



# wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 10:58 AM JST

PDB ID : 6LQS  
EMDB ID : EMD-0952  
Title : Cryo-EM structure of 90S small subunit preribosomes in transition states (State D)  
Authors : Du, Y.; Ye, K.  
Deposited on : 2020-01-14  
Resolution : 3.80 Å (reported)  
Based on initial model : 6LQP

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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), 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

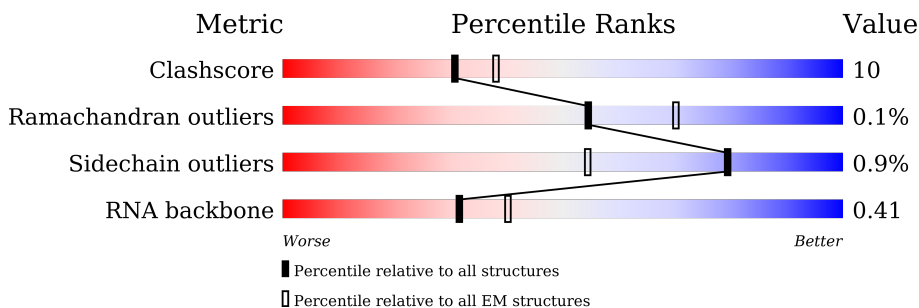
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.



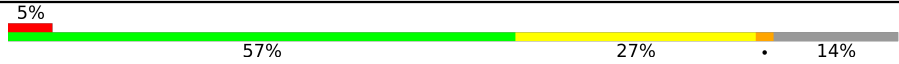

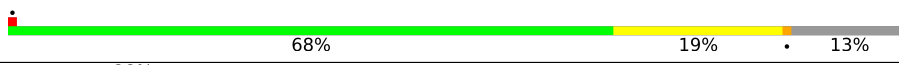

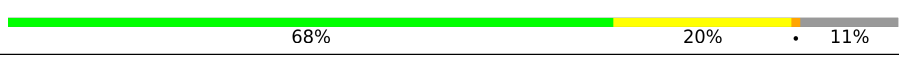
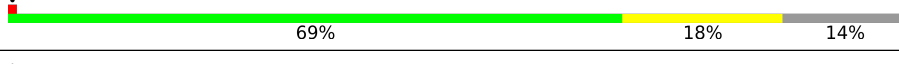
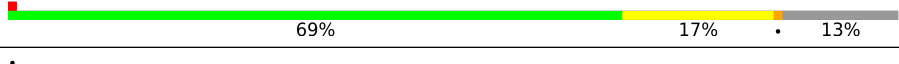

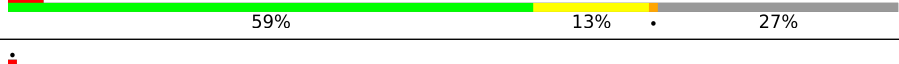

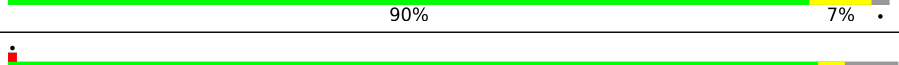
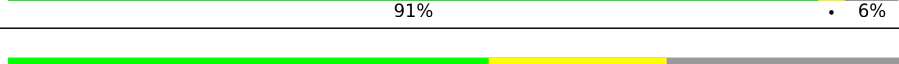

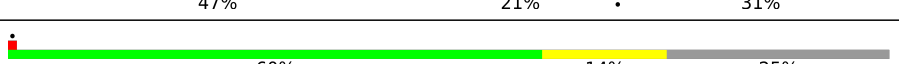

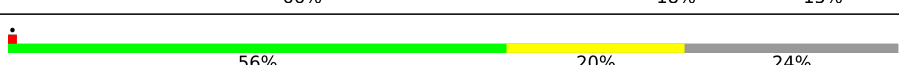
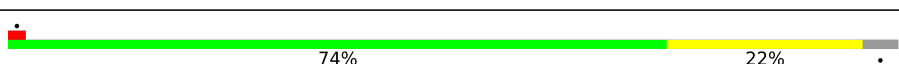
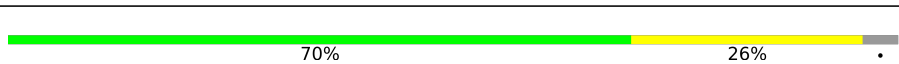
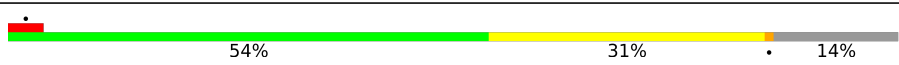



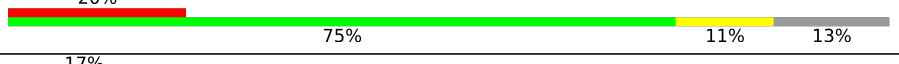


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	3A	333	
2	5A	700	
3	SA	1809	
4	SC	255	
5	SF	261	
6	SG	225	
7	SH	236	

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Mol	Chain	Length	Quality of chain
8	SI	190	
9	SJ	200	
10	SK	197	
11	SM	156	
12	SO	151	
13	SP	137	
14	SR	143	
15	SX	130	
16	SY	145	
17	SZ	135	
18	Sc	82	
19	Sd	67	
20	3B	327	
20	3C	327	
21	3D	504	
22	3E	511	
23	3F	573	
24	3G	126	
24	3H	126	
25	A4	776	
26	A5	643	
27	A8	713	
28	A9	575	
29	AE	1769	
30	AF	513	

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Mol	Chain	Length	Quality of chain
31	AG	896	
32	B1	900	
33	B2	943	
34	B3	817	
35	B8	594	
36	BE	939	
37	B6	440	
38	5B	214	
39	5C	554	
40	5D	250	
41	5E	593	
42	5F	183	
43	5G	290	
44	5H	610	
45	5I	489	
46	5J	217	
47	5K	189	
48	RD	1729	
49	RE	1237	
50	RF	297	
51	RG	252	
51	RH	252	
52	RJ	1183	
53	RK	367	
54	RN	810	

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Mol	Chain	Length	Quality of chain
55	RO	552	95% 78% 17% 5%
56	RP	2493	81% 6% 13%
57	RQ	899	22% 75%
58	RS	480	51% 36% 16% 48%
59	RT	326	6% 40% 12% 48%
60	RW	206	56% 71% 27%
61	X1	347	22% 77%
62	X2	694	20% 80%
63	R5	305	98% 68% 30%
64	R1	246	99% 70% 28%
65	R3	394	86% 61% 25% 14%
66	R6	223	100% 66% 34%
67	R2	265	100% 71% 29%
68	M3	250	86% 61% 24% 14%
69	R0	240	99% 72% 26%
70	r4	359	82% 81% 18%
71	C4	292	76% 55% 21% 24%
72	R4	1001	95% 61% 33% 5%
73	r6	733	14% 86%
74	R7	184	46% 34% 12% 54%
75	M4	1073	81% 51% 30% 19%
76	M6	186	22% 18% 78%

## 2 Entry composition

There are 79 unique types of molecules in this entry. The entry contains 238320 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 RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3A	234	4962	2220	863	1645	234	0	0

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	152	3260	1455	593	1060	152	0	0

- Molecule 3 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	1249	26609	11894	4706	8760	1249	0	0

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SC	232	1848	1168	339	337	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SF	250	1930	1232	354	341	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

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

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SH	182	1457	917	273	266	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SI	164	1310	847	222	241		0	0

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SJ	140	1104	689	211	202	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SK	171	1388	879	268	240	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SM	137	1113	715	212	183	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SO	134	1087	698	202	186	1	0	0

- Molecule 13 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SP	118	868	536	164	165	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 15 is a protein called 40S ribosomal protein S22-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SX	127	Total	C	N	O	S	0	0
			1003	640	183	177	3		

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SY	106	Total	C	N	O	S	0	0
			807	515	148	142	2		

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	SZ	123	Total	C	N	O	0	0
			986	626	188	172		

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Sc	80	Total	C	N	O	S	0	0
			603	377	109	112	5		

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 20 is a protein called rRNA 2'-O-methyltransferase fibrillar.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
20	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 21 is a protein called Nucleolar protein 56.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	3D	378	Total	C	N	O	S	0	0
			2974	1886	511	568	9		

- Molecule 22 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3E	432	Total	C	N	O	S	0	0
			3041	1895	545	592	9		

- Molecule 23 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3F	437	Total	C	N	O	S	0	0
			3498	2227	609	652	10		

- Molecule 24 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
24	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A4	664	Total	C	N	O	S	0	0
			5243	3320	912	990	21		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A5	511	Total	C	N	O	S	0	0
			3953	2507	682	751	13		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A8	548	Total	C	N	O	S	0	0
			3307	2054	608	642	3		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	A9	128	939	594	173	170	2	0	0

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AE	1534	9956	6243	1771	1923	19	0	0

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AF	479	3807	2395	685	715	12	0	0

- Molecule 31 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AG	826	6570	4181	1111	1259	19	0	0

- Molecule 32 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	B1	806	6427	4104	1099	1205	19	0	0

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	B2	825	6502	4156	1096	1223	27	0	0

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	B3	757	5919	3769	993	1130	27	0	0

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	B8	477	3764	2387	662	705	10	0	0

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BE	823	6475	4107	1119	1228	21	0	0

- Molecule 37 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	B6	374	2800	1782	501	505	12	0	0

- Molecule 38 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	5B	60	495	310	101	84	0	0

- Molecule 39 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	5C	458	3612	2276	636	689	11	0	0

- Molecule 40 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	5D	204	1733	1082	340	306	5	0	0

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	5E	193	1564	970	280	310	4	0	0

- Molecule 42 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 43 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5G	216	Total	C	N	O	S	0	0
			1732	1093	321	312	6		

- Molecule 44 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	5H	74	Total	C	N	O	0	0
			596	373	122	101		

- Molecule 45 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5I	460	Total	C	N	O	S	0	0
			3756	2349	685	706	16		

- Molecule 46 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5J	134	Total	C	N	O	S	0	0
			1127	712	205	207	3		

- Molecule 47 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5K	166	Total	C	N	O	S	0	0
			1323	849	238	226	10		

- Molecule 48 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	RD	316	Total	C	N	O	S	0	0
			2413	1541	415	452	5		

- Molecule 49 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	RE	1090	8805	5720	1452	1609	24	0	0

- Molecule 50 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	RF	241	1963	1253	335	367	8	0	0

- Molecule 51 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	RG	216	1701	1079	296	315	11	0	0
51	RH	230	1799	1142	313	333	11	0	0

- Molecule 52 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	RJ	731	5935	3812	1051	1046	26	0	0

- Molecule 53 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 54 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	RN	553	4088	2590	731	758	9	0	0

- Molecule 55 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	RO	525	3766	2412	646	696	12	0	0

- Molecule 56 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	RP	2180	12716	7827	2389	2484	16	0	0

- Molecule 57 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	RQ	226	1655	1026	314	313	2	0	0

- Molecule 58 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	RS	251	2051	1340	349	359	3	0	0

- Molecule 59 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	RT	171	1357	864	249	240	4	0	0

- Molecule 60 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	RW	150	747	447	150	150	0	0

- Molecule 61 is a protein called Unassigned helices 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	X1	80	400	240	80	80	0	0

- Molecule 62 is a protein called Unassigned helices 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	X2	141	705	423	141	141	0	0

- Molecule 63 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	R5	299	2304	1444	393	451	16	0	0

- Molecule 64 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	R1	244	1886	1177	335	366	8	0	0

- Molecule 65 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	R3	339	2588	1640	441	497	10	1	0

- Molecule 66 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	R6	223	1696	1067	285	334	10	0	0

- Molecule 67 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	R2	265	2030	1296	334	395	5	0	0

- Molecule 68 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	M3	215	1639	1024	273	332	10	0	0

- Molecule 69 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	R0	237	1792	1143	295	344	10	0	0

- Molecule 70 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	r4	293	2236	1393	403	428	12	0	0

- Molecule 71 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	C4	222	1653	1034	287	325	7	0	0

- Molecule 72 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	R4	948	7430	4693	1308	1394	35	0	0

- Molecule 73 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	r6	104	802	496	144	157	5	0	0

- Molecule 74 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	R7	85	681	428	117	132	4	0	0

- Molecule 75 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	M4	874	6814	4354	1166	1254	40	0	0

- Molecule 76 is a protein called M-phase phosphoprotein 6 homolog.

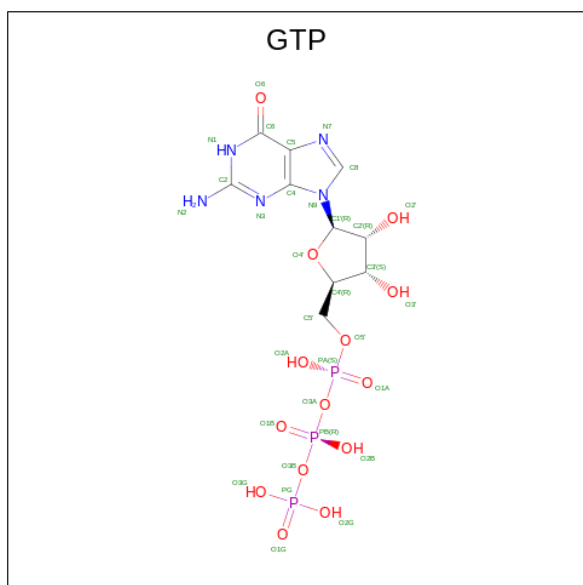
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	M6	40	275	170	51	54	0	0

- Molecule 77 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		AltConf
77	Sc	1	Total	Zn	0
			1	1	
77	5K	1	Total	Zn	0
			1	1	

- Molecule 78 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

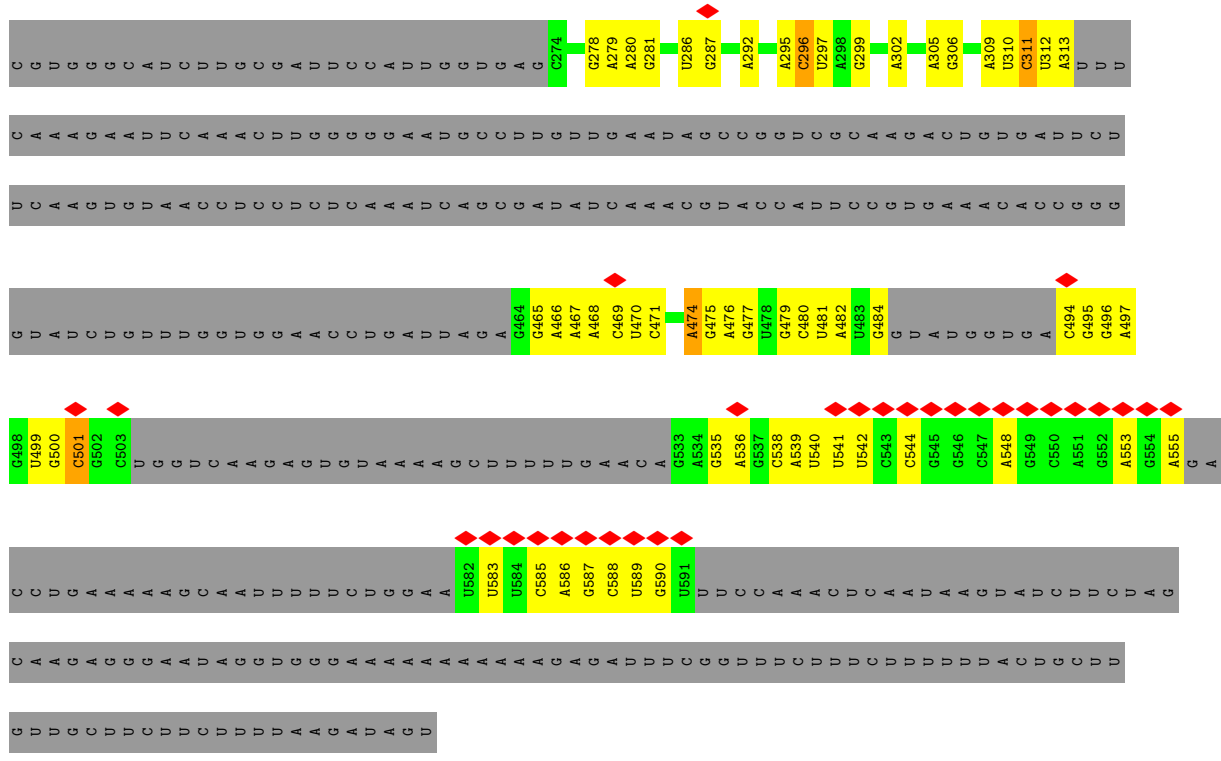


Mol	Chain	Residues	Atoms					AltConf
78	RJ	1	Total	C	N	O	P	0
			32	10	5	14	3	

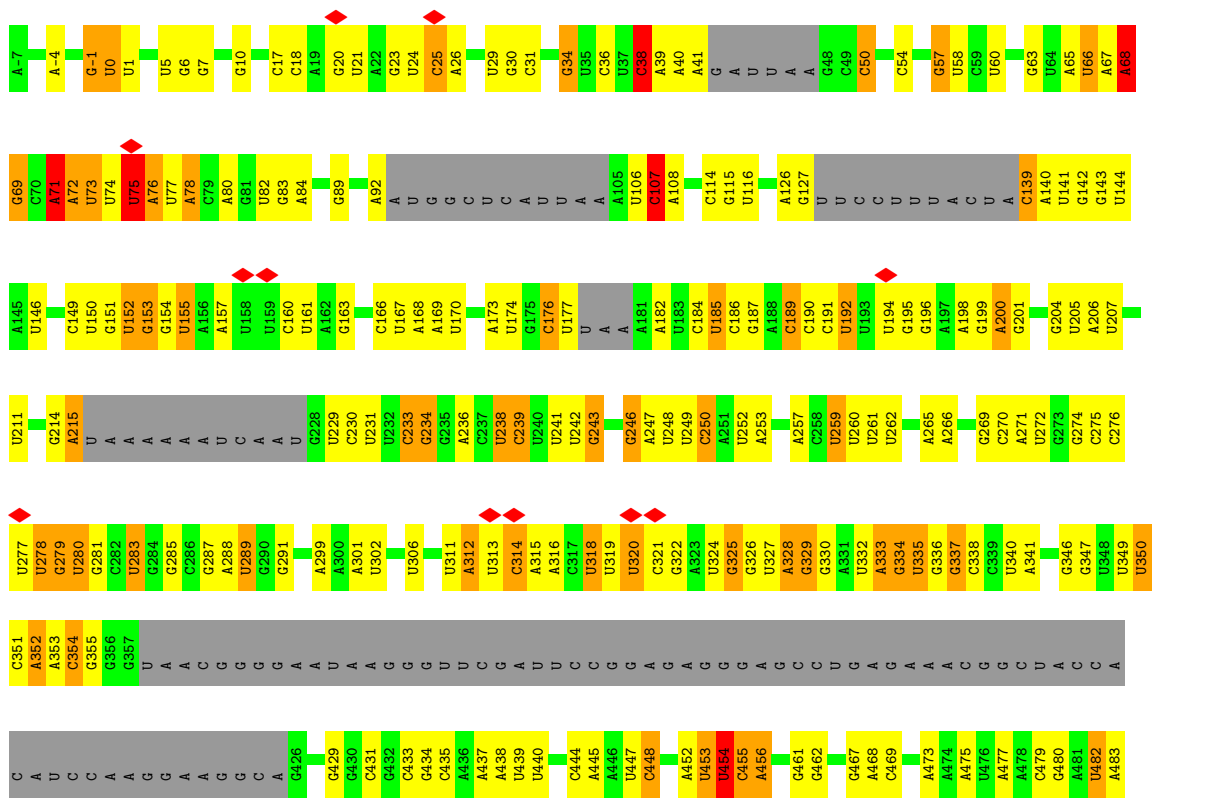
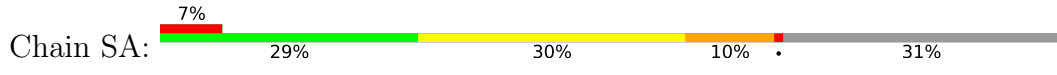
- Molecule 79 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

