wwPDB EM Validation Summary Report

Jul 13, 2023 – 07:48 PM EDT

PDB ID	:	8FKS
EMDB ID	:	EMD-29255
Title	:	Human nucleolar pre-60S ribosomal subunit (State B2)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

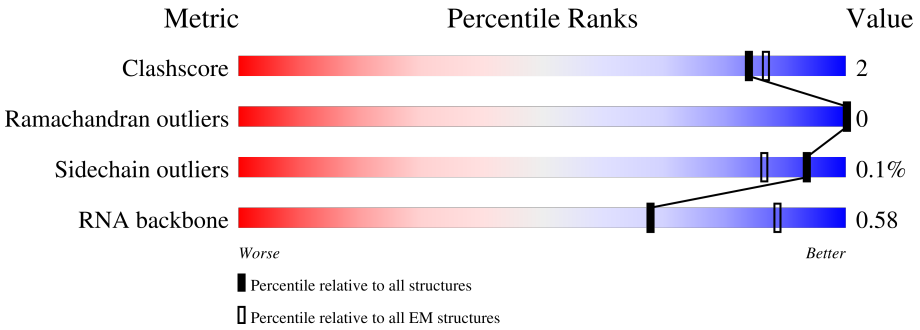
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.88 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 >=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 <=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	BA	165	28% 84% 10% 5%
2	L1	157	8% 81% 14%
3	L2	1167	94%
4	L3	5070	28% 7% 64%
5	L6	211	49% 5% 46%
6	L7	203	89% 9%
7	L8	215	59% 37%

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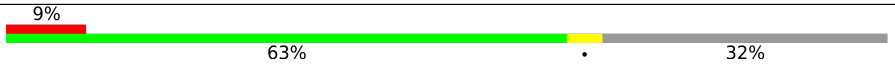
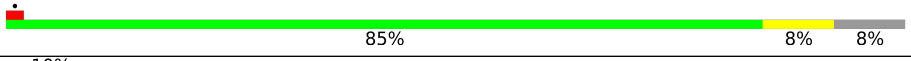
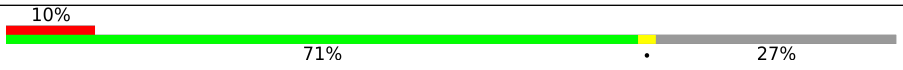
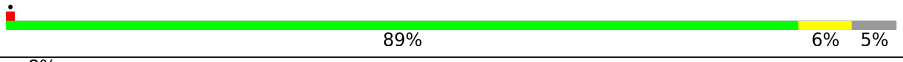
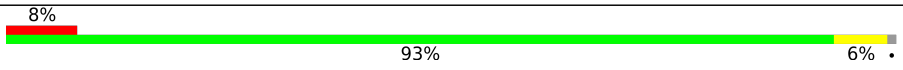
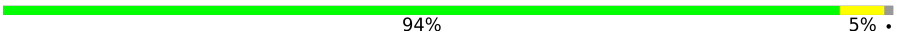
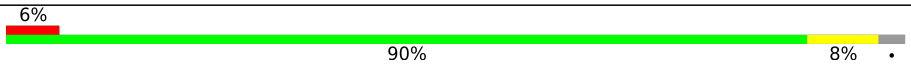
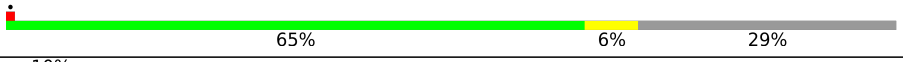
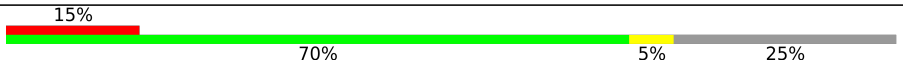
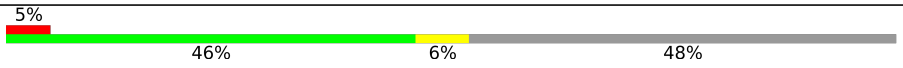
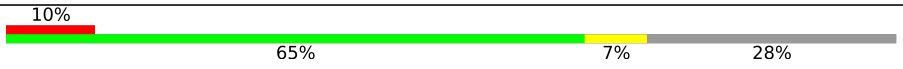
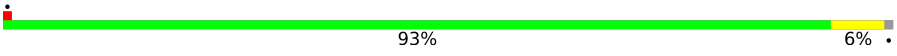
Mol	Chain	Length	Quality of chain
8	L9	204	
9	LA	184	
10	LB	188	
11	LC	176	
12	LE	160	
13	LG	140	
14	LH	156	
15	LI	145	
16	LK	148	
17	LL	137	
18	LN	403	
19	LQ	135	
20	LS	123	
21	LT	110	
22	LU	105	
23	LW	97	
24	NE	361	
25	NF	260	
26	NG	282	
27	NN	473	
28	SA	427	
29	SC	288	
30	SD	248	
31	SE	266	
32	SG	192	

