



## wwPDB EM Validation Summary Report ⓘ

Apr 23, 2024 – 03:17 pm BST

PDB ID : 6ZQB  
EMDB ID : EMD-11358  
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state B2  
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.  
Deposited on : 2020-07-09  
Resolution : 3.90 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](mailto: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:

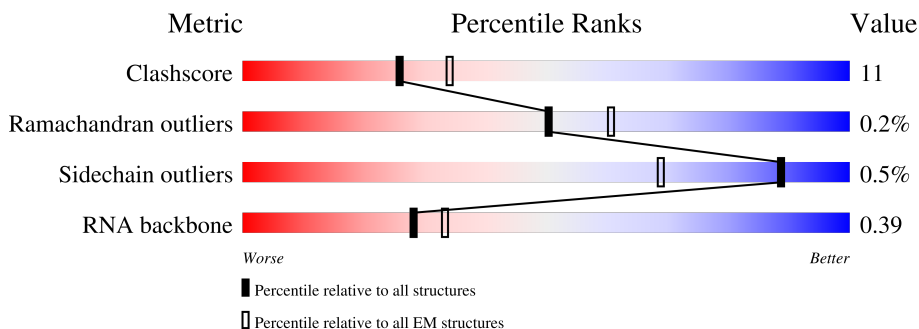
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



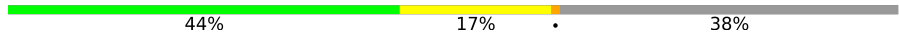









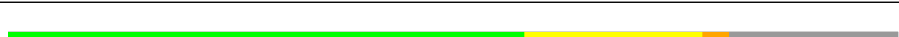


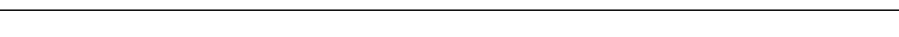
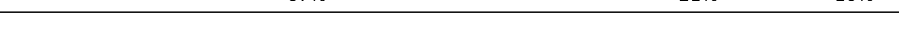
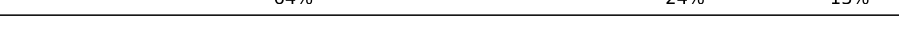



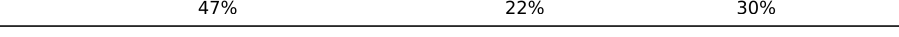





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	923	
2	UB	810	
3	UC	610	
4	UD	776	
5	UE	643	
6	UF	440	
7	UG	554	









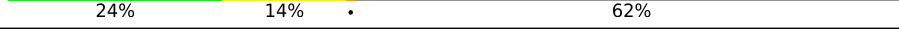

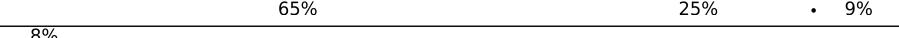
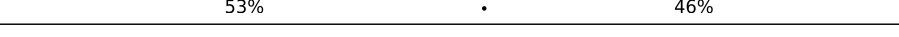

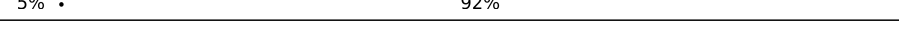

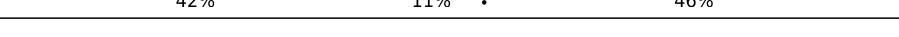
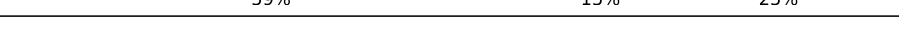

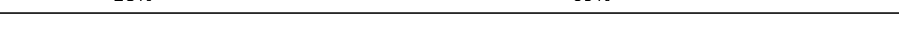






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	UH	713	
9	UI	575	
10	UJ	1769	
11	UK	250	
12	UL	943	
13	UM	817	
14	UN	145	
15	UO	513	
16	UP	214	
17	UQ	896	
18	UR	594	
19	US	552	
20	UT	2493	
21	UU	939	
22	UV	1237	
23	UX	189	
24	UZ	274	
25	CA	327	
25	CB	327	
26	CD	504	
27	CE	511	
28	CF	126	
28	CG	126	
29	CH	573	
30	CI	183	






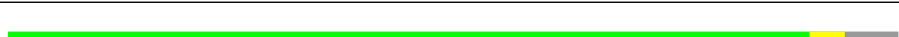
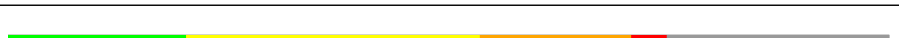
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	CJ	290	
32	CK	593	
33	CL	1183	
34	CM	367	
35	CN	297	
36	JA	1056	
36	JB	1056	
37	JC	707	
38	JE	357	
39	JF	252	
39	JG	252	
40	JH	483	
41	JJ	274	
42	JK	534	
43	JM	217	
44	JN	346	
45	JO	316	
46	JP	489	
47	JQ	206	
48	DA	255	
49	DE	261	
50	DF	225	
51	DG	236	
52	DH	190	
53	DI	200	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	DJ	197	
55	DL	156	
56	DN	151	
57	DO	137	
58	DQ	143	
59	DS	147	
60	DW	130	
61	DX	145	
62	DY	135	
63	Db	82	
64	Dc	67	
65	D2	700	
66	D3	1808	
67	D4	175	

## 2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 223151 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UA	834	6635	4223	1140	1253	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	508	3743	2373	665	696	9	0	0

- Molecule 3 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	128	1026	633	204	189	0	0

- Molecule 4 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	675	5361	3395	929	1015	22	0	0

- Molecule 5 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UE	475	3772	2400	649	710	13	0	0

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UF	293	2487	1605	435	434	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UG	533	4218	2646	758	802	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UH	441	2690	1672	492	523	3	0	0

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	UI	102	846	547	149	148	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UJ	1117	6857	4267	1252	1326	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UK	241	2016	1251	388	370	7	0	0

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	UL	842	6720	4300	1126	1267	27	0	0

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	UM	762	5957	3779	1006	1144	28	0	0

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 14, U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UN	145	1207	750	230	225	2	0	0

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UO	493	3911	2462	702	735	12	0	0

- Molecule 16 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	UP	60	495	310	101	84	0	0

- Molecule 17 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UQ	832	6662	4236	1124	1283	19	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	UR	481	3791	2399	668	714	10	0	0

- Molecule 19 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	US	481	3650	2355	611	672	12	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	UT	2234	11108	6640	2234	2234	0	0

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 21.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	UU	848	6678	4241	1149	1267	21	0	0

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	UV	1080	8725	5672	1439	1590	24	0	0

- Molecule 23 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	UX	174	1395	890	255	240	10	0	0

- Molecule 24 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	UZ	247	2006	1284	356	358	8	0	0

- Molecule 25 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	CA	242	1881	1193	338	340	10	0	0
25	CB	228	1782	1131	320	321	10	0	0

- Molecule 26 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	CD	380	2994	1898	513	574	9	0	0

- Molecule 27 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	CE	435	2985	1852	543	582	8	0	0

- Molecule 28 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CF	123	Total	C	N	O	S	0	0
			931	594	160	173	4		
28	CG	123	Total	C	N	O	S	0	0
			928	591	160	173	4		

- Molecule 29 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CH	454	Total	C	N	O	S	0	0
			3634	2311	638	675	10		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CI	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CJ	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CK	207	Total	C	N	O	S	0	0
			1667	1034	297	332	4		

- Molecule 33 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CL	781	Total	C	N	O	S	0	0
			6332	4063	1122	1117	30		

- Molecule 34 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 35 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CN	232	Total	C	N	O	S	0	0
			1893	1213	322	351	7		

- Molecule 36 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JA	812	Total	C	N	O	S	0	0
			5892	3727	1041	1099	25		
36	JB	835	Total	C	N	O		0	0
			4132	2462	835	835			

- Molecule 37 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	JC	354	Total	C	N	O	S	0	0
			2845	1795	489	552	9		

- Molecule 38 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	JE	136	Total	C	N	O	S	0	0
			1125	674	231	217	3		

- Molecule 39 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	JF	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
39	JG	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 40 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 41 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	JJ	182	Total	C	N	O	S	0	0
			1448	926	262	256	4		

- Molecule 42 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	JK	42	334	213	54	67	0	0

- Molecule 43 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	JM	135	1137	721	211	201	4	0	0

- Molecule 44 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	JN	186	1428	879	287	259	3	0	0

- Molecule 45 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	JO	236	1930	1231	342	345	12	0	0

- Molecule 46 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	JP	457	3725	2328	679	702	16	0	0

- Molecule 47 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	JQ	63	381	234	69	78	0	0

- Molecule 48 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	DA	240	1912	1209	354	345	4	0	0

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DE	245	Total	C	N	O	S	0	0
			1944	1245	360	336	3		

- Molecule 50 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DF	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 52 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	DH	184	Total	C	N	O	0	0
			1477	949	265	263		

- Molecule 53 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	DI	177	Total	C	N	O	S	0	0
			1399	869	279	249	2		

- Molecule 54 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DJ	177	Total	C	N	O	S	0	0
			1428	902	275	250	1		

- Molecule 55 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DL	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 56 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	DN	150	1192	759	224	207	2	0	0

- Molecule 57 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	DO	120	881	544	167	167	3	0	0

- Molecule 58 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	DQ	125	973	625	174	174	0	0

- Molecule 59 is a protein called 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
59	DS	104	516	308	104	104	0	0

- Molecule 60 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	DW	129	1021	650	188	180	3	0	0

- Molecule 61 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	DX	103	786	503	144	137	2	0	0

- Molecule 62 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	DY	97	767	490	138	139	0	0

- Molecule 63 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 64 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Dc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 65 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	D2	522	Total	C	N	O	P	0	0
			11138	4977	1976	3663	522		

- Molecule 66 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	D3	1198	Total	C	N	O	P	0	0
			25549	11417	4548	8386	1198		

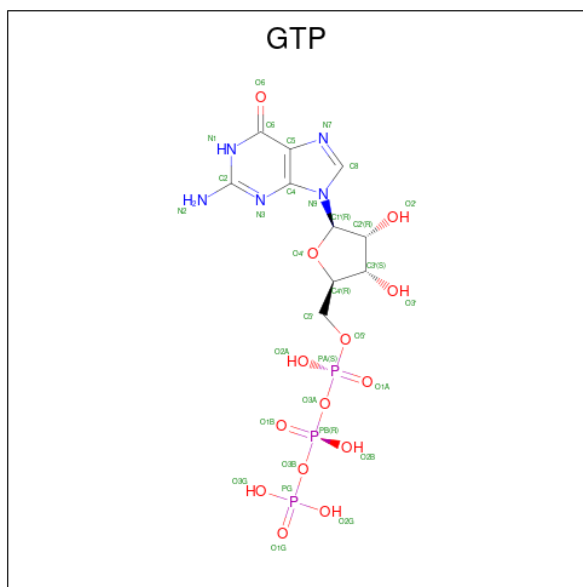
- Molecule 67 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	D4	175	Total	C	N	O	P	0	0
			3712	1661	648	1228	175		

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	UX	1	Total	Zn	0
			1	1	
68	Db	1	Total	Zn	0
			1	1	

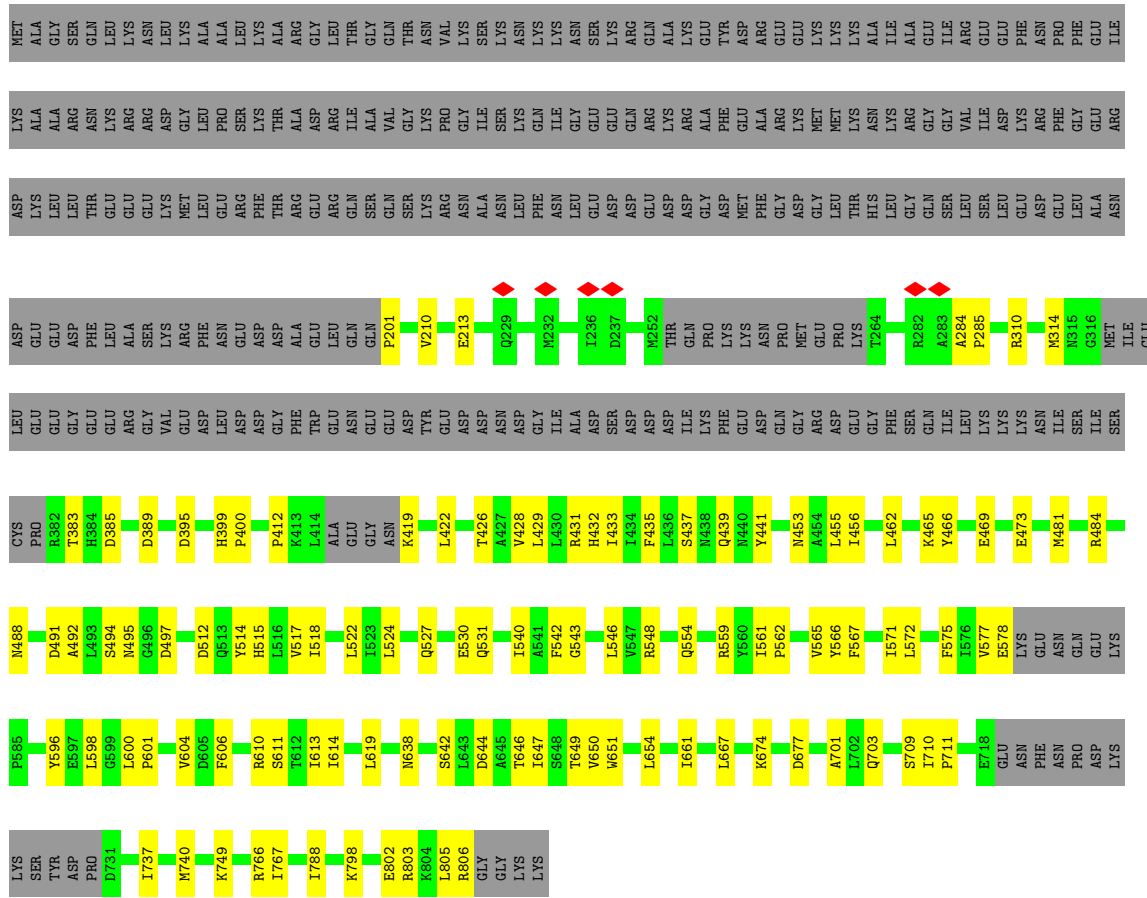
- Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



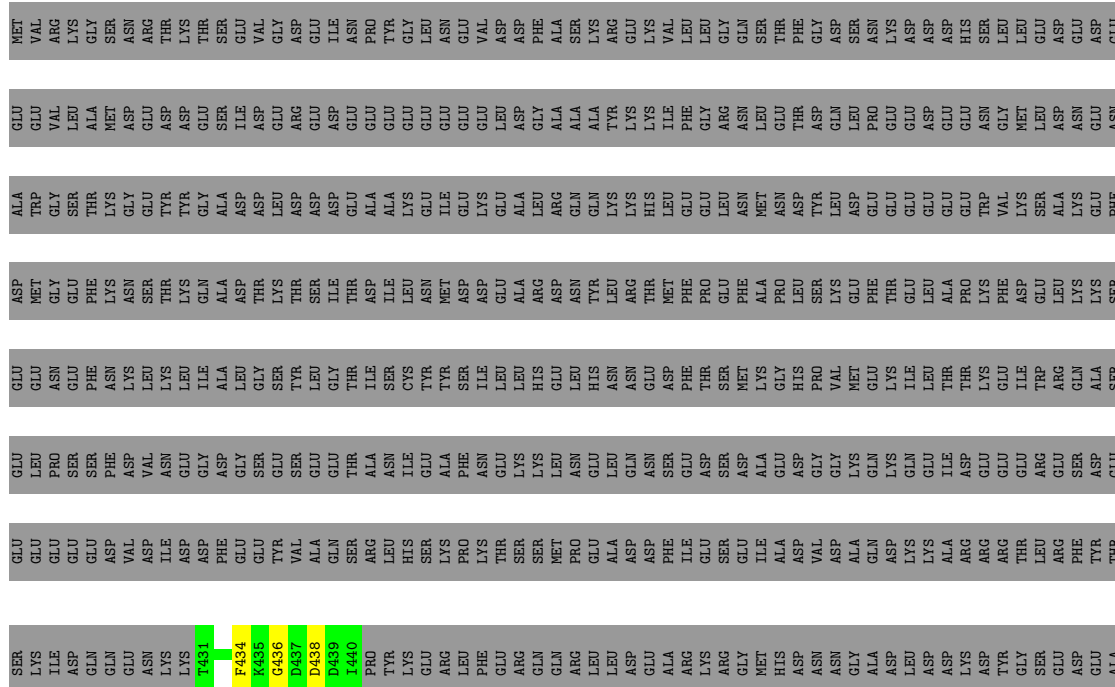
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	CL	1	32	10	5	14	3	0

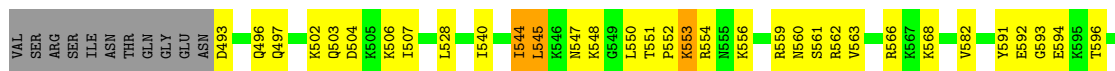




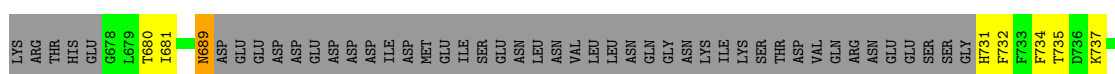
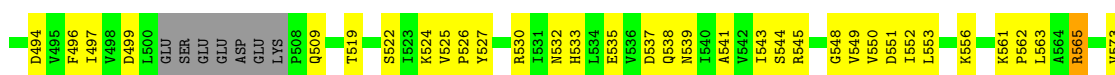
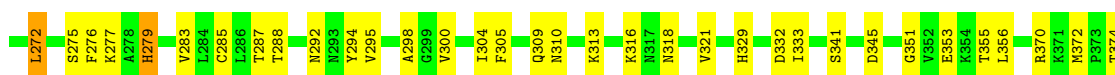
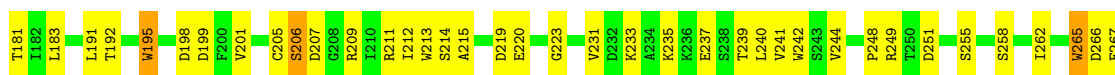
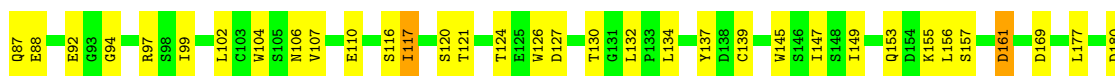
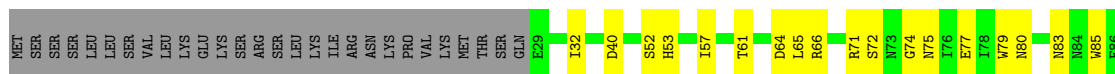


