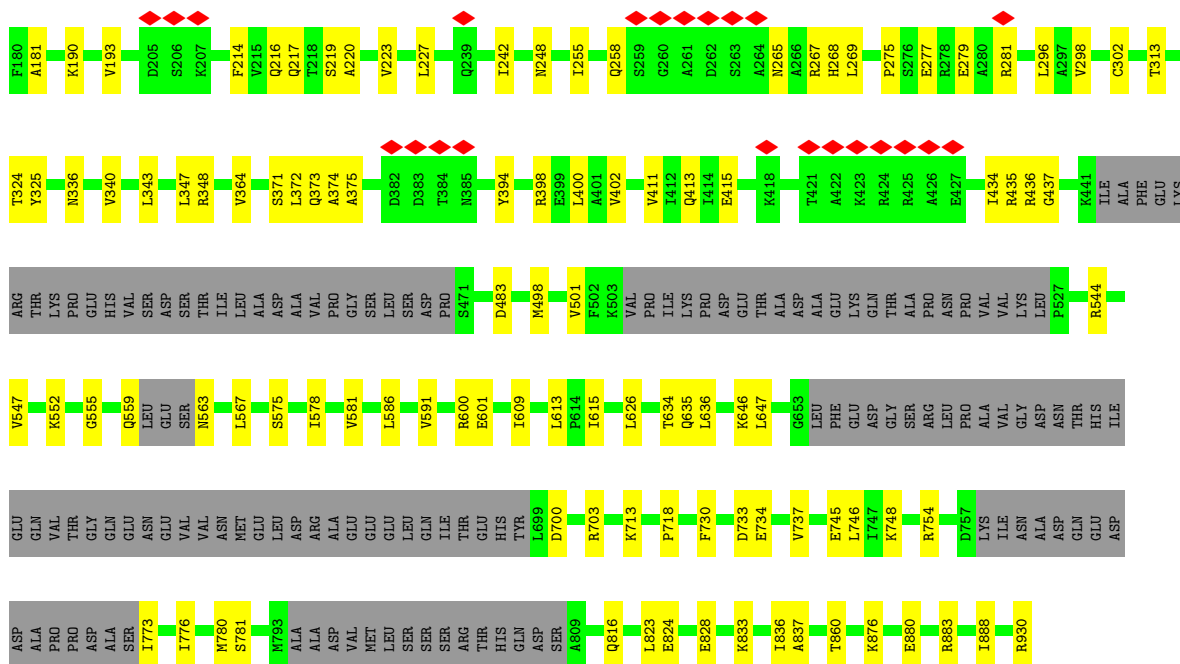


- Molecule 44: 35s rna

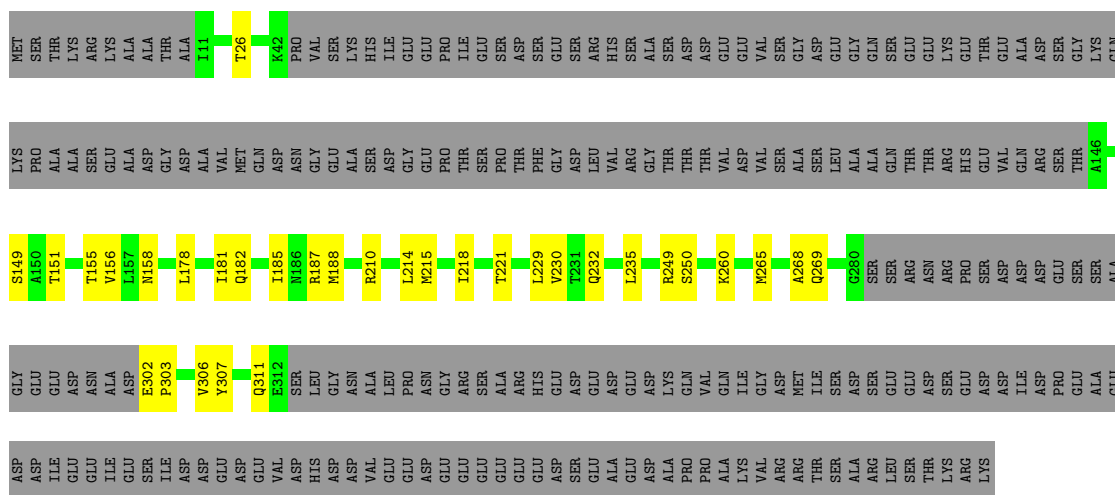
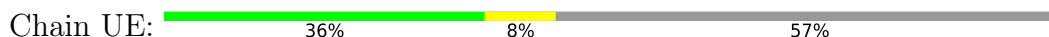