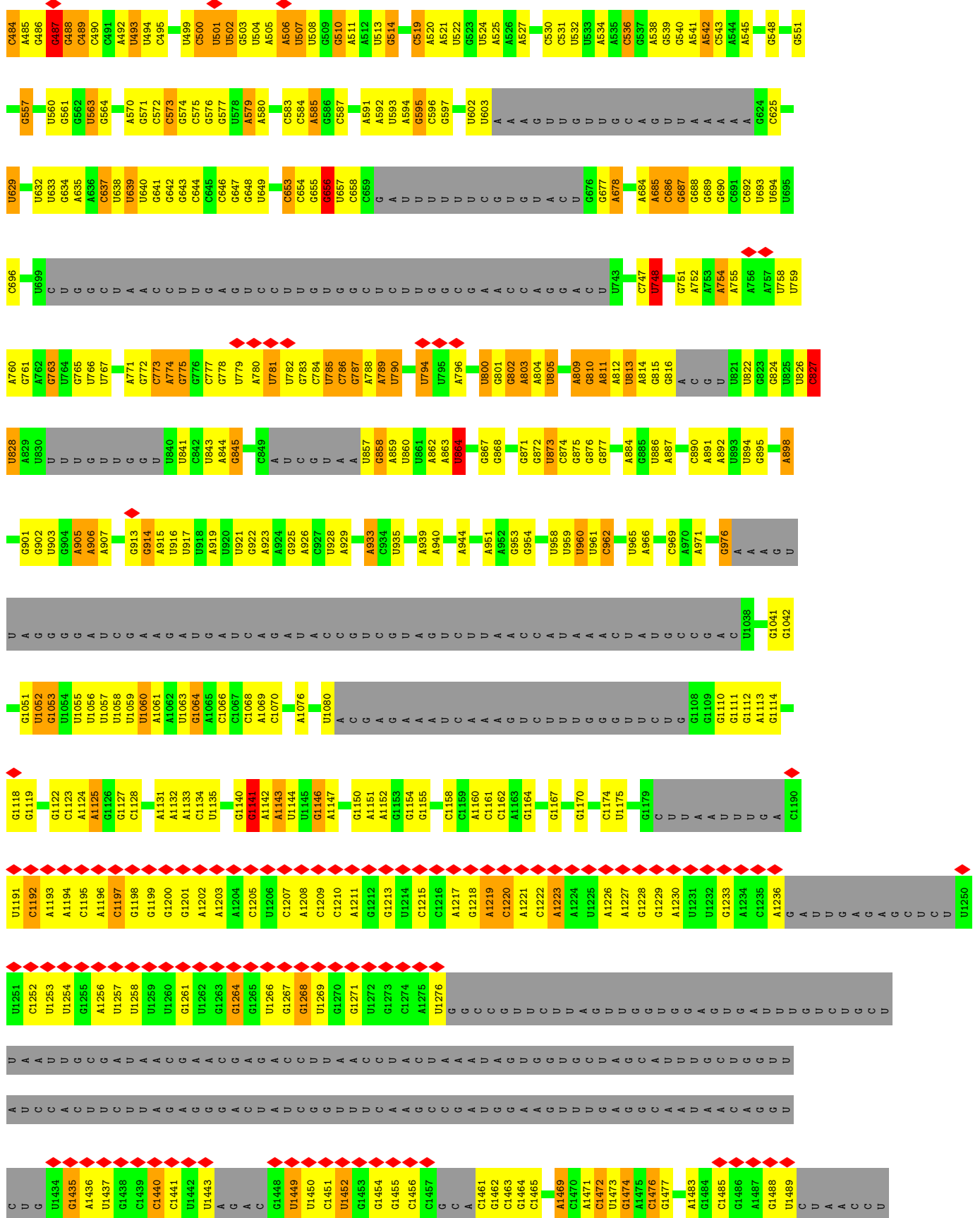
Mol	Chain	Residues	Atoms		AltConf
79	RJ	1	Total	Mg	0
			1	1	



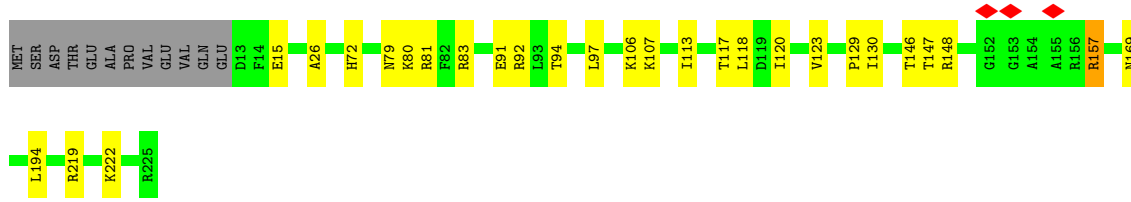


● Molecule 3: 18S pre-rRNA

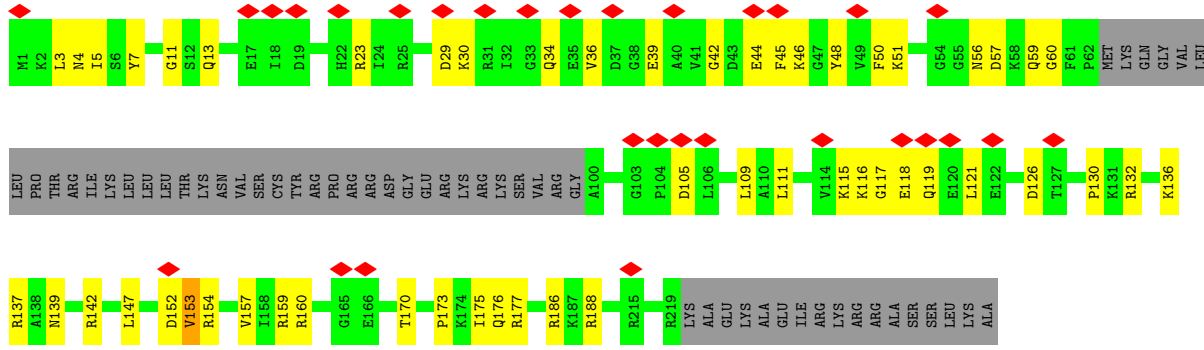




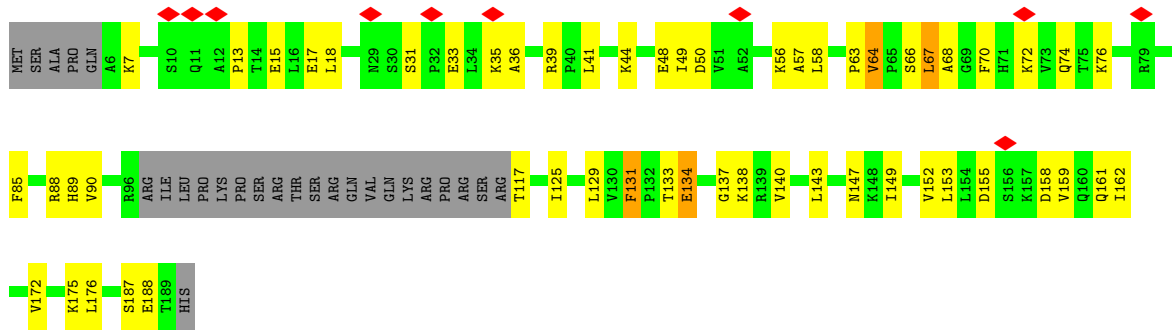




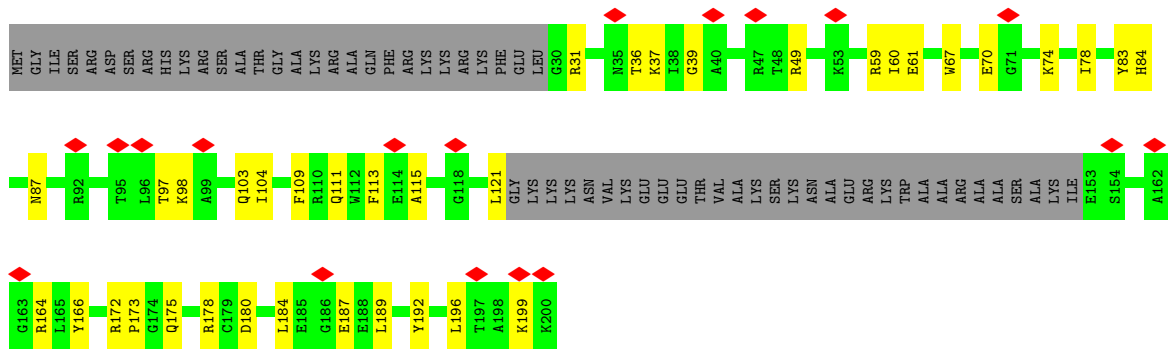
• Molecule 7: 40S ribosomal protein S6-A



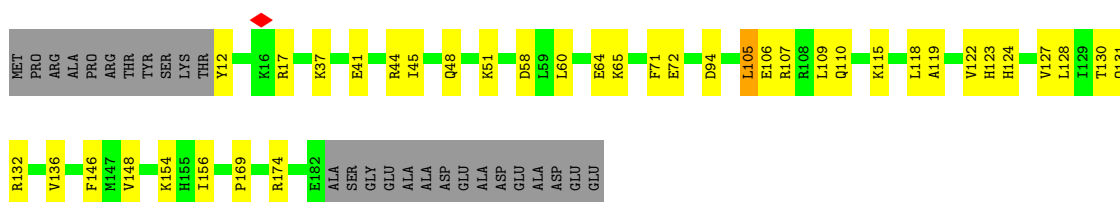
• Molecule 8: 40S ribosomal protein S7-A



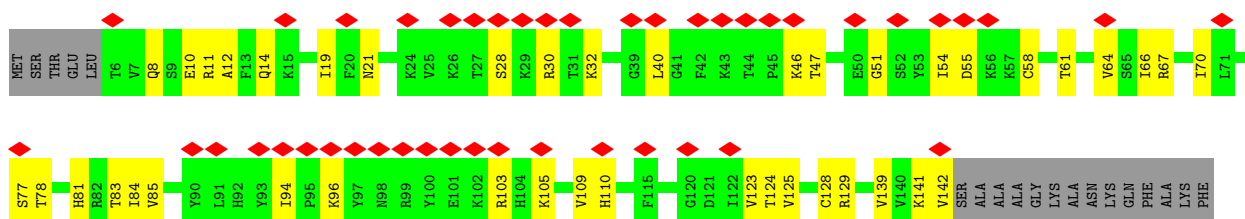
• Molecule 9: 40S ribosomal protein S8-A



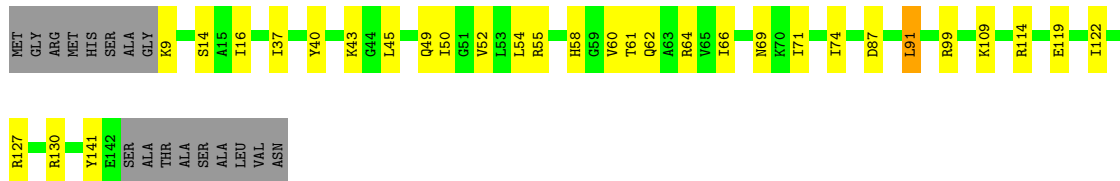
• Molecule 10: 40S ribosomal protein S9-A



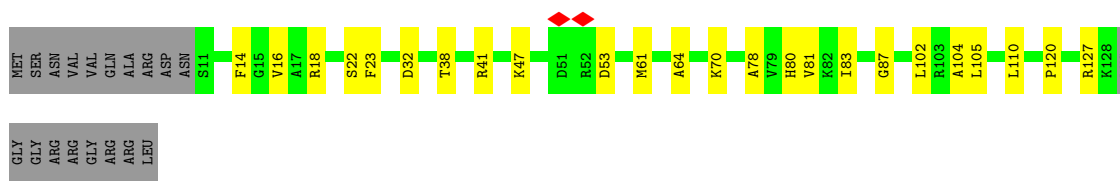
• Molecule 11: 40S ribosomal protein S11-A



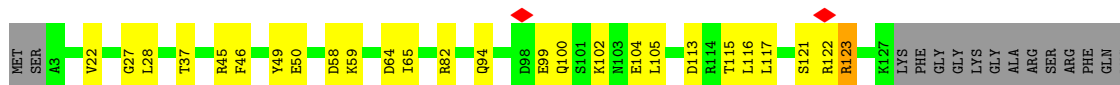
• Molecule 12: 40S ribosomal protein S13



• Molecule 13: 40S ribosomal protein S14-A



• Molecule 14: 40S ribosomal protein S16-A



SER  
TYR  
ARG

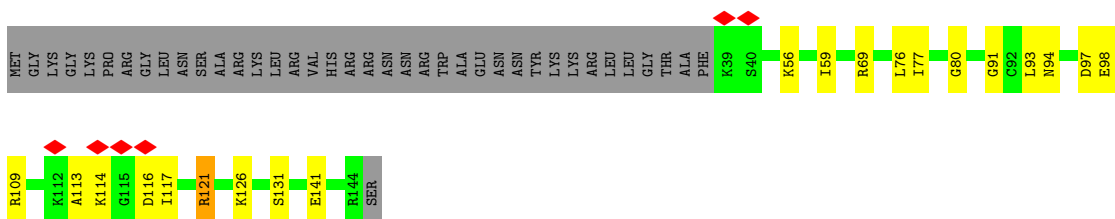
- Molecule 15: 40S ribosomal protein S22-B

Chain SX:  71% 27%



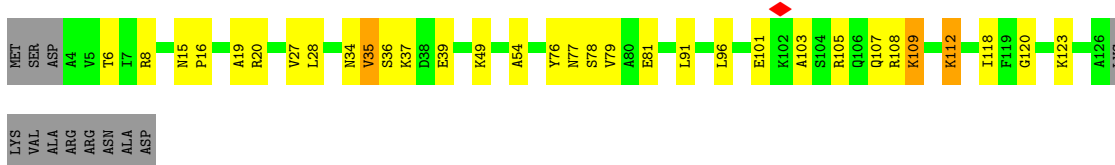
- Molecule 16: 40S ribosomal protein S23-A

Chain SY:  59% 13% 27%



- Molecule 17: 40S ribosomal protein S24-A

Chain SZ:  67% 21% 9%



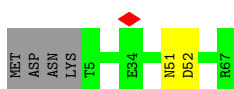
- Molecule 18: 40S ribosomal protein S27-A

Chain Sc:  90% 7%



- Molecule 19: 40S ribosomal protein S28-A

Chain Sd:  91% 6%



- Molecule 20: rRNA 2'-O-methyltransferase fibrillar



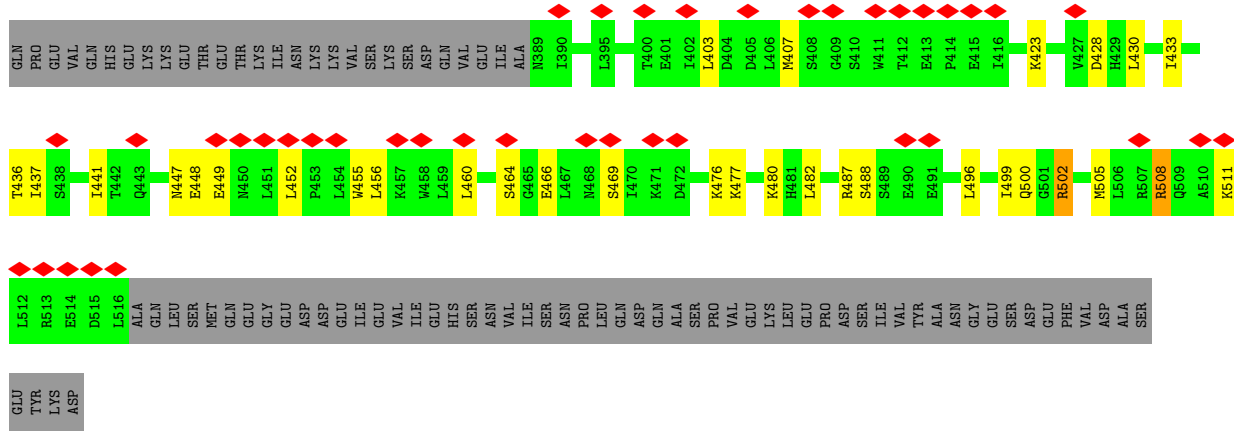




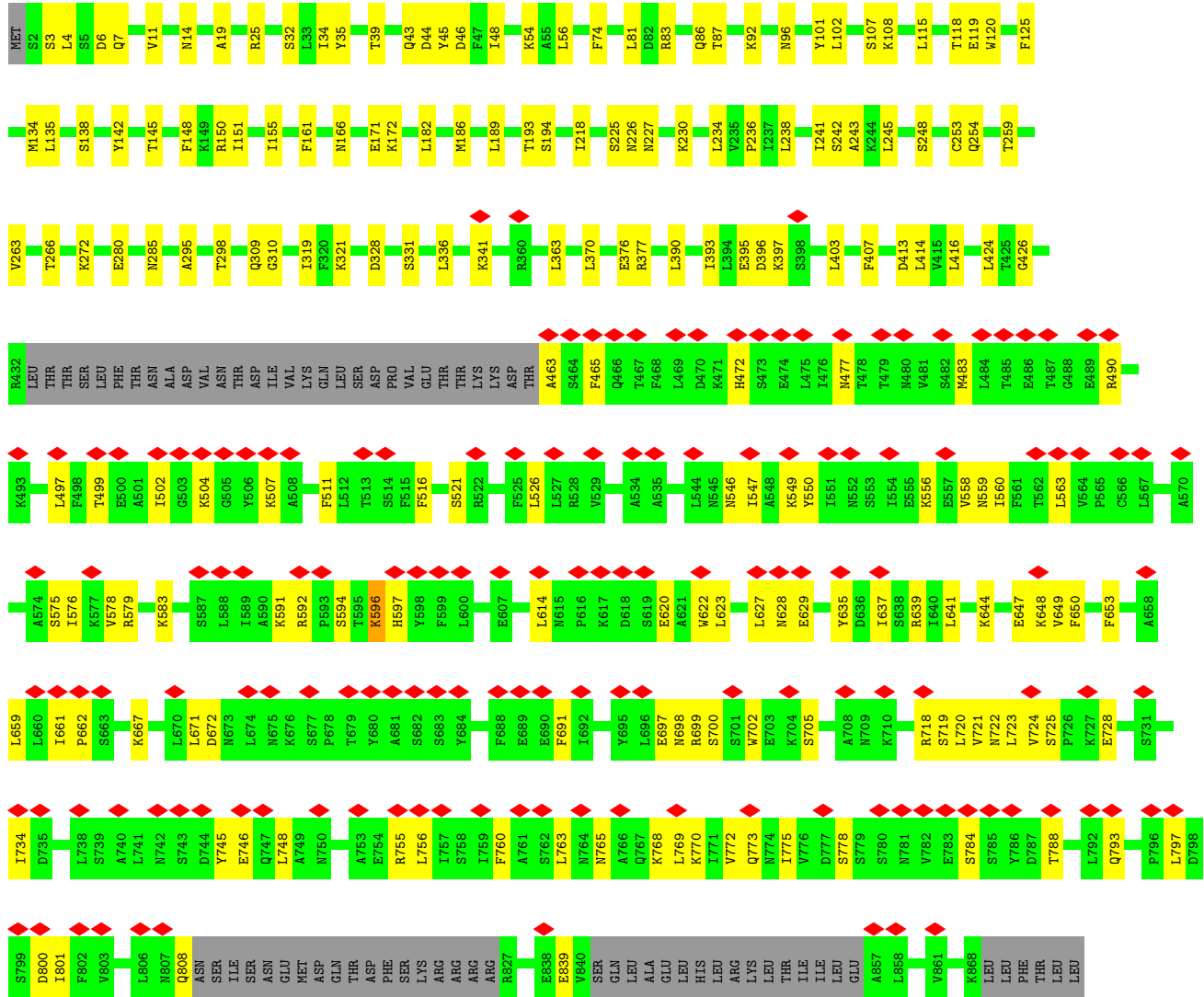
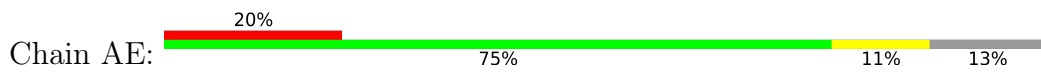