● Molecule 3: Something about silencing protein 10

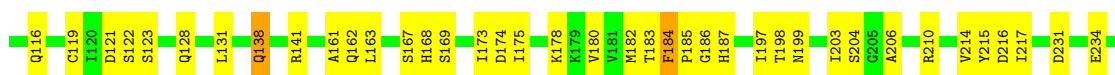




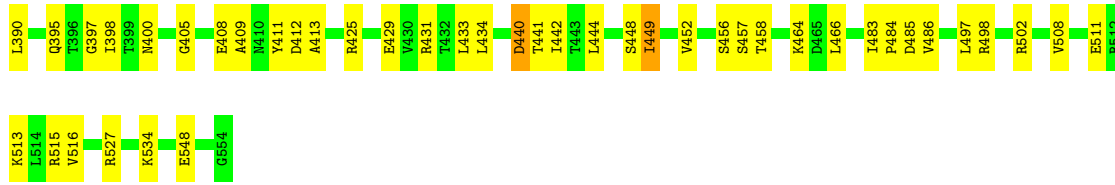
• Molecule 4: U3 small nucleolar RNA-associated protein 4



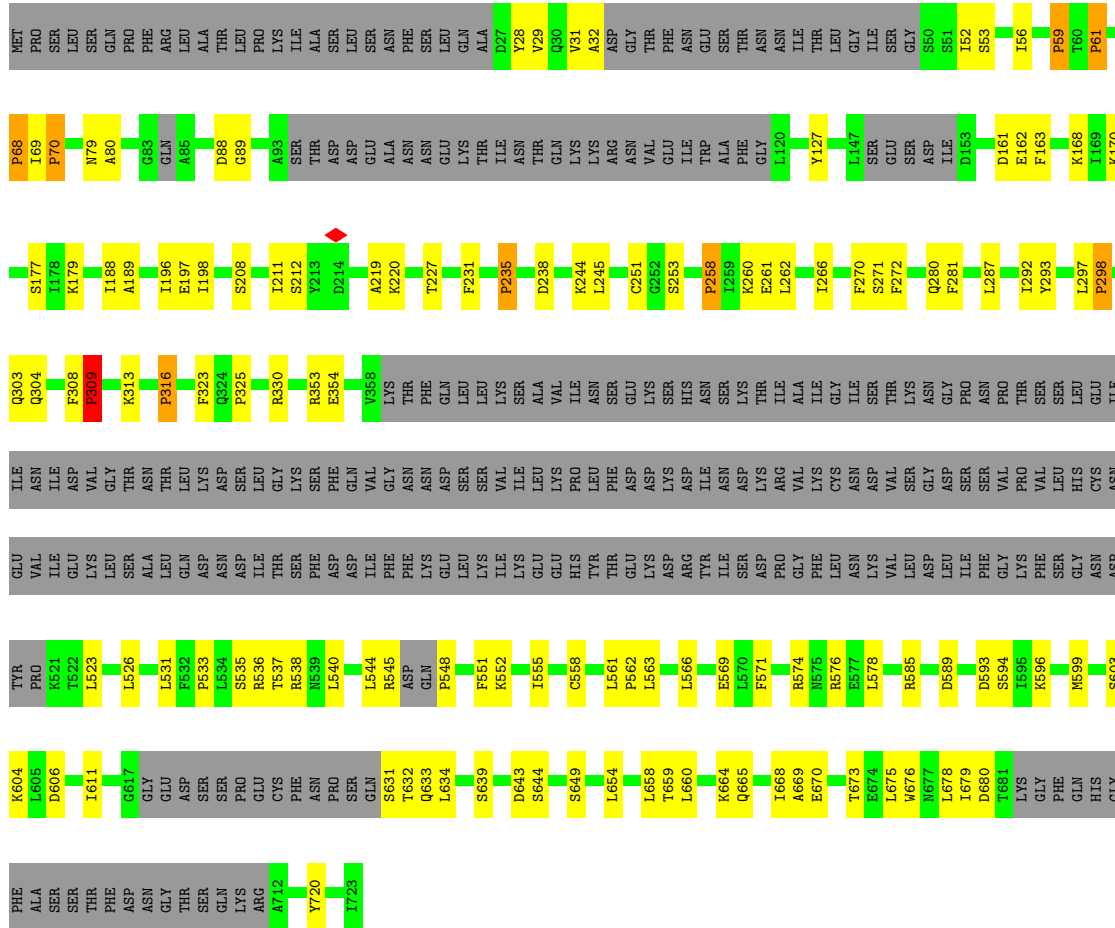
• Molecule 5: U3 small nucleolar RNA-associated protein 5



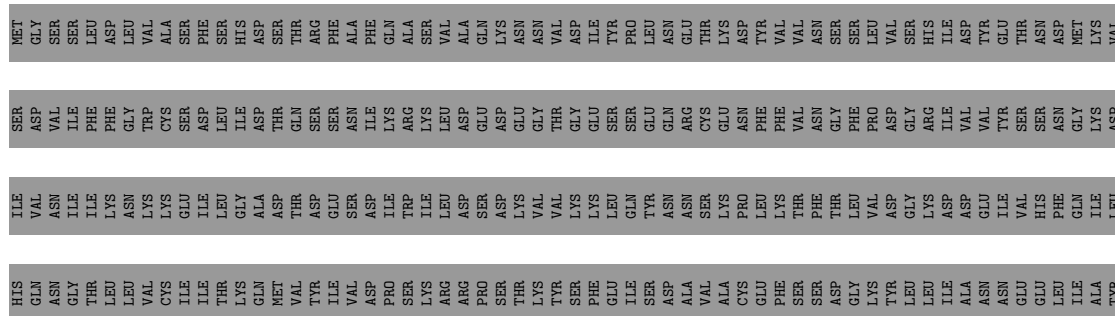




• Molecule 8: U3 small nucleolar RNA-associated protein 8

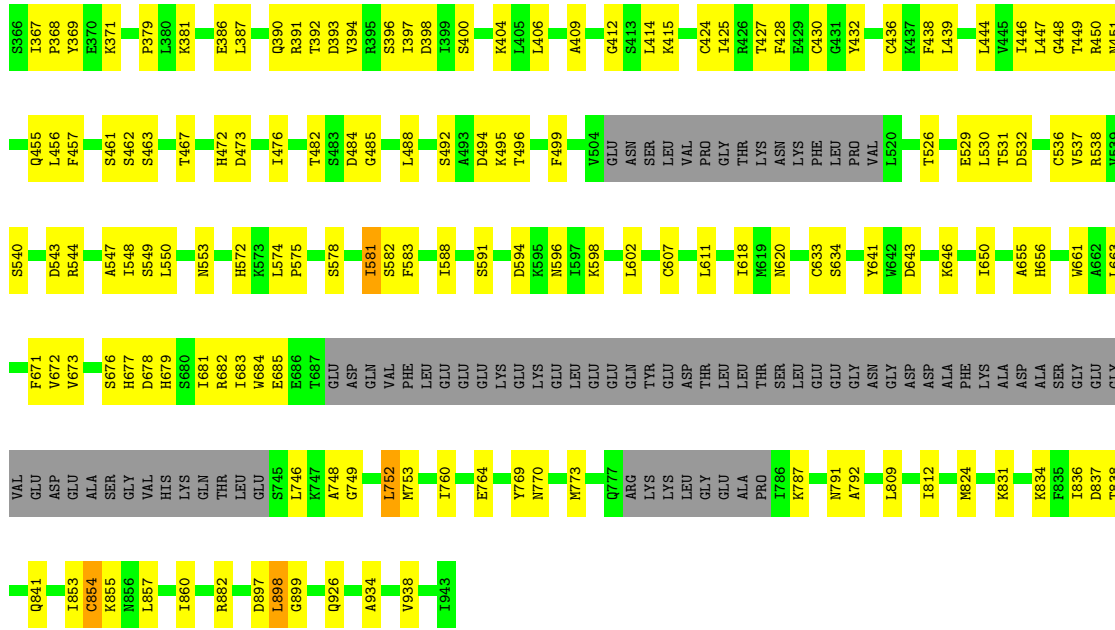


• Molecule 9: U3 small nucleolar RNA-associated protein 9

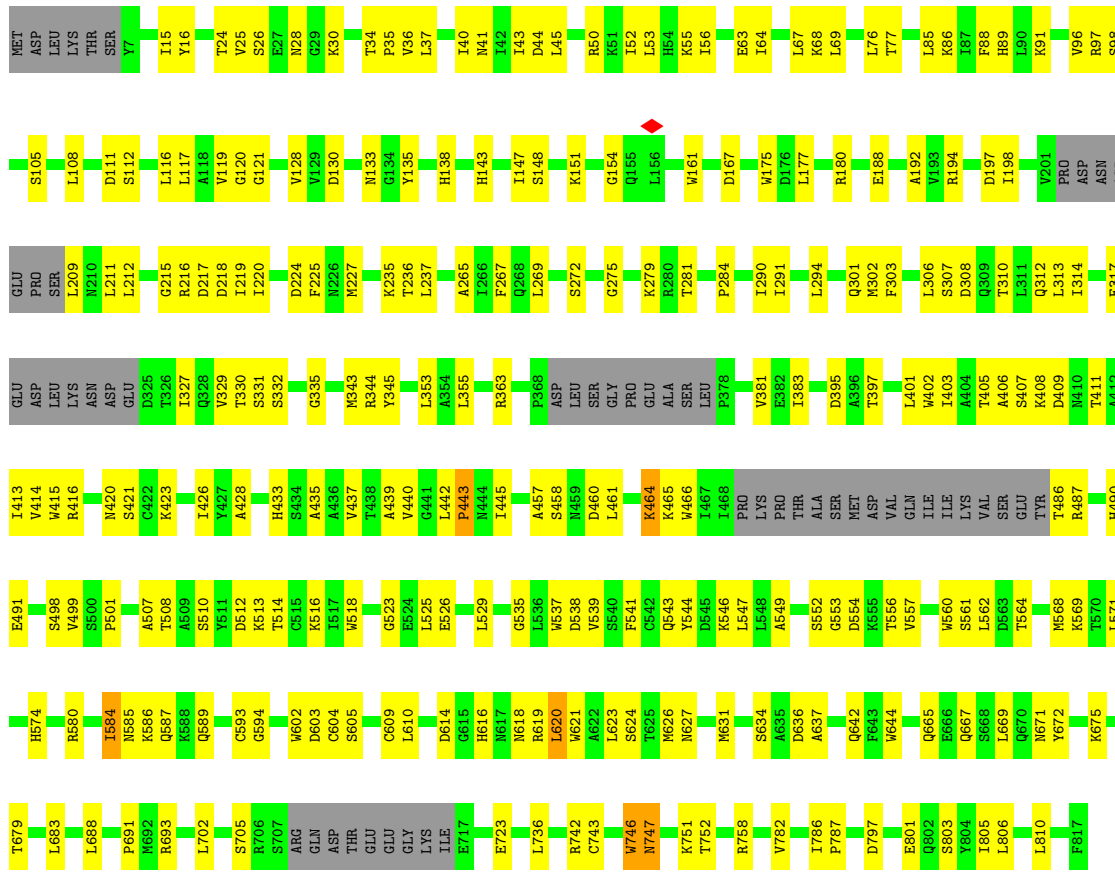








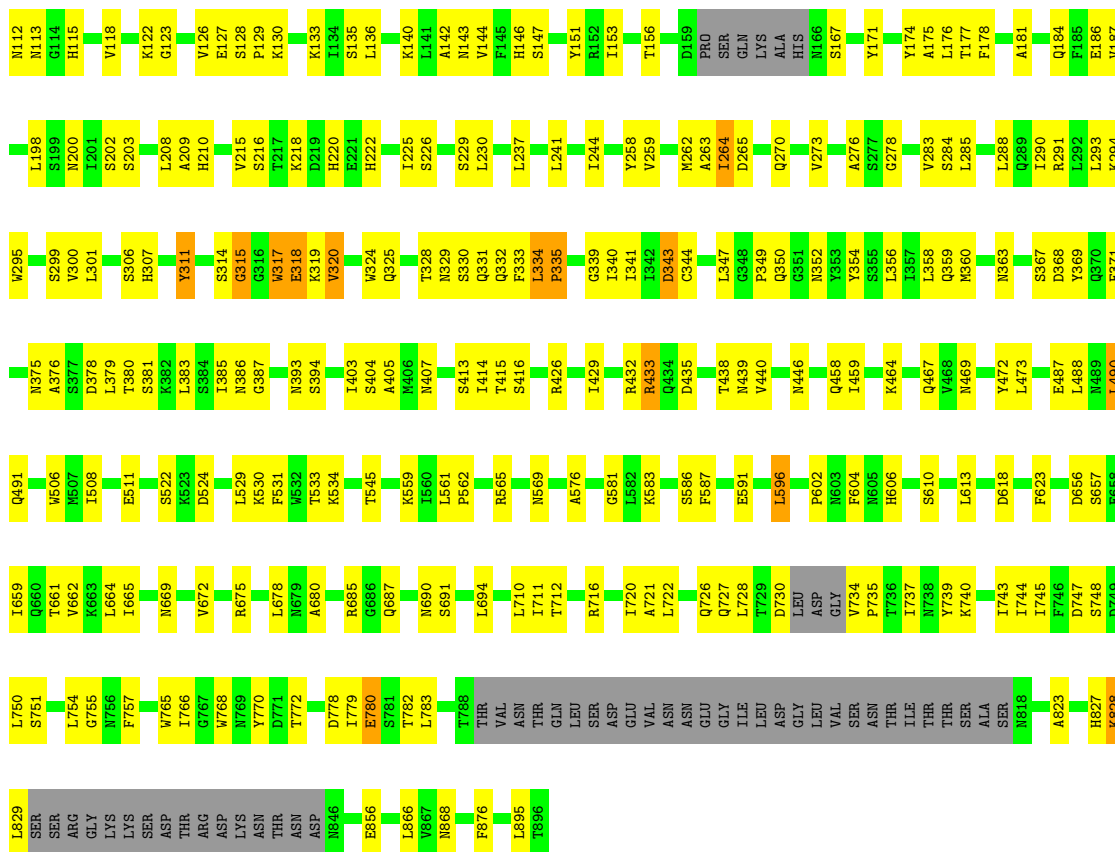
● Molecule 13: U3 small nucleolar RNA-associated protein 13



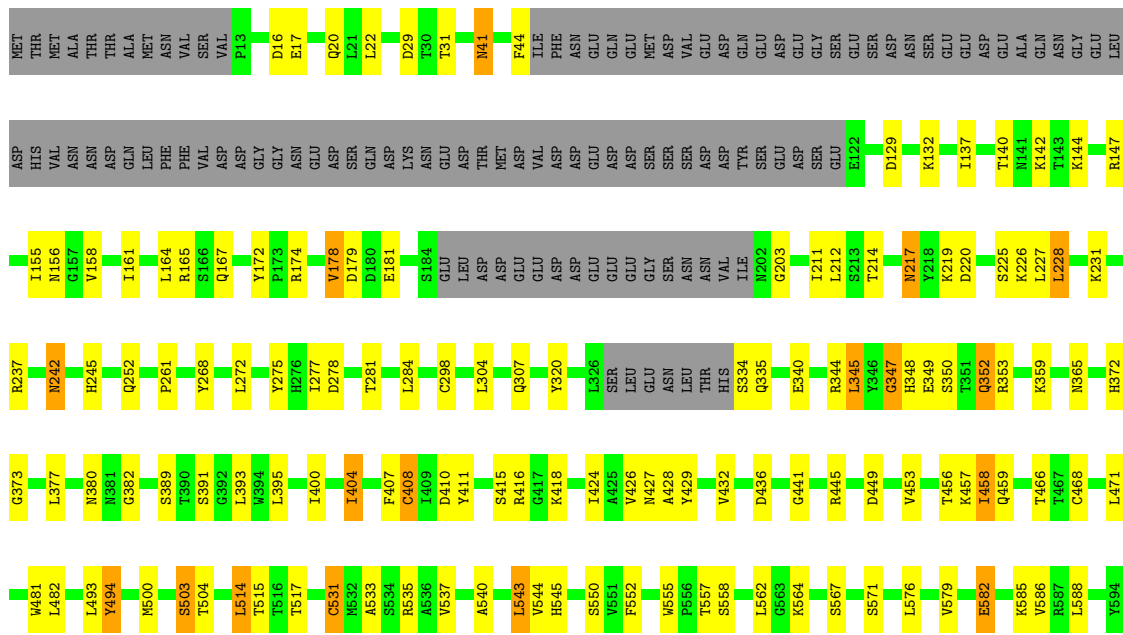
● Molecule 14: U3 small nucleolar RNA-associated protein 14, U3 small nucleolar RNA-associated protein 14