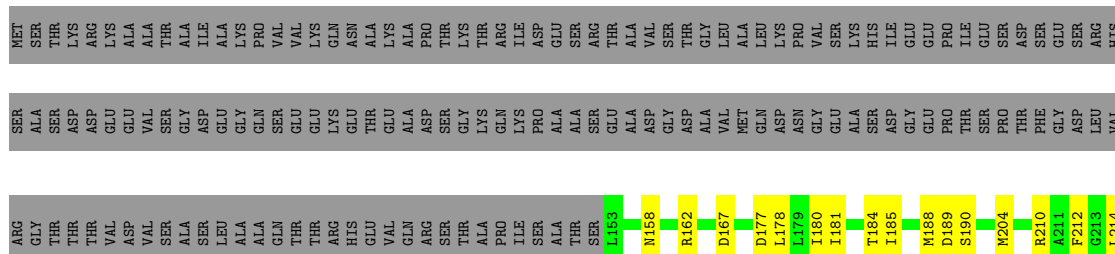


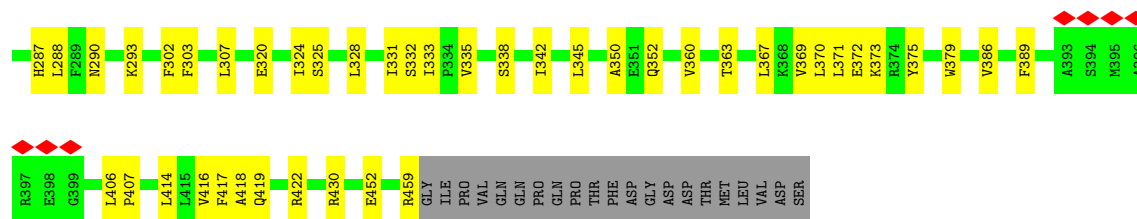


- Molecule 47: Small-subunit processome Utp12 domain-containing protein

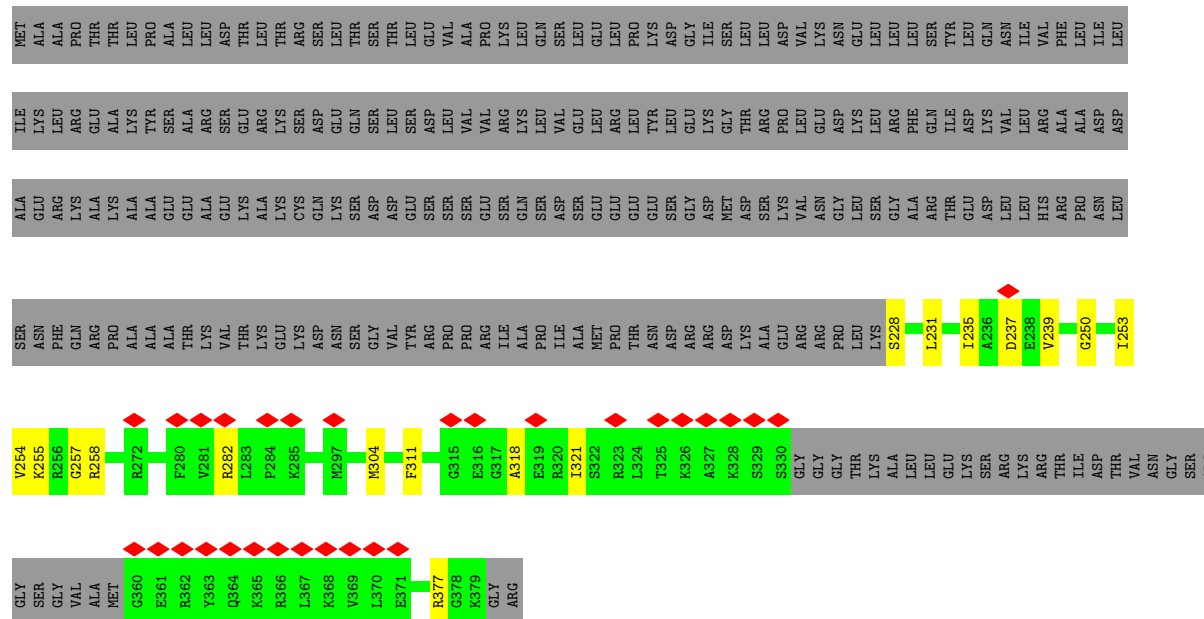


- Molecule 47: Small-subunit processome Utp12 domain-containing protein





- Molecule 51: U3 small nucleolar ribonucleoprotein protein lcp5-like protein



- Molecule 52: utp16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	501.59998, 501.59998, 501.59998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	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, ADP, MG, ZN, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	UA	0.20	0/6555	0.50	0/8909
2	UB	0.20	0/4592	0.49	0/6178
3	UC	0.17	0/638	0.45	0/845
4	UD	0.18	0/6250	0.46	0/8465
5	UF	0.20	0/2665	0.46	0/3606
6	UG	0.21	0/3838	0.50	0/5181
7	UJ	0.21	0/3471	0.49	0/4709
8	UK	0.18	0/1713	0.40	0/2266
9	UL	0.19	0/6299	0.52	2/8531 (0.0%)
10	UM	0.19	0/6680	0.50	0/9090
11	UN	0.21	0/1425	0.45	0/1913
12	UO	0.20	0/3895	0.49	0/5302
13	UQ	0.17	0/6140	0.46	2/8352 (0.0%)
14	UR	0.18	0/3560	0.46	0/4809
15	UU	0.20	0/6947	0.49	4/9452 (0.0%)
16	UX	0.20	0/1503	0.47	0/2022
17	UZ	0.20	0/1857	0.51	0/2526
18	CA	0.20	0/1814	0.46	0/2456
18	CB	0.21	0/1853	0.54	0/2511
19	CC	0.21	0/2911	0.50	0/3937
20	CD	0.21	0/3412	0.53	0/4617
21	CE	0.25	0/891	0.53	0/1214
21	CF	0.22	0/876	0.56	2/1195 (0.2%)
22	CG	0.19	0/3307	0.52	0/4462
23	CH	0.18	0/2939	0.47	0/3988
24	CI	0.19	0/6813	0.49	2/9182 (0.0%)
25	CJ	0.22	0/1462	0.46	0/1967
26	CK	0.20	0/2376	0.46	0/3214
27	CL	0.18	0/1812	0.41	0/2437
28	CM	0.20	0/3573	0.49	0/4829
29	CN	0.22	0/1797	0.51	0/2443
29	CO	0.22	0/1714	0.52	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.22	0/1655	0.58	0/2229
31	CQ	0.20	0/1436	0.47	0/1932
32	CR	0.21	0/6809	0.58	1/9215 (0.0%)
32	CS	0.21	0/6722	0.55	0/9099
33	CT	0.17	0/1053	0.45	0/1413
34	Cc	0.19	0/1485	0.45	0/2008
35	Ce	0.27	0/1298	0.75	4/1750 (0.2%)
36	Cg	0.20	0/1265	0.49	0/1694
37	Ci	0.19	0/819	0.51	0/1107
38	Cj	0.24	0/958	0.50	0/1293
39	Cm	0.23	0/1001	0.56	0/1345
40	Cn	0.15	0/712	0.41	0/954
41	Co	0.20	0/754	0.49	0/1011
42	Cp	0.21	0/461	0.50	0/620
43	CU	0.17	0/1041	0.48	0/1387
44	C1	0.12	0/28360	0.24	0/44174
45	C2	0.13	0/5434	0.23	0/8459
46	UH	0.19	0/6301	0.51	0/8526
47	UE	0.24	0/1374	0.53	0/1852
47	UI	0.26	0/1005	0.67	0/1352
48	US	0.23	0/3765	0.60	7/5100 (0.1%)
49	Cl	0.25	0/638	0.67	0/857
50	CX	0.27	0/2180	0.71	1/2956 (0.0%)
51	CY	0.21	0/986	0.58	0/1303
52	UP	0.14	0/428	0.37	0/570
All	All	0.19	0/183518	0.47	25/255139 (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	2
13	UQ	0	1
30	CP	0	1
35	Ce	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CI	753	ASN	CA-C-N	8.11	137.03	121.54
24	CI	753	ASN	C-N-CA	8.11	137.03	121.54
35	Ce	38	ALA	CA-C-N	6.68	133.73	121.70
35	Ce	38	ALA	C-N-CA	6.68	133.73	121.70
21	CF	67	HIS	CA-C-N	5.76	123.87	120.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	CP	189	MET	Peptide
35	Ce	38	ALA	Peptide
1	UA	316	ALA	Peptide
1	UA	645	ALA	Peptide
13	UQ	849	ALA	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	6411	0	6305	53	0
2	UB	4506	0	4633	57	0
3	UC	630	0	687	5	0
4	UD	6108	0	6108	71	0
5	UF	2599	0	2650	20	0
6	UG	3765	0	3800	41	0
7	UJ	3412	0	3519	34	0
8	UK	1699	0	1832	14	0
9	UL	6175	0	6188	91	0
10	UM	6545	0	6547	107	0
11	UN	1401	0	1455	10	0
12	UO	3811	0	3861	42	0
13	UQ	6012	0	6044	71	0
14	UR	3498	0	3508	20	0
15	UU	6778	0	6782	56	0
16	UX	1480	0	1554	15	0
17	UZ	1815	0	1896	17	0
18	CA	1778	0	1830	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CB	1816	0	1847	31	0
19	CC	2866	0	2960	38	0
20	CD	3355	0	3483	42	0
21	CE	879	0	918	12	0
21	CF	864	0	900	15	0
22	CG	3245	0	3262	38	0
23	CH	2888	0	2979	27	0
24	CI	6666	0	6825	100	0
25	CJ	1434	0	1482	11	0
26	CK	2329	0	2373	27	0
27	CL	1786	0	1826	19	0
28	CM	3501	0	3498	34	0
29	CN	1762	0	1807	15	0
29	CO	1683	0	1726	20	0
30	CP	1625	0	1718	27	0
31	CQ	1413	0	1479	8	0
32	CR	6677	0	6809	122	0
32	CS	6591	0	6674	143	0
33	CT	1035	0	1063	12	0
34	Cc	1464	0	1504	13	0
35	Ce	1279	0	1322	29	0
36	Cg	1248	0	1365	21	0
37	Ci	808	0	831	14	0
38	Cj	943	0	1002	8	0
39	Cm	985	0	1021	12	0
40	Cn	702	0	750	5	0
41	Co	741	0	785	12	0
42	Cp	458	0	489	7	0
43	CU	1035	0	1093	13	0
44	C1	25383	0	12859	89	0
45	C2	4869	0	2465	9	0
46	UH	6198	0	6272	82	0
47	UE	1362	0	1440	24	0
47	UI	996	0	1054	28	0
48	US	3672	0	3679	48	0
49	Cl	633	0	676	7	0
50	CX	2130	0	2219	41	0
51	CY	979	0	995	15	0
52	UP	422	0	457	4	0
53	UX	1	0	0	0	0
54	CI	32	0	12	1	0
55	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CS	27	0	12	0	0
All	All	177206	0	165130	1734	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1734 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:441:THR:HA	4:UD:456:LEU:O	1.24	1.37
12:UO:333:HIS:HA	12:UO:346:ARG:O	1.40	1.22
46:UH:555:GLY:O	46:UH:567:LEU:HA	1.39	1.19
15:UU:159:ILE:O	15:UU:172:THR:HA	1.52	1.08
12:UO:335:ALA:HA	12:UO:344:SER:O	1.55	1.06