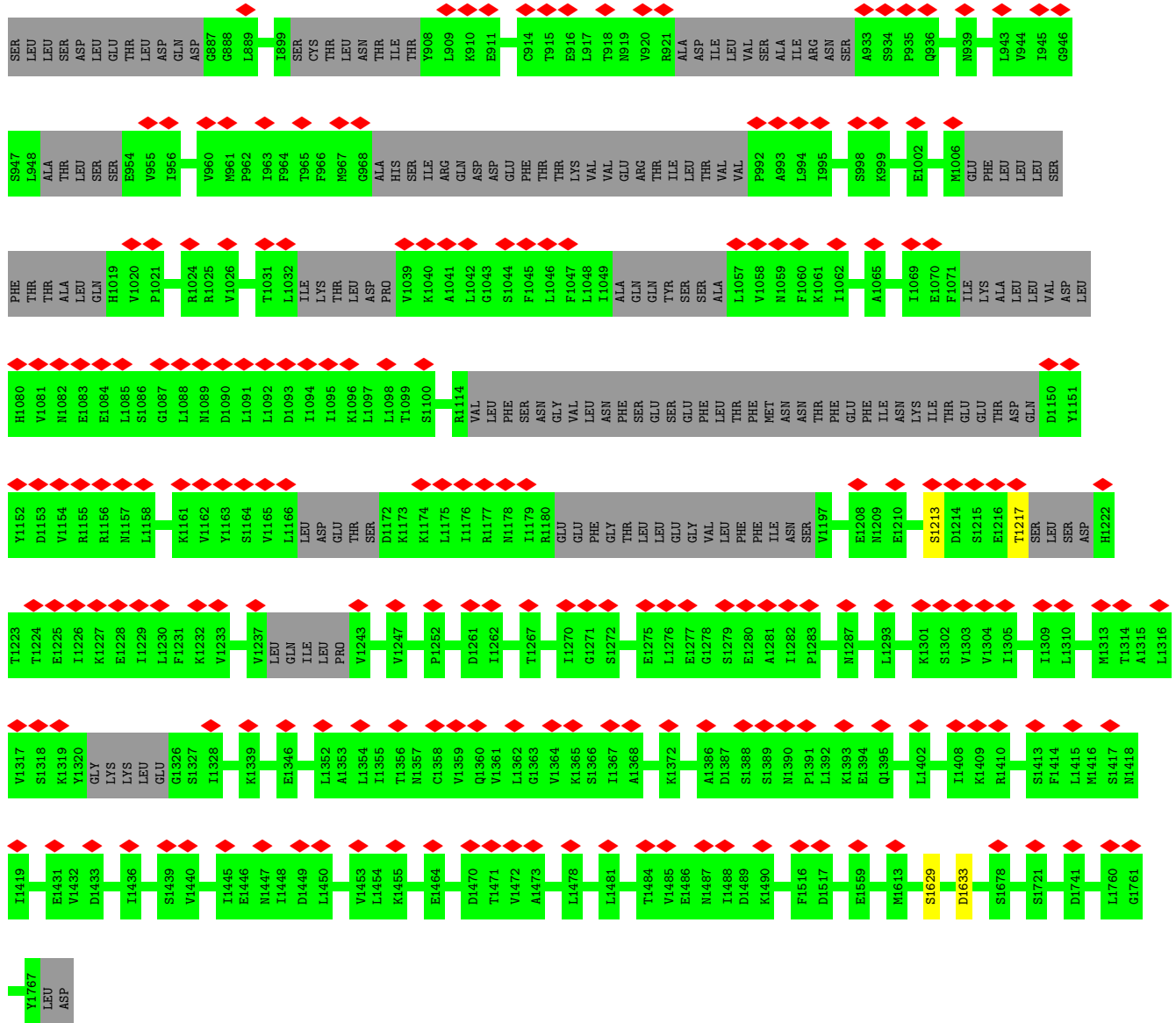




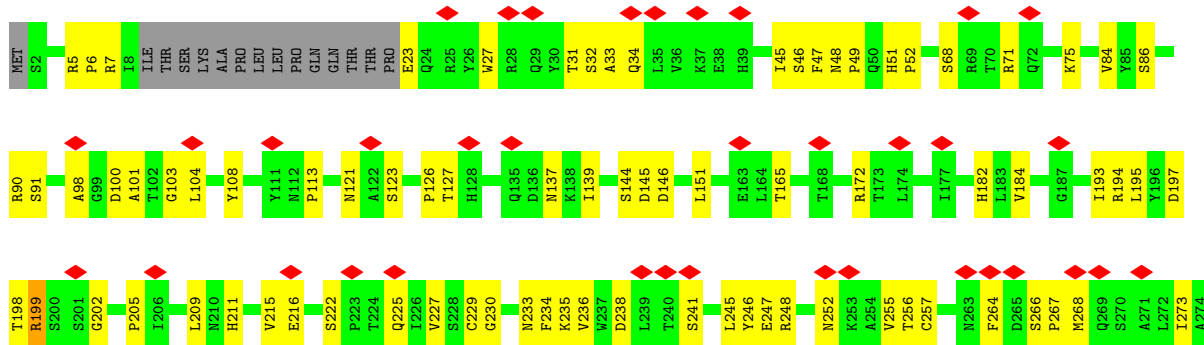


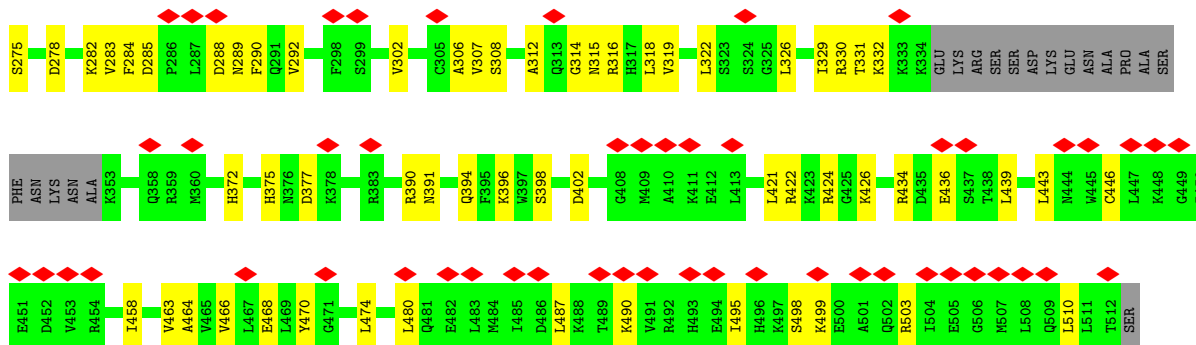
• Molecule 29: U3 small nucleolar RNA-associated protein 10



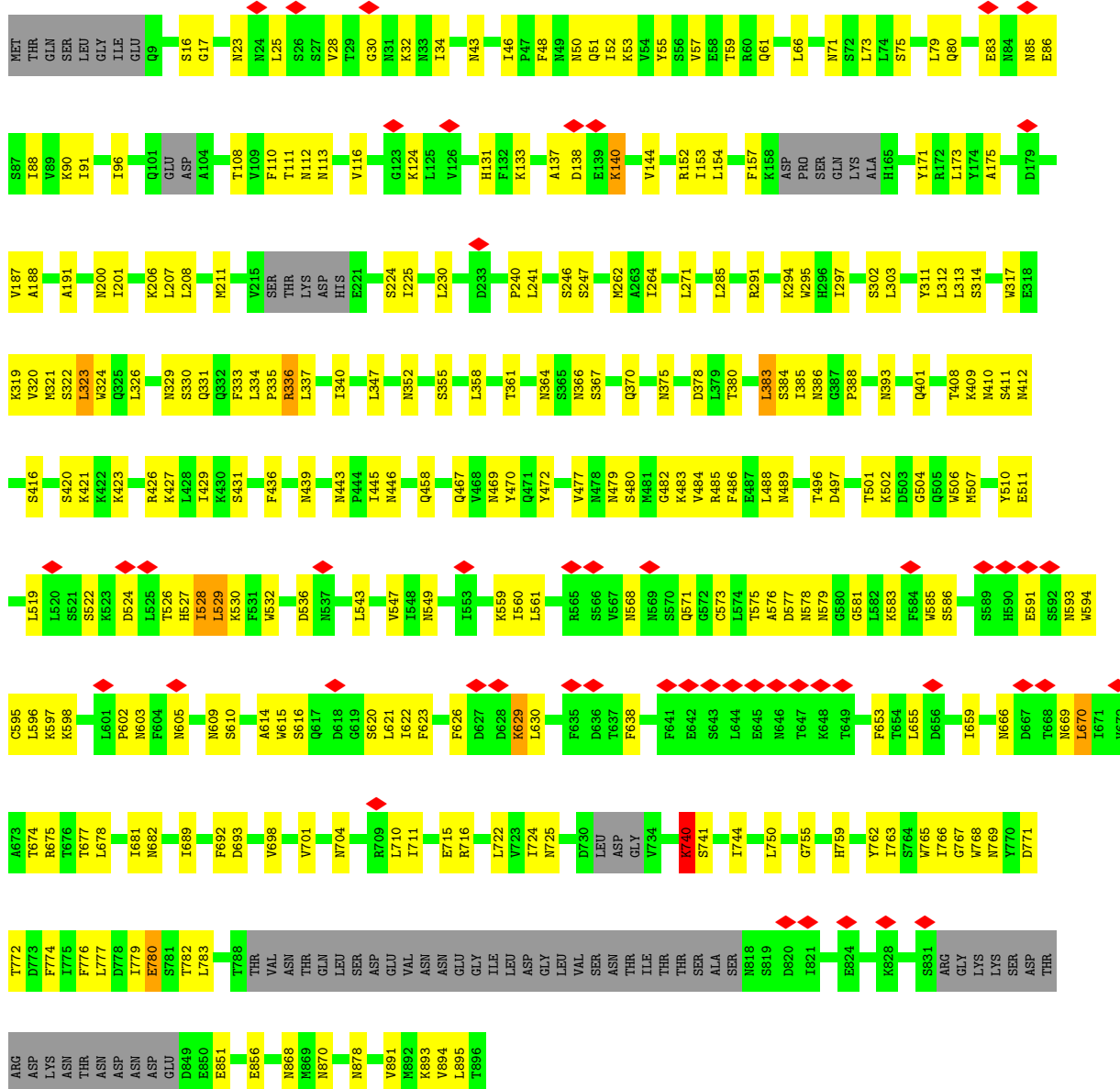


• Molecule 30: U3 small nucleolar RNA-associated protein 15





• Molecule 31: NET1-associated nuclear protein 1



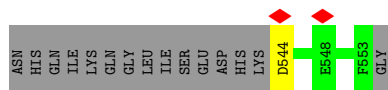




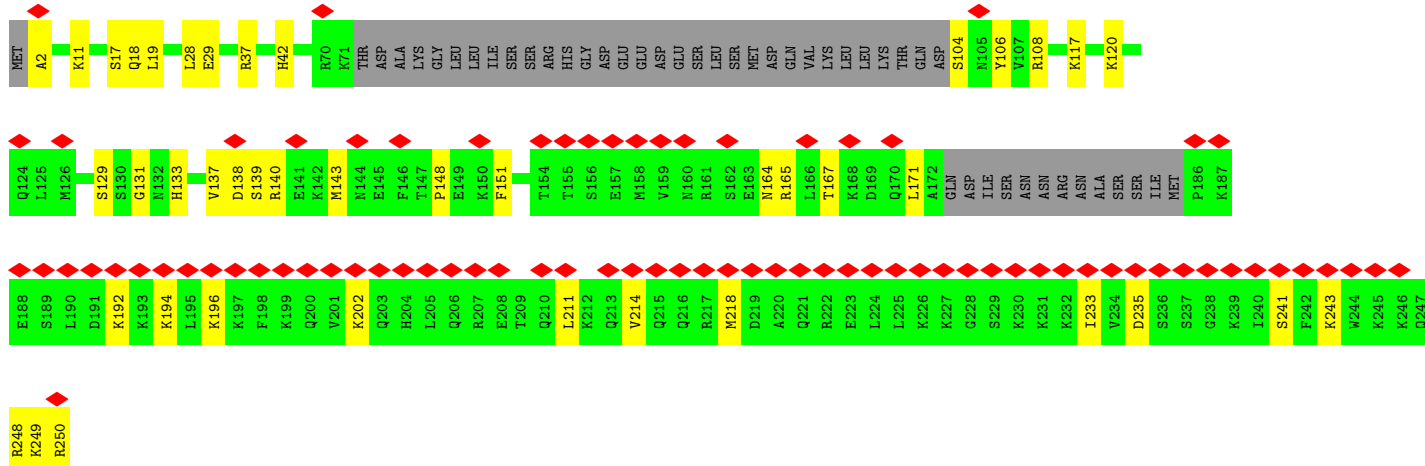




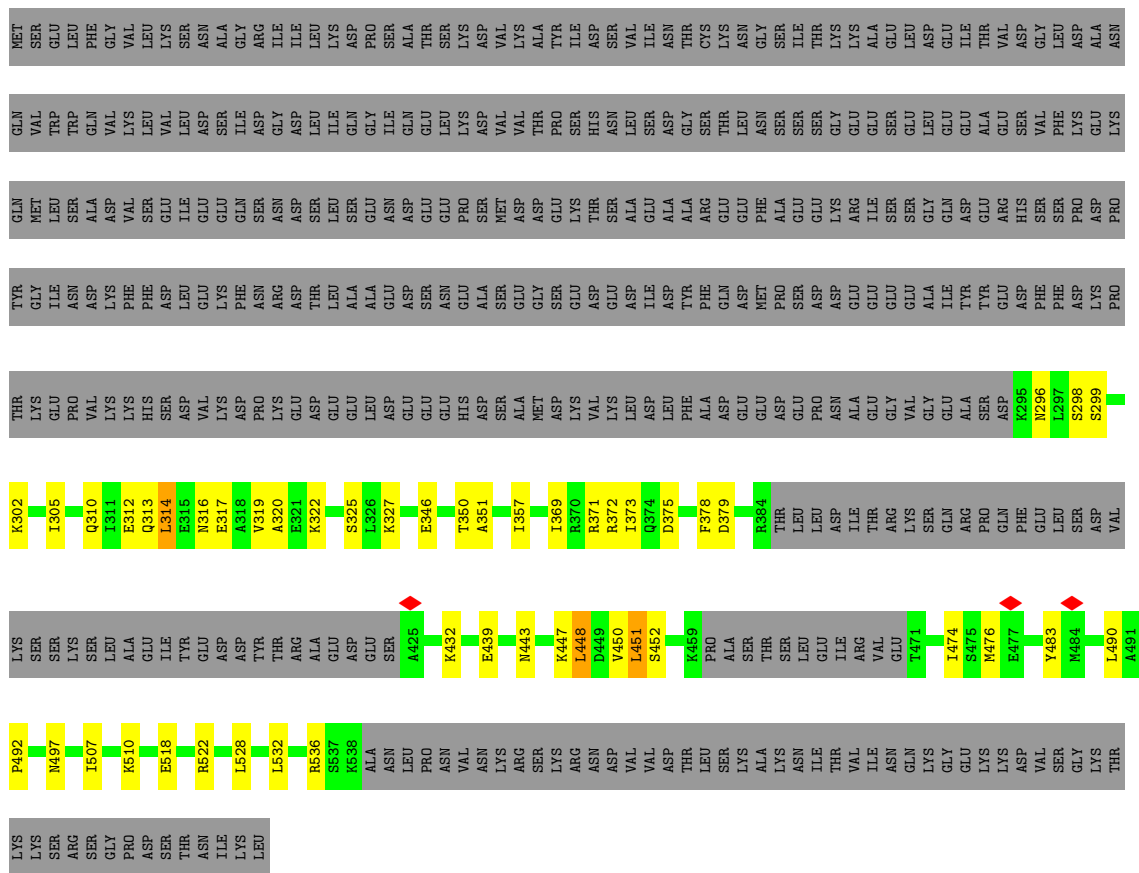




• Molecule 40: U3 small nucleolar RNA-associated protein 11



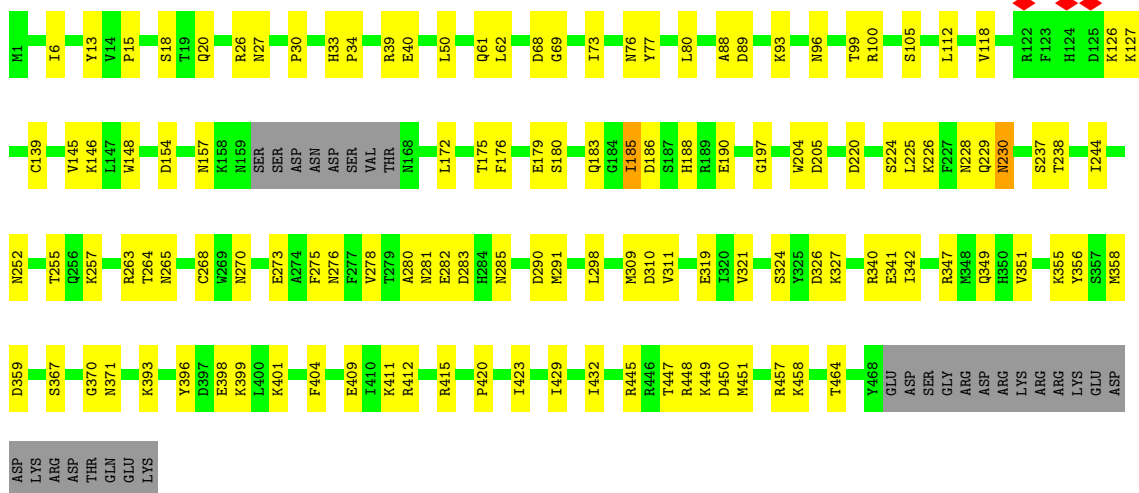
• Molecule 41: U3 small nucleolar RNA-associated protein MPP10



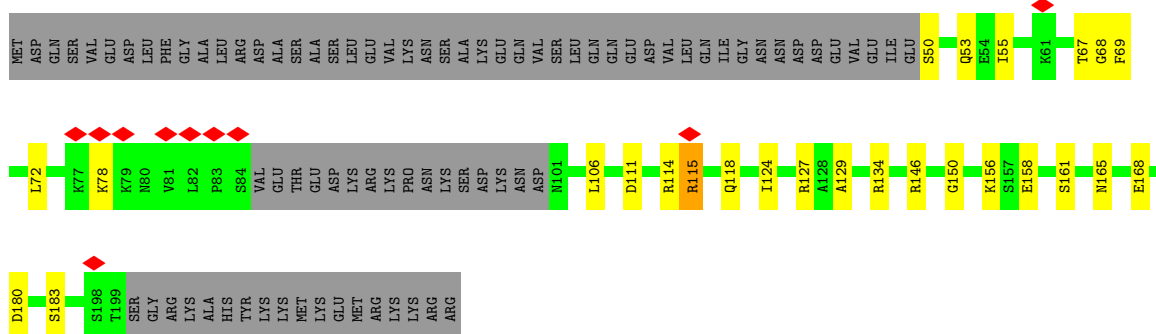




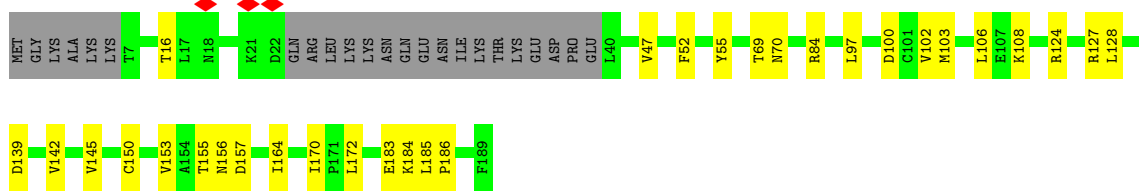
• Molecule 45: Protein SOF1



• Molecule 46: rRNA-processing protein FCF2



• Molecule 47: rRNA-processing protein FCF1



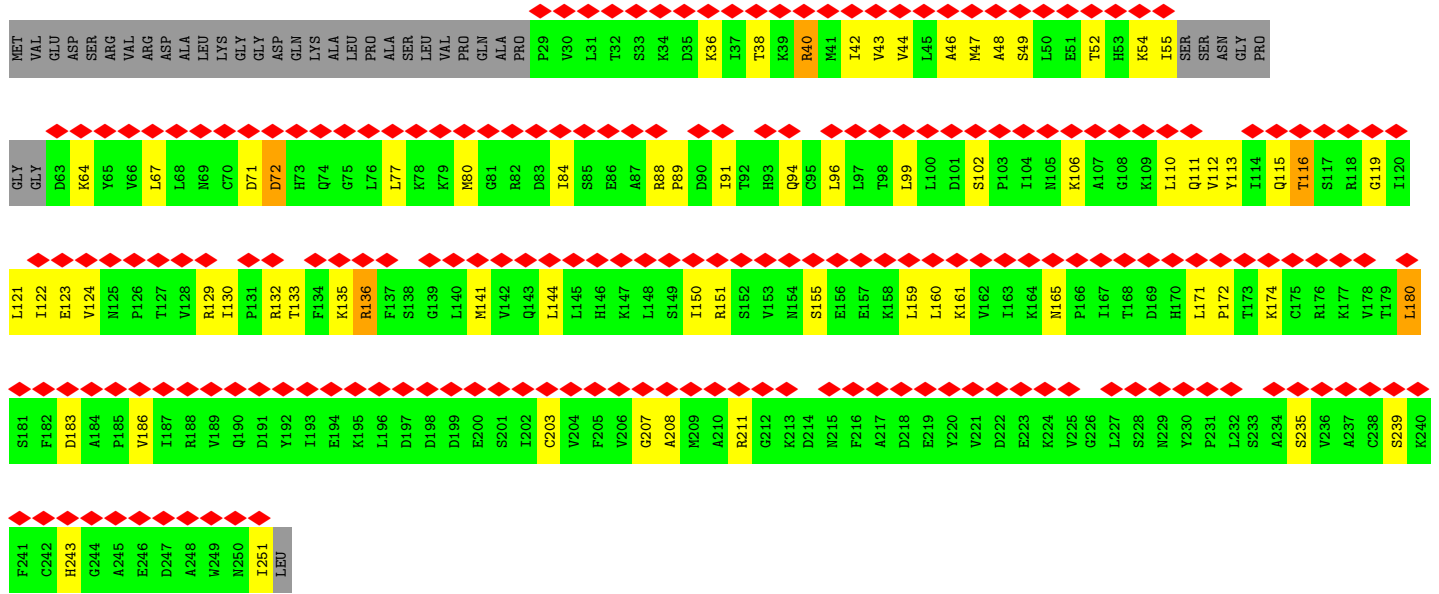
• Molecule 48: rRNA biogenesis protein RRP5