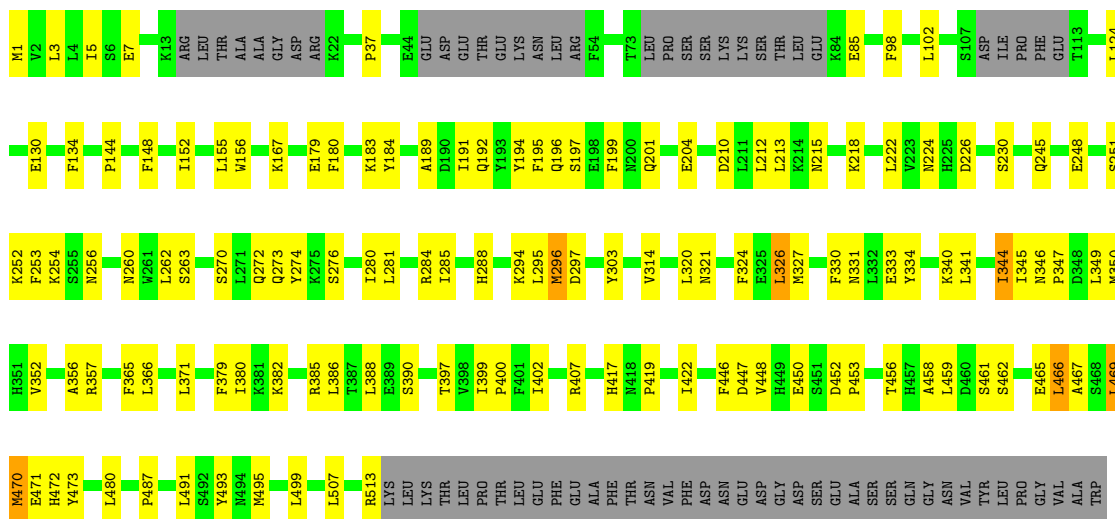


• Molecule 18: U3 small nucleolar RNA-associated protein 18

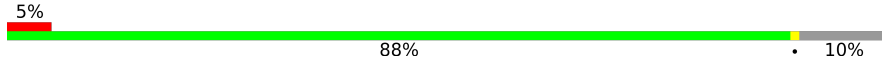


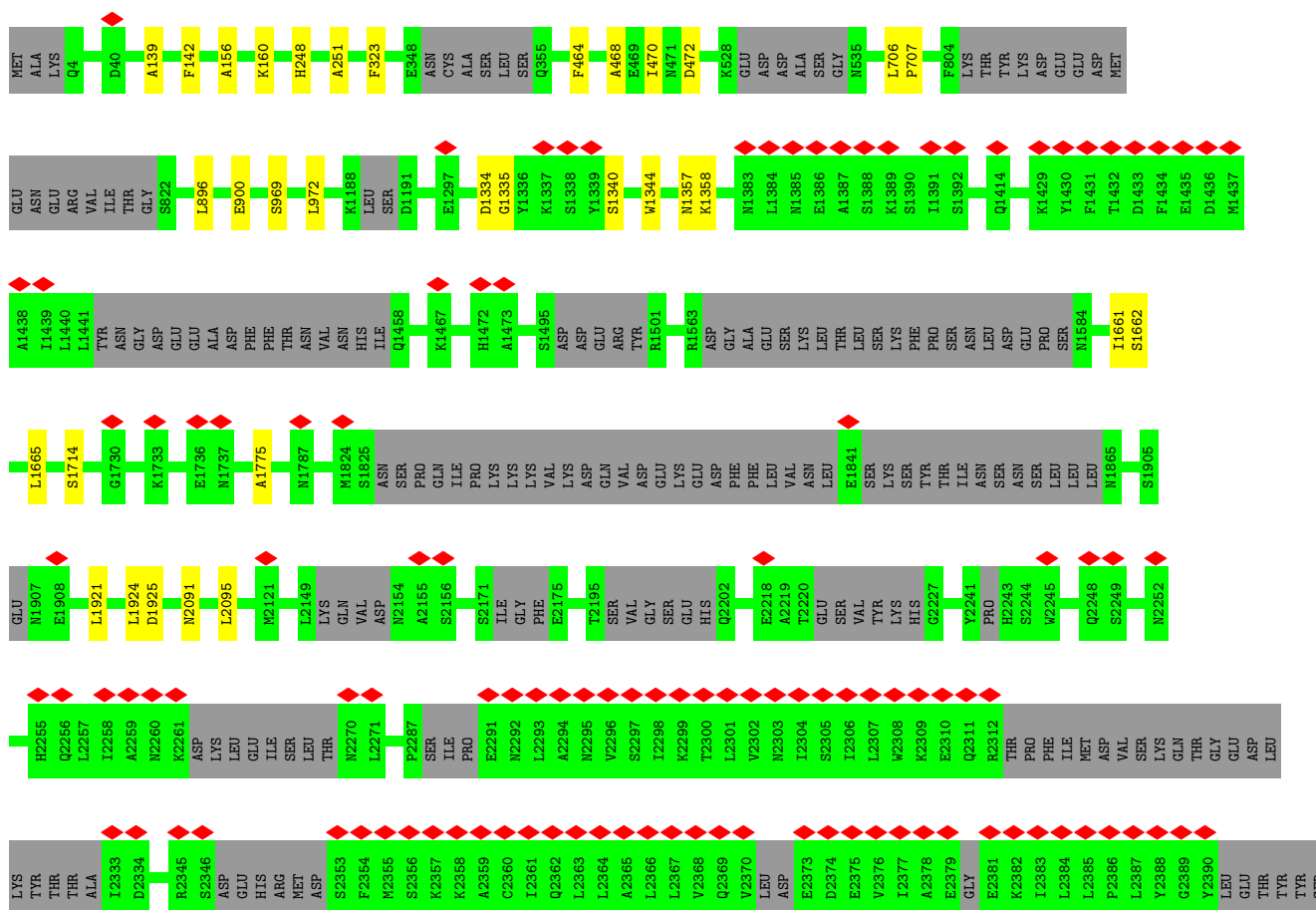
• Molecule 19: Nucleolar complex protein 4

Chain US:  63% 23% 13%

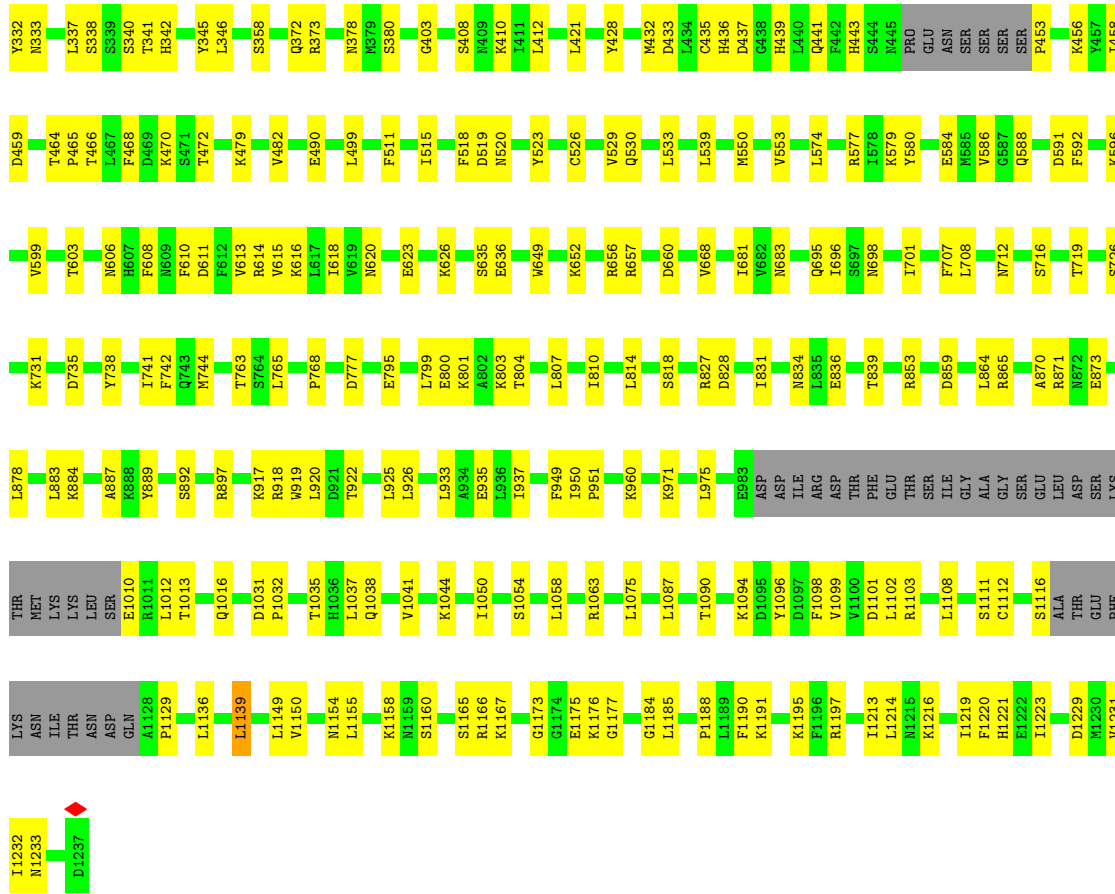


• Molecule 20: U3 small nucleolar RNA-associated protein 20

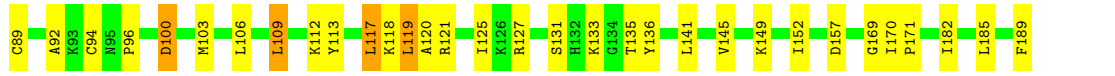
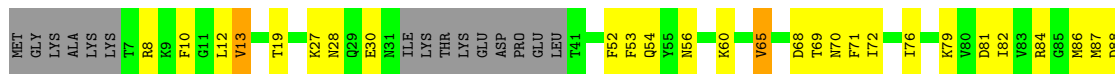
Chain UT:  5% 88% 10%



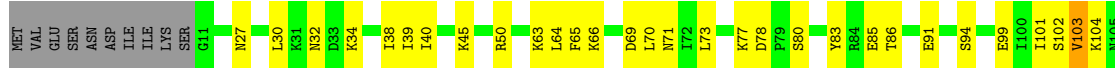




• Molecule 23: rRNA-processing protein FCF1

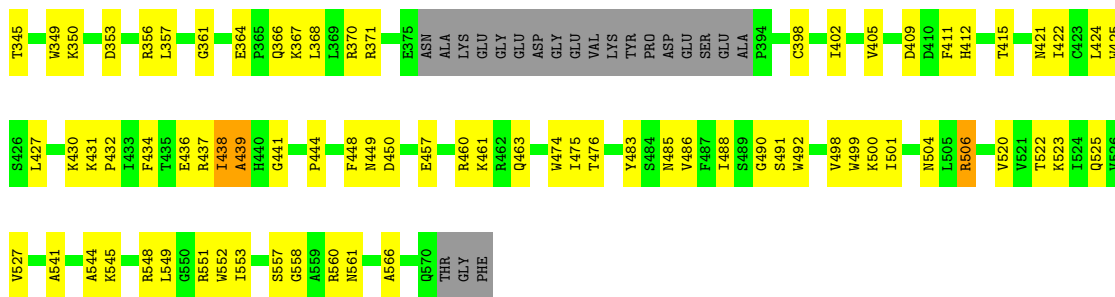


• Molecule 24: Ribosome biogenesis protein UTP30

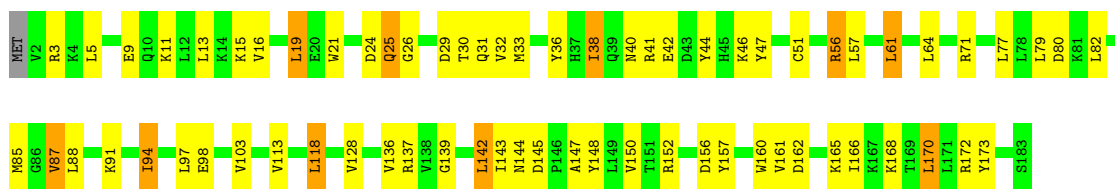




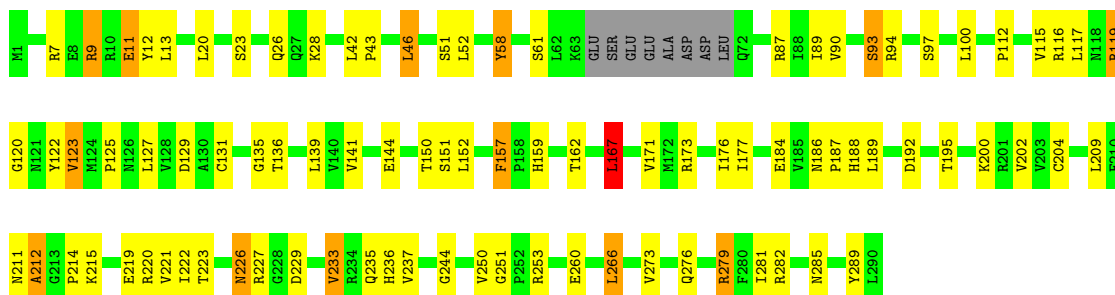




• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3



• Molecule 31: U3 small nucleolar ribonucleoprotein protein IMP4

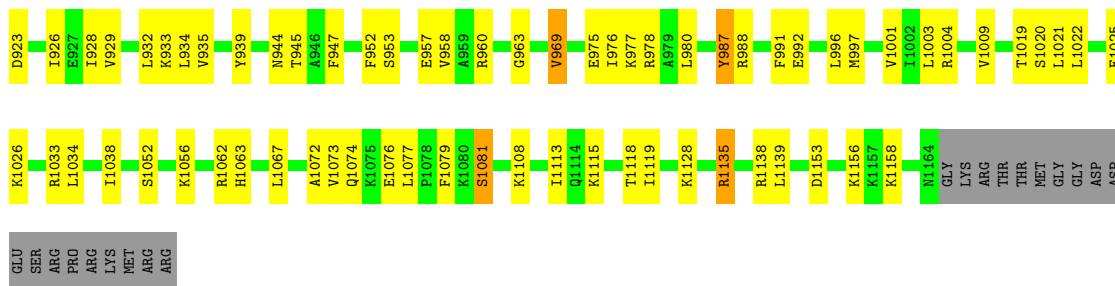


• Molecule 32: U3 small nucleolar RNA-associated protein MPP10

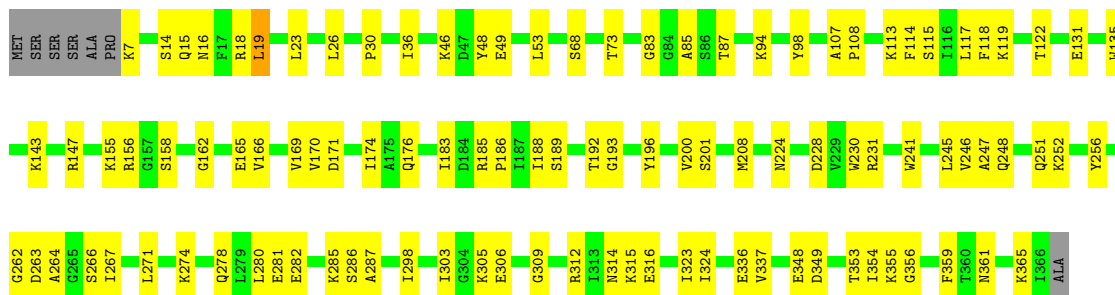




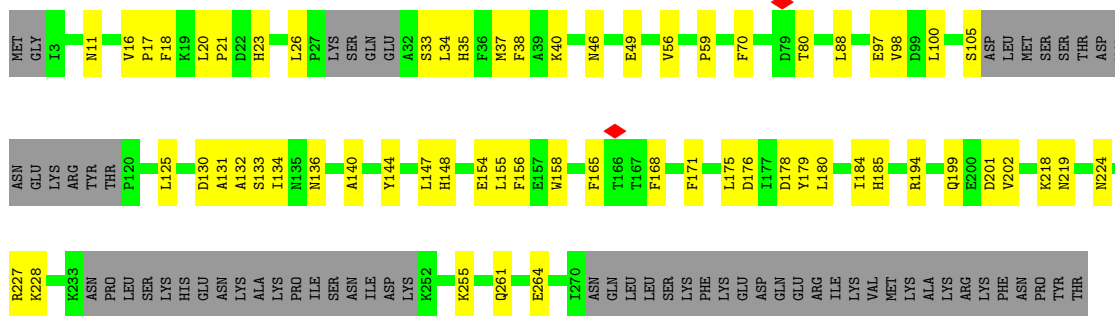




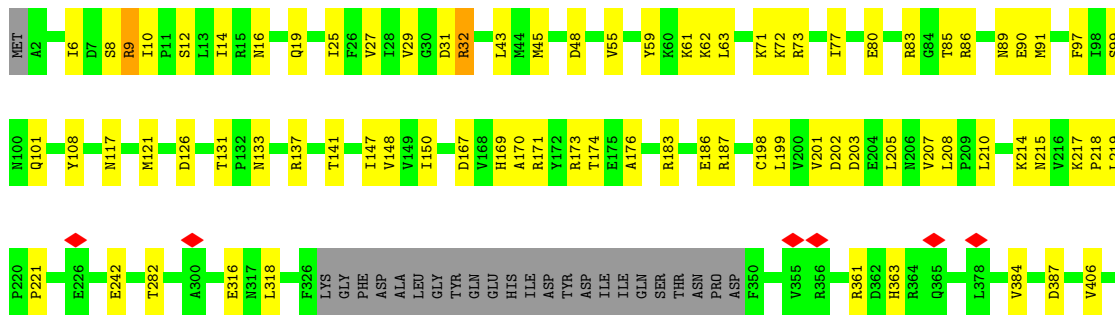
• Molecule 34: RNA 3'-terminal phosphate cyclase-like protein