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	834/904 (92%)	802 (96%)	32 (4%)	0	100	100
2	UB	556/907 (61%)	538 (97%)	18 (3%)	0	100	100
3	UC	77/648 (12%)	75 (97%)	2 (3%)	0	100	100
4	UD	761/884 (86%)	731 (96%)	30 (4%)	0	100	100
5	UF	325/414 (78%)	319 (98%)	6 (2%)	0	100	100
6	UG	475/558 (85%)	460 (97%)	14 (3%)	1 (0%)	43	76
7	UJ	445/1802 (25%)	435 (98%)	10 (2%)	0	100	100
8	UK	211/270 (78%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	UL	767/962 (80%)	728 (95%)	39 (5%)	0	100	100
10	UM	835/912 (92%)	794 (95%)	41 (5%)	0	100	100
11	UN	171/708 (24%)	166 (97%)	5 (3%)	0	100	100
12	UO	497/557 (89%)	476 (96%)	20 (4%)	1 (0%)	43	76
13	UQ	775/960 (81%)	738 (95%)	36 (5%)	1 (0%)	48	80
14	UR	436/618 (71%)	427 (98%)	9 (2%)	0	100	100
15	UU	896/1049 (85%)	859 (96%)	37 (4%)	0	100	100
16	UX	188/193 (97%)	178 (95%)	10 (5%)	0	100	100
17	UZ	229/391 (59%)	216 (94%)	13 (6%)	0	100	100
18	CA	238/313 (76%)	230 (97%)	8 (3%)	0	100	100
18	CB	235/313 (75%)	226 (96%)	9 (4%)	0	100	100
19	CC	383/523 (73%)	369 (96%)	14 (4%)	0	100	100
20	CD	444/582 (76%)	428 (96%)	16 (4%)	0	100	100
21	CE	119/127 (94%)	113 (95%)	6 (5%)	0	100	100
21	CF	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
22	CG	402/630 (64%)	386 (96%)	16 (4%)	0	100	100
23	CH	383/411 (93%)	370 (97%)	13 (3%)	0	100	100
24	CI	829/1163 (71%)	801 (97%)	27 (3%)	1 (0%)	48	80
25	CJ	177/183 (97%)	175 (99%)	2 (1%)	0	100	100
26	CK	295/297 (99%)	287 (97%)	8 (3%)	0	100	100
27	CL	225/785 (29%)	217 (96%)	7 (3%)	1 (0%)	30	65
28	CM	443/446 (99%)	428 (97%)	15 (3%)	0	100	100
29	CN	222/252 (88%)	211 (95%)	11 (5%)	0	100	100
29	CO	211/252 (84%)	203 (96%)	8 (4%)	0	100	100
30	CP	197/322 (61%)	192 (98%)	5 (2%)	0	100	100
31	CQ	178/259 (69%)	174 (98%)	4 (2%)	0	100	100
32	CR	836/1073 (78%)	807 (96%)	29 (4%)	0	100	100
32	CS	826/1073 (77%)	791 (96%)	35 (4%)	0	100	100
33	CT	127/203 (63%)	122 (96%)	5 (4%)	0	100	100
34	Cc	188/212 (89%)	180 (96%)	7 (4%)	1 (0%)	24	60
35	Ce	155/203 (76%)	141 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Cg	157/190 (83%)	157 (100%)	0	0	100	100
37	Ci	113/150 (75%)	111 (98%)	2 (2%)	0	100	100
38	Cj	124/143 (87%)	119 (96%)	5 (4%)	0	100	100
39	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
40	Cn	92/145 (63%)	90 (98%)	2 (2%)	0	100	100
41	Co	90/136 (66%)	82 (91%)	7 (8%)	1 (1%)	11	43
42	Cp	59/68 (87%)	53 (90%)	6 (10%)	0	100	100
43	CU	127/311 (41%)	122 (96%)	5 (4%)	0	100	100
46	UH	787/930 (85%)	766 (97%)	21 (3%)	0	100	100
47	UE	172/410 (42%)	158 (92%)	14 (8%)	0	100	100
47	UI	126/410 (31%)	122 (97%)	4 (3%)	0	100	100
48	US	443/549 (81%)	425 (96%)	16 (4%)	2 (0%)	24	60
49	Cl	78/156 (50%)	70 (90%)	8 (10%)	0	100	100
50	CX	265/480 (55%)	249 (94%)	16 (6%)	0	100	100
51	CY	119/381 (31%)	118 (99%)	1 (1%)	0	100	100
52	UP	52/364 (14%)	48 (92%)	4 (8%)	0	100	100
All	All	18635/27439 (68%)	17922 (96%)	704 (4%)	9 (0%)	100	100

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	Cc	88	GLY
6	UG	56	PRO
12	UO	130	GLN
48	US	241	GLU
13	UQ	447	SER

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	662/774 (86%)	662 (100%)	0	100	100
2	UB	474/788 (60%)	473 (100%)	1 (0%)	87	92
3	UC	67/536 (12%)	67 (100%)	0	100	100
4	UD	657/738 (89%)	656 (100%)	1 (0%)	87	92
5	UF	250/341 (73%)	250 (100%)	0	100	100
6	UG	386/474 (81%)	386 (100%)	0	100	100
7	UJ	355/1526 (23%)	355 (100%)	0	100	100
8	UK	162/227 (71%)	162 (100%)	0	100	100
9	UL	667/821 (81%)	667 (100%)	0	100	100
10	UM	712/770 (92%)	712 (100%)	0	100	100
11	UN	146/576 (25%)	146 (100%)	0	100	100
12	UO	403/456 (88%)	403 (100%)	0	100	100
13	UQ	651/817 (80%)	651 (100%)	0	100	100
14	UR	360/523 (69%)	360 (100%)	0	100	100
15	UU	677/863 (78%)	677 (100%)	0	100	100
16	UX	152/167 (91%)	152 (100%)	0	100	100
17	UZ	186/329 (56%)	186 (100%)	0	100	100
18	CA	175/228 (77%)	175 (100%)	0	100	100
18	CB	195/228 (86%)	194 (100%)	1 (0%)	81	89
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	344/489 (70%)	344 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	331 (100%)	0	100	100
23	CH	303/320 (95%)	302 (100%)	1 (0%)	86	91
24	CI	681/1009 (68%)	680 (100%)	1 (0%)	88	93
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	245 (100%)	0	100	100
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	364 (100%)	0	100	100
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	CP	177/287 (62%)	177 (100%)	0	100	100
31	CQ	151/215 (70%)	151 (100%)	0	100	100
32	CR	731/916 (80%)	731 (100%)	0	100	100
32	CS	722/916 (79%)	722 (100%)	0	100	100
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Cc	149/178 (84%)	149 (100%)	0	100	100
35	Ce	137/177 (77%)	137 (100%)	0	100	100
36	Cg	123/162 (76%)	123 (100%)	0	100	100
37	Ci	78/117 (67%)	78 (100%)	0	100	100
38	Cj	92/115 (80%)	92 (100%)	0	100	100
39	Cm	103/113 (91%)	103 (100%)	0	100	100
40	Cn	70/116 (60%)	70 (100%)	0	100	100
41	Co	79/115 (69%)	79 (100%)	0	100	100
42	Cp	47/61 (77%)	47 (100%)	0	100	100
43	CU	106/260 (41%)	106 (100%)	0	100	100
46	UH	674/788 (86%)	673 (100%)	1 (0%)	88	93
47	UE	148/346 (43%)	148 (100%)	0	100	100
47	UI	108/346 (31%)	108 (100%)	0	100	100
48	US	404/493 (82%)	404 (100%)	0	100	100
49	Cl	71/135 (53%)	71 (100%)	0	100	100
50	CX	227/411 (55%)	227 (100%)	0	100	100
51	CY	100/322 (31%)	100 (100%)	0	100	100
52	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	15443/23152 (67%)	15437 (100%)	6 (0%)	100	100

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	CH	269	GLN
24	CI	737	GLN
46	UH	373	GLN
4	UD	673	ASN
2	UB	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
32	CS	261	GLN
48	US	468	HIS
34	Cc	103	HIS
46	UH	216	GLN
10	UM	579	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	C1	1171/2350 (49%)	224 (19%)	13 (1%)
45	C2	225/274 (82%)	51 (22%)	1 (0%)
All	All	1396/2624 (53%)	275 (19%)	14 (1%)

5 of 275 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	C1	4	G
44	C1	14	G
44	C1	16	U
44	C1	17	C
44	C1	18	G

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	C1	1087	G
44	C1	1163	A
45	C2	255	U
44	C1	2177	G
44	C1	2219	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	UA	646	1	8,9,10	1.53	1 (12%)	8,12,14	1.56	2 (25%)
14	SEP	UR	139	14	8,9,10	1.53	1 (12%)	8,12,14	1.64	2 (25%)

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
1	SEP	UA	646	1	-	0/5/8/10	-
14	SEP	UR	139	14	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	646	SEP	P-O1P	3.35	1.61	1.50
14	UR	139	SEP	P-O1P	3.34	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	UR	139	SEP	P-OG-CB	-3.05	109.89	118.30
14	UR	139	SEP	OG-CB-CA	2.95	111.01	108.14
1	UA	646	SEP	P-OG-CB	-2.84	110.47	118.30
1	UA	646	SEP	OG-CB-CA	2.78	110.85	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
56	ADP	CS	1101	-	27,29,29	1.36	4 (14%)	42,45,45	1.95	11 (26%)
54	GTP	CI	1201	55	30,34,34	0.83	1 (3%)	46,54,54	1.70	12 (26%)

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
56	ADP	CS	1101	-	-	3/16/32/32	0/3/3/3
54	GTP	CI	1201	55	-	6/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CS	1101	ADP	C5-C4	4.55	1.47	1.39
56	CS	1101	ADP	C5-C6	2.74	1.48	1.41
56	CS	1101	ADP	C8-N7	2.48	1.36	1.31
54	CI	1201	GTP	C2-N3	2.18	1.38	1.33
56	CS	1101	ADP	C5-N7	-2.12	1.35	1.39

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	CS	1101	ADP	C5-C4-N3	-6.21	118.65	126.75
54	CI	1201	GTP	C5-C4-N3	-4.93	120.46	128.46
56	CS	1101	ADP	N3-C4-N9	4.84	135.06	127.08
54	CI	1201	GTP	C2-N3-C4	4.42	120.18	112.30
56	CS	1101	ADP	C2-N3-C4	3.90	120.96	111.75