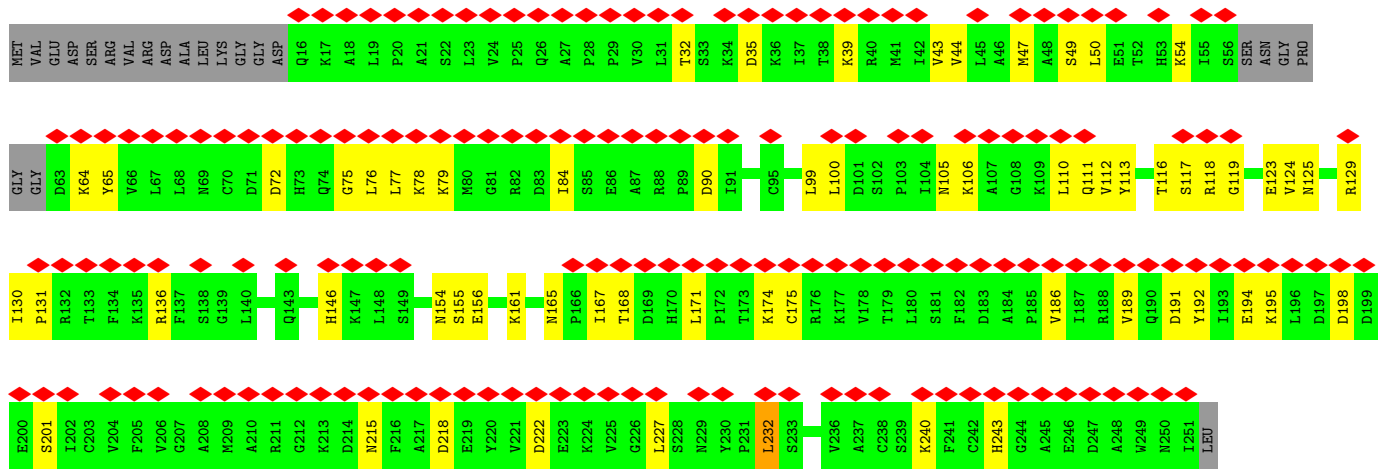




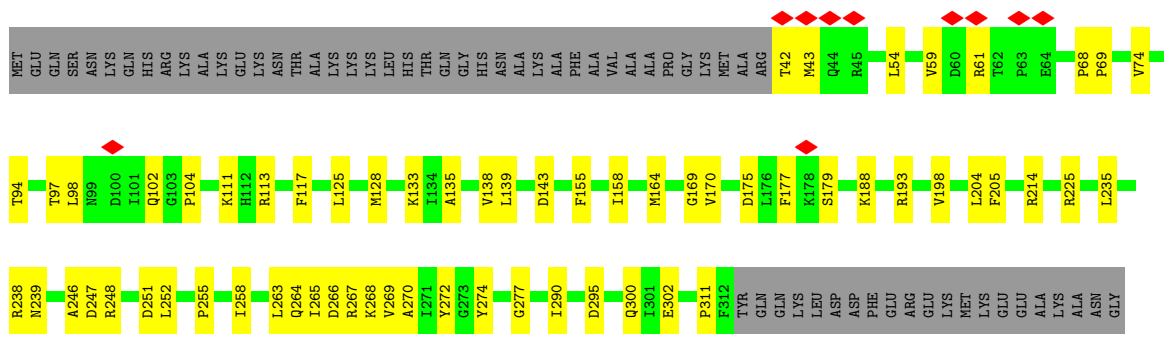




• Molecule 51: Ribosomal RNA small subunit methyltransferase NEP1

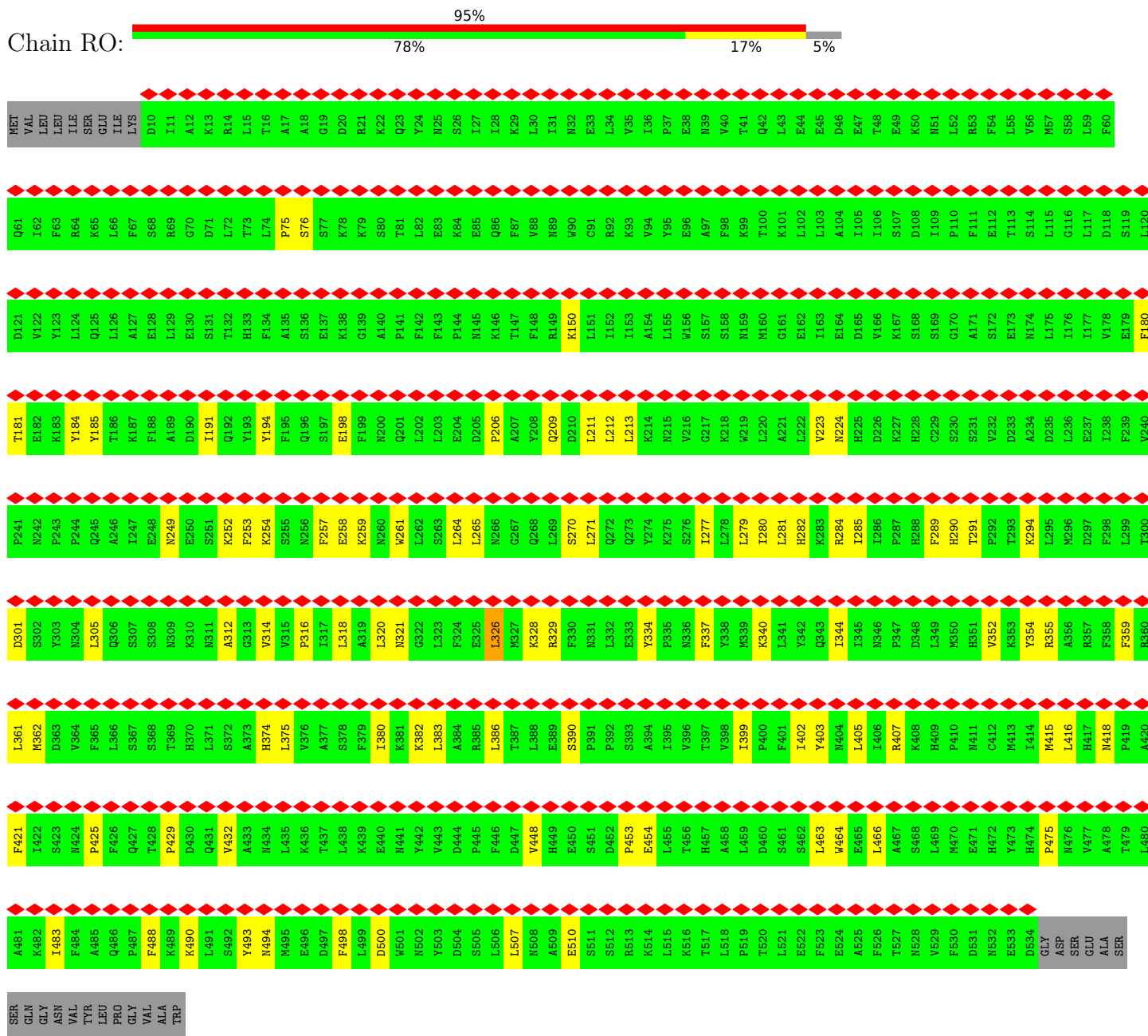


• Molecule 52: Ribosome biogenesis protein BMS1

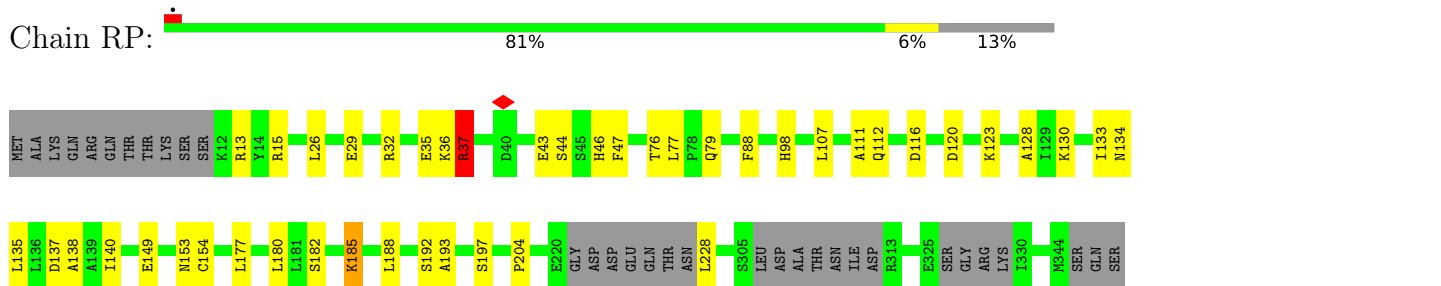


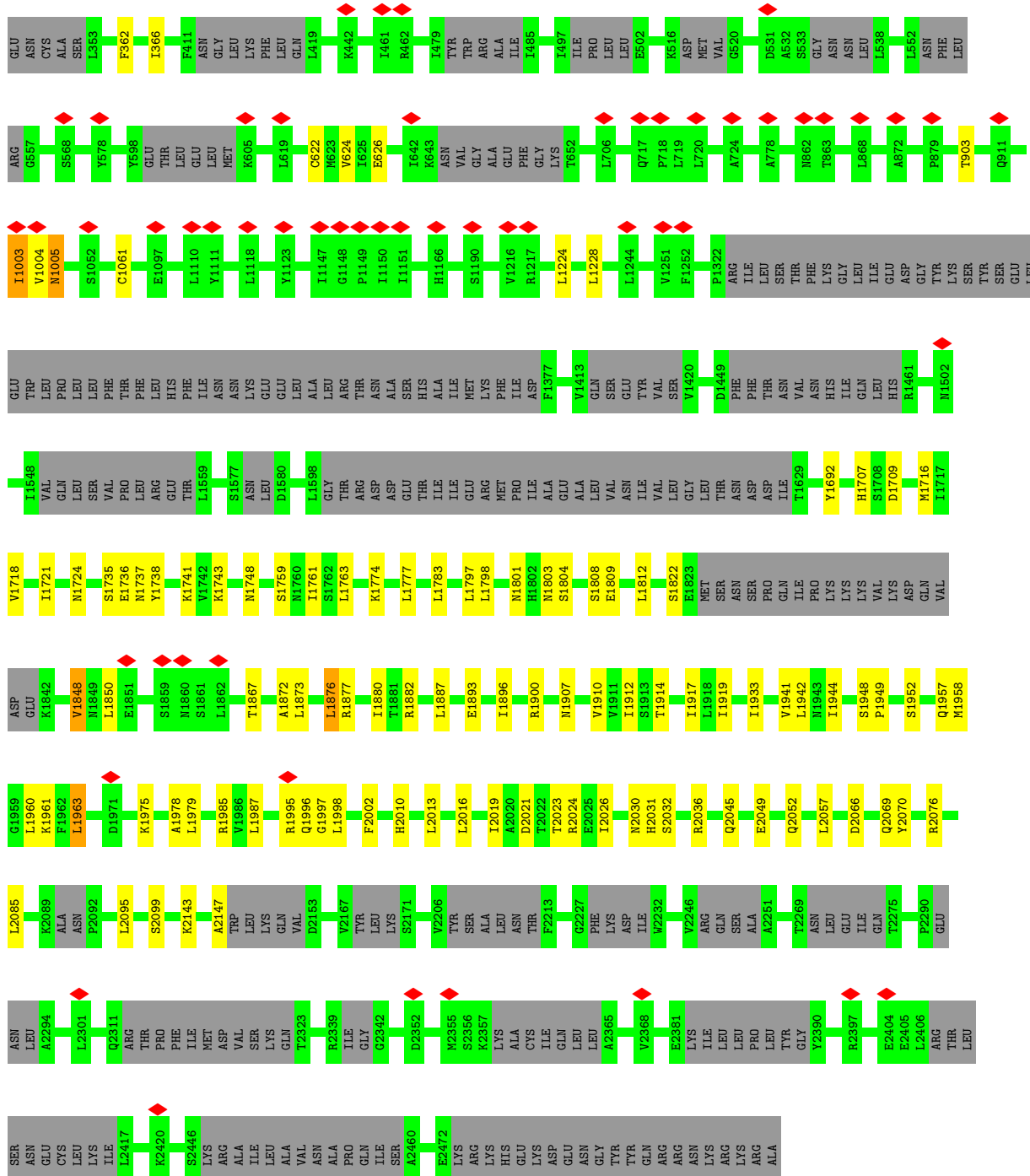






• Molecule 56: U3 small nucleolar RNA-associated protein 20

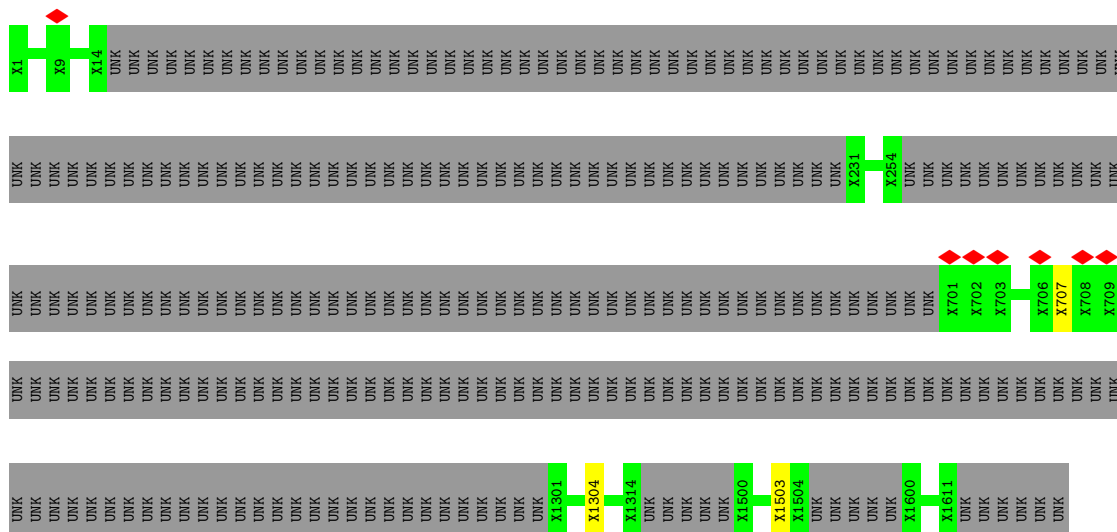




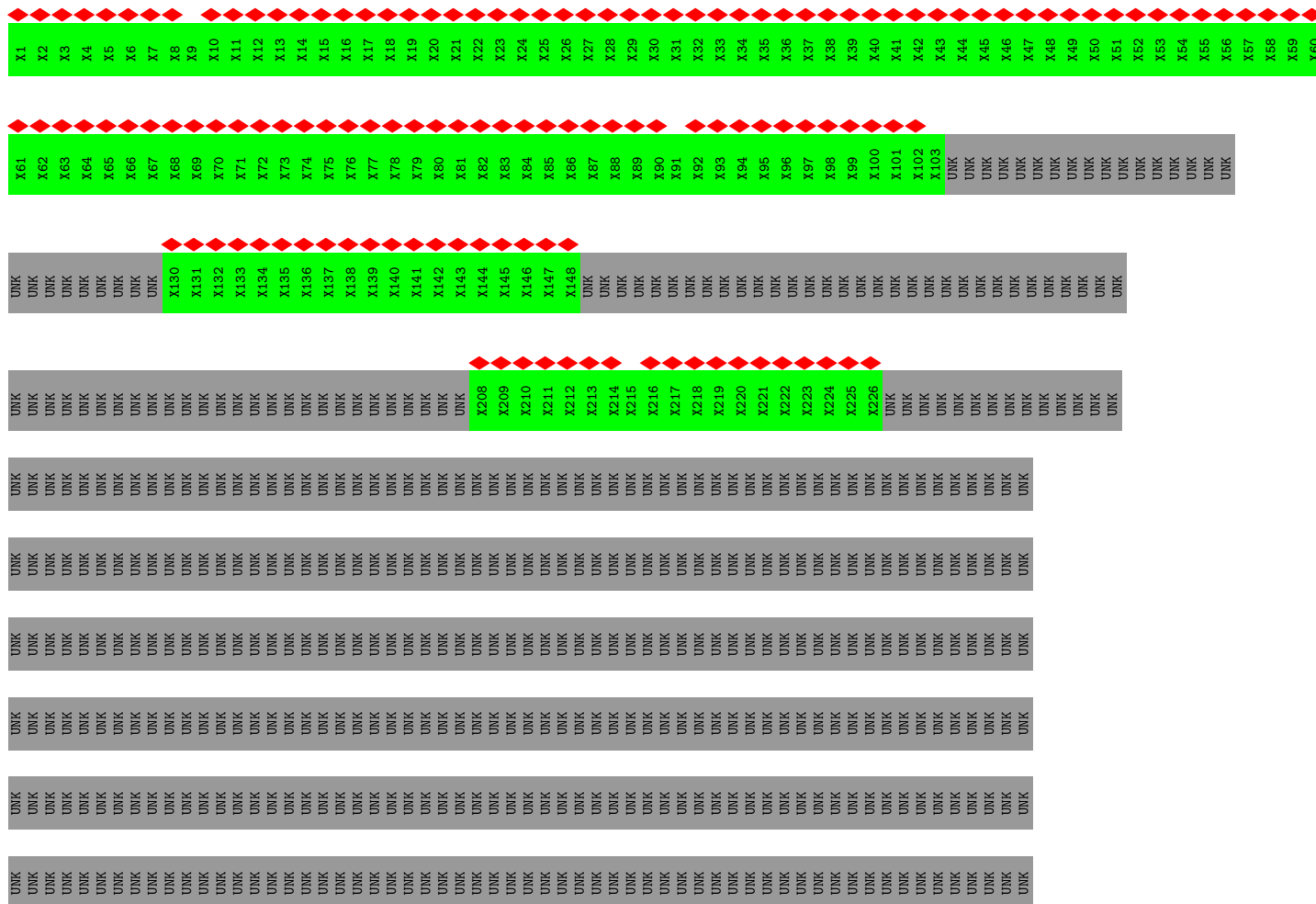




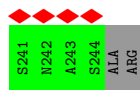




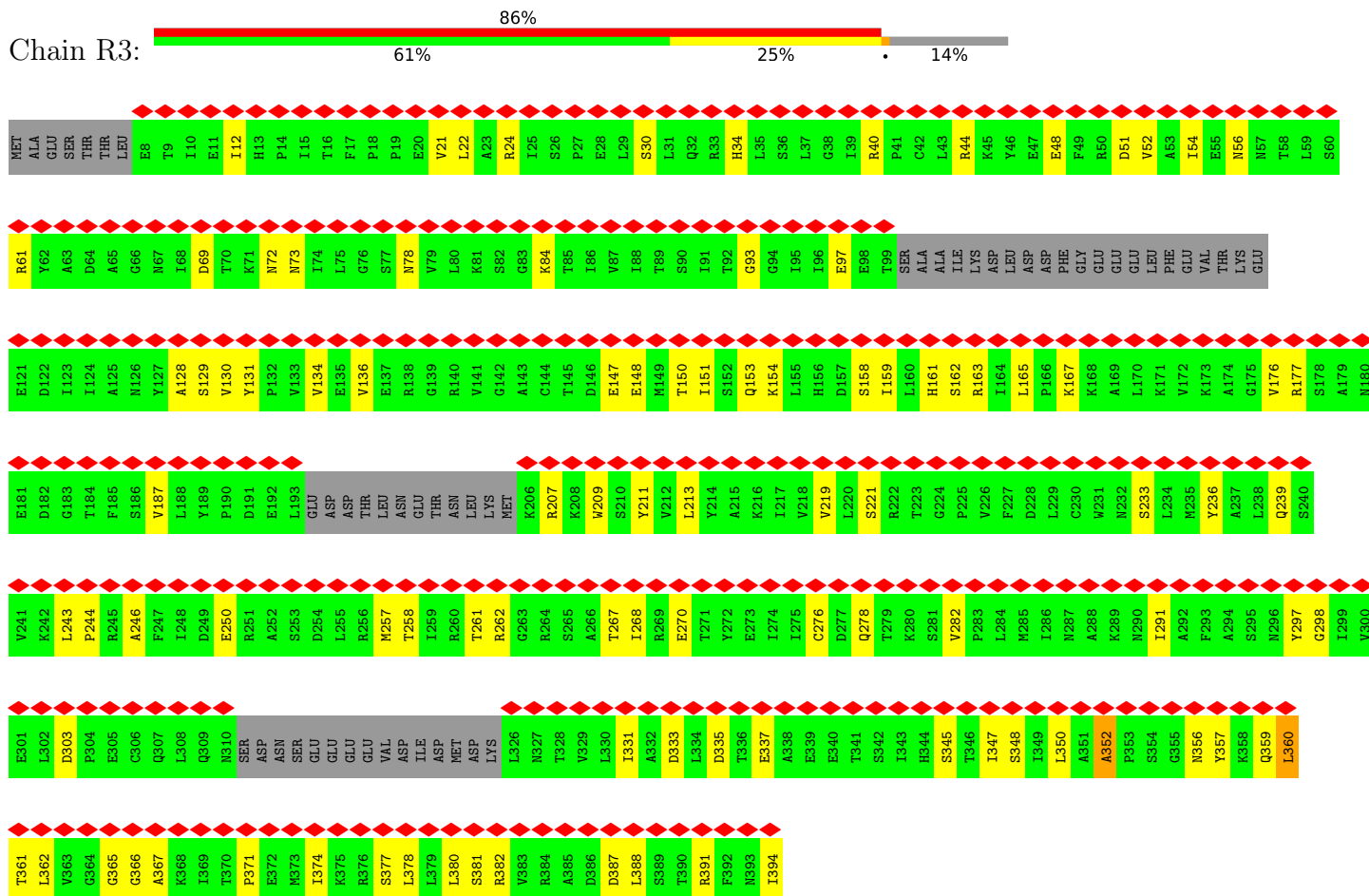
• Molecule 62: Unassigned helices 2



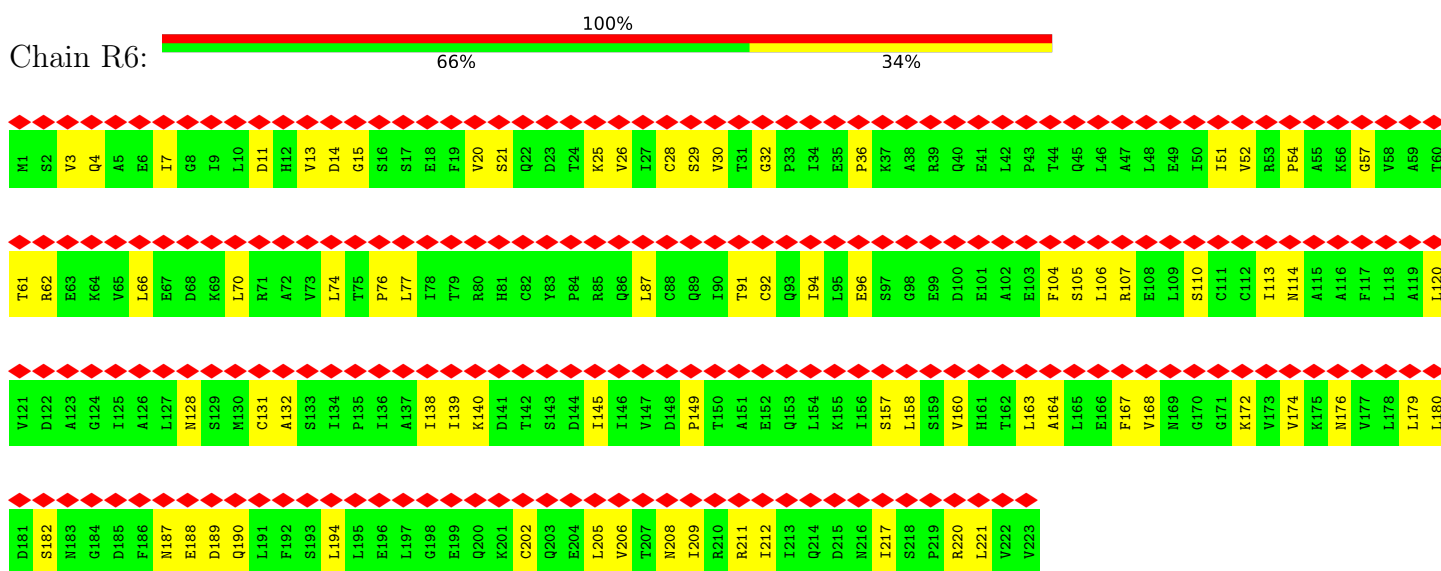




• Molecule 65: Exosome complex component RRP43



• Molecule 66: Exosome complex component RRP46







GLY	T241	ALA	A186	T187	F188	S189	V190	S191	Q192	A193	S194	S195	D196	L197	G198	E199	T200	F201	R202	G203	I204	I205	R206	S207	Q208	D209	V210	R211	S212	T213	D214	R215	D216	R217	V218	K219	V220	I221	E222	C223	F224	K225	P226	G227	D228	I229	V230	R231	A232	Q233	V234	L235	S236	L237	G238	D239	G240
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T242	N243	Y244	L245	T246	A248	R249	N250	D251	L252	G253	V255	F256	A257	R258	A259	N261	G262	A263	G264	G265	L266	M267	Y268	A269	T270	D271	V272	Q273	M274	M275	T276	S277	P278	V279	T280	G281	C282	T283	E284	K285	R286	K287	C288	A289	K290	P291	PHE
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• Molecule 72: Exosome complex exonuclease DIS3



MET	R9	R10	K11	R12	L13	A14	D15	G16	L17	S18	V19	T20	Q21	K22	V23	F24	V25	R26	S27	R28	N29	G30	G31	A32	T33	K34	I35	V36	R37	E38	H39	Y40	L41	R42	D44	S43	I45	P46	C47	L48	S49	R50	F51	D52	C52	T53	K54	C55	P56	Q57	I58	V59	L60
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P61	D62	A63	Q64	N65	E66	L67	P68	R69	F70	I71	L72	S73	D74	S75	P76	L77	E78	L79	S80	A81	P82	I83	G84	R85	H86	Y87	V88	V89	L90	D91	T92	N93	V94	V95	L96	Q97	A98	I99	D100	L101	L102	E103	N104	P105	N106	C107	F108	D109	L110	C52	V111	I112	V113	P114	Q115	I116	V117	L118	D119	E120
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V121	R122	M123	K124	S125	Y126	P127	V128	Y129	T130	R131	L132	R133	T134	L135	C136	R137	D138	S139	D140	D141	H142	K143	R144	F145	I146	V147	F148	H149	N150	E151	F152	S153	L154	H155	T156	F157	V158	E159	R160	L161	P162	M163	E164	T165	I166	M167	D168	R169	N170	D171	R172	A173	I174	R175	K176	T177	Q178	Q179	V180
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Y181	S182	E183	H184	L185	P187	Y188	D189	I190	M191	V192	V193	L194	V195	T196	D197	R199	L200	N201	H202	E203	A204	A205	G206	G207	L208	E208	V209	E210	S211	N212	I213	L214	S215	T216	K216	S217	L218	V219	Q220	Y221	I222	E223	L224	L225	G228	N227	A228	D229	D230	I231	R232	D233	L234	I235	P236	Q237	MET	ASP	SER
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PHE	T249	F250	S251	D252	F253	T254	F255	P256	Y258	Y259	S260	A262	R263	V264	G266	G267	L268	K269	N270	G271	V272	Y274	Q275	G276	N277	L278	Q279	L280	S281	E282	Y283	N284	F285	L286	E287	G288	S289	V290	A291	L292	P293	R294	F295	S296	K297	P298	V299	L300
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I301	V302	G303	Q304	K305	N306	L307	N308	R309	A310	F311	N312	G313	D314	Q315	V316	I317	V318	E319	L320	L321	Q323	S324	E325	V326	K327	A328	SER	ILE	VAL	LEU	ASP	SER	GLU	HIS	PHE	ASP	VAL	ASN	ASP	ASN	PRO	ASP	ILE	GLU	ALA	GLY	ASP	ASP	ASP	ASN	ASN	GLU	SER	SER	SER
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ASN	THR	THR	V364	I365	S366	D367	K368	Q369	R370	R371	L372	L373	A374	K375	D376	A377	M378	I379	A380	Q381	R382	S383	K384	K385	I386	Q387	K447	R448	I449	V450	V451	S452	V453	Y454	I455	S456	W456	R457	R458	S399	W400	R401	Q402	Y403	V404	G405	O406	L407	A408	P409	S410	S411	V412	D413	P414	Q415	S416	S417	S418	T419	Q420	E480
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M421	V422	F423	V424	L425	L426	M427	D428	K429	C430	L431	P432	K433	V434	R435	L436	R437	T438	R439	R440	A441	A442	E443	L444	L445	D446	K447	R448	I449	V450	V451	S452	V453	Y454	I455	S456	W456	R457	R458	S399	W400	R401	Q402	Y403	V404	G405	O406	L407	A408	P409	S410	S411	V412	D413	P414	Q415	S416	S417	S418	T419	Q420	E480
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T481	F482	A483	L484	L485	L486	E487	H488	D489	V490	E491	Y492	R493	P494	F495	S496	K497	K498	V499	L500	E501	C502	L503	P504	A505	E506	G507	H508	D509	W510	K511	A512	P513	T514	A515	L516	D517	D518	P519	E520	A521	V522	S523	K524	D525	P526	L527	L528	T529	K530	R531	K532	D533	L534	R535	E536	K537	L538	I539	C540
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S541	I542	D543	P544	P545	G546	C547	V548	D549	I550	D551	D552	A553	L554	H555	A556	K557	K558	L559	P560	N561	G562	M563	W564	E565	V566	G567	V568	H569	I570	A571	D572	V573	T574	H575	F576	V577	D578	P579	G580	T581	A582	L583	D584	A585	E586	G587	S588	A589	R590	G591	T592	S593	V594	E595	L596	V597	D598	K599	R600
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I601	D602	M603	L604	P605	M606	L607	L608	G609	T610	D611	L612	C613	S614	L615	K616	Y618	V619	D620	R621	F622	A623	F624	S625	V626	I627	W628	E629	L630	D631	D632	S633	A634	M635	I636	V637	M638	V639	N640	F641	M642	K643	S644	V645	I646	R647	S648	R649	E650	A651	F652	S653	Y654	E655	Q656	A657	L658	L659	R660
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E301	ASN	F302	GLN	A303	ILE	E304	GLY	K305	ASP	I306	PRO	C307	ASN	K308	THR	I309	THR	H310	ASP	S311	SER	Q312	GLY	P313	LYS	C314	GLY	H315	GLN	I316	TYR	V317	LYS	Y318	GLY	T319	GLY	N320	ALA	F321	LYS	P323	ASP	T324	ALA	P325	LYS	L326	ASP	Q327	LYS	H328	LYS	Y329	LYS	L330	LYS	F331	LYS	P332	LYS	A333	ASP	M400	ASP	H334	ASP	G335	ASP	D336	ASP	G337	ASP	I338	ASP	Y339	ASP	L340	ASP	V341	ASP	P408	ASP	V409	ASP	D343	ASP	E344	ASP	K345	ASP	S346	ASP	T347	ASP	F348	ASP	R349	ASP	K350	ASP	E351	ASP	N352	ASP	F353	ASP	Q354	ASP	K355	ASP	A356	ASP	M357	ASP	A358	ASP	S359	ASP	I360	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
S361	ASN	L422	GLN	A423	ILE	L424	GLY	K425	ASP	M426	PRO	S427	ASN	K428	THR	L429	THR	D430	ASP	F431	SER	N432	GLY	S433	LYS	D434	GLY	H435	GLN	I436	TYR	V437	LYS	Y438	GLY	T439	GLY	N440	ALA	F441	LYS	K442	ASP	I443	ASP	F444	ALA	N445	LYS	L446	ASP	Q447	LYS	H448	LYS	Y449	LYS	L450	LYS	L451	LYS	P452	LYS	E453	ASP	M400	ASP	H454	ASP	G455	ASP	D456	ASP	G457	ASP	I458	ASP	Y459	ASP	L460	ASP	V461	ASP	P408	ASP	V409	ASP	D463	ASP	E464	ASP	K465	ASP	S466	ASP	T467	ASP	F468	ASP	R469	ASP	K470	ASP	E471	ASP	N472	ASP	F473	ASP	Q474	ASP	K475	ASP	A476	ASP	M477	ASP	A478	ASP	S479	ASP	I480	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