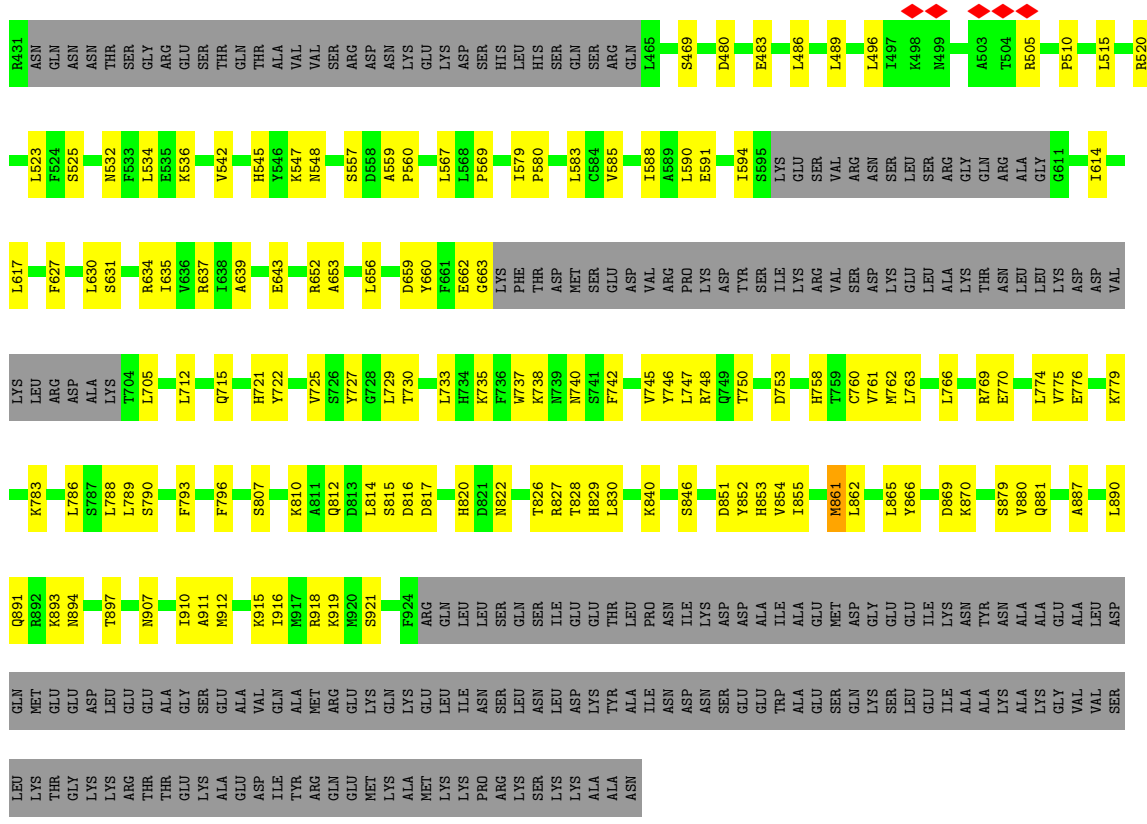


• Molecule 35: Ribosomal RNA-processing protein 7

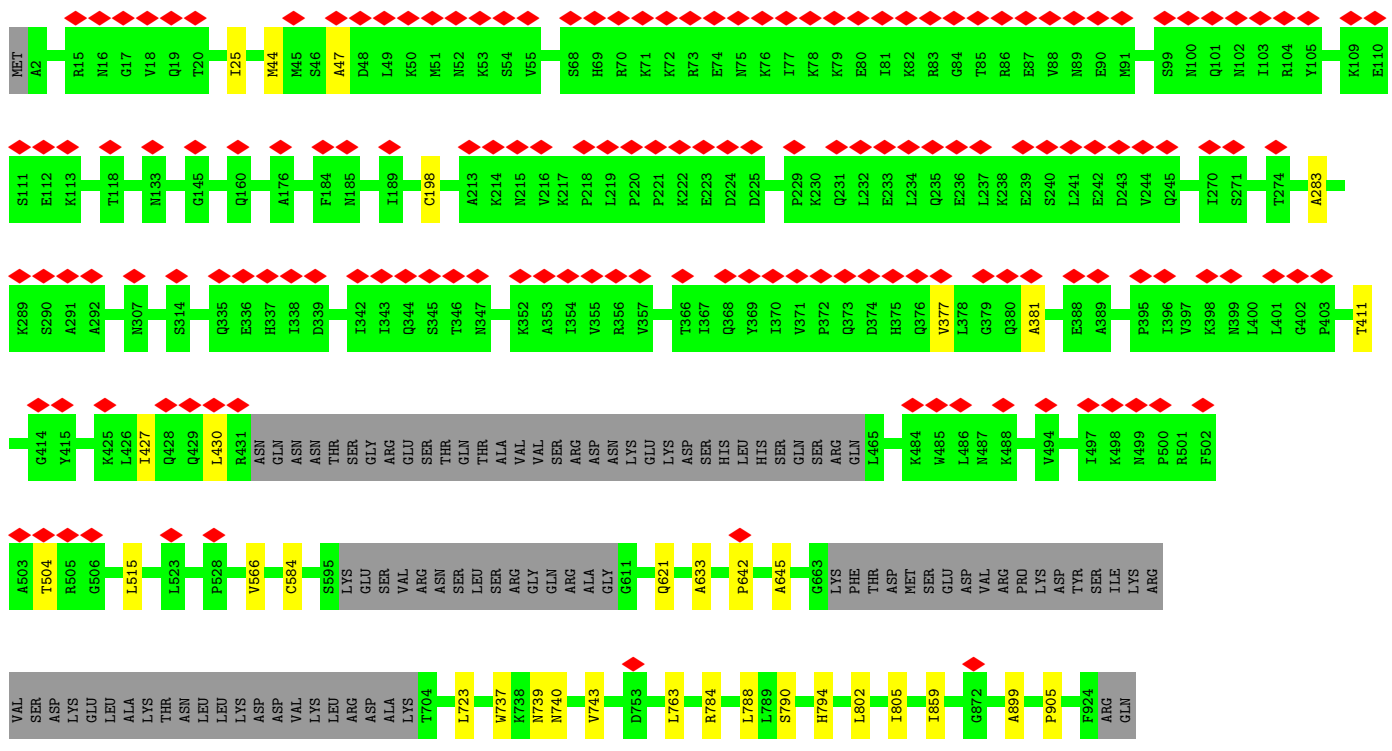
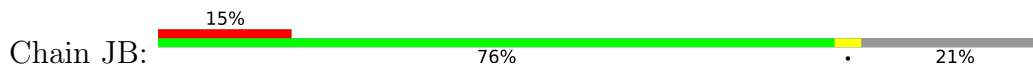


• Molecule 36: RNA cytidine acetyltransferase



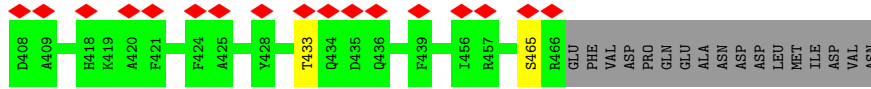


● Molecule 36: RNA cytidine acetyltransferase

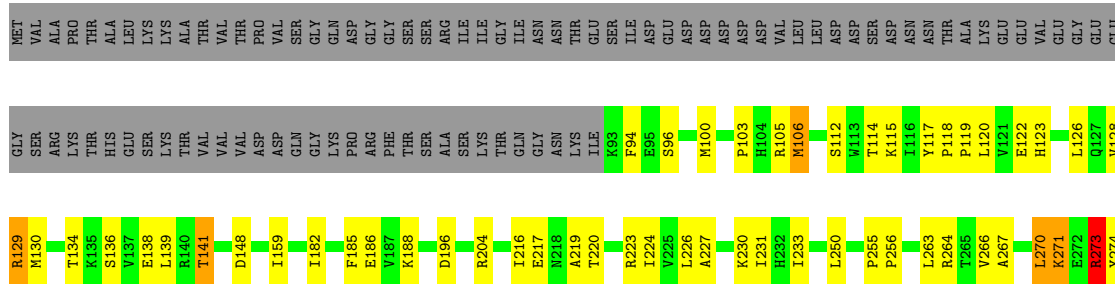




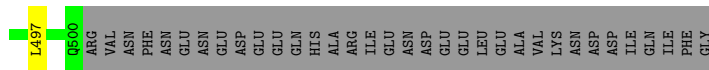




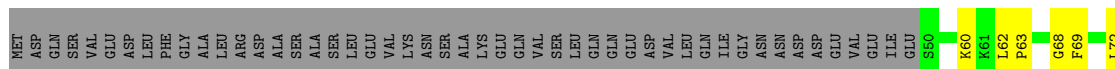
• Molecule 41: Pre-rRNA-processing protein PNO1



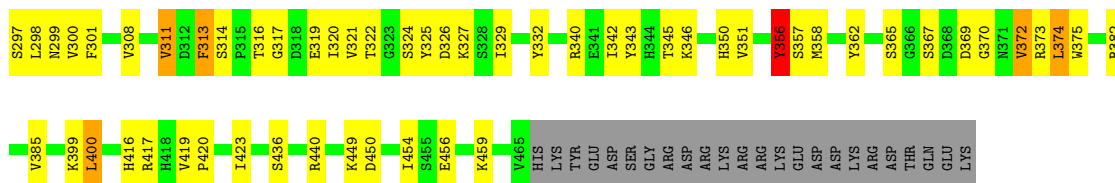
• Molecule 42: Protein BFR2



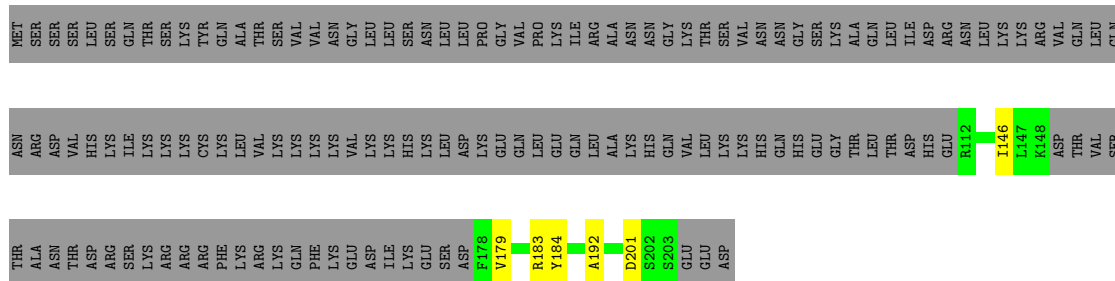
• Molecule 43: rRNA-processing protein FCF2



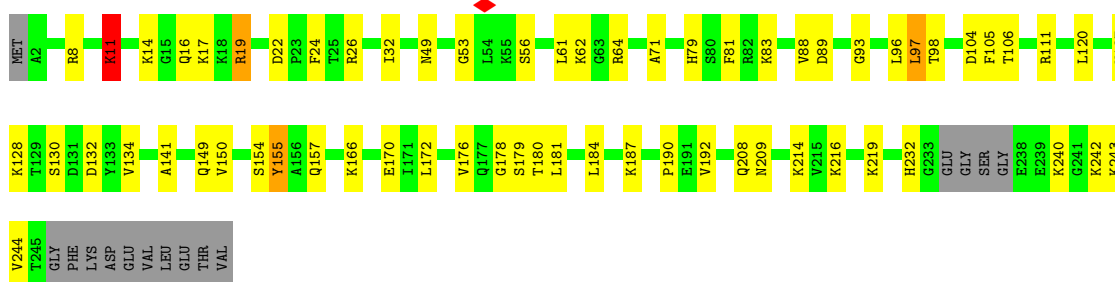




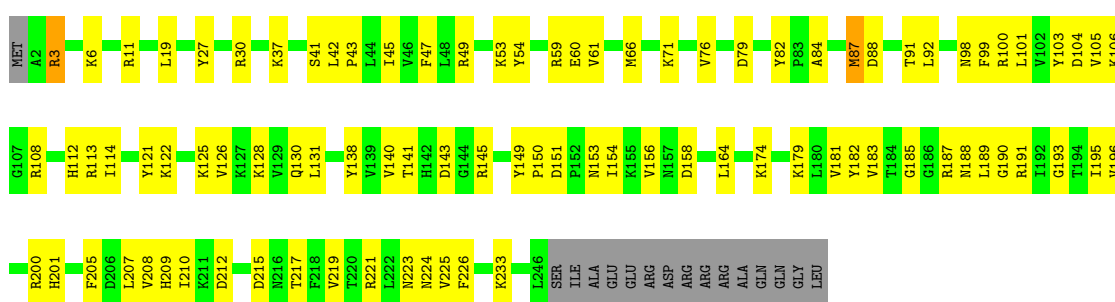
• Molecule 47: Regulator of rDNA transcription protein 14



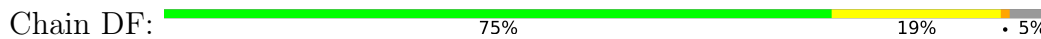
• Molecule 48: 40S ribosomal protein S1-A



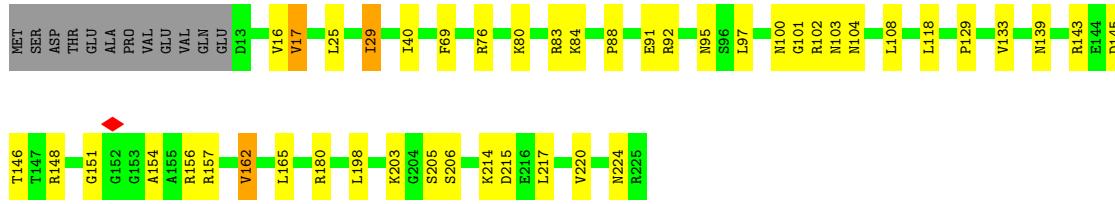
• Molecule 49: 40S ribosomal protein S4-A



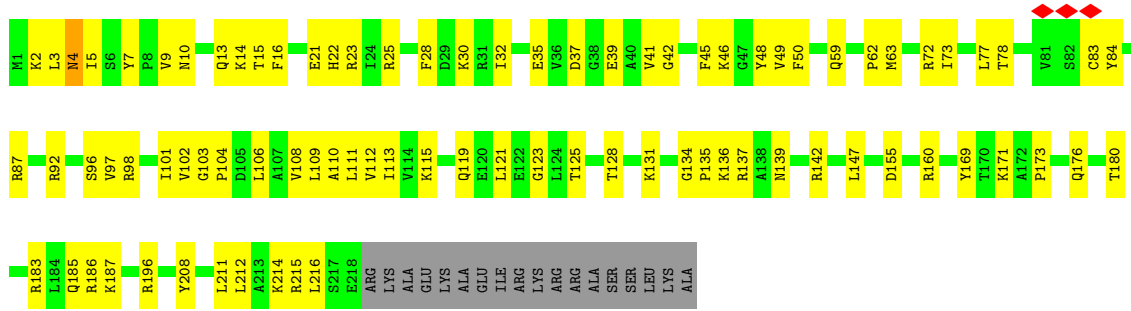
• Molecule 50: Rps5p



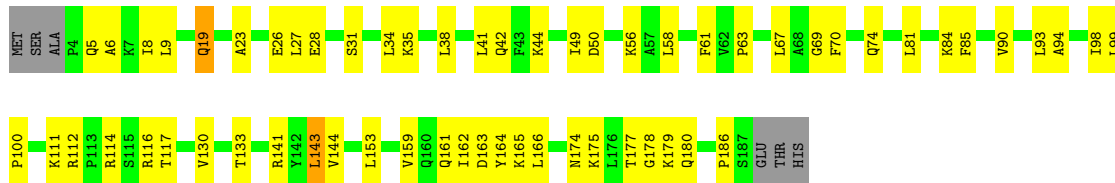




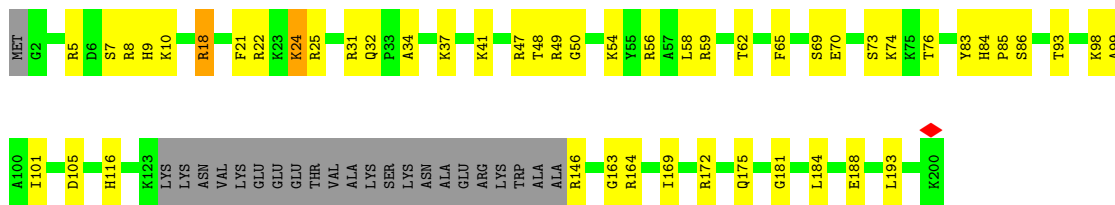
• Molecule 51: 40S ribosomal protein S6-A



• Molecule 52: 40S ribosomal protein S7-A

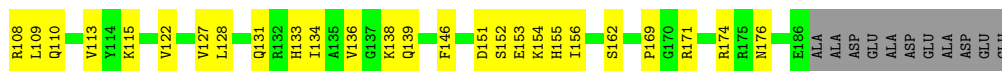


• Molecule 53: 40S ribosomal protein S8-A

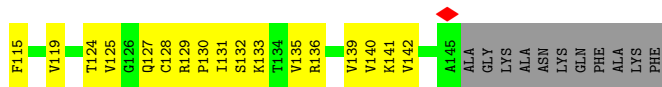


• Molecule 54: 40S ribosomal protein S9-A

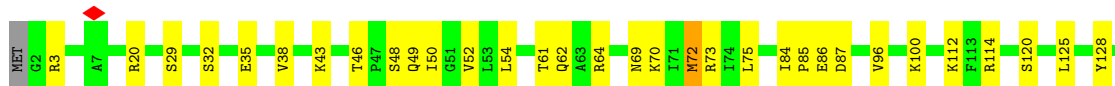
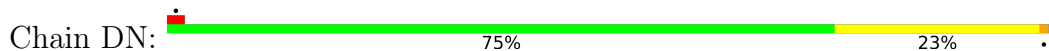




• Molecule 55: 40S ribosomal protein S11-A



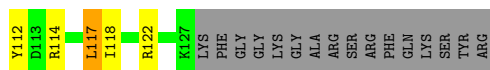
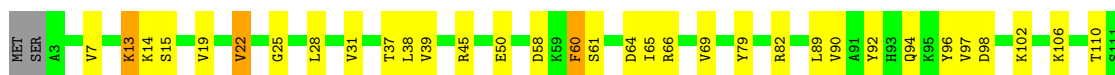
• Molecule 56: 40S ribosomal protein S13



• Molecule 57: 40S ribosomal protein S14-A

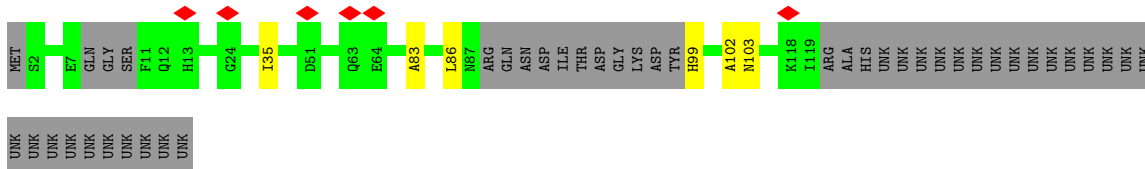


• Molecule 58: 40S ribosomal protein S16-A



• Molecule 59: 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18

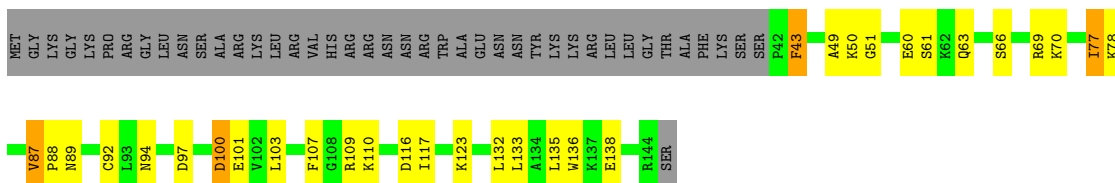




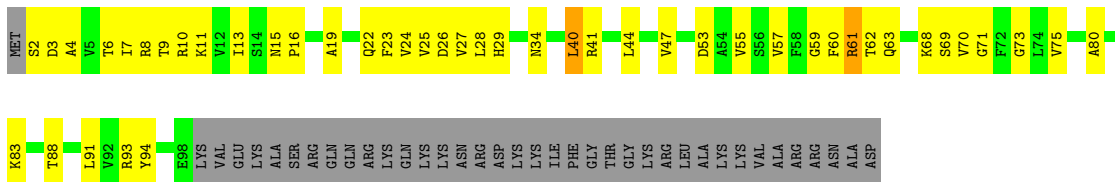
- Molecule 60: 40S ribosomal protein S22-A