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

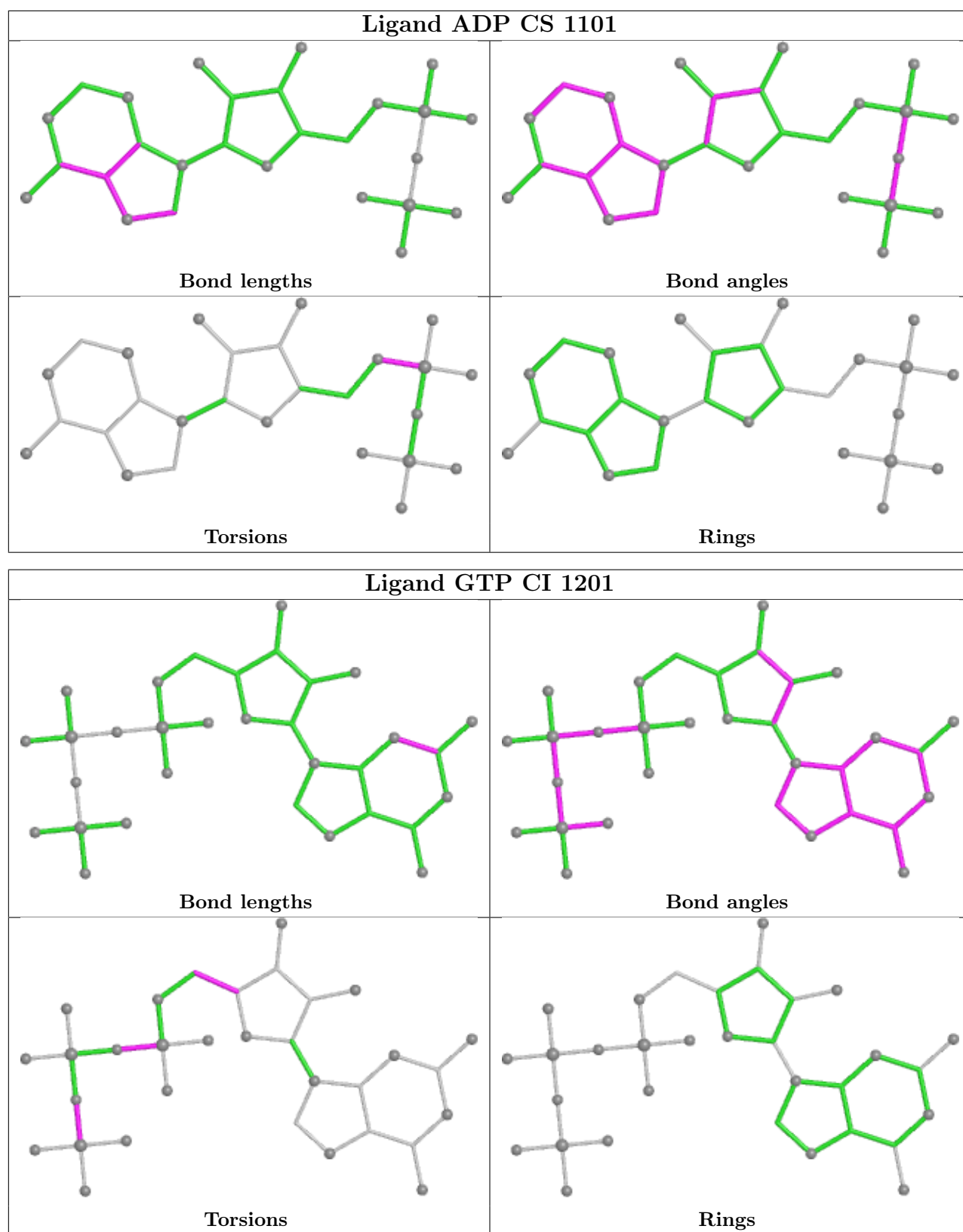
Mol	Chain	Res	Type	Atoms
54	CI	1201	GTP	PB-O3B-PG-O3G
56	CS	1101	ADP	C5'-O5'-PA-O1A
56	CS	1101	ADP	C5'-O5'-PA-O2A
54	CI	1201	GTP	O4'-C4'-C5'-O5'
54	CI	1201	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CI	1201	GTP	1	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

There are no chain breaks in this entry.

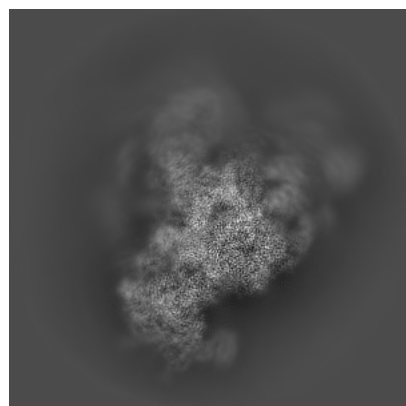
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66685. These allow visual inspection of the internal detail of the map and identification of artifacts.

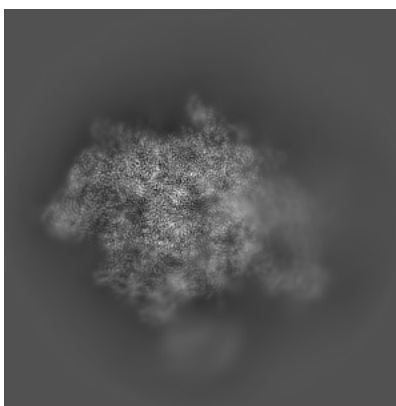
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

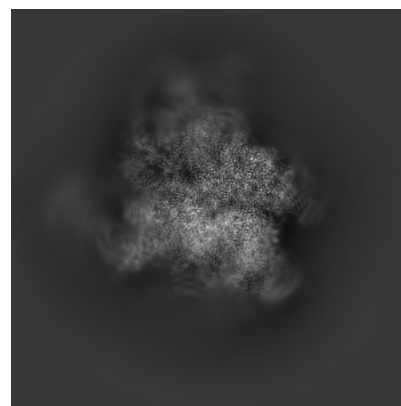
6.1.1 Primary map



X

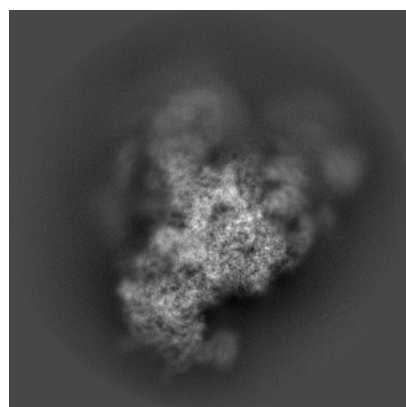


Y

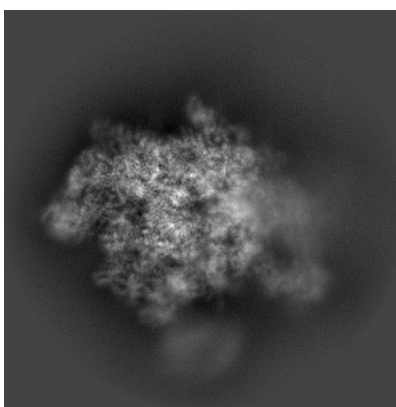


Z

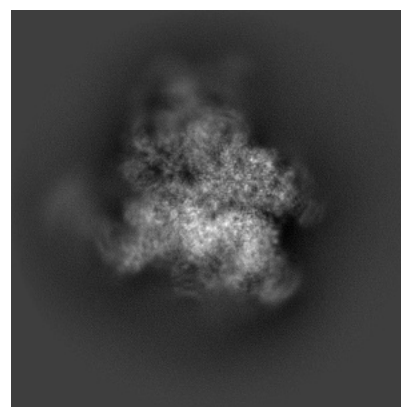
6.1.2 Raw map



X



Y

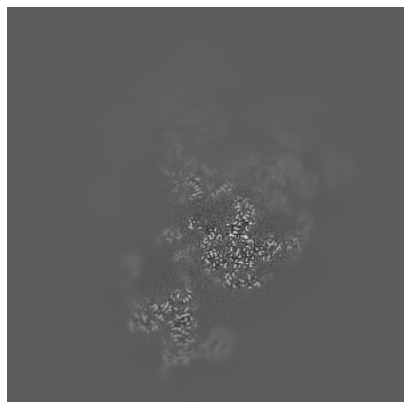


Z

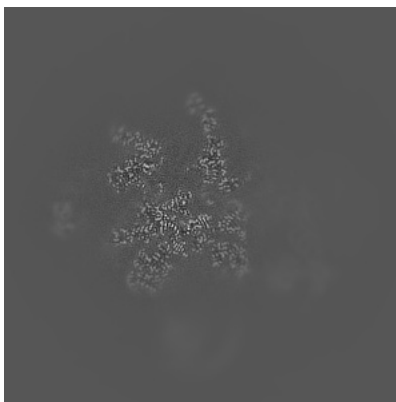
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