P481	GLN	I482	VAL	L483	VAL	K484	LEU	E485	LEU	V486	LEU	I487	LEU	E488	LEU	L489	LEU	D490	LEU	F491	SER	Q492	LEU	S493	LEU	G494	LEU	F495	LEU	L496	LEU	K497	LEU	V498	LEU	L499	LEU	F500	LEU	L440	ALA	T441	LYS	K442	ASP	I443	ASP	F444	ALA	N445	LYS	L446	ASP	Q447	LYS	H448	LYS	Y449	LYS	L450	LYS	L451	LYS	P452	LYS	E453	ASP	M400	ASP	H454	ASP	G455	ASP	D456	ASP	G457	ASP	I458	ASP	Y459	ASP	L460	ASP	V461	ASP	P408	ASP	V409	ASP	D463	ASP	E464	ASP	K465	ASP	S466	ASP	T467	ASP	F468	ASP	R469	ASP	K470	ASP	E471	ASP	N472	ASP	F473	ASP	Q474	ASP	K475	ASP	A476	ASP	M477	ASP	A478	ASP	S479	ASP	I480	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
S541	GLN	G542	VAL	R543	VAL	A544	LEU	G545	LEU	R546	LEU	S547	LEU	G548	LEU	L549	LEU	D550	LEU	F551	SER	R552	LEU	G553	LEU	I554	LEU	V555	LEU	L556	LEU	M557	LEU	M558	LEU	L559	LEU	D560	LEU	E561	LEU	K562	ASP	M563	ASP	E564	ALA	F565	LYS	P566	LYS	Q567	LYS	S568	LYS	G569	LYS	L570	LYS	L571	LYS	P572	LYS	E573	ASP	M574	ASP	K575	ASP	G576	ASP	Q577	ASP	D578	ASP	L579	ASP	D580	ASP	S581	ASP	E582	ASP	F583	ASP	H584	ASP	L585	ASP	G586	ASP	Y587	ASP	N588	ASP	M589	ASP	L590	ASP	E591	ASP	N592	ASP	L593	ASP	G594	ASP	R595	ASP	V596	ASP	E597	ASP	G598	ASP	I599	ASP	S600	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
P601	LEU	E602	LEU	F603	LEU	M604	LEU	L605	LEU	E606	LEU	H607	LEU	S608	LEU	F609	LEU	D610	LEU	F611	SER	R612	LEU	G613	LEU	Q614	LEU	V615	LEU	L616	LEU	S617	LEU	V618	LEU	P619	LEU	D620	LEU	M621	LEU	E622	LEU	K623	LEU	L624	LEU	A625	LEU	G626	LEU	H627	LEU	S628	LEU	G629	LEU	L630	LEU	L631	LEU	P632	LEU	E633	LEU	M634	LEU	K635	LEU	L636	LEU	H637	LEU	S638	LEU	V639	LEU	P640	LEU	D641	LEU	F642	LEU	G643	LEU	M644	LEU	L645	LEU	E646	LEU	H647	LEU	S648	LEU	V649	LEU	P650	LEU	D651	LEU	F652	LEU	G653	LEU	M654	LEU	L655	LEU	E656	LEU	H657	LEU	S658	LEU	V659	LEU	P660	LEU	D661	LEU	F662	LEU	G663	LEU	M664	LEU	L665	LEU	E666	LEU	H667	LEU	S668	LEU	V669	LEU	P670	LEU	D671	LEU	F672	LEU	G673	LEU	M674	LEU	L675	LEU	E676	LEU	H677	LEU	S678	LEU	V679	LEU	P680	LEU	D681	LEU	F682	LEU	G683	LEU	M684	LEU	L685	LEU	E686	LEU	H687	LEU	S688	LEU	V689	LEU	P690	LEU	D691	LEU	F692	LEU	G693	LEU	M694	LEU	L695	LEU	E696	LEU	H697	LEU	S698	LEU	V699	LEU	P700	LEU	D701	LEU	F702	LEU	G703	LEU	M704	LEU	L705	LEU	E706	LEU	H707	LEU	S708	LEU	V709	LEU	P710	LEU	D711	LEU	F712	LEU	G713	LEU	M714	LEU	L715	LEU	E716	LEU	H717	LEU	S718	LEU	V719	LEU	P720	LEU	D721	LEU	F722	LEU	G723	LEU	M724	LEU	L725	LEU	E726	LEU	H727	LEU	S728	LEU	V729	LEU	P730	LEU	D731	LEU	F732	LEU	G733	LEU	M734	LEU	L735	LEU	E736	LEU	H737	LEU	S738	LEU	V739	LEU	P740	LEU	D741	LEU	F742	LEU	G743	LEU	M744	LEU	L745	LEU	E746	LEU	H747	LEU	S748	LEU	V749	LEU	P750	LEU	D751	LEU	F752	LEU	G753	LEU	M754	LEU	L755	LEU	E756	LEU	H757	LEU	S758	LEU	V759	LEU	P760	LEU	D761	LEU	F762	LEU	G763	LEU	M764	LEU	L765	LEU	E766	LEU	H767	LEU	S768	LEU	V769	LEU	P770	LEU	D771	LEU	F772	LEU	G773	LEU	M774	LEU	L775	LEU	E776	LEU	H777	LEU	S778	LEU	V779	LEU	P780	LEU	D781	LEU	F782	LEU	G783	LEU	M784	LEU	L785	LEU	E786	LEU	H787	LEU	S788	LEU	V789	LEU	P790	LEU	D791	LEU	F792	LEU	G793	LEU	M794	LEU	L795	LEU	E796	LEU	H797	LEU	S798	LEU	V799	LEU	P800	LEU	D801	LEU	F802	LEU	G803	LEU	M804	LEU	L805	LEU	E806	LEU	H807	LEU	S808	LEU	V809	LEU	P810	LEU	D811	LEU	F812	LEU	G813	LEU	M814	LEU	L815	LEU	E816	LEU	H817	LEU	S818	LEU	V819	LEU	P820	LEU	D821	LEU	F822	LEU	G823	LEU	M824	LEU	L825	LEU	E826	LEU	H827	LEU	S828	LEU	V829	LEU	P830	LEU	D831	LEU	F832	LEU	G833	LEU	M834	LEU	L835	LEU	E836	LEU	H837	LEU	S838	LEU	V839	LEU	P840	LEU	D841	LEU	F842	LEU	G843	LEU	M844	LEU	L845	LEU	E846	LEU	H847	LEU	S848	LEU	V849	LEU	P850	LEU	D851	LEU	F852	LEU	G853	LEU	M854	LEU	L855	LEU	E856	LEU	H857	LEU	S858	LEU	V859	LEU	P860	LEU	D861	LEU	F862	LEU	G863	LEU	M864	LEU	L865	LEU	E866	LEU	H867	LEU	S868	LEU	V869	LEU	P870	LEU	D871	LEU	F872	LEU	G873	LEU	M874	LEU	L875	LEU	E876	LEU	H877	LEU	S878	LEU	V879	LEU	P880	LEU	D881	LEU	F882	LEU	G883	LEU	M884	LEU	L885	LEU	E886	LEU	H887	LEU	S888	LEU	V889	LEU	P890	LEU	D891	LEU	F892	LEU	G893	LEU	M894	LEU	L895	LEU	E896	LEU	H897	LEU	S898	LEU	V899	LEU	P900	LEU	D901	LEU	F902	LEU	G903	LEU	M904	LEU	L905	LEU	E906	LEU	H907	LEU	S908	LEU	V909	LEU	P910	LEU	D911	LEU	F912	LEU	G913	LEU	M914	LEU	L915	LEU	E916	LEU	H917	LEU	S918	LEU	V919	LEU	P920	LEU	D921	LEU	F922	LEU	G923	LEU	M924	LEU	L925	LEU	E926	LEU	H927	LEU	S928	LEU	V929	LEU	P930	LEU	D931	LEU	F932	LEU	G933	LEU	M934	LEU	L935	LEU	E936	LEU	H937	LEU	S938	LEU	V939	LEU	P940	LEU	D941	LEU	F942	LEU	G943	LEU	M944	LEU	L945	LEU	E946	LEU	H947	LEU	S948	LEU	V949	LEU	P950	LEU	D951	LEU	F952	LEU	G953	LEU	M954	LEU	L955	LEU	E956	LEU	H957	LEU	S958	LEU	V959	LEU	P960	LEU	D961	LEU	F962	LEU	G963	LEU	M964	LEU	L965	LEU	E966	LEU	H967	LEU	S968	LEU	V969	LEU	P970	LEU	D971	LEU	F972	LEU	G973	LEU	M974	LEU	L975	LEU	E976	LEU	H977	LEU	S978	LEU	V979	LEU	P980	LEU	D981	LEU	F982	LEU	G983	LEU	M984	LEU	L985	LEU	E986	LEU	H987	LEU	S988	LEU	V989	LEU	P990	LEU	D991	LEU	F992	LEU	G993	LEU	M994	LEU	L995	LEU	E996	LEU	H997	LEU	S998	LEU	V999	LEU	P1000	LEU	D1001	LEU	F1002	LEU	G1003	LEU	M1004	LEU	L1005	LEU	E1006	LEU	H1007	LEU	S1008	LEU	V1009	LEU	P1010	LEU	D1011	LEU	F1012	LEU	G1013	LEU	M1014	LEU	L1015	LEU	E1016	LEU	H1017	LEU	S1018	LEU	V1019	LEU	P1020	LEU	D1021	LEU	F1022	LEU	G1023	LEU	M1024	LEU	L1025	LEU	E1026	LEU	H1027	LEU	S1028	LEU	V1029	LEU	P1030	LEU	D1031	LEU	F1032	LEU	G1033	LEU	M1034	LEU	L1035	LEU	E1036	LEU	H1037	LEU	S1038	LEU	V1039	LEU	P1040	LEU	D1041	LEU	F1042	LEU	G1043	LEU	M1044	LEU	L1045	LEU	E1046	LEU	H1047	LEU	S1048	LEU	V1049	LEU	P1050	LEU	D1051	LEU	F1052	LEU	G1053	LEU	M1054	LEU	L1055	LEU	E1056	LEU	H1057	LEU	S1058	LEU	V1059	LEU	P1060	LEU	D1061	LEU	F1062	LEU	G1063	LEU	M1064	LEU	L1065	LEU	E1066	LEU	H1067	LEU	S1068	LEU	V1069	LEU	P1070	LEU	D1071	LEU	F1072	LEU	G1073	LEU	M1074	LEU	L1075	LEU	E1076	LEU	H1077	LEU	S1078	LEU	V1079	LEU	P1080	LEU	D1081	LEU	F1082	LEU	G1083	LEU	M1084	LEU	L1085	LEU	E1086	LEU	H1087	LEU	S1088	LEU	V1089	LEU	P1090	LEU	D1091	LEU	F1092	LEU	G1093	LEU	M1094	LEU	L1095	LEU	E1096	LEU	H1097	LEU	S1098	LEU	V1099	LEU	P1100	LEU	D1101	LEU	F1102	LEU	G1103	LEU	M1104	LEU	L1105	LEU	E1106	LEU	H1107	LEU	S1108	LEU	V1109	LEU	P1110	LEU	D1111	LEU	F1112	LEU	G1113	LEU	M1114	LEU	L1115	LEU	E1116	LEU	H1117	LEU	S1118	LEU	V1119	LEU	P1120	LEU	D1121	LEU	F1122	LEU	G1123	LEU	M1124	LEU	L1125	LEU	E1126	LEU	H1127	LEU	S1128	LEU	V1129	LEU	P1130	LEU	D1131	LEU	F1132	LEU	G1133	LEU	M1134	LEU	L1135	LEU	E1136	LEU	H1137	LEU	S1138	LEU	V1139	LEU	P1140	LEU	D1141	LEU	F1142	LEU	G1143	LEU	M1144	LEU	L1145	LEU	E1146	LEU	H1147	LEU	S1148	LEU	V1149	LEU	P1150	LEU	D1151	LEU	F1152	LEU	G1153	LEU	M1154	LEU	L1155	LEU	E1156	LEU	H1157	LEU	S1158	LEU	V1159	LEU	P1160	LEU	D1161	LEU	F1162	LEU	G1163	LEU	M1164	LEU	L1165	LEU	E1