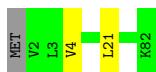
- Molecule 61: 40S ribosomal protein S23-A



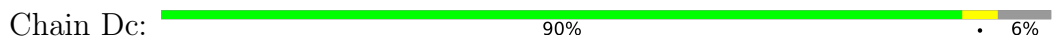
- Molecule 62: 40S ribosomal protein S24-A



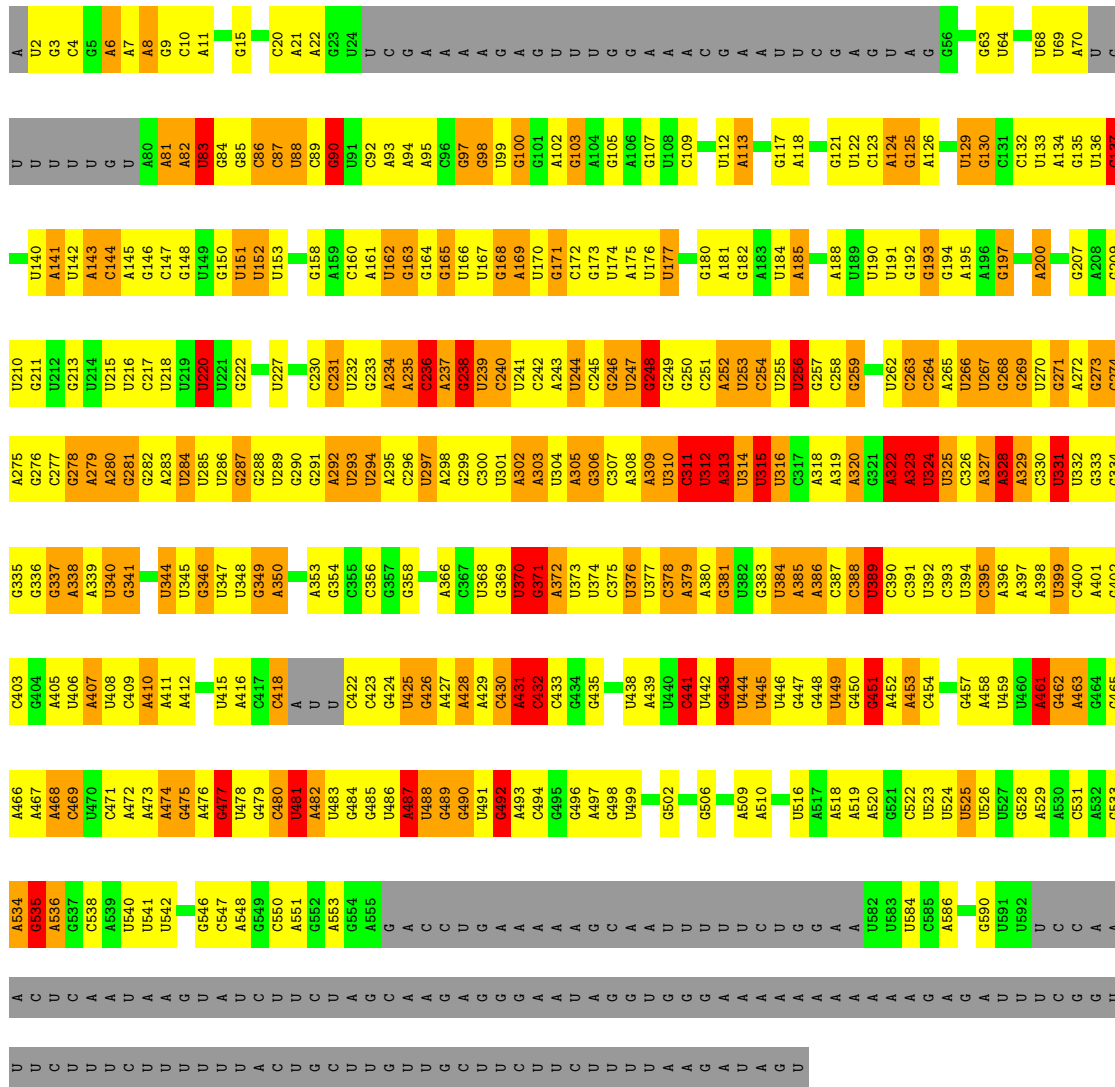
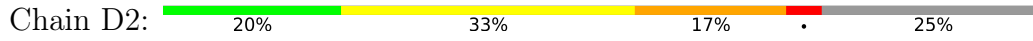
- Molecule 63: 40S ribosomal protein S27-A



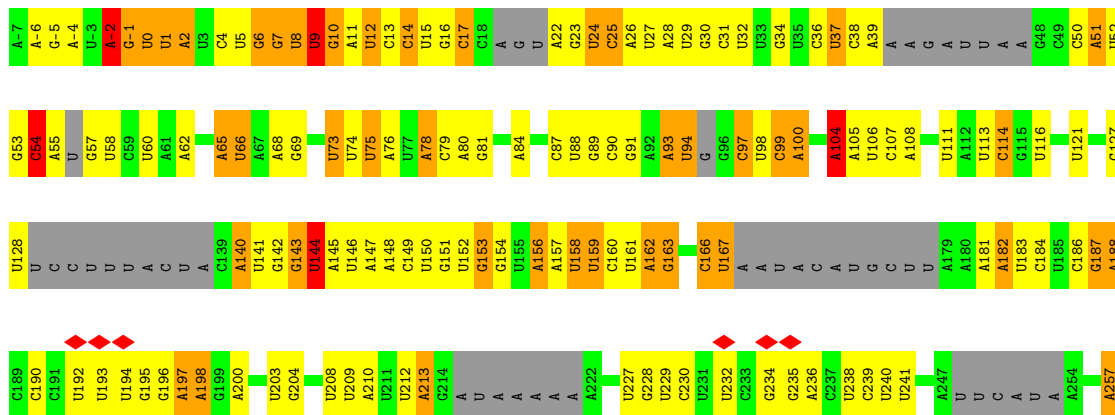
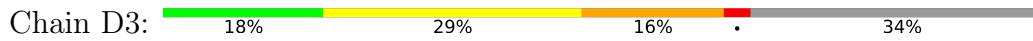
- Molecule 64: 40S ribosomal protein S28-A



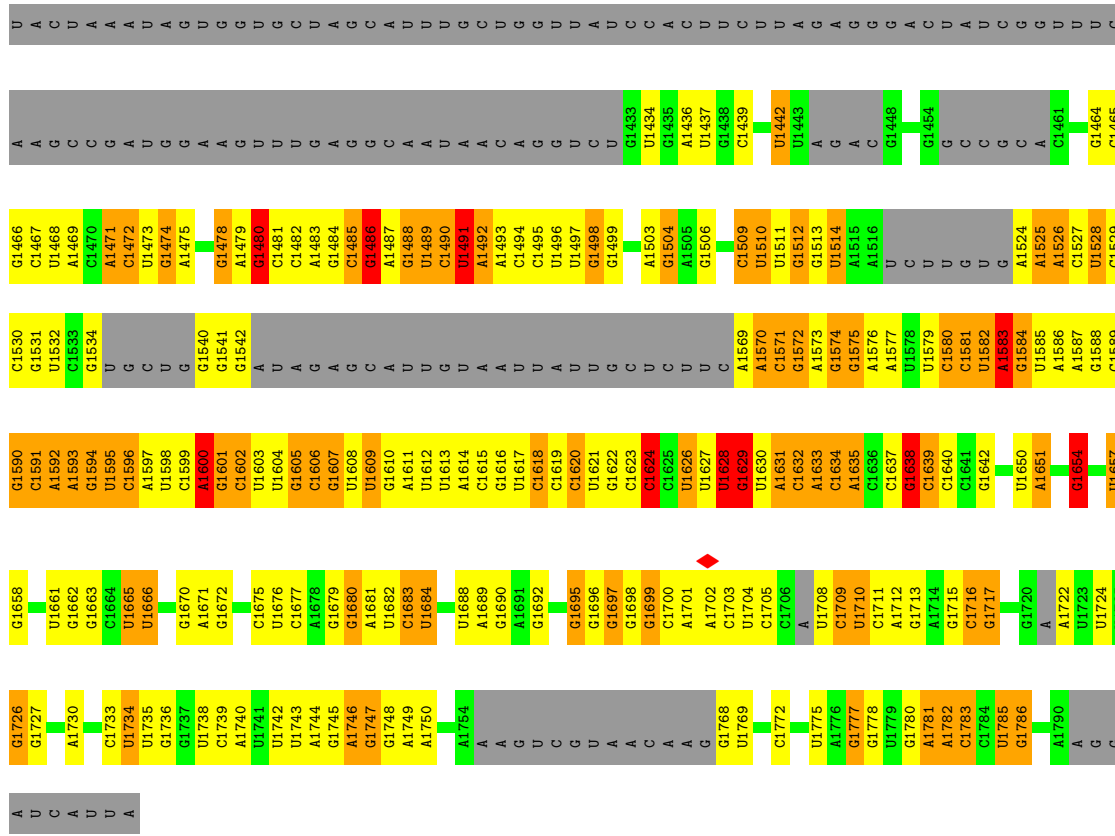
- Molecule 65: 5ETS RNA



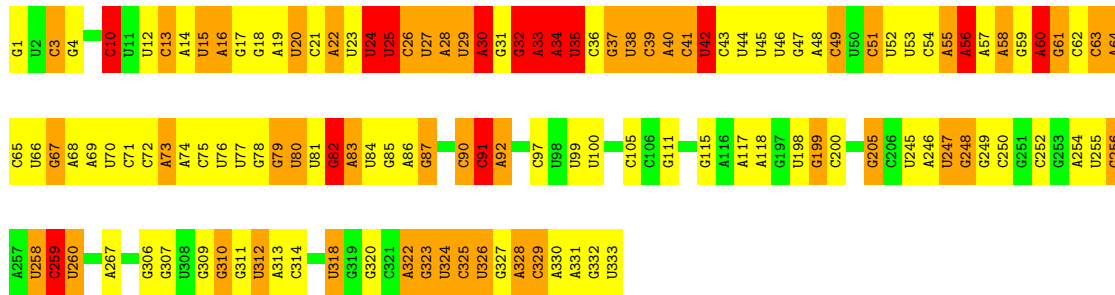
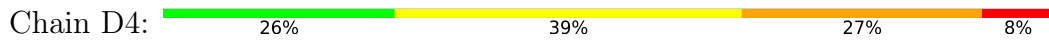
• Molecule 66: 18S rRNA







● Molecule 67: U3 snoRNA



## 4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32213	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	1.71	109/6780 (1.6%)	1.08	35/9175 (0.4%)
2	UB	0.51	0/3796	0.61	6/5137 (0.1%)
3	UC	1.03	1/1034 (0.1%)	0.86	2/1365 (0.1%)
4	UD	0.95	15/5461 (0.3%)	0.82	6/7395 (0.1%)
5	UE	1.07	8/3840 (0.2%)	0.88	6/5208 (0.1%)
6	UF	1.03	4/2538 (0.2%)	0.84	5/3405 (0.1%)
7	UG	1.60	70/4302 (1.6%)	1.11	26/5805 (0.4%)
8	UH	0.39	0/2703	0.68	11/3703 (0.3%)
9	UI	0.50	0/861	0.80	2/1156 (0.2%)
10	UJ	0.85	11/6903 (0.2%)	0.75	14/9474 (0.1%)
11	UK	1.26	14/2042 (0.7%)	0.96	1/2704 (0.0%)
12	UL	0.76	2/6851 (0.0%)	0.79	6/9246 (0.1%)
13	UM	0.71	5/6058 (0.1%)	0.80	6/8201 (0.1%)
14	UN	1.22	8/1231 (0.6%)	0.93	6/1661 (0.4%)
15	UO	1.10	12/3993 (0.3%)	0.90	10/5413 (0.2%)
16	UP	0.56	0/499	0.84	0/659
17	UQ	0.96	10/6794 (0.1%)	0.86	12/9203 (0.1%)
18	UR	1.50	36/3875 (0.9%)	1.02	17/5254 (0.3%)
19	US	0.61	0/3736	0.75	7/5086 (0.1%)
20	UT	0.28	0/11085	0.52	0/15445
21	UU	1.49	68/6815 (1.0%)	0.98	17/9213 (0.2%)
22	UV	0.50	0/8933	0.60	3/12081 (0.0%)
23	UX	1.50	16/1418 (1.1%)	1.07	5/1906 (0.3%)
24	UZ	0.70	1/2041 (0.0%)	0.74	1/2745 (0.0%)
25	CA	1.43	14/1917 (0.7%)	1.00	6/2588 (0.2%)
25	CB	0.73	0/1815	0.77	1/2448 (0.0%)
26	CD	0.96	3/3041 (0.1%)	0.85	7/4098 (0.2%)
27	CE	0.88	4/3012 (0.1%)	0.79	0/4091
28	CF	1.33	6/944 (0.6%)	0.97	5/1284 (0.4%)
28	CG	0.93	0/941	1.00	5/1281 (0.4%)
29	CH	0.61	1/3705 (0.0%)	0.68	1/4983 (0.0%)
30	CI	1.84	39/1559 (2.5%)	1.21	19/2097 (0.9%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	CJ	1.36	21/2337 (0.9%)	1.04	13/3148 (0.4%)
32	CK	1.06	2/1685 (0.1%)	0.98	6/2261 (0.3%)
33	CL	1.18	27/6471 (0.4%)	0.92	19/8708 (0.2%)
34	CM	0.85	0/2832	0.78	3/3825 (0.1%)
35	CN	0.44	0/1934	0.59	1/2604 (0.0%)
36	JA	0.48	0/5994	0.65	1/8139 (0.0%)
36	JB	0.30	0/4128	0.57	0/5747
37	JC	0.51	0/2908	0.71	1/3938 (0.0%)
38	JE	0.55	0/1139	0.75	2/1512 (0.1%)
39	JF	0.51	0/1727	0.70	1/2329 (0.0%)
39	JG	0.82	0/1828	0.83	3/2470 (0.1%)
40	JH	0.24	0/1293	0.37	0/1801
41	JJ	0.65	1/1475 (0.1%)	0.77	4/1987 (0.2%)
42	JK	0.49	0/342	0.71	1/462 (0.2%)
43	JM	1.02	2/1156 (0.2%)	0.88	2/1536 (0.1%)
44	JN	1.15	4/1435 (0.3%)	0.96	4/1907 (0.2%)
45	JO	1.01	3/1961 (0.2%)	0.89	3/2631 (0.1%)
46	JP	1.64	70/3802 (1.8%)	1.06	17/5118 (0.3%)
47	JQ	0.41	0/385	0.57	0/529
48	DA	1.00	2/1937 (0.1%)	0.90	2/2593 (0.1%)
49	DE	0.46	0/1985	0.63	1/2675 (0.0%)
50	DF	1.23	4/1690 (0.2%)	0.93	7/2285 (0.3%)
51	DG	0.45	0/1779	0.62	0/2379
52	DH	0.58	0/1502	0.74	2/2023 (0.1%)
53	DI	0.46	0/1422	0.63	1/1899 (0.1%)
54	DJ	1.14	5/1450 (0.3%)	0.92	1/1941 (0.1%)
55	DL	0.40	0/1155	0.60	0/1557
56	DN	0.82	0/1215	0.70	1/1638 (0.1%)
57	DO	0.98	0/892	0.79	0/1202
58	DQ	1.70	18/990 (1.8%)	1.04	2/1335 (0.1%)
59	DS	0.31	0/513	0.59	0/711
60	DW	1.18	3/1038 (0.3%)	0.93	1/1395 (0.1%)
61	DX	1.27	1/798 (0.1%)	0.99	2/1065 (0.2%)
62	DY	0.60	0/780	0.88	2/1049 (0.2%)
63	Db	0.91	0/620	0.84	2/838 (0.2%)
64	Dc	1.26	2/499 (0.4%)	1.05	2/670 (0.3%)
65	D2	2.24	658/12457 (5.3%)	1.69	374/19407 (1.9%)
66	D3	1.84	889/28553 (3.1%)	1.49	518/44437 (1.2%)
67	D4	2.61	329/4142 (7.9%)	1.84	155/6435 (2.4%)
All	All	1.26	2498/230772 (1.1%)	1.04	1402/321696 (0.4%)

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	4
4	UD	0	7
5	UE	0	1
6	UF	0	3
7	UG	0	4
10	UJ	0	3
12	UL	0	4
13	UM	0	2
14	UN	0	1
15	UO	0	1
17	UQ	0	4
18	UR	0	3
20	UT	0	7
21	UU	0	4
23	UX	0	1
26	CD	0	1
27	CE	0	1
30	CI	0	1
31	CJ	0	2
32	CK	0	1
34	CM	0	1
36	JA	0	1
36	JB	0	3
37	JC	0	2
38	JE	0	2
43	JM	0	1
44	JN	0	1
46	JP	0	4
48	DA	0	3
49	DE	0	1
52	DH	0	1
58	DQ	0	2
59	DS	0	1
60	DW	0	1
61	DX	0	3
All	All	0	82

The worst 5 of 2498 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	CL	1081	SER	CA-CB	-16.22	1.28	1.52

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	280	A	N9-C4	-13.97	1.29	1.37
67	D4	61	G	C5-C4	-12.91	1.29	1.38
66	D3	584	C	N1-C6	-12.87	1.29	1.37
67	D4	61	G	N7-C5	-12.51	1.31	1.39

The worst 5 of 1402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	D2	312	U	O4'-C1'-N1	19.10	123.48	108.20
13	UM	443	PRO	N-CD-CG	-16.65	78.23	103.20
67	D4	27	U	N3-C2-O2	-15.30	111.49	122.20
65	D2	233	G	N3-C4-C5	14.71	135.96	128.60
21	UU	494	LEU	CB-CG-CD2	-14.58	86.21	111.00