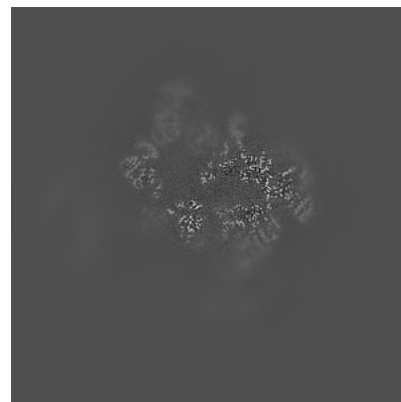
6.2.1 Primary map



X Index: 240

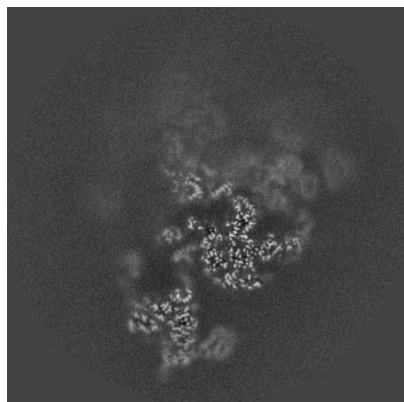


Y Index: 240

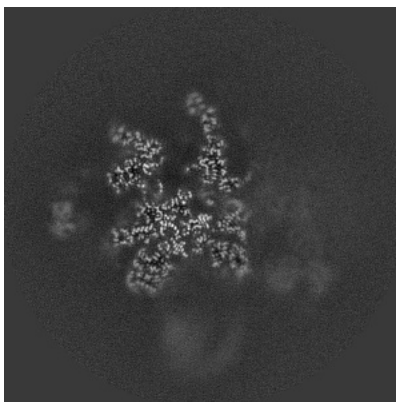


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

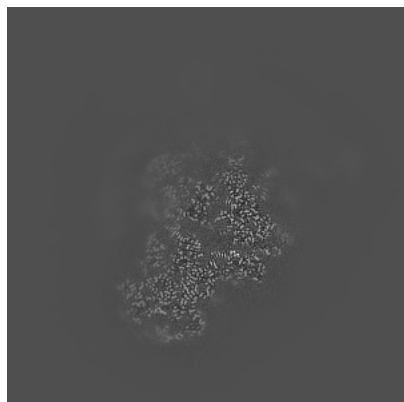


Z Index: 240

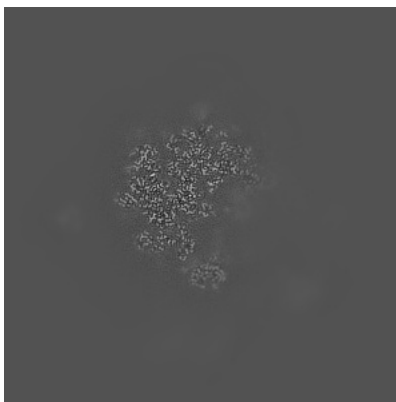
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

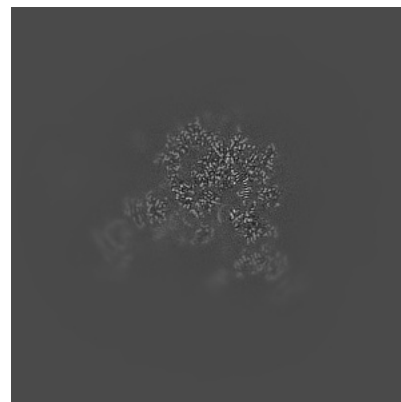
6.3.1 Primary map



X Index: 283

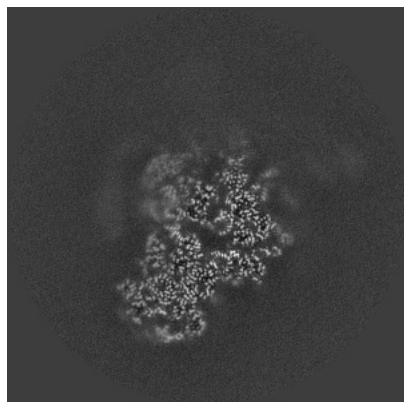


Y Index: 274

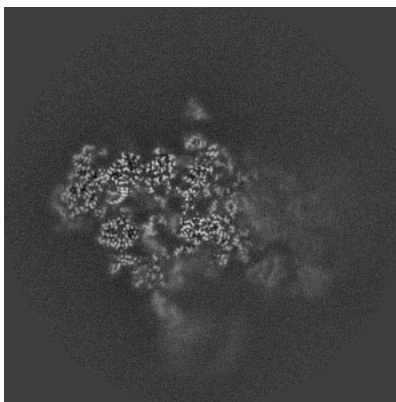


Z Index: 181

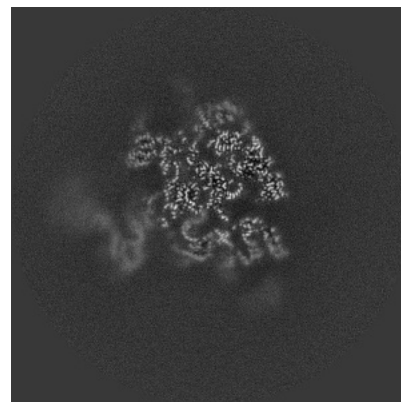
6.3.2 Raw map



X Index: 283



Y Index: 222

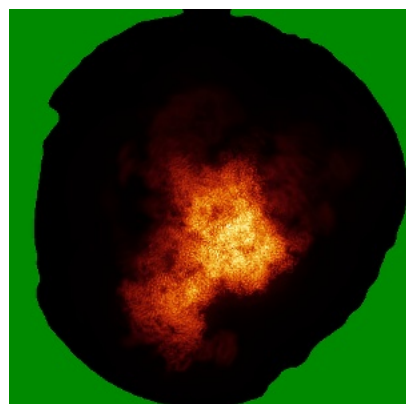


Z Index: 204

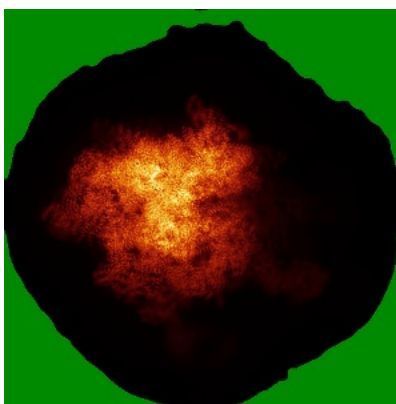
The images above show the largest variance slices of the map in three orthogonal directions.

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

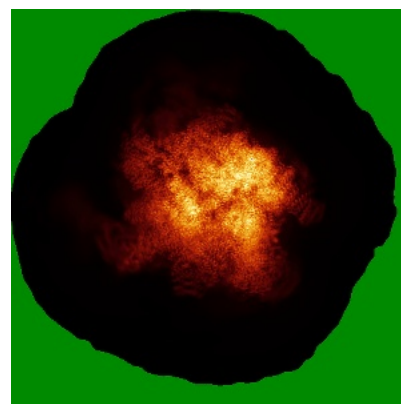
6.4.1 Primary map



X

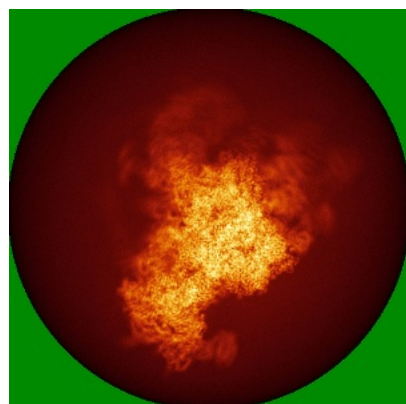


Y

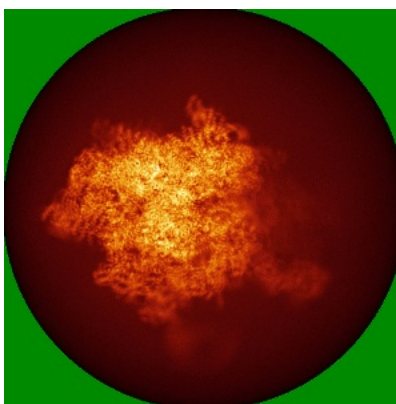


Z

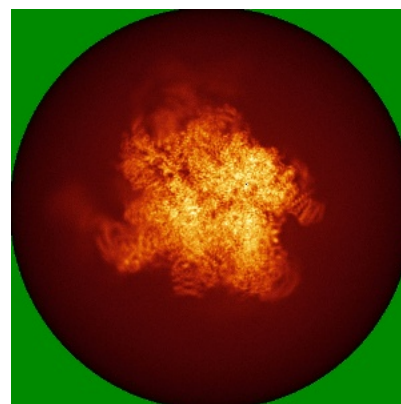
6.4.2 Raw map



X



Y



Z

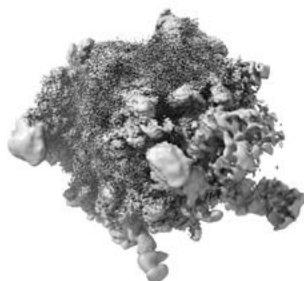
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

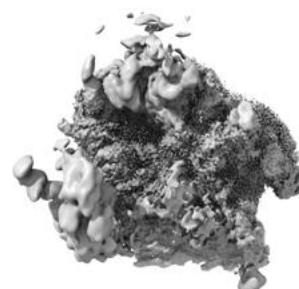
6.5.1 Primary map



X



Y



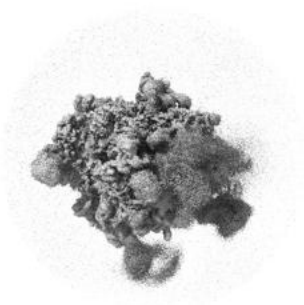
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