## 4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75404	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	597.632, 597.632, 597.632	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	3A	0.66	0/5532	1.21	32/8585 (0.4%)
2	5A	0.52	0/3643	1.20	23/5663 (0.4%)
3	SA	0.65	0/29737	1.18	205/46285 (0.4%)
4	SC	0.46	0/1874	0.71	3/2512 (0.1%)
5	SF	0.41	0/1969	0.70	3/2661 (0.1%)
6	SG	0.44	0/1690	0.63	0/2285
7	SH	0.31	0/1477	0.58	1/1977 (0.1%)
8	SI	0.41	0/1330	0.71	1/1792 (0.1%)
9	SJ	0.31	0/1124	0.61	0/1510
10	SK	0.51	0/1410	0.66	2/1888 (0.1%)
11	SM	0.31	0/1139	0.57	0/1535
12	SO	0.44	0/1109	0.64	0/1495
13	SP	0.42	0/879	0.63	0/1186
14	SR	0.53	0/990	0.69	1/1335 (0.1%)
15	SX	0.49	0/1020	0.66	0/1371
16	SY	0.42	0/819	0.60	0/1093
17	SZ	0.52	0/1000	0.65	0/1334
18	Sc	0.45	0/613	0.73	1/828 (0.1%)
19	Sd	0.49	0/499	0.71	1/670 (0.1%)
20	3B	0.56	0/1901	0.66	1/2567 (0.0%)
20	3C	0.36	0/1796	0.63	1/2424 (0.0%)
21	3D	0.45	0/3020	0.66	4/4066 (0.1%)
22	3E	0.38	0/3072	0.61	2/4169 (0.0%)
23	3F	0.50	0/3569	0.67	0/4806
24	3G	0.40	0/928	0.72	0/1262
24	3H	0.53	0/928	0.68	1/1262 (0.1%)
25	A4	0.36	0/5338	0.64	1/7230 (0.0%)
26	A5	0.45	0/4021	0.63	1/5462 (0.0%)
27	A8	0.27	0/3328	0.60	0/4565
28	A9	0.27	0/951	0.68	2/1287 (0.2%)
29	AE	0.34	0/10050	0.54	1/13739 (0.0%)
30	AF	0.32	0/3885	0.61	2/5261 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	AG	0.34	0/6699	0.64	5/9077 (0.1%)
32	B1	0.56	0/6570	0.67	1/8892 (0.0%)
33	B2	0.42	0/6628	0.67	1/8954 (0.0%)
34	B3	0.37	0/6014	0.71	4/8137 (0.0%)
35	B8	0.43	0/3848	0.65	2/5218 (0.0%)
36	BE	0.55	0/6606	0.66	1/8935 (0.0%)
37	B6	0.45	0/2849	0.56	0/3853
38	5B	0.26	0/499	0.62	0/659
39	5C	0.53	0/3690	0.65	0/4991
40	5D	0.33	0/1757	0.57	0/2320
41	5E	0.40	0/1580	0.67	2/2115 (0.1%)
42	5F	0.50	0/1559	0.66	1/2097 (0.0%)
43	5G	0.51	0/1768	0.66	0/2392
44	5H	0.45	0/601	0.63	1/789 (0.1%)
45	5I	0.64	0/3835	0.67	2/5162 (0.0%)
46	5J	0.35	0/1147	0.57	0/1531
47	5K	0.51	0/1346	0.63	0/1812
48	RD	0.31	0/2454	0.59	0/3310
49	RE	0.37	0/9015	0.63	7/12195 (0.1%)
50	RF	0.37	0/2004	0.64	2/2697 (0.1%)
51	RG	0.29	0/1727	0.63	1/2329 (0.0%)
51	RH	0.28	0/1828	0.61	0/2470
52	RJ	0.45	0/6067	0.62	2/8170 (0.0%)
53	RK	0.41	0/2832	0.63	0/3825
54	RN	0.30	0/4146	0.58	0/5604
55	RO	0.29	0/3849	0.60	1/5261 (0.0%)
56	RP	0.31	0/12777	0.51	4/17558 (0.0%)
57	RQ	0.44	0/1682	0.60	0/2286
58	RS	0.34	0/2104	0.70	2/2854 (0.1%)
59	RT	0.33	0/1379	0.62	0/1853
60	RW	0.23	0/745	0.38	0/1038
63	R5	0.57	0/2340	0.64	1/3161 (0.0%)
64	R1	0.54	0/1910	0.68	0/2579
65	R3	0.50	0/2628	0.69	2/3569 (0.1%)
66	R6	0.54	0/1714	0.70	0/2328
67	R2	0.51	0/2069	0.69	0/2817
68	M3	0.53	0/1661	0.65	0/2243
69	R0	0.55	0/1828	0.69	0/2486
70	r4	0.52	0/2269	0.66	0/3066
71	C4	0.48	0/1676	0.66	0/2277
72	R4	0.42	0/7575	0.61	3/10290 (0.0%)
73	r6	0.47	0/810	0.58	0/1091
74	R7	0.39	0/686	0.57	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	M4	0.50	0/6945	0.67	3/9400 (0.0%)
76	M6	0.43	0/277	0.66	0/371
All	All	0.47	0/244634	0.76	337/339083 (0.1%)

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
4	SC	0	4
7	SH	0	1
8	SI	0	4
12	SO	0	1
18	Sc	0	2
19	Sd	0	1
20	3C	0	1
23	3F	0	1
26	A5	0	1
27	A8	0	6
29	AE	0	1
30	AF	0	1
31	AG	0	5
32	B1	0	1
33	B2	0	2
34	B3	0	5
38	5B	0	1
41	5E	0	1
45	5I	0	3
49	RE	0	3
50	RF	0	3
51	RH	0	1
52	RJ	0	1
53	RK	0	1
55	RO	0	4
56	RP	0	11
57	RQ	0	2
59	RT	0	1
64	R1	0	1
65	R3	0	3
66	R6	0	1
67	R2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	M3	0	2
70	r4	0	1
71	C4	0	1
72	R4	0	1
75	M4	0	3
All	All	0	83

There are no bond length outliers.

The worst 5 of 337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	27	U	C2-N1-C1'	11.58	131.59	117.70
1	3A	27	U	N1-C2-O2	11.42	130.79	122.80
1	3A	27	U	N3-C2-O2	-10.83	114.62	122.20
3	SA	453	U	N3-C2-O2	-10.59	114.79	122.20
3	SA	453	U	N1-C2-O2	9.83	129.68	122.80

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	SC	135	LEU	Peptide
4	SC	16	GLN	Peptide
4	SC	177	GLN	Peptide
4	SC	208	GLN	Peptide
7	SH	152	ASP	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	3A	4962	0	2519	58	0
2	5A	3260	0	1643	34	0
3	SA	26609	0	13415	315	0
4	SC	1848	0	1940	41	0
5	SF	1930	0	1950	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	SG	1669	0	1724	21	0
7	SH	1457	0	1504	39	0
8	SI	1310	0	1374	36	0
9	SJ	1104	0	1107	28	0
10	SK	1388	0	1467	28	0
11	SM	1113	0	1181	29	0
12	SO	1087	0	1152	26	0
13	SP	868	0	894	18	0
14	SR	973	0	1029	19	0
15	SX	1003	0	1040	24	0
16	SY	807	0	865	16	0
17	SZ	986	0	1042	19	0
18	Sc	603	0	621	0	0
19	Sd	497	0	535	0	0
20	3B	1865	0	1910	46	0
20	3C	1763	0	1805	48	0
21	3D	2974	0	3001	53	0
22	3E	3041	0	2831	68	0
23	3F	3498	0	3515	80	0
24	3G	916	0	964	17	0
24	3H	916	0	964	23	0
25	A4	5243	0	5216	195	0
26	A5	3953	0	3894	86	0
27	A8	3307	0	2316	45	0
28	A9	939	0	898	25	0
29	AE	9956	0	7969	130	0
30	AF	3807	0	3791	89	0
31	AG	6570	0	6473	189	0
32	B1	6427	0	6329	127	0
33	B2	6502	0	6493	156	0
34	B3	5919	0	6007	146	0
35	B8	3764	0	3757	84	0
36	BE	6475	0	6453	156	0
37	B6	2800	0	2517	43	0
38	5B	495	0	561	10	0
39	5C	3612	0	3578	66	0
40	5D	1733	0	1815	36	0
41	5E	1564	0	1592	41	0
42	5F	1530	0	1572	30	0
43	5G	1732	0	1744	37	0
44	5H	596	0	661	8	0
45	5I	3756	0	3708	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	5J	1127	0	1150	17	0
47	5K	1323	0	1401	20	0
48	RD	2413	0	2264	29	0
49	RE	8805	0	8911	192	0
50	RF	1963	0	1942	42	0
51	RG	1701	0	1767	49	0
51	RH	1799	0	1872	46	0
52	RJ	5935	0	6100	130	0
53	RK	2781	0	2878	79	0
54	RN	4088	0	3798	62	0
55	RO	3766	0	3269	63	0
56	RP	12716	0	8235	90	0
57	RQ	1655	0	1461	22	0
58	RS	2051	0	2096	46	0
59	RT	1357	0	1426	23	0
60	RW	747	0	312	2	0
61	X1	400	0	99	3	0
62	X2	705	0	151	0	0
63	R5	2304	0	2265	61	0
64	R1	1886	0	1904	51	0
65	R3	2588	0	2607	70	0
66	R6	1696	0	1744	46	0
67	R2	2030	0	2047	51	0
68	M3	1639	0	1592	42	0
69	R0	1792	0	1747	41	0
70	r4	2236	0	2215	0	0
71	C4	1653	0	1616	41	0
72	R4	7430	0	7346	218	0
73	r6	802	0	776	0	0
74	R7	681	0	707	13	0
75	M4	6814	0	6792	224	0
76	M6	275	0	254	6	0
77	5K	1	0	0	0	0
77	Sc	1	0	0	0	0
78	RJ	32	0	12	0	0
79	RJ	1	0	0	0	0
All	All	238320	0	212092	4259	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 10.

The worst 5 of 4259 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)
25:A4:741:LEU:HD11	25:A4:744:VAL:CG2	1.48	1.42
25:A4:740:PRO:O	25:A4:756:GLU:HG2	1.44	1.16
25:A4:741:LEU:HD11	25:A4:744:VAL:HG21	1.16	1.13
25:A4:741:LEU:HD21	25:A4:744:VAL:HG23	1.39	1.04
25:A4:741:LEU:CD1	25:A4:744:VAL:CG2	2.39	1.00

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	
4	SC	230/255 (90%)	190 (83%)	39 (17%)	1 (0%)	34	70
5	SF	248/261 (95%)	211 (85%)	37 (15%)	0	100	100
6	SG	211/225 (94%)	194 (92%)	17 (8%)	0	100	100
7	SH	178/236 (75%)	158 (89%)	17 (10%)	3 (2%)	9	43
8	SI	160/190 (84%)	136 (85%)	24 (15%)	0	100	100
9	SJ	136/200 (68%)	113 (83%)	23 (17%)	0	100	100
10	SK	169/197 (86%)	155 (92%)	14 (8%)	0	100	100
11	SM	135/156 (86%)	119 (88%)	16 (12%)	0	100	100
12	SO	132/151 (87%)	119 (90%)	13 (10%)	0	100	100
13	SP	116/137 (85%)	103 (89%)	13 (11%)	0	100	100
14	SR	123/143 (86%)	110 (89%)	13 (11%)	0	100	100
15	SX	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
16	SY	104/145 (72%)	91 (88%)	13 (12%)	0	100	100
17	SZ	121/135 (90%)	104 (86%)	17 (14%)	0	100	100
18	Sc	78/82 (95%)	66 (85%)	12 (15%)	0	100	100
19	Sd	61/67 (91%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
20	3C	221/327 (68%)	204 (92%)	17 (8%)	0	100	100
21	3D	372/504 (74%)	343 (92%)	29 (8%)	0	100	100
22	3E	428/511 (84%)	389 (91%)	39 (9%)	0	100	100
23	3F	431/573 (75%)	365 (85%)	65 (15%)	1 (0%)	47	79
24	3G	119/126 (94%)	109 (92%)	10 (8%)	0	100	100
24	3H	119/126 (94%)	112 (94%)	6 (5%)	1 (1%)	19	57
25	A4	650/776 (84%)	583 (90%)	67 (10%)	0	100	100
26	A5	501/643 (78%)	453 (90%)	48 (10%)	0	100	100
27	A8	534/713 (75%)	423 (79%)	109 (20%)	2 (0%)	34	70
28	A9	126/575 (22%)	114 (90%)	12 (10%)	0	100	100
29	AE	1496/1769 (85%)	1372 (92%)	124 (8%)	0	100	100
30	AF	473/513 (92%)	427 (90%)	46 (10%)	0	100	100
31	AG	812/896 (91%)	694 (86%)	118 (14%)	0	100	100
32	B1	800/900 (89%)	720 (90%)	80 (10%)	0	100	100
33	B2	813/943 (86%)	731 (90%)	82 (10%)	0	100	100
34	B3	733/817 (90%)	608 (83%)	123 (17%)	2 (0%)	41	74
35	B8	469/594 (79%)	423 (90%)	45 (10%)	1 (0%)	47	79
36	BE	817/939 (87%)	746 (91%)	71 (9%)	0	100	100
37	B6	368/440 (84%)	343 (93%)	25 (7%)	0	100	100
38	5B	58/214 (27%)	52 (90%)	6 (10%)	0	100	100
39	5C	452/554 (82%)	400 (88%)	52 (12%)	0	100	100
40	5D	198/250 (79%)	172 (87%)	25 (13%)	1 (0%)	29	66
41	5E	187/593 (32%)	173 (92%)	14 (8%)	0	100	100
42	5F	180/183 (98%)	165 (92%)	15 (8%)	0	100	100
43	5G	214/290 (74%)	196 (92%)	18 (8%)	0	100	100
44	5H	72/610 (12%)	63 (88%)	9 (12%)	0	100	100
45	5I	456/489 (93%)	422 (92%)	33 (7%)	1 (0%)	47	79
46	5J	130/217 (60%)	121 (93%)	9 (7%)	0	100	100
47	5K	162/189 (86%)	149 (92%)	13 (8%)	0	100	100
48	RD	310/1729 (18%)	278 (90%)	32 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	RE	1080/1237 (87%)	996 (92%)	84 (8%)	0	100	100
50	RF	233/297 (78%)	203 (87%)	30 (13%)	0	100	100
51	RG	212/252 (84%)	193 (91%)	19 (9%)	0	100	100
51	RH	226/252 (90%)	208 (92%)	18 (8%)	0	100	100
52	RJ	719/1183 (61%)	649 (90%)	69 (10%)	1 (0%)	51	83
53	RK	358/367 (98%)	335 (94%)	23 (6%)	0	100	100
54	RN	539/810 (66%)	482 (89%)	57 (11%)	0	100	100
55	RO	523/552 (95%)	473 (90%)	49 (9%)	1 (0%)	47	79
56	RP	2112/2493 (85%)	1903 (90%)	203 (10%)	6 (0%)	41	74
57	RQ	220/899 (24%)	197 (90%)	23 (10%)	0	100	100
58	RS	247/480 (52%)	218 (88%)	29 (12%)	0	100	100
59	RT	165/326 (51%)	152 (92%)	13 (8%)	0	100	100
60	RW	146/206 (71%)	140 (96%)	6 (4%)	0	100	100
63	R5	297/305 (97%)	276 (93%)	21 (7%)	0	100	100
64	R1	242/246 (98%)	225 (93%)	17 (7%)	0	100	100
65	R3	332/394 (84%)	304 (92%)	27 (8%)	1 (0%)	41	74
66	R6	221/223 (99%)	208 (94%)	13 (6%)	0	100	100
67	R2	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
68	M3	209/250 (84%)	190 (91%)	19 (9%)	0	100	100
69	R0	235/240 (98%)	216 (92%)	19 (8%)	0	100	100
70	r4	287/359 (80%)	262 (91%)	25 (9%)	0	100	100
71	C4	214/292 (73%)	198 (92%)	16 (8%)	0	100	100
72	R4	942/1001 (94%)	875 (93%)	67 (7%)	0	100	100
73	r6	98/733 (13%)	91 (93%)	7 (7%)	0	100	100
74	R7	83/184 (45%)	82 (99%)	1 (1%)	0	100	100
75	M4	866/1073 (81%)	806 (93%)	60 (7%)	0	100	100
76	M6	36/186 (19%)	32 (89%)	4 (11%)	0	100	100
All	All	26369/36145 (73%)	23774 (90%)	2573 (10%)	22 (0%)	54	83

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	B8	226	LYS

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Mol	Chain	Res	Type
55	RO	75	PRO
24	3H	6	PRO
27	A8	309	PRO
56	RP	37	ARG

### 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	
4	SC	205/224 (92%)	203 (99%)	2 (1%)	76	86
5	SF	199/222 (90%)	196 (98%)	3 (2%)	65	81
6	SG	180/191 (94%)	179 (99%)	1 (1%)	86	92
7	SH	153/201 (76%)	152 (99%)	1 (1%)	84	91
8	SI	145/170 (85%)	144 (99%)	1 (1%)	84	91
9	SJ	114/161 (71%)	114 (100%)	0	100	100
10	SK	147/166 (89%)	146 (99%)	1 (1%)	84	91
11	SM	124/137 (90%)	122 (98%)	2 (2%)	62	79
12	SO	117/128 (91%)	114 (97%)	3 (3%)	46	69
13	SP	90/105 (86%)	89 (99%)	1 (1%)	73	85
14	SR	105/119 (88%)	104 (99%)	1 (1%)	76	86
15	SX	108/111 (97%)	108 (100%)	0	100	100
16	SY	88/120 (73%)	86 (98%)	2 (2%)	50	72
17	SZ	103/113 (91%)	98 (95%)	5 (5%)	25	55
18	Sc	69/71 (97%)	66 (96%)	3 (4%)	29	58
19	Sd	56/60 (93%)	56 (100%)	0	100	100
20	3B	201/240 (84%)	201 (100%)	0	100	100
20	3C	190/240 (79%)	187 (98%)	3 (2%)	62	79
21	3D	322/435 (74%)	320 (99%)	2 (1%)	86	92
22	3E	265/433 (61%)	263 (99%)	2 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	3F	382/503 (76%)	374 (98%)	8 (2%)	53	74
24	3G	100/104 (96%)	100 (100%)	0	100	100
24	3H	100/104 (96%)	100 (100%)	0	100	100
25	A4	593/713 (83%)	585 (99%)	8 (1%)	69	82
26	A5	431/574 (75%)	428 (99%)	3 (1%)	84	91
27	A8	174/657 (26%)	170 (98%)	4 (2%)	50	72
28	A9	89/533 (17%)	86 (97%)	3 (3%)	37	64
29	AE	708/1633 (43%)	705 (100%)	3 (0%)	91	95
30	AF	424/454 (93%)	420 (99%)	4 (1%)	78	88
31	AG	750/826 (91%)	744 (99%)	6 (1%)	81	89
32	B1	707/789 (90%)	703 (99%)	4 (1%)	86	92
33	B2	712/832 (86%)	701 (98%)	11 (2%)	65	81
34	B3	665/719 (92%)	657 (99%)	8 (1%)	71	84
35	B8	421/529 (80%)	419 (100%)	2 (0%)	88	94
36	BE	721/819 (88%)	713 (99%)	8 (1%)	73	85
37	B6	251/414 (61%)	248 (99%)	3 (1%)	71	84
38	5B	57/196 (29%)	56 (98%)	1 (2%)	59	77
39	5C	394/480 (82%)	390 (99%)	4 (1%)	76	86
40	5D	192/234 (82%)	191 (100%)	1 (0%)	88	94
41	5E	175/535 (33%)	174 (99%)	1 (1%)	86	92
42	5F	171/172 (99%)	171 (100%)	0	100	100
43	5G	191/258 (74%)	191 (100%)	0	100	100
44	5H	63/538 (12%)	63 (100%)	0	100	100
45	5I	415/443 (94%)	408 (98%)	7 (2%)	60	78
46	5J	124/200 (62%)	121 (98%)	3 (2%)	49	71
47	5K	148/169 (88%)	147 (99%)	1 (1%)	84	91
48	RD	226/1544 (15%)	225 (100%)	1 (0%)	91	95
49	RE	994/1125 (88%)	986 (99%)	8 (1%)	81	89
50	RF	221/274 (81%)	216 (98%)	5 (2%)	50	72
51	RG	195/222 (88%)	191 (98%)	4 (2%)	53	74
51	RH	206/222 (93%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	RJ	649/1039 (62%)	644 (99%)	5 (1%)	81	89
53	RK	307/312 (98%)	302 (98%)	5 (2%)	62	79
54	RN	379/732 (52%)	375 (99%)	4 (1%)	73	85
55	RO	329/506 (65%)	327 (99%)	2 (1%)	86	92
56	RP	550/2307 (24%)	545 (99%)	5 (1%)	78	88
57	RQ	149/808 (18%)	149 (100%)	0	100	100
58	RS	225/421 (53%)	219 (97%)	6 (3%)	44	69
59	RT	148/282 (52%)	148 (100%)	0	100	100
63	R5	255/266 (96%)	255 (100%)	0	100	100
64	R1	210/218 (96%)	207 (99%)	3 (1%)	67	81
65	R3	282/349 (81%)	281 (100%)	1 (0%)	91	95
66	R6	195/197 (99%)	195 (100%)	0	100	100
67	R2	236/240 (98%)	236 (100%)	0	100	100
68	M3	181/219 (83%)	180 (99%)	1 (1%)	86	92
69	R0	194/209 (93%)	193 (100%)	1 (0%)	88	94
70	r4	243/311 (78%)	242 (100%)	1 (0%)	91	95
71	C4	174/240 (72%)	172 (99%)	2 (1%)	73	85
72	R4	812/901 (90%)	808 (100%)	4 (0%)	88	94
73	r6	89/671 (13%)	89 (100%)	0	100	100
74	R7	76/168 (45%)	75 (99%)	1 (1%)	69	82
75	M4	729/953 (76%)	725 (100%)	4 (0%)	88	94
76	M6	25/168 (15%)	25 (100%)	0	100	100
All	All	20418/31979 (64%)	20229 (99%)	189 (1%)	79	88