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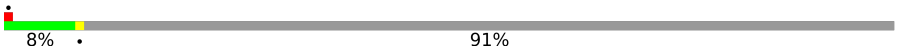
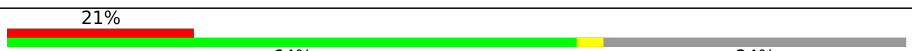
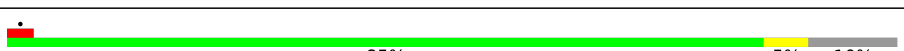
Mol	Chain	Length	Quality of chain
33	SH	293	
34	SI	255	
35	SJ	847	
36	SK	245	
37	SL	490	
38	SM	588	
39	SN	306	
40	SO	353	
41	SQ	239	
42	SR	634	
43	SS	746	
44	ST	365	
45	SV	163	
46	SW	670	
47	SZ	178	

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 108693 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 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	156	1176	731	221	220	4	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	152	3234	1443	571	1068	152	0	0

- Molecule 3 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L2	69	1468	653	263	483	69	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L3	1824	39106	17411	7173	12698	1824	0	0

- Molecule 5 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L6	114	936	583	206	146	1	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L7	184	1507	976	290	237	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L9	183	Total	C	N	O	S	0	0
			1546	974	325	243	4		

- Molecule 9 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	121	Total	C	N	O	S	0	0
			981	616	182	176	7		

- Molecule 10 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 11 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 12 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	LE	108	Total	C	N	O	0	0
			702	430	138	134		

- Molecule 13 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LG	114	Total	C	N	O	S	0	0
			844	532	155	152	5		

- Molecule 14 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	LH	36	Total	C	N	O	0	0
			284	182	60	42		

- Molecule 15 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 16 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LK	108	Total	C	N	O	S	0	0
			642	388	137	115	2		

- Molecule 17 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LL	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 18 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LN	377	Total	C	N	O	S	0	0
			3044	1937	566	527	14		

- Molecule 19 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 20 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 21 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 22 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LU	102	Total	C	N	O	S	1	0
			840	526	180	129	5		

- Molecule 23 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LW	69	Total	C	N	O	S	0	0
			563	346	126	86	5		

- Molecule 24 is a protein called Surfeit locus protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NE	156	Total	C	N	O	S	0	0
			1331	810	293	226	2		

- Molecule 25 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NF	195	Total	C	N	O	S	0	0
			1588	1010	302	267	9		

- Molecule 26 is a protein called RRP15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NG	89	Total	C	N	O	S	0	0
			738	456	145	133	4		

- Molecule 27 is a protein called Suppressor of SWI4 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NN	244	Total	C	N	O	S	0	0
			1950	1230	371	338	11		

- Molecule 28 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SA	329	Total	C	N	O	S	0	0
			2645	1675	522	435	13		

- Molecule 29 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SC	207	Total	C	N	O	S	0	0
			1663	1073	314	273	3		

- Molecule 30 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SD	212	Total	C	N	O	S	0	0
			1755	1127	334	285	9		