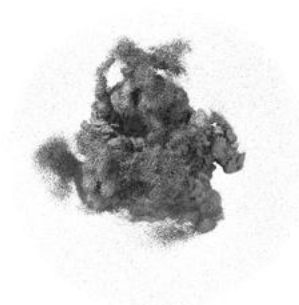
6.5.2 Raw map



X



Y



Z

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

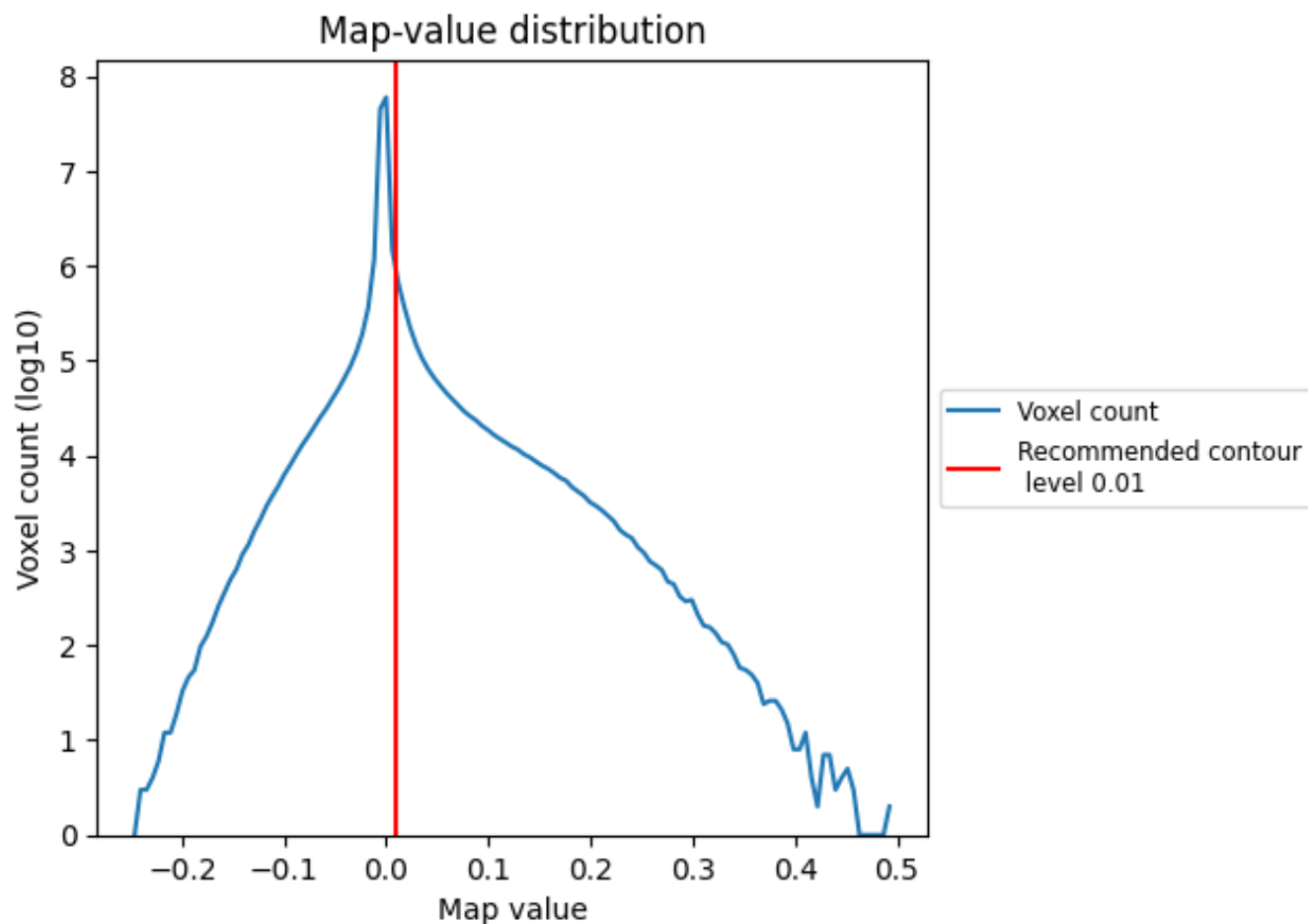
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

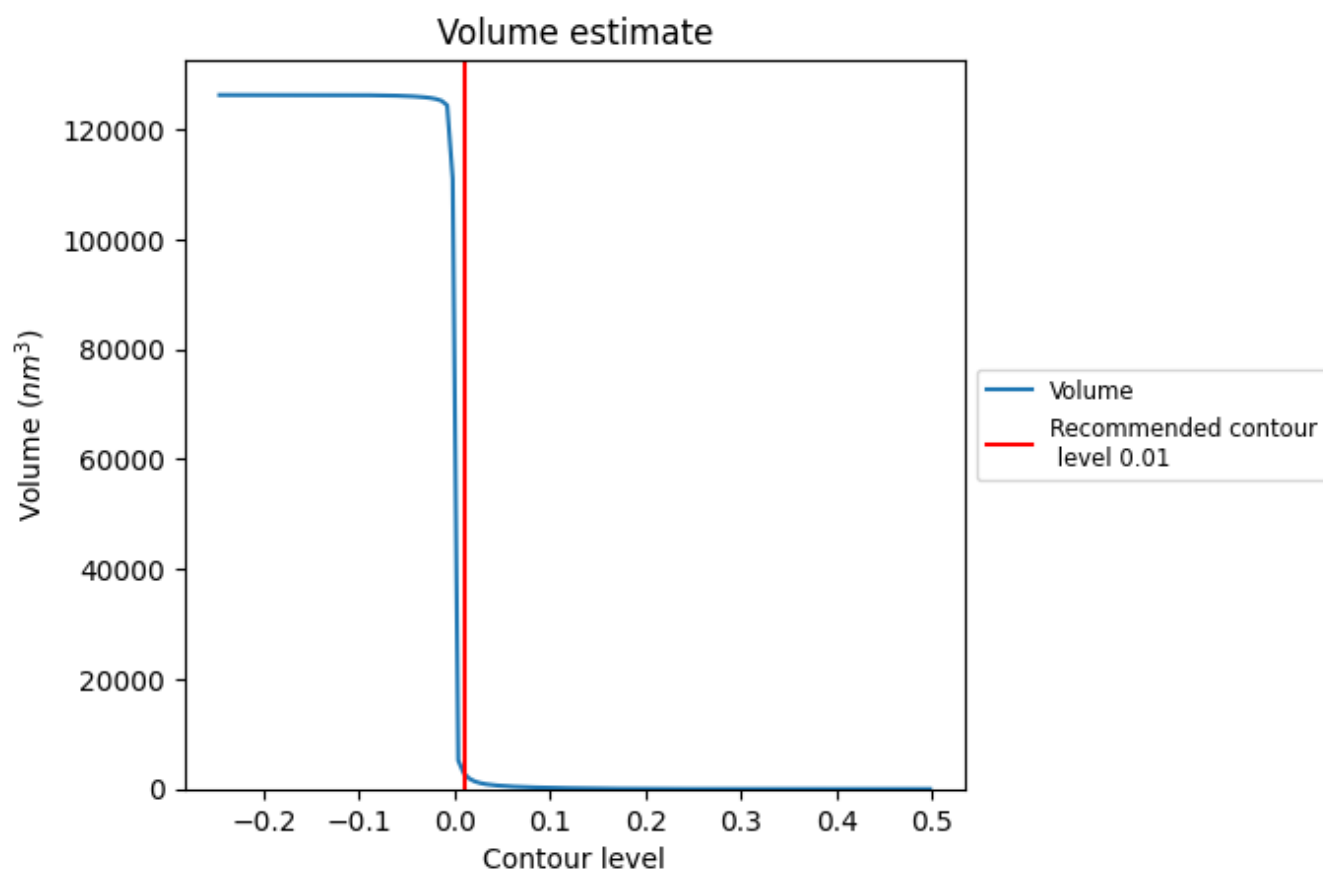
This section contains the results of statistical analysis of the map.

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.