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	5I	100	ARG
51	RG	136	ARG
45	5I	255	THR
49	RE	316	ARG
53	RK	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 286 such sidechains are listed below:



Mol	Chain	Res	Type
56	RP	115	HIS
57	RQ	836	ASN
72	R4	29	ASN
33	B2	195	GLN
32	B1	837	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	222/333 (66%)	86 (38%)	3 (1%)
2	5A	144/700 (20%)	62 (43%)	2 (1%)
3	SA	1227/1809 (67%)	466 (37%)	20 (1%)
All	All	1593/2842 (56%)	614 (38%)	25 (1%)

5 of 614 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	4	G
1	3A	12	U
1	3A	15	U
1	3A	24	U
1	3A	25	U

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	SA	579	A
3	SA	685	A
3	SA	1754	A
3	SA	637	C
3	SA	773	C

## 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

Of 4 ligands modelled in this entry, 3 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
78	GTP	RJ	1201	79	26,34,34	1.18	2 (7%)	32,54,54	1.78	7 (21%)

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
78	GTP	RJ	1201	79	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	RJ	1201	GTP	C5-C6	-4.13	1.39	1.47
78	RJ	1201	GTP	C2-N3	2.02	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	RJ	1201	GTP	PA-O3A-PB	-5.07	115.43	132.83
78	RJ	1201	GTP	PB-O3B-PG	-3.88	119.52	132.83
78	RJ	1201	GTP	C5-C6-N1	3.52	120.16	113.95
78	RJ	1201	GTP	C8-N7-C5	3.16	109.02	102.99
78	RJ	1201	GTP	C2-N1-C6	-3.14	119.31	125.10

There are no chirality outliers.

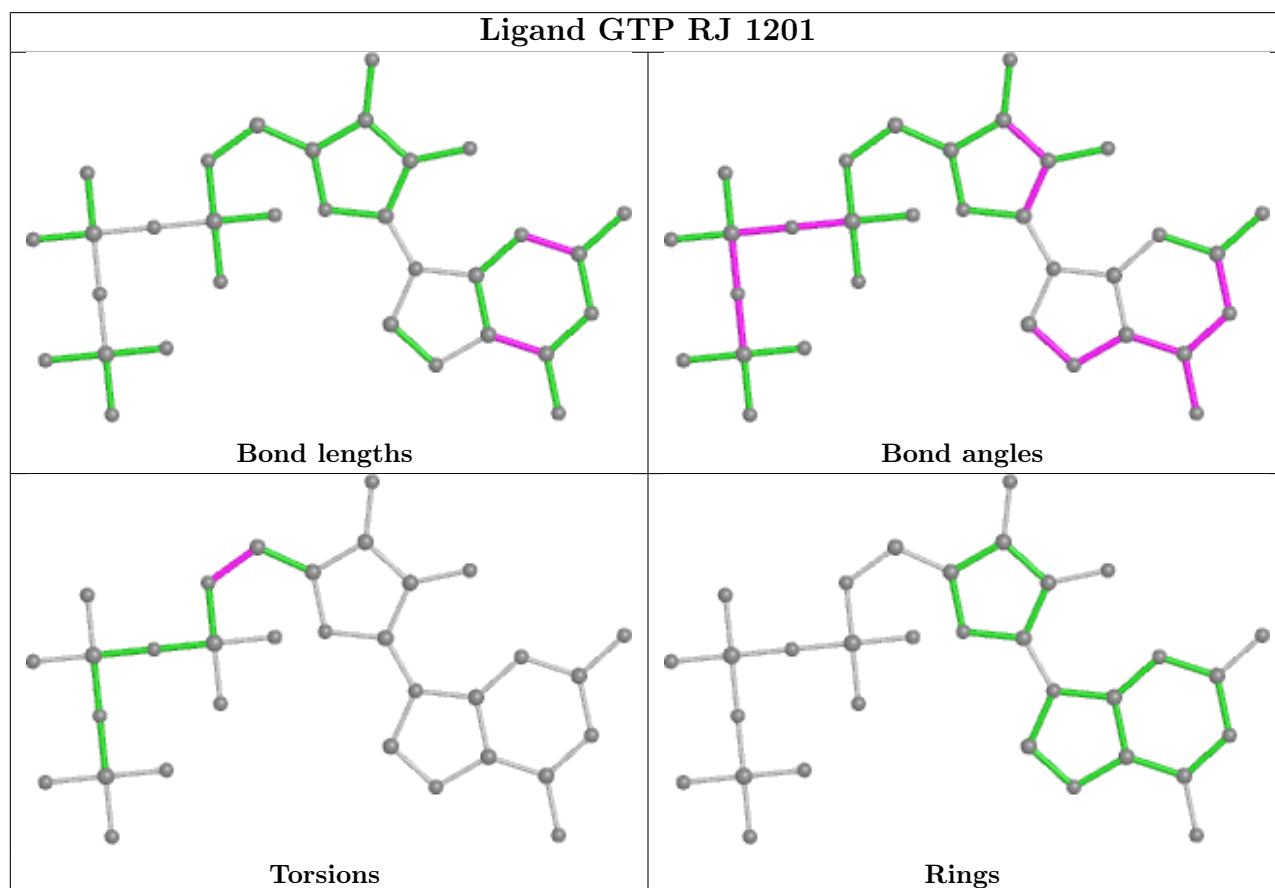
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
78	RJ	1201	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no chain breaks in this entry.

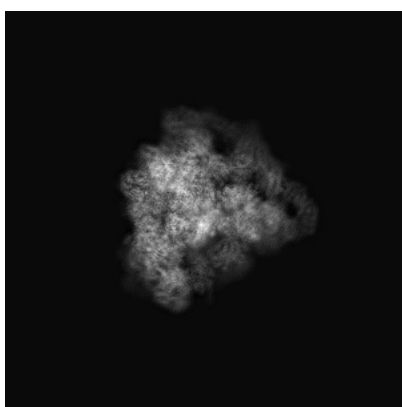
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0952. These allow visual inspection of the internal detail of the map and identification of artifacts.

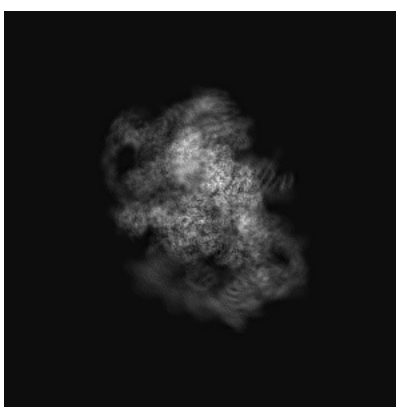
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

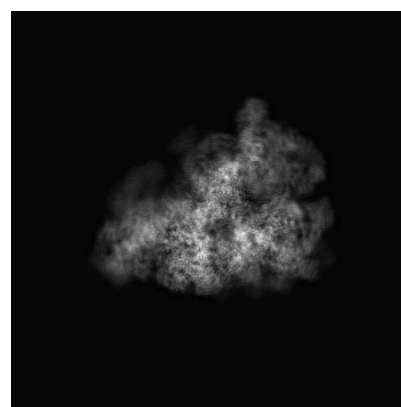
#### 6.1.1 Primary map



X



Y

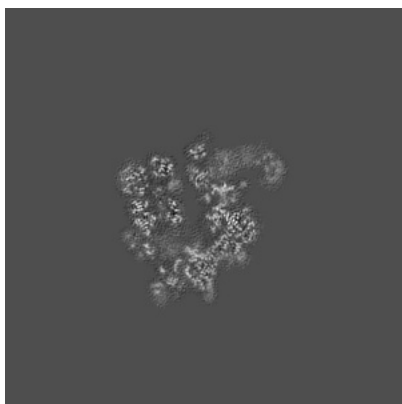


Z

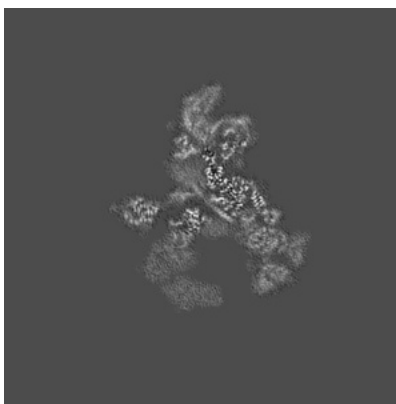
The images above show the map projected in three orthogonal directions.

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

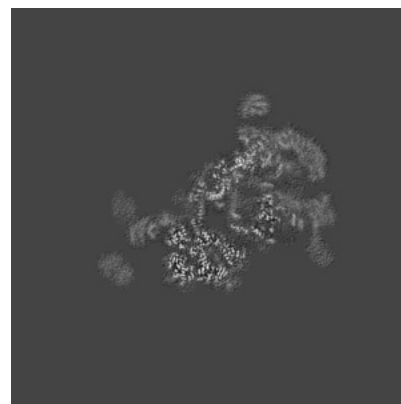
#### 6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

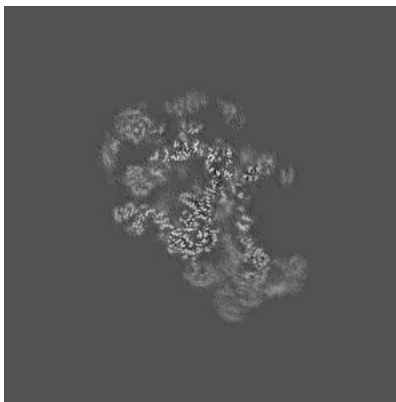
The images above show central slices of the map in three orthogonal directions.

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

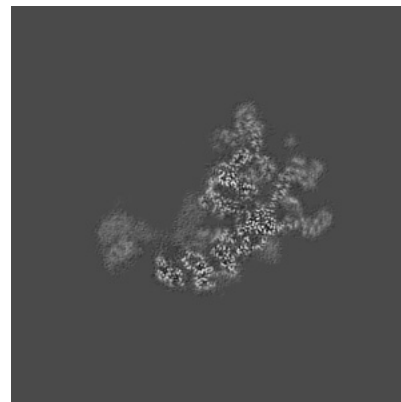
### 6.3.1 Primary map



X Index: 212



Y Index: 189

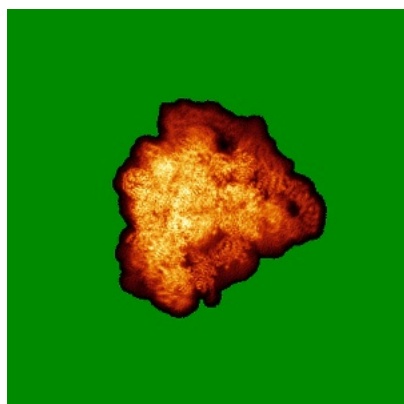


Z Index: 245

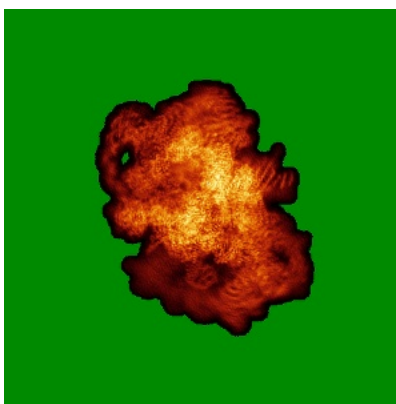
The images above show the largest variance slices of the map in three orthogonal directions.

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

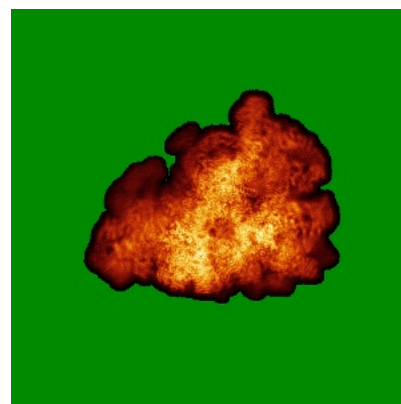
### 6.4.1 Primary map



X



Y

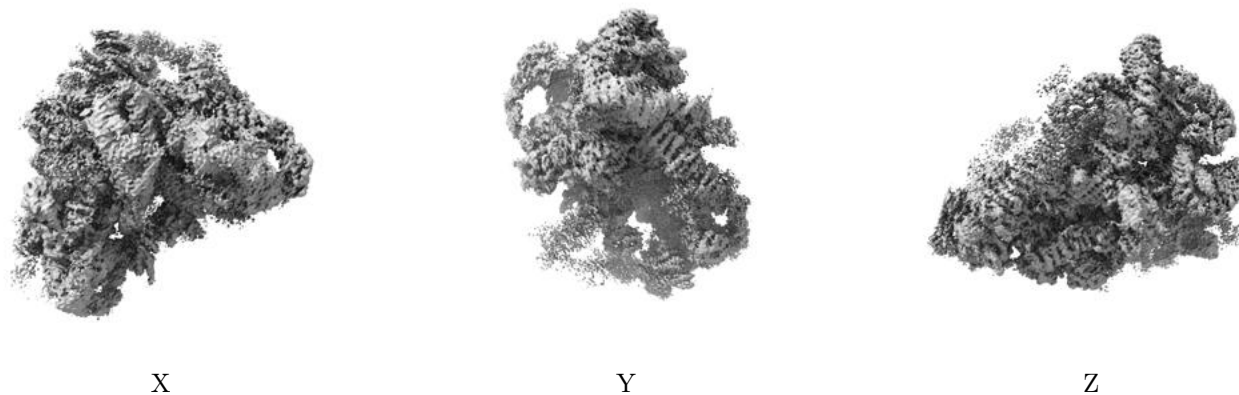


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

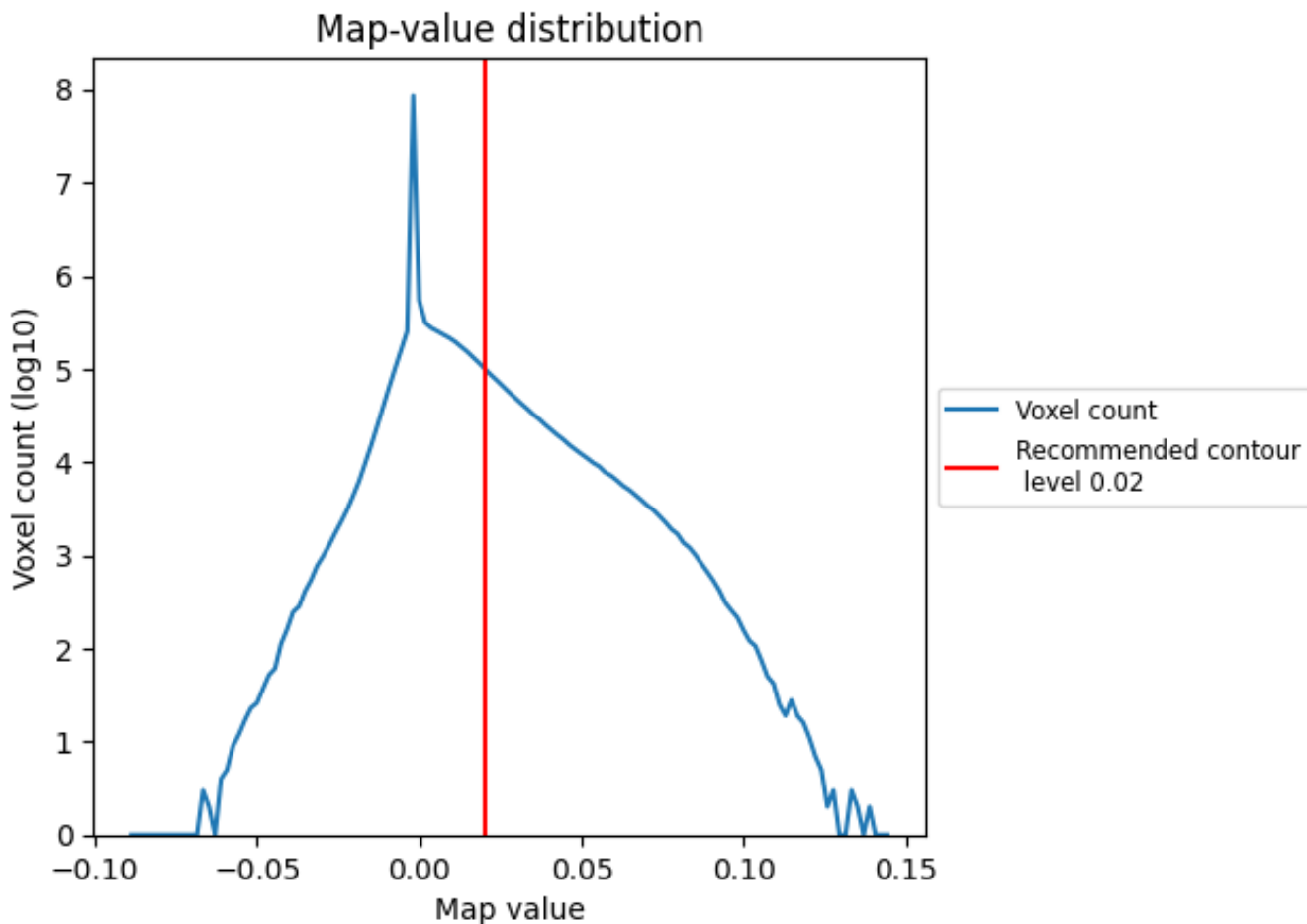
## 6.6 Mask visualisation [i](#)

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.

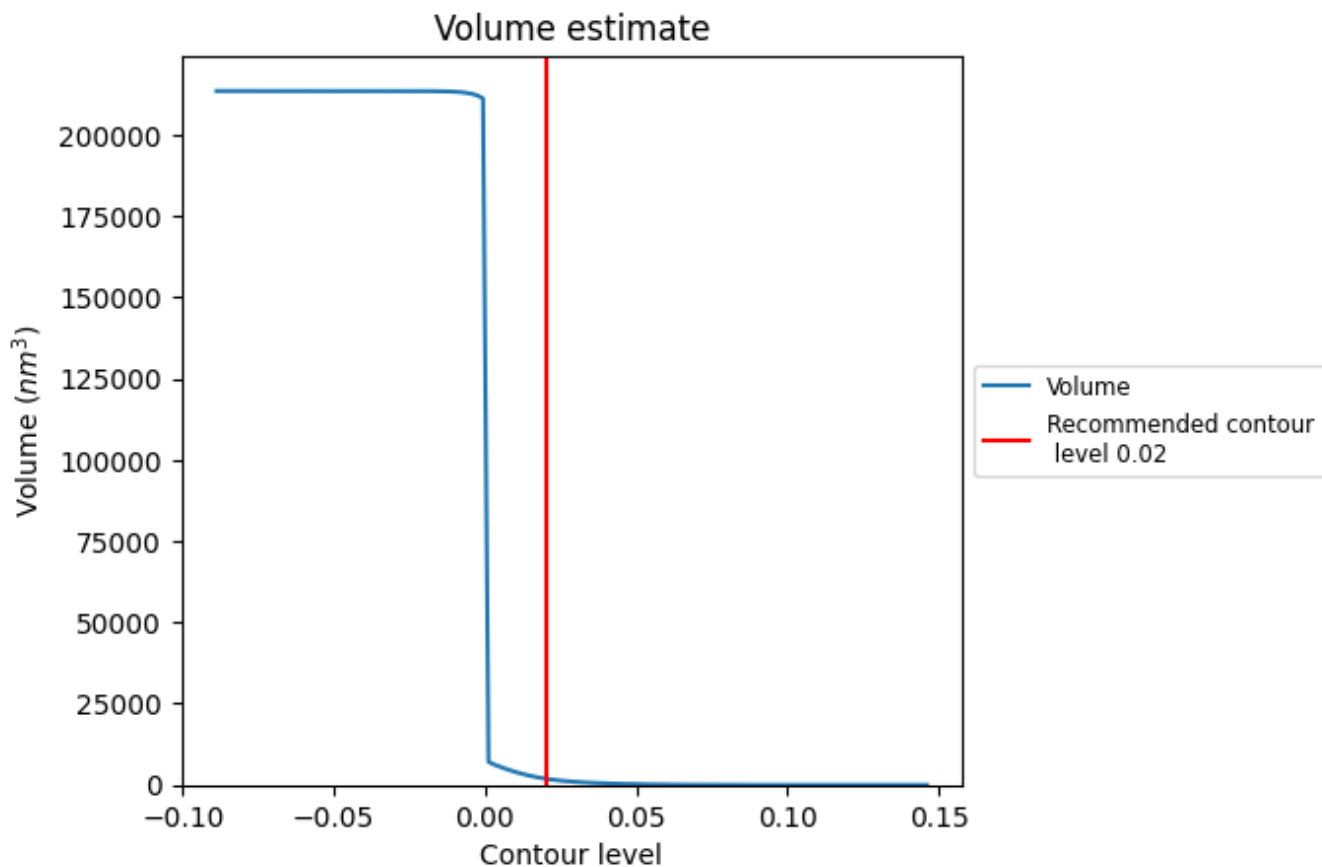
### 7.1 Map-value distribution [i](#)



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.