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UA	157	ASP	Peptide
1	UA	202	ASP	Peptide
1	UA	288	ASP	Peptide
1	UA	516	SER	Peptide
4	UD	117	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	6635	0	6524	147	0
2	UB	3743	0	3445	80	0
3	UC	1026	0	1080	40	0
4	UD	5361	0	5364	141	0
5	UE	3772	0	3806	99	0
6	UF	2487	0	2533	59	0
7	UG	4218	0	4223	94	0
8	UH	2690	0	1931	69	0
9	UI	846	0	904	39	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	UJ	6857	0	5023	85	0
11	UK	2016	0	2093	59	0
12	UL	6720	0	6753	196	0
13	UM	5957	0	5992	182	0
14	UN	1207	0	1201	26	0
15	UO	3911	0	3906	119	0
16	UP	495	0	561	13	0
17	UQ	6662	0	6588	173	0
18	UR	3791	0	3772	89	0
19	US	3650	0	3365	102	0
20	UT	11108	0	4748	16	0
21	UU	6678	0	6652	131	0
22	UV	8725	0	8841	190	0
23	UX	1395	0	1474	40	0
24	UZ	2006	0	2118	54	0
25	CA	1881	0	1928	31	0
25	CB	1782	0	1826	54	0
26	CD	2994	0	3018	81	0
27	CE	2985	0	2703	59	0
28	CF	931	0	983	18	0
28	CG	928	0	976	34	0
29	CH	3634	0	3662	112	0
30	CI	1530	0	1572	36	0
31	CJ	2296	0	2325	64	0
32	CK	1667	0	1701	50	0
33	CL	6332	0	6516	190	0
34	CM	2781	0	2878	73	0
35	CN	1893	0	1875	37	0
36	JA	5892	0	5420	146	0
36	JB	4132	0	1819	17	0
37	JC	2845	0	2761	91	0
38	JE	1125	0	1101	46	0
39	JF	1701	0	1767	42	0
39	JG	1799	0	1872	48	0
40	JH	1295	0	570	2	0
41	JJ	1448	0	1524	43	0
42	JK	334	0	313	12	0
43	JM	1137	0	1187	28	0
44	JN	1428	0	1425	25	0
45	JO	1930	0	2025	38	0
46	JP	3725	0	3679	100	0
47	JQ	381	0	255	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	DA	1912	0	2023	53	0
49	DE	1944	0	2030	69	0
50	DF	1669	0	1724	31	0
51	DG	1755	0	1846	68	0
52	DH	1477	0	1568	49	0
53	DI	1399	0	1431	47	0
54	DJ	1428	0	1506	48	0
55	DL	1129	0	1196	35	0
56	DN	1192	0	1255	27	0
57	DO	881	0	910	21	0
58	DQ	973	0	1029	23	0
59	DS	516	0	222	12	0
60	DW	1021	0	1060	24	0
61	DX	786	0	843	20	0
62	DY	767	0	787	53	0
63	Db	610	0	629	0	0
64	Dc	497	0	535	0	0
65	D2	11138	0	5569	138	0
66	D3	25549	0	12882	423	0
67	D4	3712	0	1876	51	0
68	Db	1	0	0	0	0
68	UX	1	0	0	0	0
69	CL	32	0	12	3	0
All	All	223151	0	191511	4355	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 11.

The worst 5 of 4355 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)
33:CL:80:THR:CG2	33:CL:141:LEU:CD2	2.05	1.33
12:UL:349:SER:HA	12:UL:369:TYR:O	1.21	1.30
1:UA:315:GLU:OE1	41:JJ:273:ARG:HG3	1.34	1.28
7:UG:132:GLY:HA3	7:UG:150:LEU:O	1.24	1.26
13:UM:30:LYS:HA	13:UM:45:LEU:O	1.37	1.21

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	830/923 (90%)	730 (88%)	99 (12%)	1 (0%)	51	84
2	UB	496/810 (61%)	458 (92%)	35 (7%)	3 (1%)	25	63
3	UC	124/610 (20%)	113 (91%)	10 (8%)	1 (1%)	19	57
4	UD	663/776 (85%)	585 (88%)	78 (12%)	0	100	100
5	UE	465/643 (72%)	401 (86%)	63 (14%)	1 (0%)	47	79
6	UF	283/440 (64%)	273 (96%)	10 (4%)	0	100	100
7	UG	529/554 (96%)	471 (89%)	58 (11%)	0	100	100
8	UH	423/713 (59%)	305 (72%)	94 (22%)	24 (6%)	1	21
9	UI	98/575 (17%)	92 (94%)	6 (6%)	0	100	100
10	UJ	1093/1769 (62%)	1038 (95%)	55 (5%)	0	100	100
11	UK	237/250 (95%)	217 (92%)	19 (8%)	1 (0%)	34	71
12	UL	828/943 (88%)	733 (88%)	94 (11%)	1 (0%)	51	84
13	UM	750/817 (92%)	666 (89%)	84 (11%)	0	100	100
14	UN	141/145 (97%)	124 (88%)	16 (11%)	1 (1%)	22	60
15	UO	489/513 (95%)	433 (88%)	55 (11%)	1 (0%)	47	79
16	UP	58/214 (27%)	57 (98%)	1 (2%)	0	100	100
17	UQ	820/896 (92%)	720 (88%)	98 (12%)	2 (0%)	47	79
18	UR	473/594 (80%)	432 (91%)	40 (8%)	1 (0%)	47	79
19	US	471/552 (85%)	421 (89%)	49 (10%)	1 (0%)	47	79
20	UT	2189/2493 (88%)	2067 (94%)	122 (6%)	0	100	100
21	UU	842/939 (90%)	737 (88%)	105 (12%)	0	100	100
22	UV	1068/1237 (86%)	1006 (94%)	62 (6%)	0	100	100
23	UX	170/189 (90%)	151 (89%)	18 (11%)	1 (1%)	25	63
24	UZ	245/274 (89%)	217 (89%)	28 (11%)	0	100	100
25	CA	238/327 (73%)	220 (92%)	18 (8%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	CB	224/327 (68%)	197 (88%)	27 (12%)	0	100	100
26	CD	376/504 (75%)	351 (93%)	25 (7%)	0	100	100
27	CE	431/511 (84%)	394 (91%)	37 (9%)	0	100	100
28	CF	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
28	CG	121/126 (96%)	111 (92%)	10 (8%)	0	100	100
29	CH	446/573 (78%)	399 (90%)	45 (10%)	2 (0%)	34	71
30	CI	180/183 (98%)	162 (90%)	18 (10%)	0	100	100
31	CJ	278/290 (96%)	247 (89%)	30 (11%)	1 (0%)	34	71
32	CK	203/593 (34%)	177 (87%)	25 (12%)	1 (0%)	29	67
33	CL	771/1183 (65%)	704 (91%)	63 (8%)	4 (0%)	29	67
34	CM	358/367 (98%)	334 (93%)	24 (7%)	0	100	100
35	CN	224/297 (75%)	210 (94%)	14 (6%)	0	100	100
36	JA	802/1056 (76%)	717 (89%)	85 (11%)	0	100	100
36	JB	827/1056 (78%)	736 (89%)	91 (11%)	0	100	100
37	JC	350/707 (50%)	308 (88%)	42 (12%)	0	100	100
38	JE	134/357 (38%)	119 (89%)	14 (10%)	1 (1%)	22	60
39	JF	212/252 (84%)	201 (95%)	11 (5%)	0	100	100
39	JG	226/252 (90%)	215 (95%)	11 (5%)	0	100	100
40	JH	257/483 (53%)	244 (95%)	13 (5%)	0	100	100
41	JJ	180/274 (66%)	166 (92%)	13 (7%)	1 (1%)	25	63
42	JK	40/534 (8%)	30 (75%)	10 (25%)	0	100	100
43	JM	129/217 (59%)	113 (88%)	15 (12%)	1 (1%)	19	57
44	JN	178/346 (51%)	154 (86%)	19 (11%)	5 (3%)	5	34
45	JO	232/316 (73%)	215 (93%)	17 (7%)	0	100	100
46	JP	453/489 (93%)	412 (91%)	41 (9%)	0	100	100
47	JQ	59/206 (29%)	49 (83%)	9 (15%)	1 (2%)	9	43
48	DA	236/255 (92%)	207 (88%)	29 (12%)	0	100	100
49	DE	243/261 (93%)	224 (92%)	19 (8%)	0	100	100
50	DF	211/225 (94%)	188 (89%)	23 (11%)	0	100	100
51	DG	216/236 (92%)	203 (94%)	13 (6%)	0	100	100
52	DH	182/190 (96%)	160 (88%)	22 (12%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	DI	173/200 (86%)	160 (92%)	13 (8%)	0	100	100
54	DJ	175/197 (89%)	160 (91%)	15 (9%)	0	100	100
55	DL	138/156 (88%)	125 (91%)	13 (9%)	0	100	100
56	DN	148/151 (98%)	127 (86%)	21 (14%)	0	100	100
57	DO	118/137 (86%)	107 (91%)	10 (8%)	1 (1%)	19	57
58	DQ	123/143 (86%)	114 (93%)	9 (7%)	0	100	100
59	DS	98/147 (67%)	89 (91%)	9 (9%)	0	100	100
60	DW	127/130 (98%)	106 (84%)	21 (16%)	0	100	100
61	DX	101/145 (70%)	89 (88%)	12 (12%)	0	100	100
62	DY	95/135 (70%)	79 (83%)	16 (17%)	0	100	100
63	Db	79/82 (96%)	66 (84%)	13 (16%)	0	100	100
64	Dc	61/67 (91%)	52 (85%)	9 (15%)	0	100	100
All	All	24359/32678 (74%)	22000 (90%)	2302 (10%)	57 (0%)	50	79

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	UB	399	HIS
8	UH	59	PRO
8	UH	61	PRO
8	UH	68	PRO
8	UH	127	TYR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	730/812 (90%)	729 (100%)	1 (0%)	93	97
2	UB	345/732 (47%)	345 (100%)	0	100	100
3	UC	107/538 (20%)	103 (96%)	4 (4%)	34	60
4	UD	615/713 (86%)	612 (100%)	3 (0%)	88	93

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	UE	428/574 (75%)	426 (100%)	2 (0%)	88	93
6	UF	277/414 (67%)	275 (99%)	2 (1%)	84	90
7	UG	462/480 (96%)	462 (100%)	0	100	100
8	UH	150/657 (23%)	149 (99%)	1 (1%)	84	90
9	UI	97/533 (18%)	97 (100%)	0	100	100
10	UJ	390/1633 (24%)	388 (100%)	2 (0%)	88	93
11	UK	226/234 (97%)	223 (99%)	3 (1%)	69	82
12	UL	746/832 (90%)	745 (100%)	1 (0%)	93	97
13	UM	665/719 (92%)	663 (100%)	2 (0%)	92	95
14	UN	135/135 (100%)	135 (100%)	0	100	100
15	UO	437/454 (96%)	435 (100%)	2 (0%)	88	93
16	UP	57/196 (29%)	56 (98%)	1 (2%)	59	77
17	UQ	769/826 (93%)	763 (99%)	6 (1%)	81	89
18	UR	424/529 (80%)	421 (99%)	3 (1%)	84	90
19	US	360/506 (71%)	360 (100%)	0	100	100
21	UU	743/819 (91%)	740 (100%)	3 (0%)	91	94
22	UV	985/1125 (88%)	980 (100%)	5 (0%)	88	93
23	UX	156/169 (92%)	155 (99%)	1 (1%)	86	91
24	UZ	230/256 (90%)	228 (99%)	2 (1%)	78	87
25	CA	202/240 (84%)	200 (99%)	2 (1%)	76	86
25	CB	192/240 (80%)	191 (100%)	1 (0%)	88	93
26	CD	326/435 (75%)	325 (100%)	1 (0%)	92	95
27	CE	244/433 (56%)	244 (100%)	0	100	100
28	CF	102/104 (98%)	102 (100%)	0	100	100
28	CG	101/104 (97%)	100 (99%)	1 (1%)	76	86
29	CH	395/503 (78%)	393 (100%)	2 (0%)	88	93
30	CI	171/172 (99%)	170 (99%)	1 (1%)	86	91
31	CJ	251/258 (97%)	249 (99%)	2 (1%)	81	89
32	CK	187/535 (35%)	187 (100%)	0	100	100
33	CL	690/1039 (66%)	684 (99%)	6 (1%)	78	87
34	CM	307/312 (98%)	306 (100%)	1 (0%)	92	95

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	CN	212/274 (77%)	212 (100%)	0	100	100
36	JA	549/934 (59%)	545 (99%)	4 (1%)	84	90
37	JC	318/636 (50%)	318 (100%)	0	100	100
38	JE	119/315 (38%)	118 (99%)	1 (1%)	81	89
39	JF	195/222 (88%)	195 (100%)	0	100	100
39	JG	206/222 (93%)	206 (100%)	0	100	100
41	JJ	159/238 (67%)	156 (98%)	3 (2%)	57	75
42	JK	35/482 (7%)	35 (100%)	0	100	100
43	JM	124/200 (62%)	123 (99%)	1 (1%)	81	89
44	JN	141/304 (46%)	141 (100%)	0	100	100
45	JO	215/289 (74%)	213 (99%)	2 (1%)	78	87
46	JP	412/443 (93%)	412 (100%)	0	100	100
47	JQ	22/192 (12%)	21 (96%)	1 (4%)	27	56
48	DA	212/224 (95%)	209 (99%)	3 (1%)	67	81
49	DE	209/222 (94%)	206 (99%)	3 (1%)	67	81
50	DF	180/191 (94%)	180 (100%)	0	100	100
51	DG	187/201 (93%)	186 (100%)	1 (0%)	88	93
52	DH	164/170 (96%)	162 (99%)	2 (1%)	71	83
53	DI	142/161 (88%)	141 (99%)	1 (1%)	84	90
54	DJ	151/166 (91%)	150 (99%)	1 (1%)	84	90
55	DL	125/137 (91%)	125 (100%)	0	100	100
56	DN	127/128 (99%)	127 (100%)	0	100	100
57	DO	91/105 (87%)	91 (100%)	0	100	100
58	DQ	105/119 (88%)	105 (100%)	0	100	100
60	DW	110/111 (99%)	110 (100%)	0	100	100
61	DX	85/120 (71%)	83 (98%)	2 (2%)	49	69
62	DY	81/113 (72%)	81 (100%)	0	100	100
63	Db	70/71 (99%)	70 (100%)	0	100	100
64	Dc	56/60 (93%)	56 (100%)	0	100	100
All	All	17504/25311 (69%)	17418 (100%)	86 (0%)	89	93

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	CL	119	GLU
45	JO	280	LYS
33	CL	960	ARG
38	JE	356	ARG
48	DA	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
19	US	200	ASN
26	CD	23	GLN
52	DH	170	GLN
19	US	256	ASN
24	UZ	117	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
65	D2	518/700 (74%)	166 (32%)	9 (1%)
66	D3	1172/1808 (64%)	423 (36%)	28 (2%)
67	D4	169/175 (96%)	62 (36%)	2 (1%)
All	All	1859/2683 (69%)	651 (35%)	39 (2%)

5 of 651 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
65	D2	6	A
65	D2	7	A
65	D2	8	A
65	D2	9	G
65	D2	15	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
66	D3	1572	G
66	D3	1746	A
66	D3	1573	A
66	D3	1620	C
67	D4	24	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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
69	GTP	CL	2001	-	26,34,34	0.93	1 (3%)	32,54,54	1.49	5 (15%)

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
69	GTP	CL	2001	-	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	CL	2001	GTP	C6-N1	-2.56	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	CL	2001	GTP	PA-O3A-PB	-3.97	119.20	132.83
69	CL	2001	GTP	PB-O3B-PG	-3.56	120.62	132.83
69	CL	2001	GTP	C3'-C2'-C1'	3.11	105.67	100.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	CL	2001	GTP	C5-C6-N1	2.35	118.11	113.95
69	CL	2001	GTP	C8-N7-C5	2.26	107.29	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

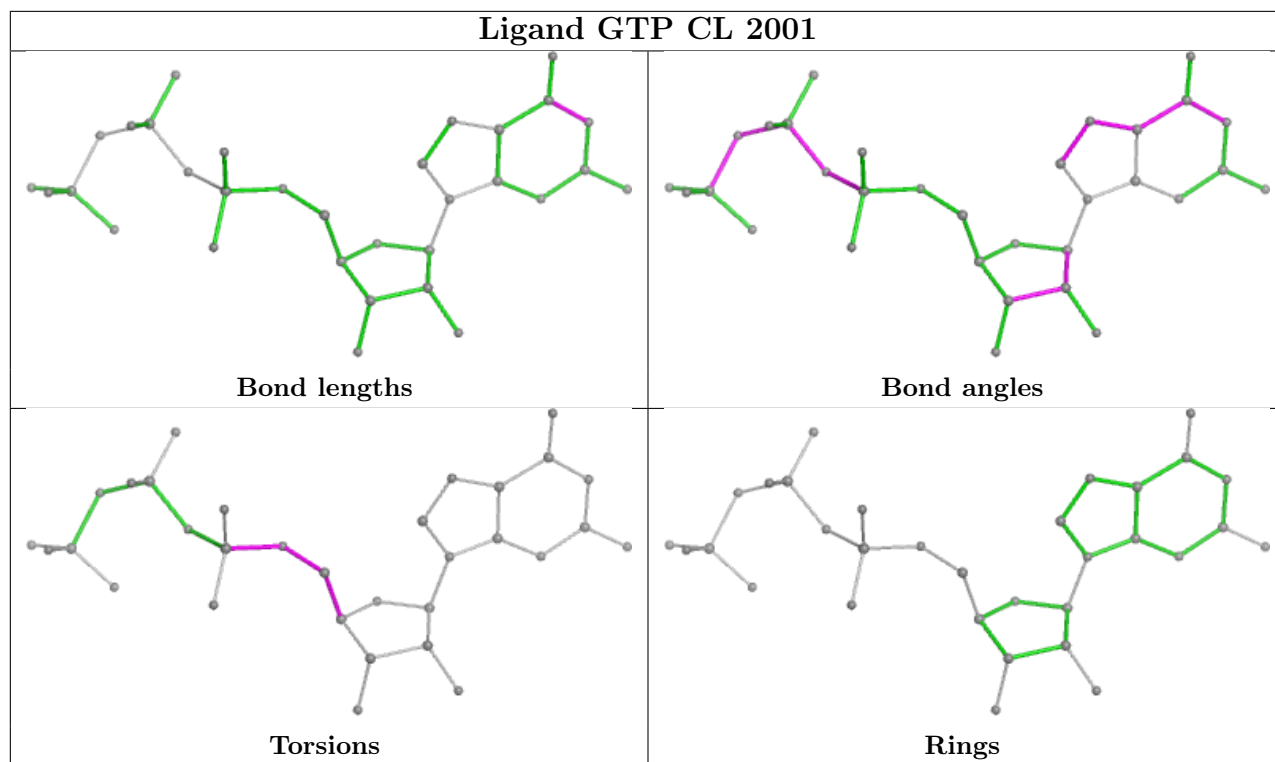
Mol	Chain	Res	Type	Atoms
69	CL	2001	GTP	C5'-O5'-PA-O1A
69	CL	2001	GTP	C3'-C4'-C5'-O5'
69	CL	2001	GTP	C4'-C5'-O5'-PA
69	CL	2001	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	CL	2001	GTP	3	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	D4	5
14	UN	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UN	349:SER	C	827:GLN	N	110.52
1	D4	118:A	O3'	197:G	P	24.98
1	D4	267:A	O3'	304:U	P	18.78
1	D4	106:C	O3'	111:G	P	16.51
1	D4	206:C	O3'	245:U	P	14.23

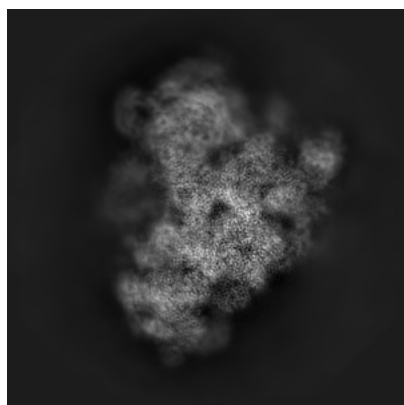
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11358. These allow visual inspection of the internal detail of the map and identification of artifacts.