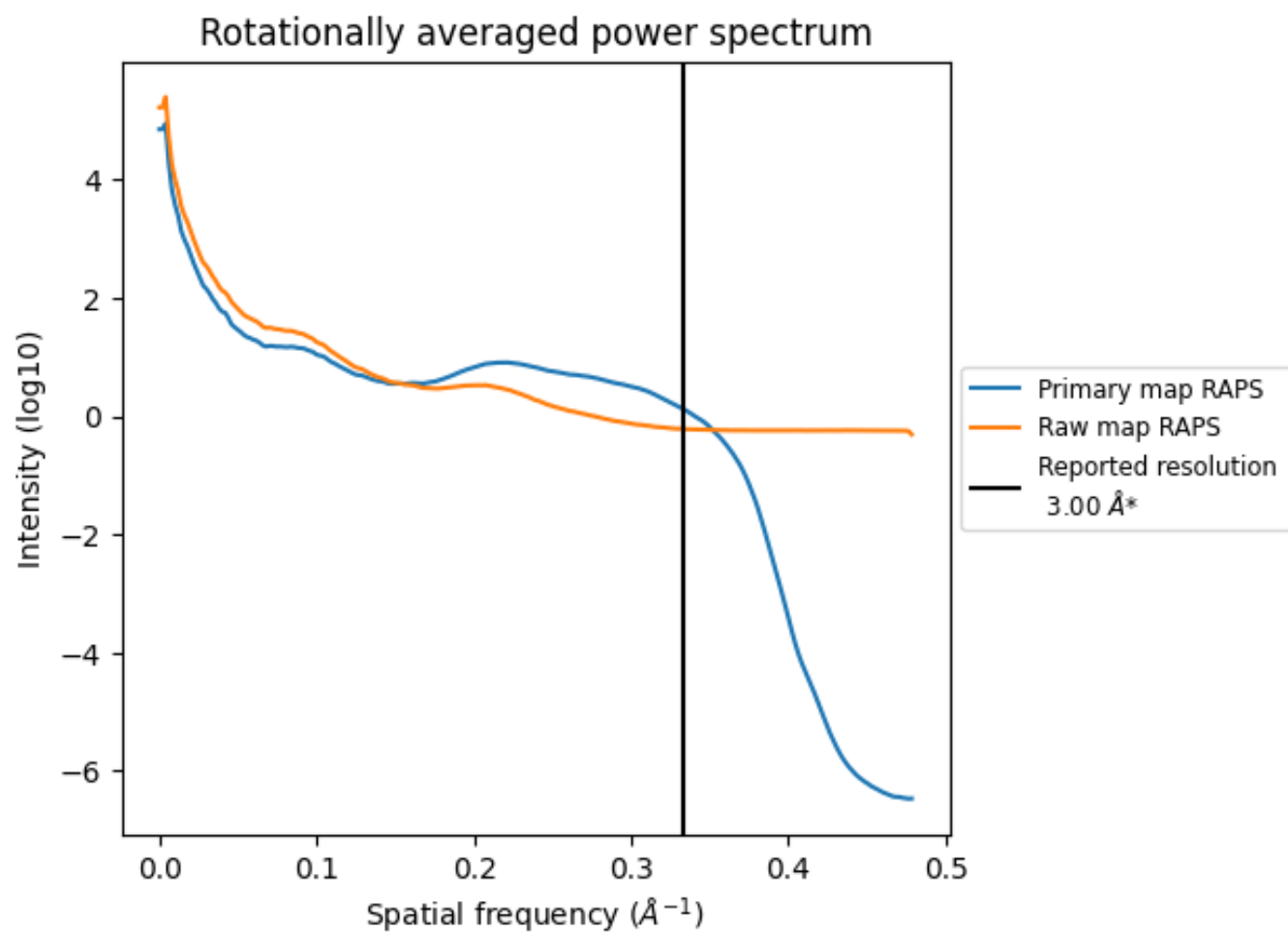
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2794 nm^3 ; this corresponds to an approximate mass of 2524 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 ⓘ

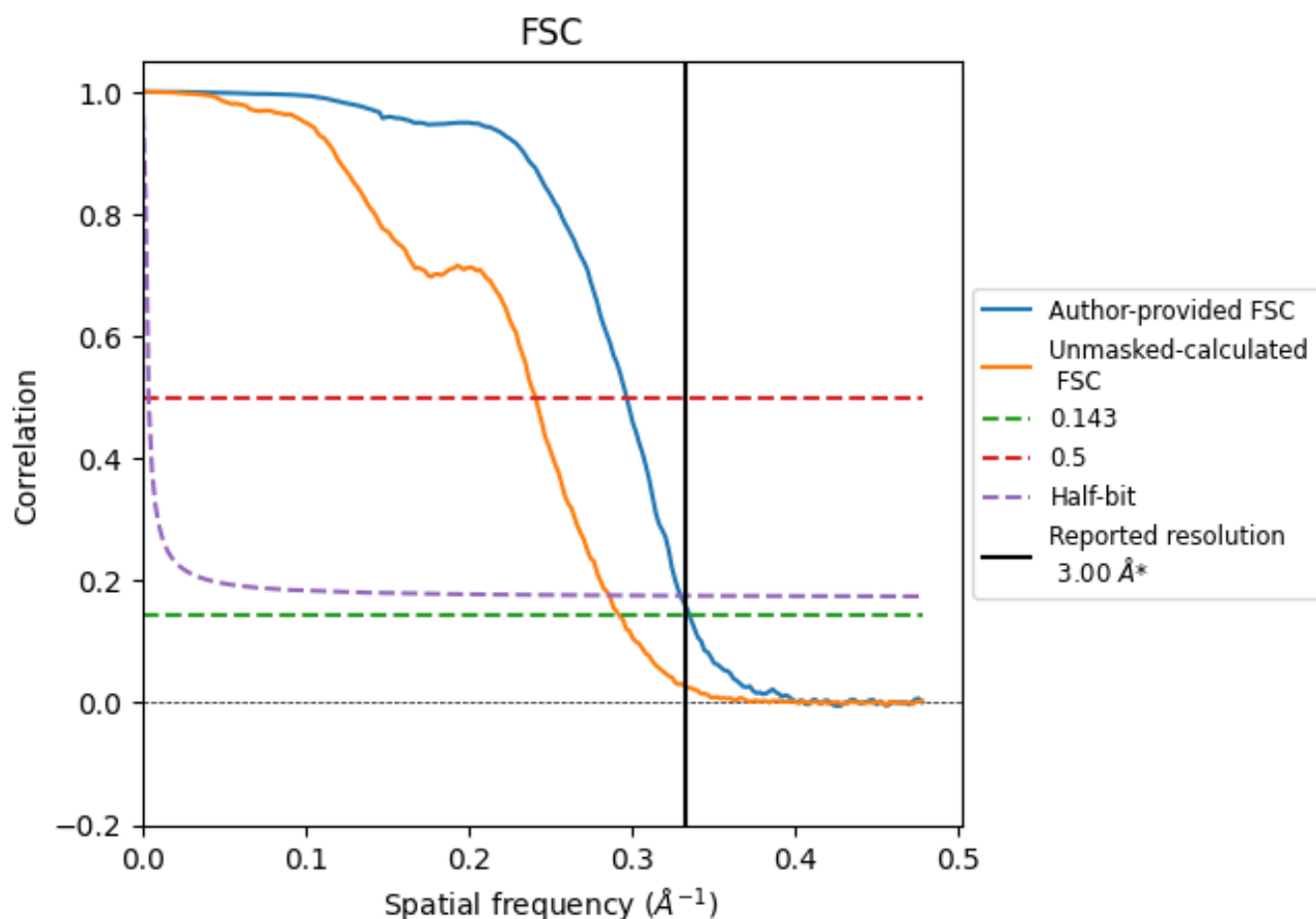


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

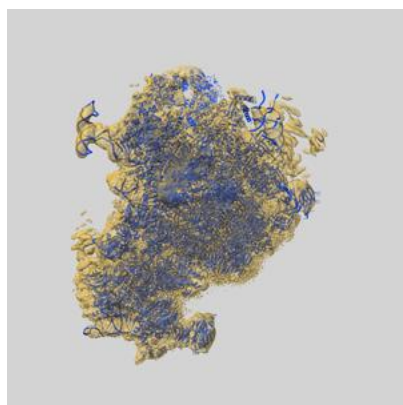
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.36	3.03
Unmasked-calculated*	3.42	4.14	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.0 by more than 10 %

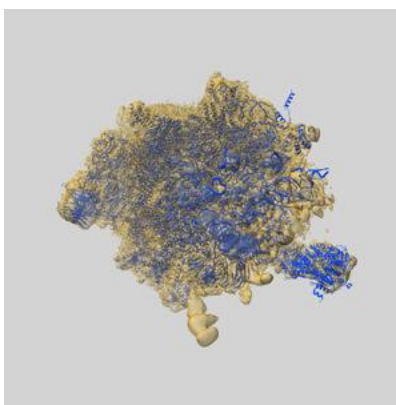
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66685 and PDB model 9XAF. Per-residue inclusion information can be found in section 3 on page 16.