- Molecule 31 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SE	186	Total	C	N	O	S	0	0
			1498	951	290	253	4		

- Molecule 32 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SG	190	Total	C	N	O	S	1	0
			1526	961	287	272	6		

- Molecule 33 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SH	150	Total	C	N	O	S	0	0
			1267	819	224	220	4		

- Molecule 34 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SI	207	Total	C	N	O	S	1	0
			1732	1121	326	281	4		

- Molecule 35 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	SJ	72	Total	C	N	O	0	0
			609	385	114	110		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 37 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 38 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SM	437	Total	C	N	O	S	0	0
			3452	2229	603	609	11		

- Molecule 39 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SN	173	Total	C	N	O	S	0	0
			1350	849	251	243	7		

- Molecule 40 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SO	296	Total	C	N	O	S	0	0
			2460	1583	446	416	15		

- Molecule 41 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 42 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SR	428	Total	C	N	O	S	0	0
			3524	2248	617	644	15		

- Molecule 43 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	SS	235	Total	C	N	O	P	S	0	0
			1955	1238	348	360	2	7		

- Molecule 44 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	ST	43	Total	C	N	O	S	0	0
			323	199	63	60	1		

- Molecule 45 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SV	137	Total	C	N	O	S	0	0
			1171	745	227	189	10		

- Molecule 46 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SW	445	Total	C	N	O	S	0	0
			3560	2288	609	646	17		

- Molecule 47 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	L1	4	Total	Mg	0
			4	4	
48	L2	1	Total	Mg	0
			1	1	
48	L3	51	Total	Mg	0
			51	51	

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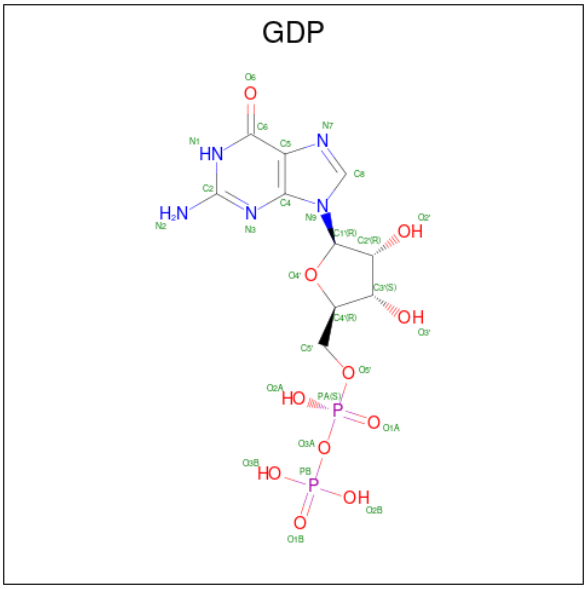
Mol	Chain	Residues	Atoms	AltConf
48	L9	1	Total Mg 1 1	0
48	LN	1	Total Mg 1 1	0
48	LQ	1	Total Mg 1 1	0
48	LT	1	Total Mg 1 1	0
48	SA	1	Total Mg 1 1	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
49	LW	1	Total Zn 1 1	0
49	SV	1	Total Zn 1 1	0

- Molecule 50 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	AltConf
50	SR	1	Total C N O P 28 10 5 11 2	0