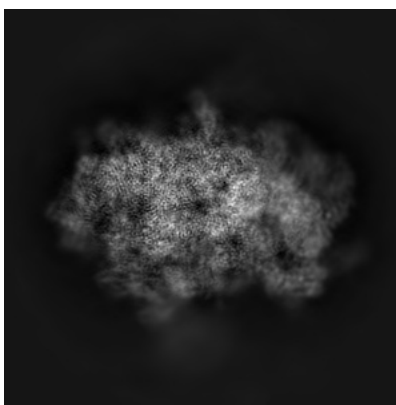
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

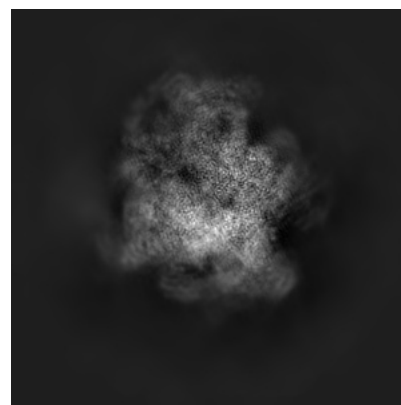
#### 6.1.1 Primary map



X



Y

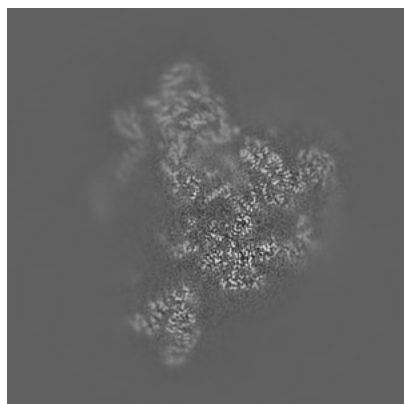


Z

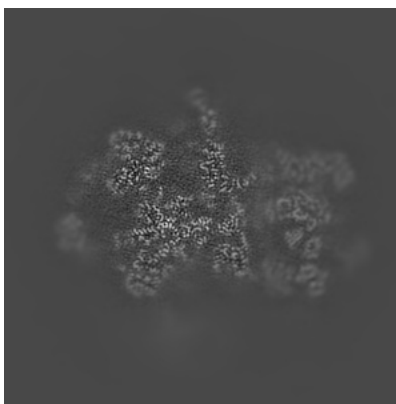
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

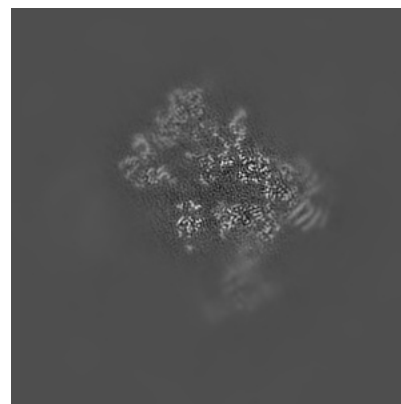
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

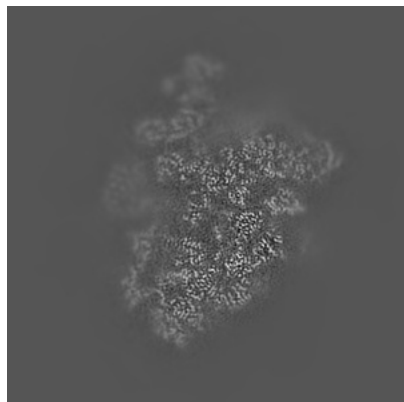


Z Index: 240

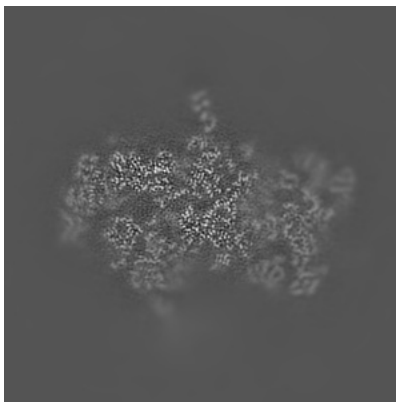
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

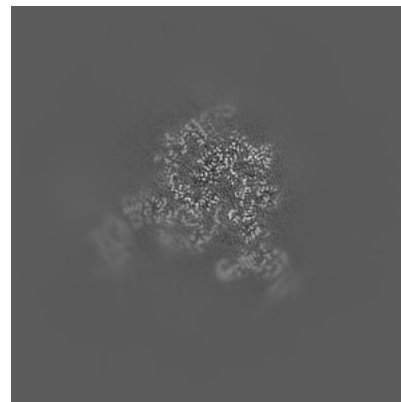
### 6.3.1 Primary map



X Index: 270



Y Index: 225

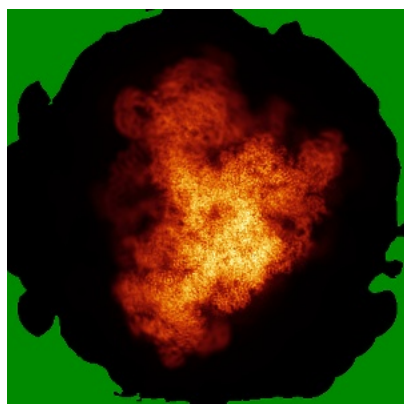


Z Index: 182

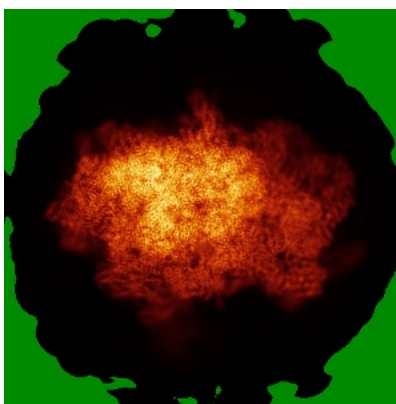
The images above show the largest variance slices of the map in three orthogonal directions.

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

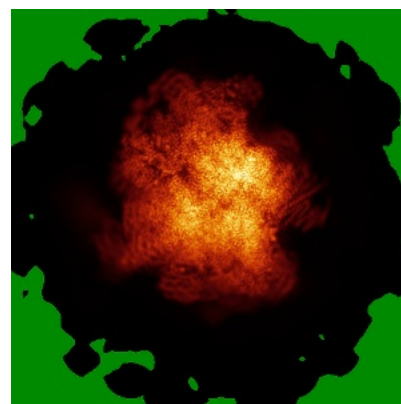
### 6.4.1 Primary map



X



Y



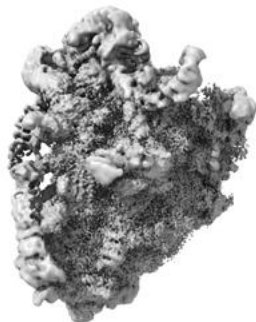
Z

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.

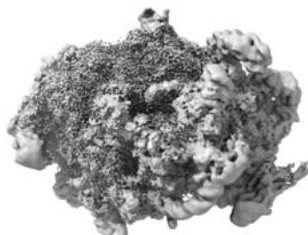


## 6.5 Orthogonal surface views [i](#)

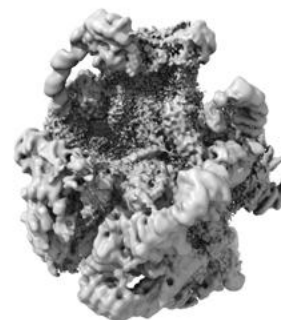
### 6.5.1 Primary map



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.

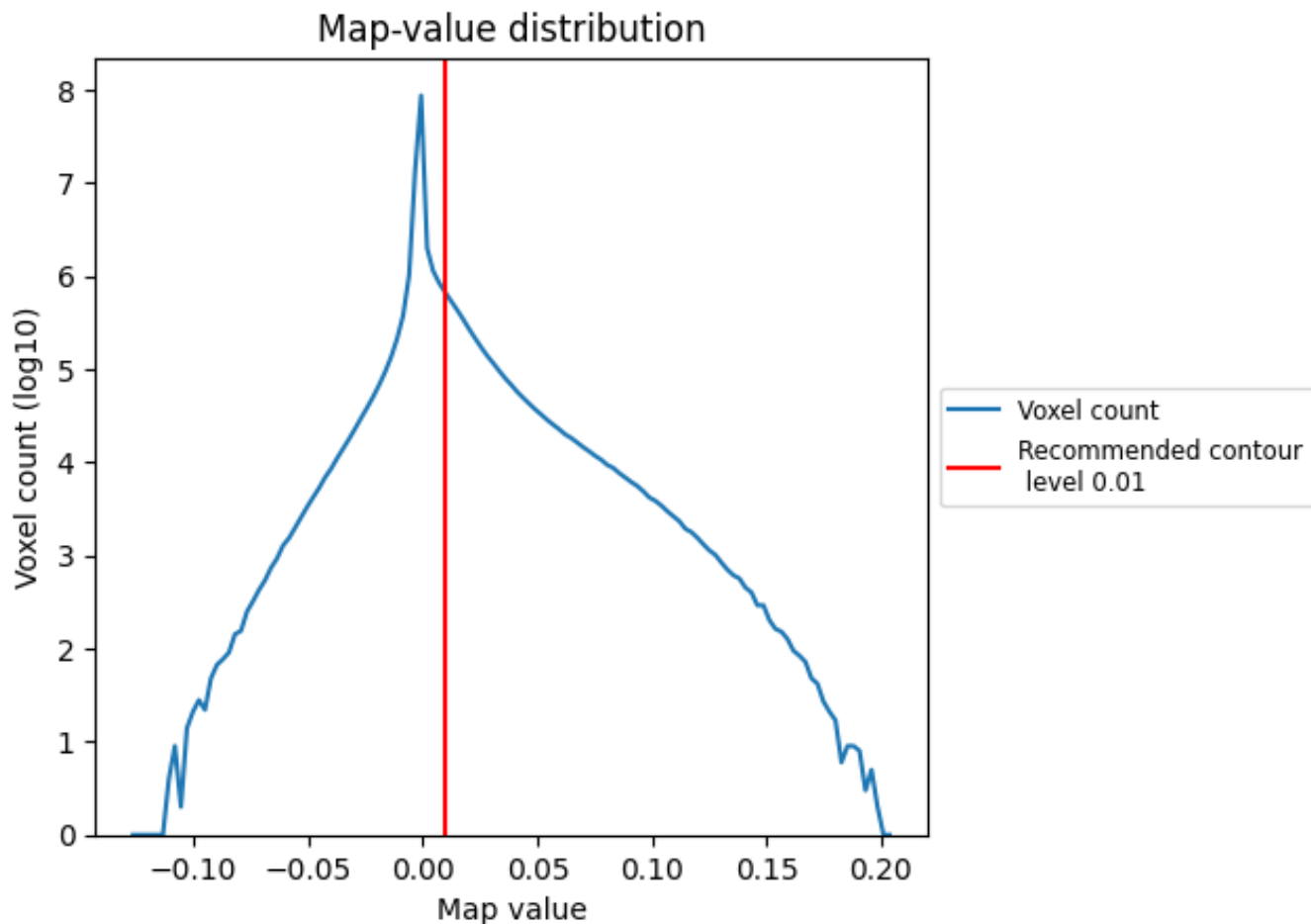
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

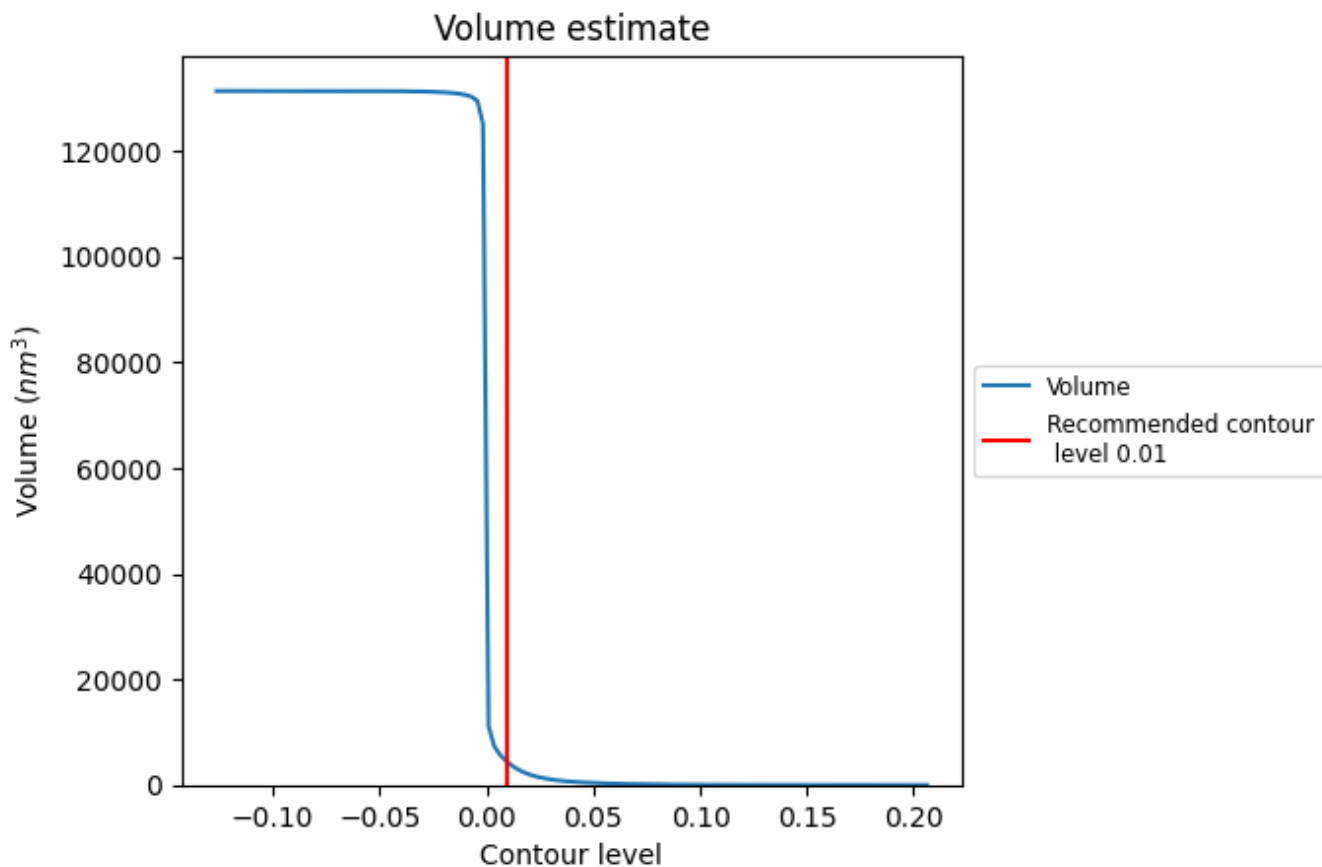
This section contains the results of statistical analysis of the map.