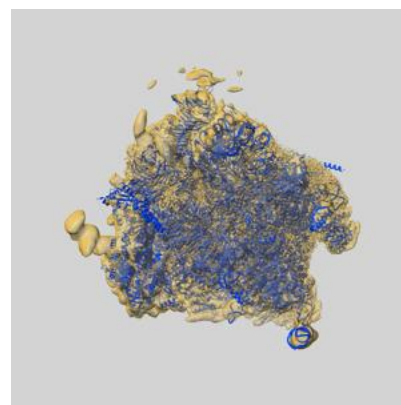
9.1 Map-model overlay [i](#)



X



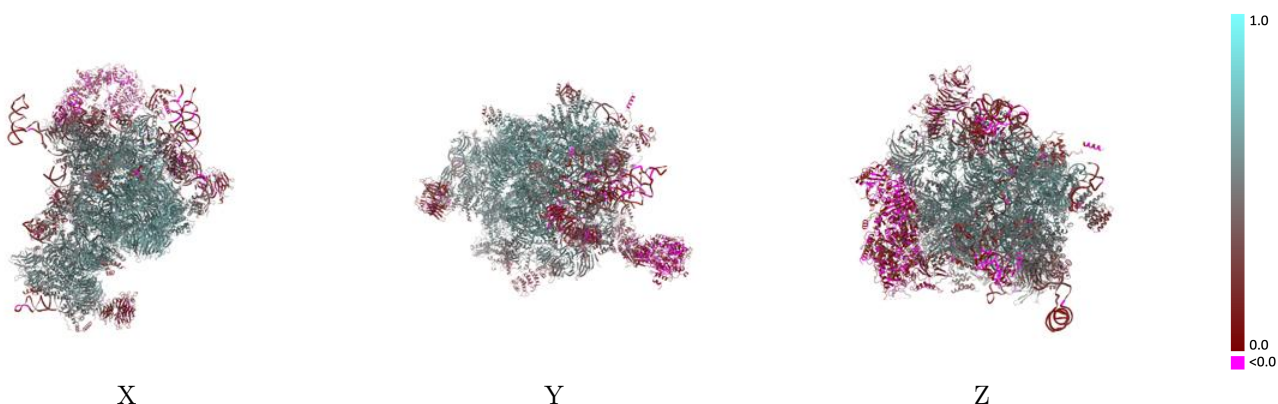
Y



Z

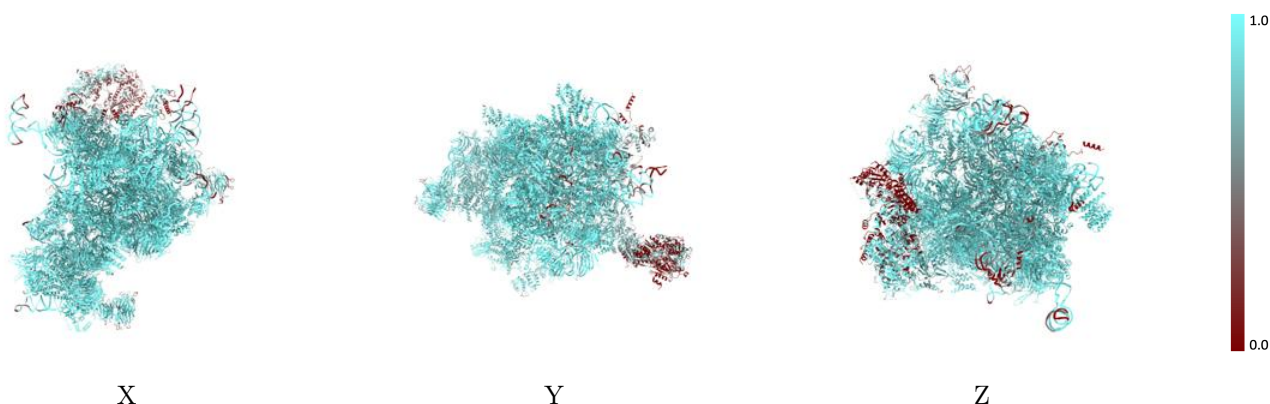
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



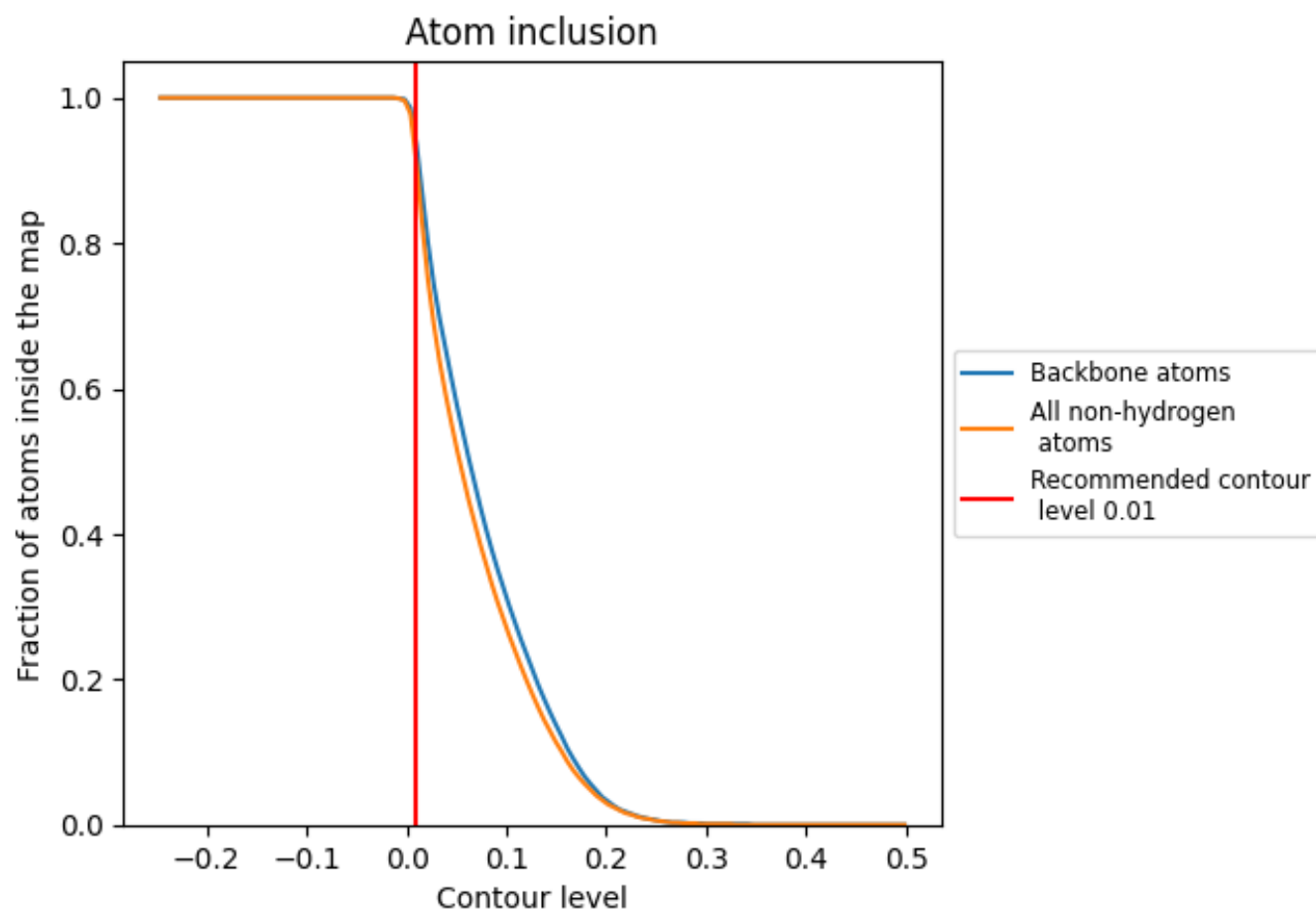
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.4550
C1	 0.9230	 0.4330
C2	 0.9330	 0.4340
CA	 0.9890	 0.6110
CB	 0.9250	 0.4460
CC	 0.9670	 0.4950
CD	 0.9360	 0.4470
CE	 0.9760	 0.5920
CF	 0.9660	 0.4830
CG	 0.8970	 0.3850
CH	 0.9770	 0.5300
CI	 0.9350	 0.4910
CJ	 0.9950	 0.6620
CK	 0.9940	 0.6300
CL	 0.9820	 0.5940
CM	 0.9890	 0.6140
CN	 0.9740	 0.5440
CO	 0.9210	 0.4170
CP	 0.8510	 0.1740
CQ	 0.9540	 0.4250
CR	 0.6840	 0.1420
CS	 0.3290	 0.0540
CT	 0.9820	 0.5940
CU	 0.8730	 0.4490
CX	 0.9080	 0.1540
CY	 0.6130	 0.2790
Cc	 0.9860	 0.6110
Ce	 0.6390	 0.2540
Cg	 0.9530	 0.5150
Ci	 0.8950	 0.1860
Cj	 0.9910	 0.6380
Cl	 0.9500	 0.4500
Cm	 0.9300	 0.4690
Cn	 0.9900	 0.5800
Co	 0.3010	 0.0390



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Chain	Atom inclusion	Q-score
Cp	 0.9930	 0.6030
UA	 0.9930	 0.6410
UB	 0.9630	 0.4580
UC	 0.9740	 0.5460
UD	 0.9810	 0.5480
UE	 0.9660	 0.5270
UF	 0.9720	 0.4880
UG	 0.9770	 0.6100
UH	 0.8920	 0.2960
UI	 0.9530	 0.4250
UJ	 0.9790	 0.5650
UK	 0.9770	 0.5880
UL	 0.9760	 0.5130
UM	 0.8320	 0.2490
UN	 0.8530	 0.5180
UO	 0.9880	 0.5910
UP	 0.9800	 0.5210
UQ	 0.9840	 0.5590
UR	 0.9930	 0.6240
US	 0.9610	 0.4640
UU	 0.9900	 0.6210
UX	 0.9710	 0.5710
UZ	 0.9780	 0.4810