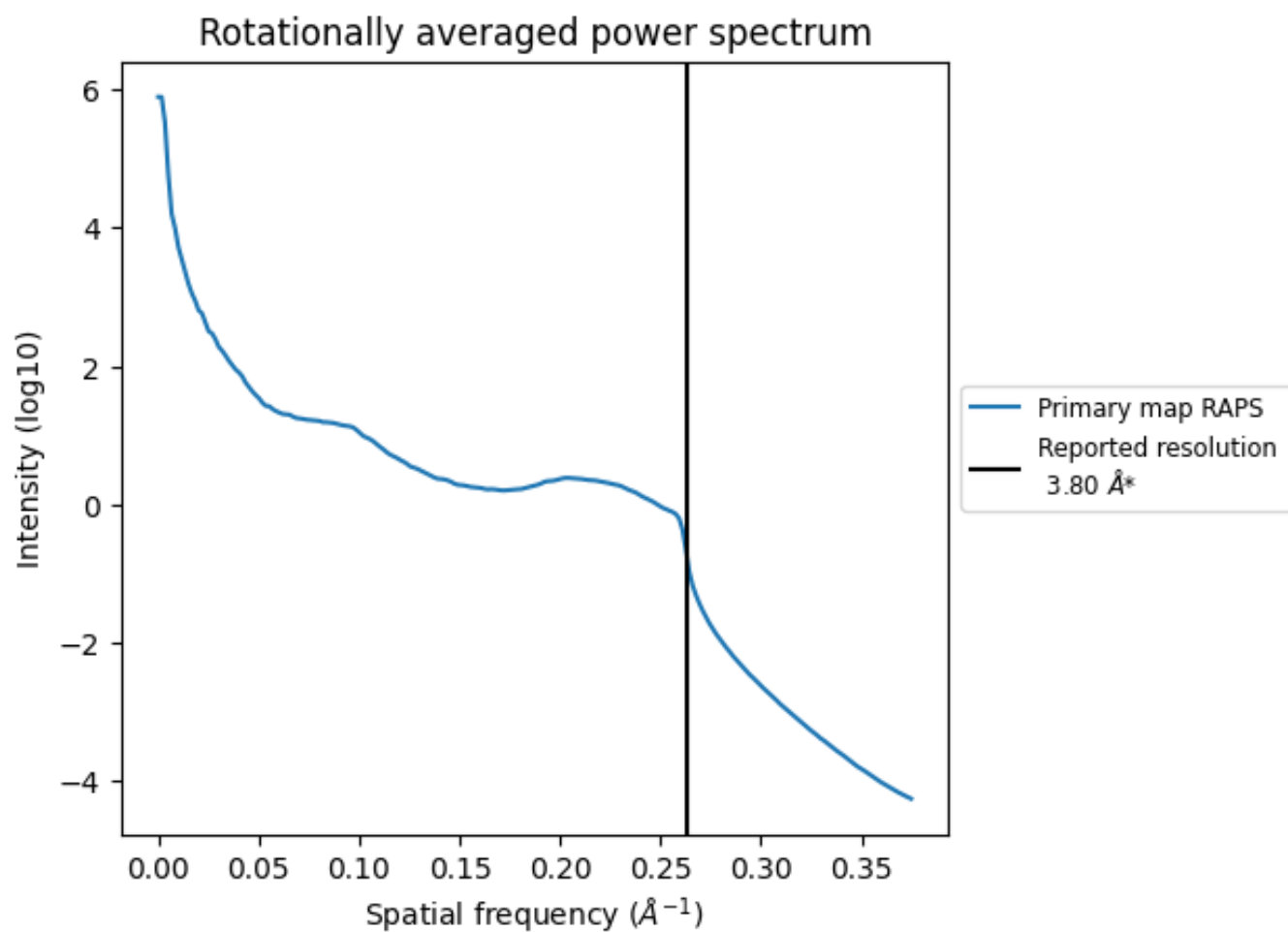
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1925 nm<sup>3</sup>; this corresponds to an approximate mass of 1739 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](#)

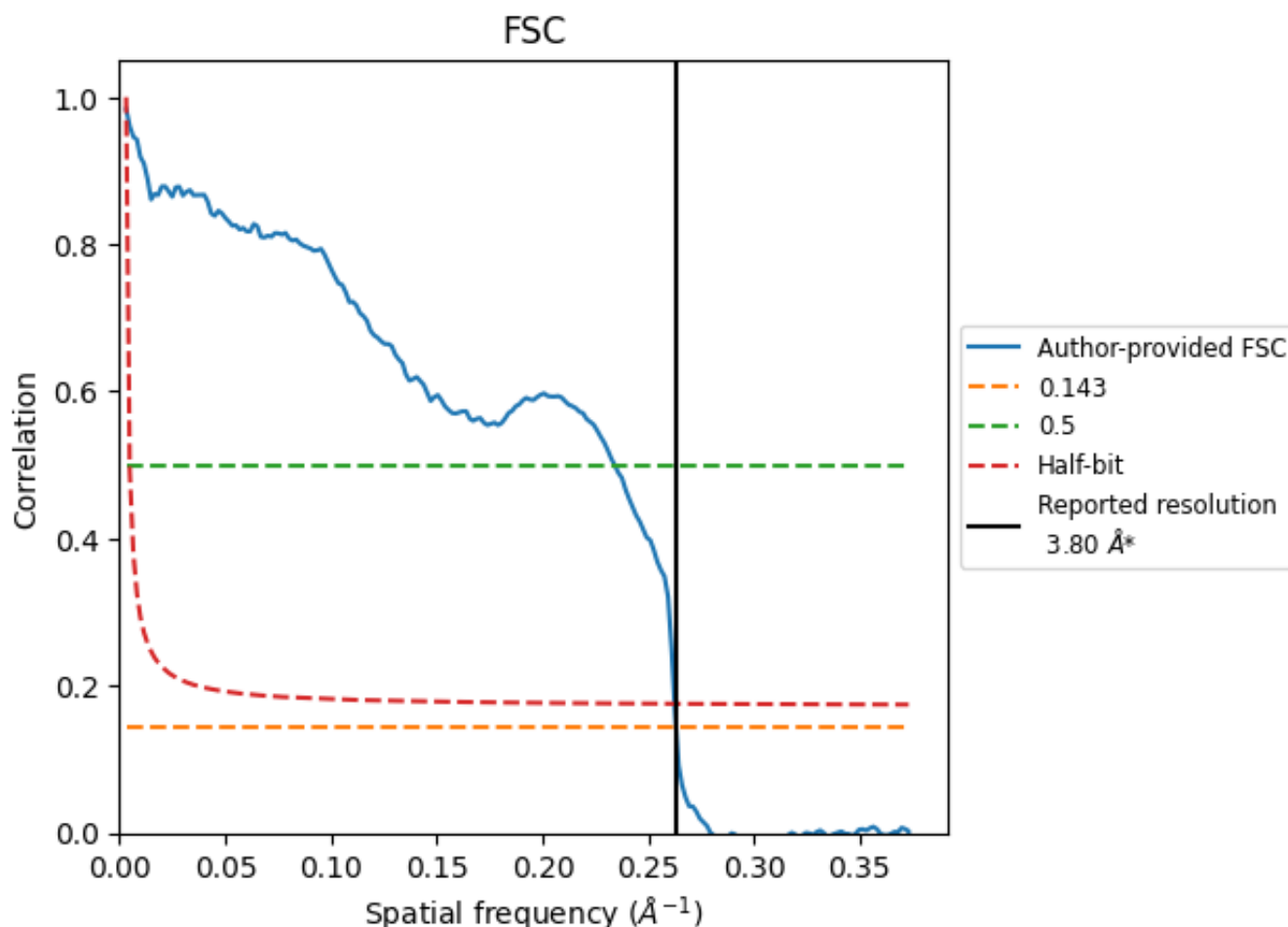


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

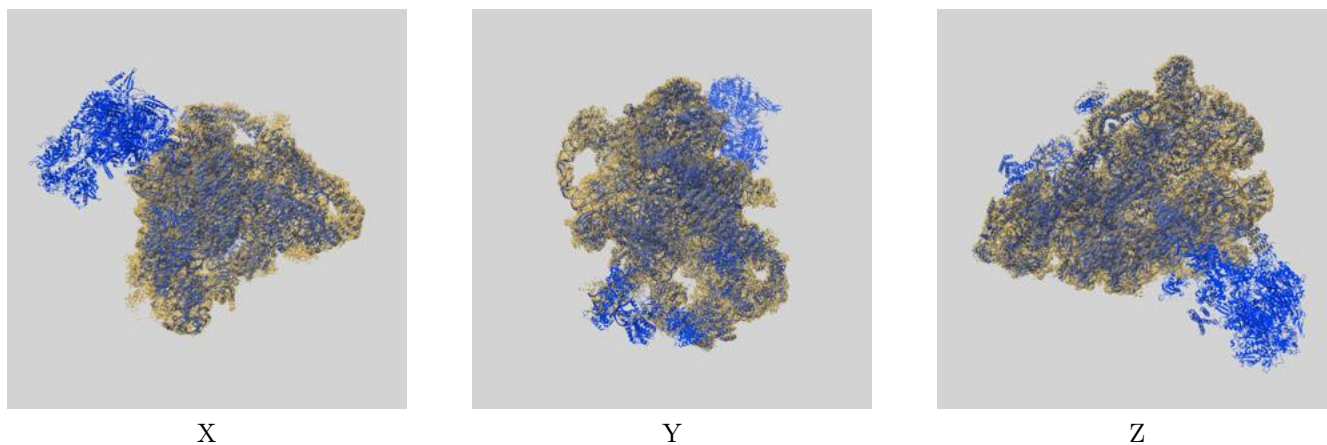
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.27	3.81
Unmasked-calculated*	-	-	-

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

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

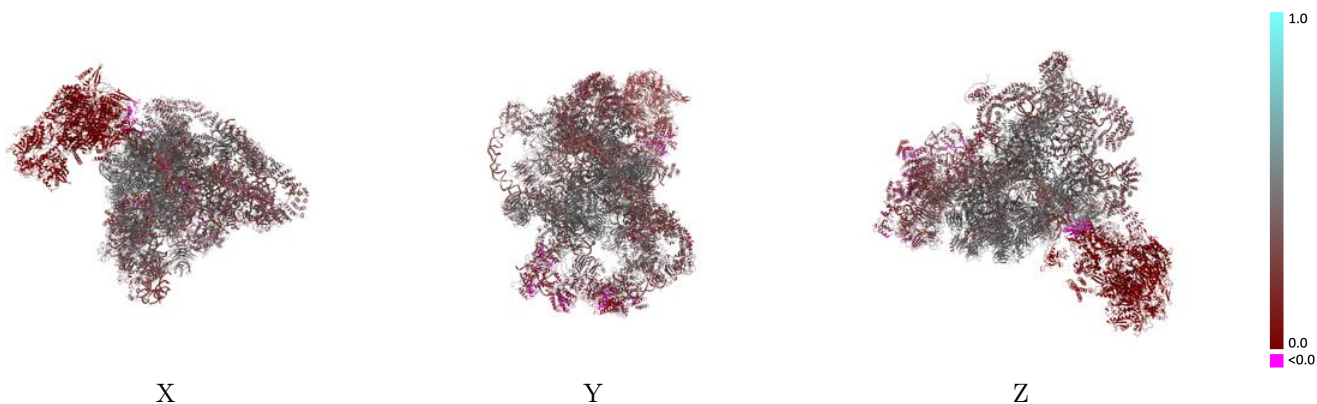
This section contains information regarding the fit between EMDB map EMD-0952 and PDB model 6LQS. Per-residue inclusion information can be found in section 3 on page 18.

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



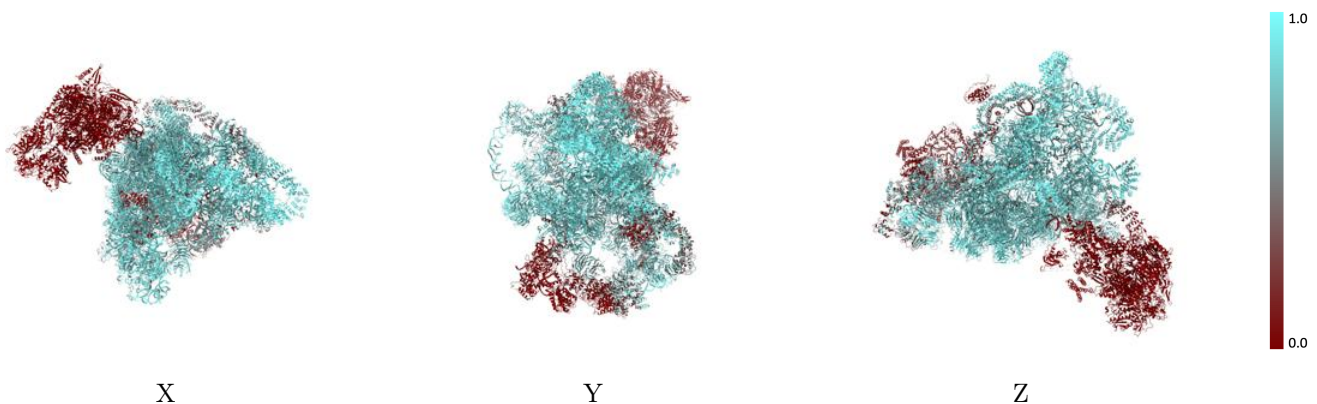
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



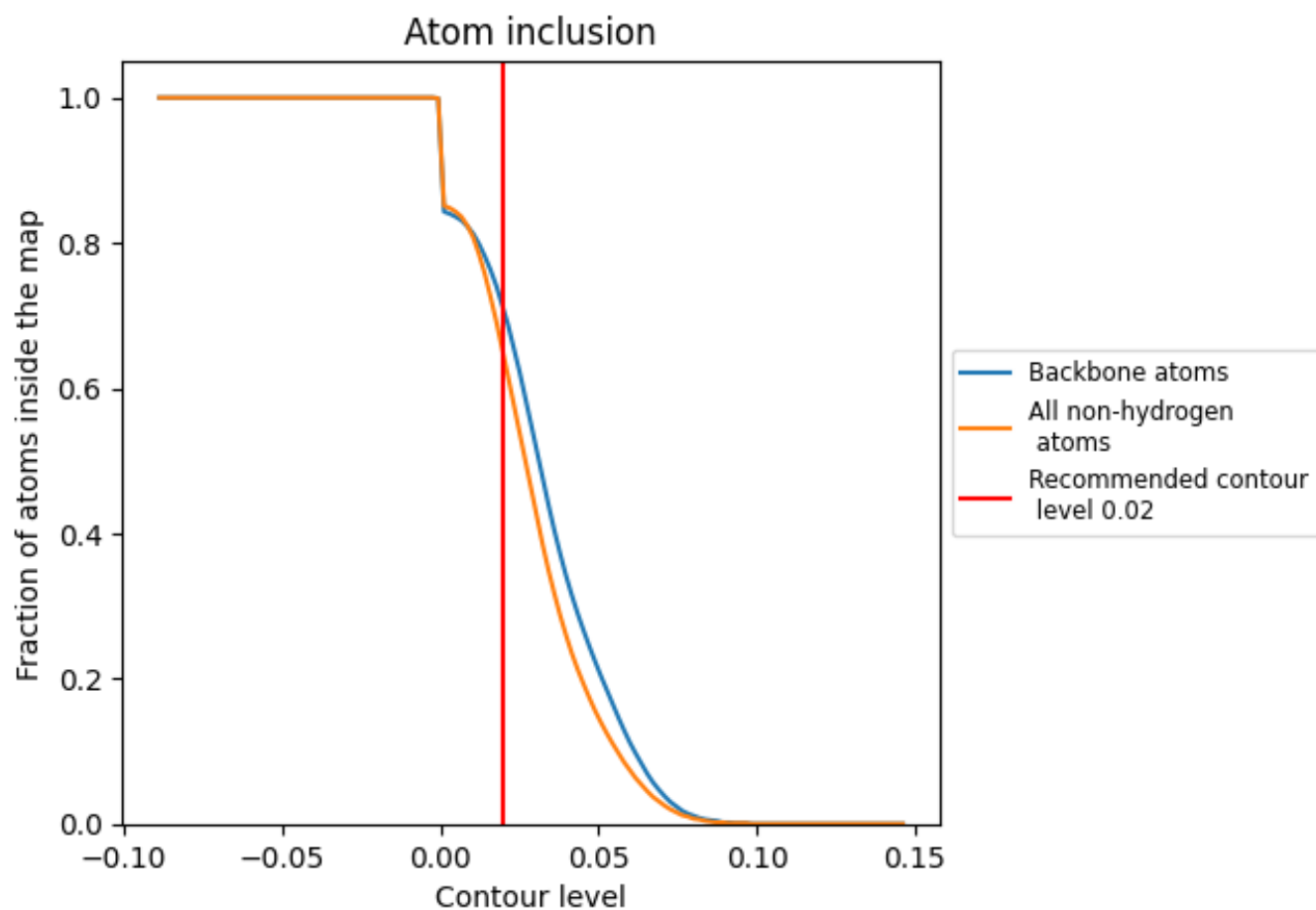
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)

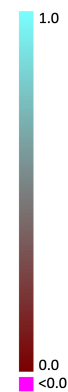


At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.3160
3A	 0.7970	 0.3500
3B	 0.8650	 0.4750
3C	 0.7380	 0.3690
3D	 0.8620	 0.4290
3E	 0.8280	 0.3910
3F	 0.8760	 0.4550
3G	 0.8010	 0.3890
3H	 0.8550	 0.4590
5A	 0.7230	 0.2890
5B	 0.4290	 0.3480
5C	 0.8620	 0.4790
5D	 0.5030	 0.3770
5E	 0.8250	 0.4170
5F	 0.8530	 0.4590
5G	 0.8430	 0.4690
5H	 0.8860	 0.4730
5I	 0.9090	 0.4910
5J	 0.7600	 0.4050
5K	 0.8640	 0.4790
A4	 0.7920	 0.3530
A5	 0.7020	 0.3800
A8	 0.3990	 0.2010
A9	 0.5750	 0.2150
AE	 0.6750	 0.3380
AF	 0.6480	 0.2880
AG	 0.7940	 0.3350
B1	 0.8910	 0.4750
B2	 0.8750	 0.4080
B3	 0.8640	 0.3710
B6	 0.8660	 0.4110
B8	 0.8570	 0.4480
BE	 0.9020	 0.4730
C4	 0.0000	 0.0000
M3	 0.0000	 0.0000



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Chain	Atom inclusion	Q-score
M4	0.0000	-0.0040
M6	0.0000	0.0000
R0	0.0000	0.0000
R1	0.0000	0.0000
R2	0.0000	0.0000
R3	0.0000	0.0000
R4	0.0000	0.0000
R5	0.0000	0.0000
R6	0.0000	0.0000
R7	0.0000	0.0000
RD	0.3260	0.2790
RE	0.8000	0.3500
RF	0.7710	0.3320
RG	0.1070	0.2420
RH	0.2340	0.2920
RJ	0.8410	0.4200
RK	0.8420	0.4100
RN	0.1150	0.1960
RO	0.0210	0.1810
RP	0.8800	0.3400
RQ	0.7950	0.4200
RS	0.0490	0.1750
RT	0.6990	0.3620
RW	0.2640	0.3010
SA	0.8380	0.3440
SC	0.8500	0.4530
SF	0.8280	0.3990
SG	0.8520	0.4490
SH	0.6680	0.3150
SI	0.7830	0.3650
SJ	0.6470	0.2950
SK	0.8750	0.4690
SM	0.5590	0.2910
SO	0.8750	0.4310
SP	0.8570	0.4260
SR	0.8830	0.4690
SX	0.8700	0.4550
SY	0.8140	0.4470
SZ	0.8770	0.4470
Sc	0.9040	0.4690
Sd	0.8850	0.4670
X1	0.8530	0.3890

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Chain	Atom inclusion	Q-score
X2	 0.0840	 0.2990
r4	 0.0000	 0.0000
r6	 0.0000	 0.0000