### 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.

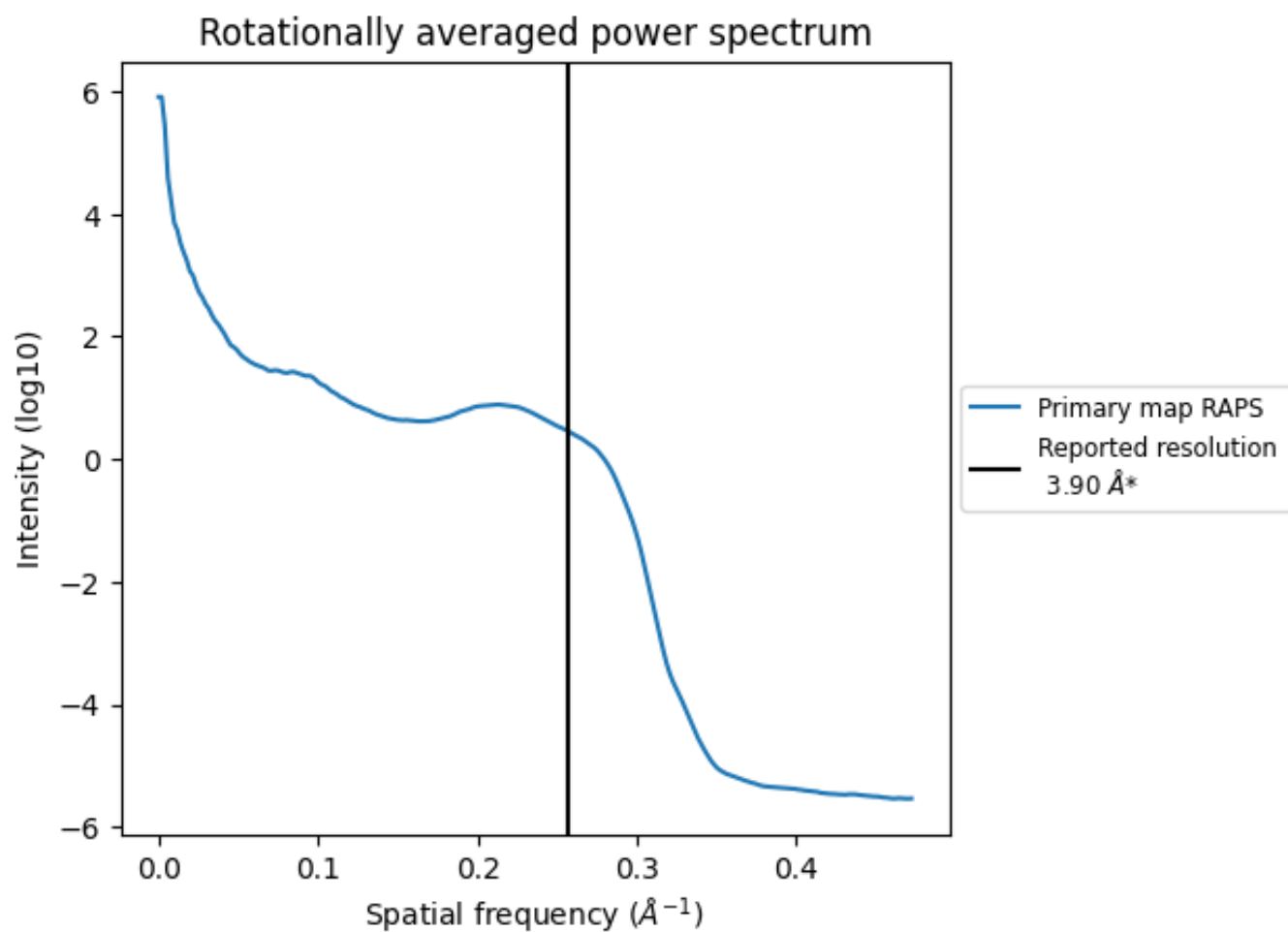
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4278  $\text{nm}^3$ ; this corresponds to an approximate mass of 3864 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

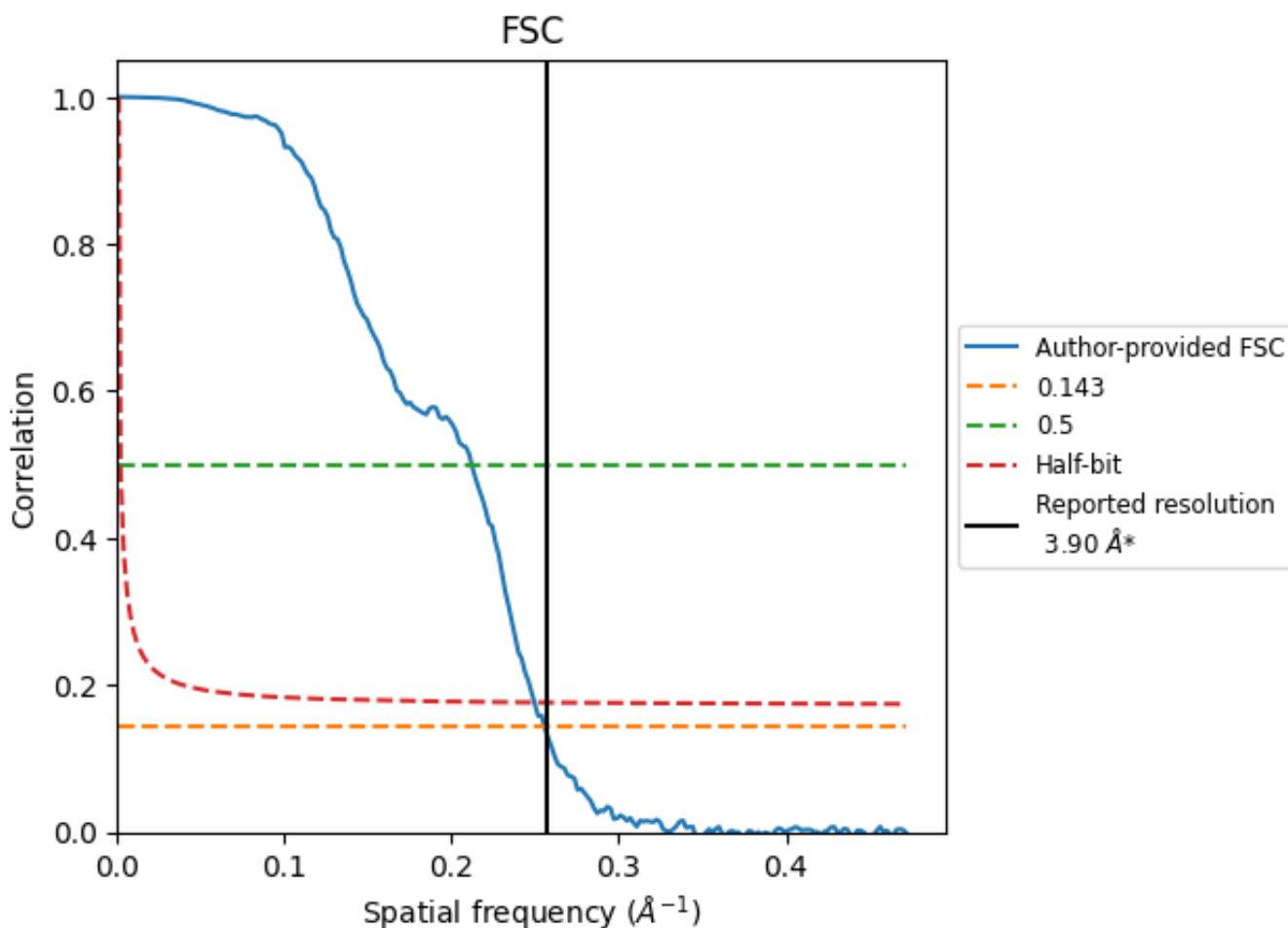


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

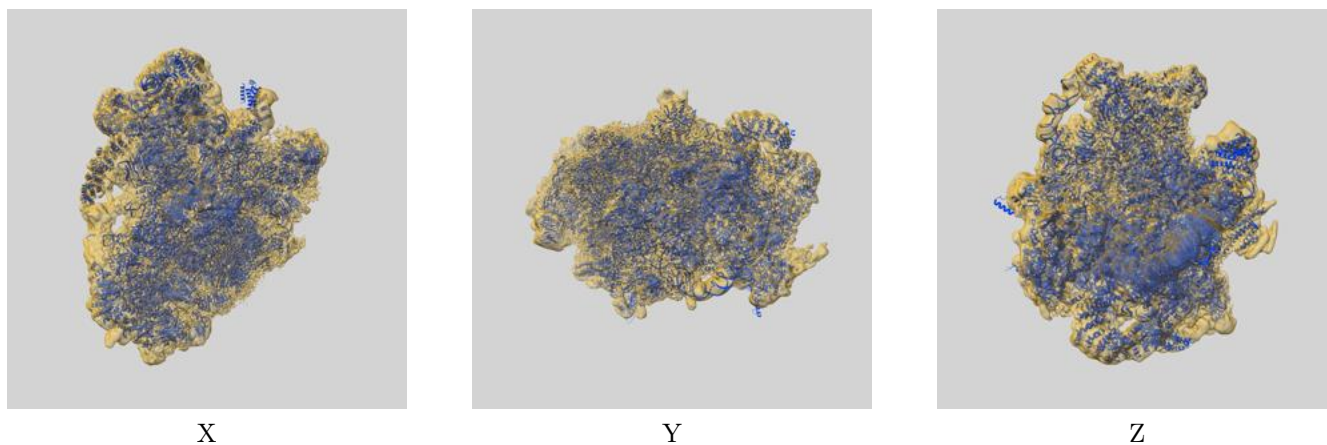
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.72	4.01
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

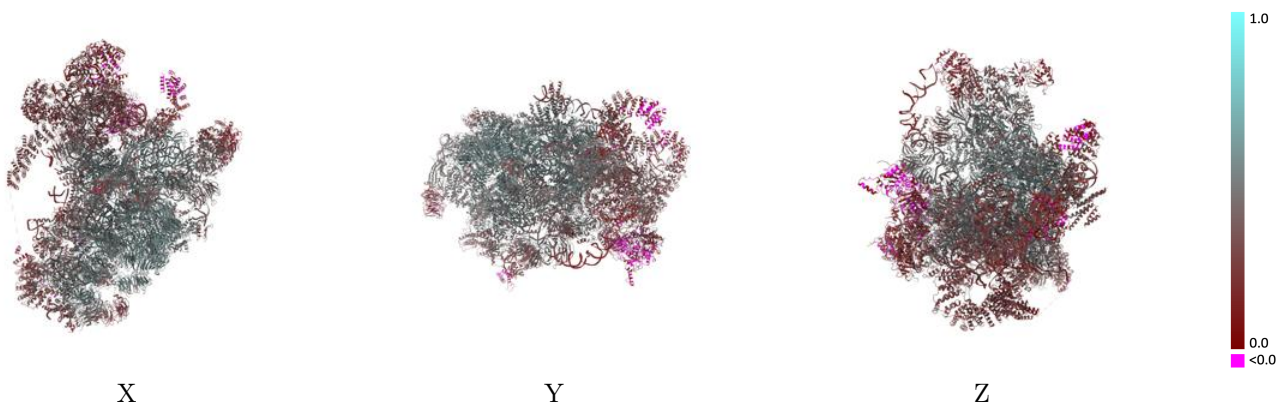
This section contains information regarding the fit between EMDB map EMD-11358 and PDB model 6ZQB. Per-residue inclusion information can be found in section 3 on page 17.

### 9.1 Map-model overlay [i](#)



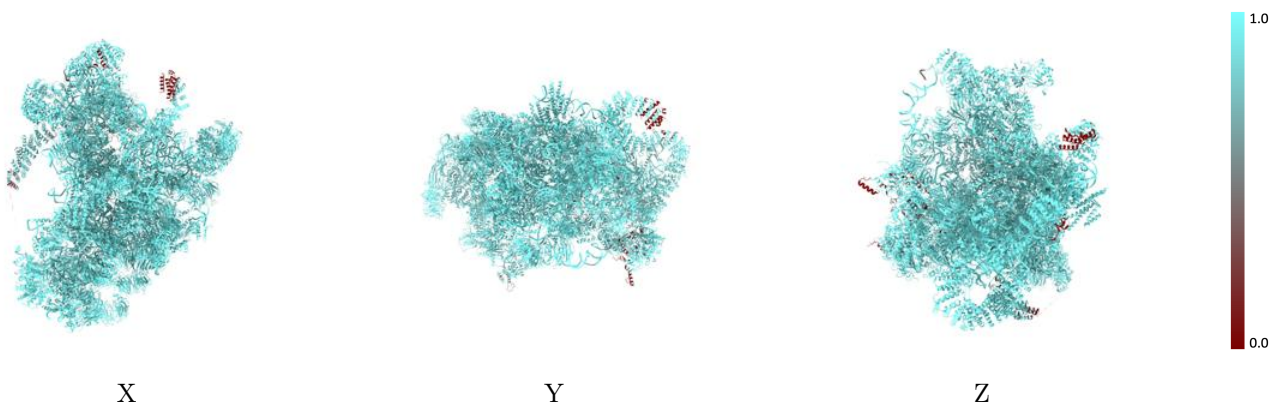
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

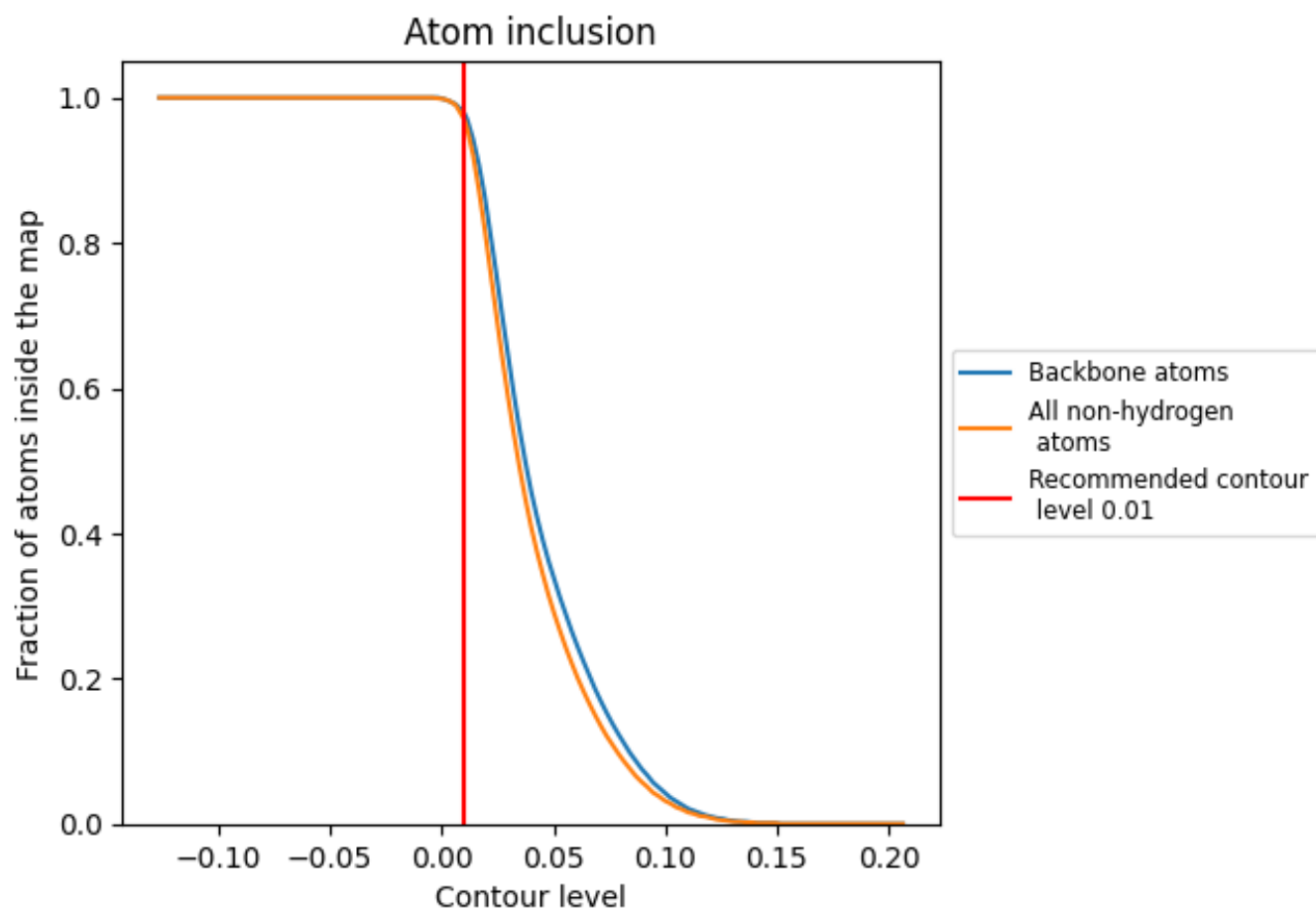
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 98% of all backbone atoms, 97% 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	 0.9700	 0.4180
CA	 0.9850	 0.5400
CB	 0.9790	 0.4490
CD	 0.9810	 0.4390
CE	 0.9870	 0.4440
CF	 0.9880	 0.5340
CG	 0.9830	 0.4950
CH	 0.9690	 0.4040
CI	 0.9870	 0.5690
CJ	 0.9840	 0.5330
CK	 0.9830	 0.4980
CL	 0.9800	 0.4960
CM	 0.9880	 0.4760
CN	 0.9400	 0.2930
D2	 0.9930	 0.4430
D3	 0.9800	 0.3870
D4	 0.9970	 0.4560
DA	 0.9620	 0.4930
DE	 0.9710	 0.3350
DF	 0.9870	 0.5290
DG	 0.9460	 0.2890
DH	 0.9570	 0.3480
DI	 0.9700	 0.3140
DJ	 0.9820	 0.5030
DL	 0.9690	 0.3070
DN	 0.9610	 0.4690
DO	 0.9940	 0.5030
DQ	 0.9920	 0.5580
DS	 0.8970	 0.2850
DW	 0.9810	 0.5160
DX	 0.9850	 0.5290
DY	 0.9410	 0.2750
Db	 0.9820	 0.5160
Dc	 0.9900	 0.5280
JA	 0.9490	 0.2970



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion	Q-score
JB	 0.7950	 0.1190
JC	 0.9370	 0.3250
JE	 0.9340	 0.3590
JF	 0.9640	 0.3740
JG	 0.9800	 0.4690
JH	 0.8460	 0.1060
JJ	 0.9770	 0.4150
JK	 0.9670	 0.2650
JM	 0.9750	 0.4760
JN	 0.9810	 0.5150
JO	 0.9840	 0.4700
JP	 0.9900	 0.5540
JQ	 0.9290	 0.3940
UA	 0.9910	 0.5600
UB	 0.9620	 0.3210
UC	 0.9800	 0.4710
UD	 0.9850	 0.4520
UE	 0.9900	 0.4920
UF	 0.9750	 0.4290
UG	 0.9890	 0.5480
UH	 0.9820	 0.2700
UI	 0.9810	 0.3370
UJ	 0.9280	 0.3780
UK	 0.9840	 0.4860
UL	 0.9820	 0.4370
UM	 0.9760	 0.4100
UN	 0.9850	 0.5020
UO	 0.9900	 0.5010
UP	 0.9650	 0.4030
UQ	 0.9900	 0.4770
UR	 0.9930	 0.5470
US	 0.9700	 0.3530
UT	 0.9300	 0.2440
UU	 0.9950	 0.5490
UV	 0.9510	 0.3270
UX	 0.9880	 0.5520
UZ	 0.9840	 0.4270