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

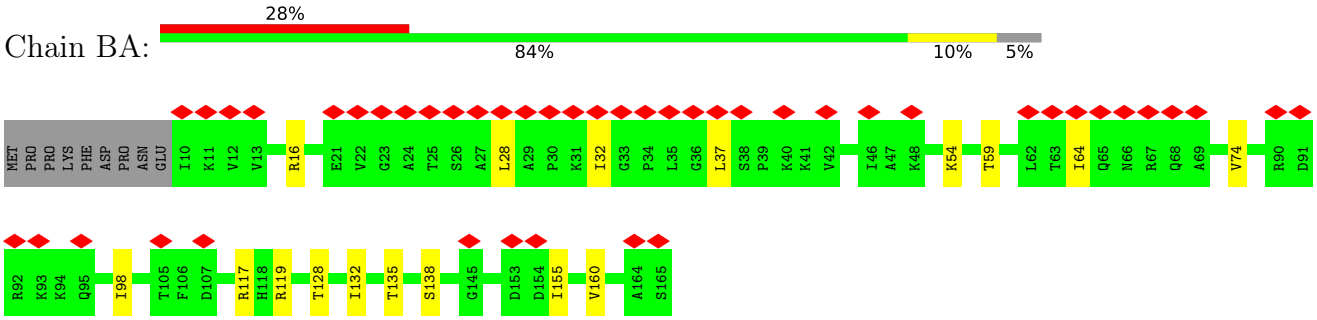
Mol	Chain	Residues	Atoms	AltConf
51	SR	1	Total K 1 1	0

3 Residue-property plots (i)

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

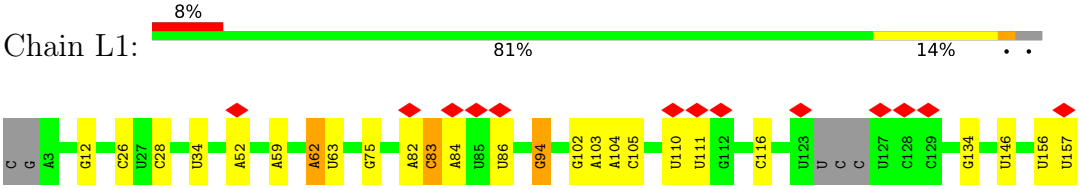
• Molecule 1: 60S ribosomal protein L12

Chain BA:



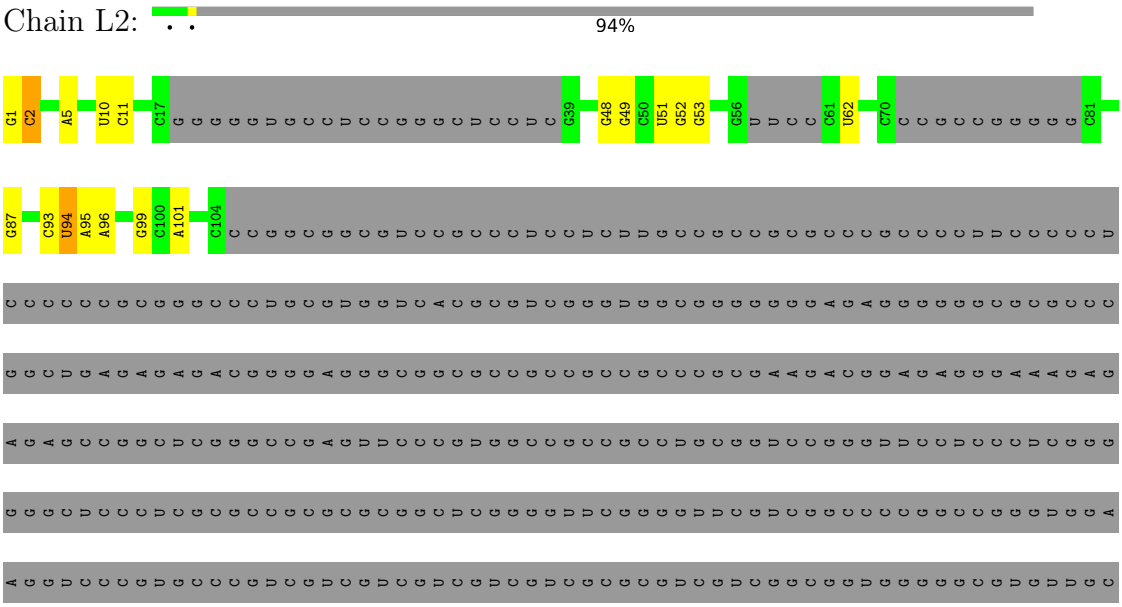
• Molecule 2: 5.8S rRNA

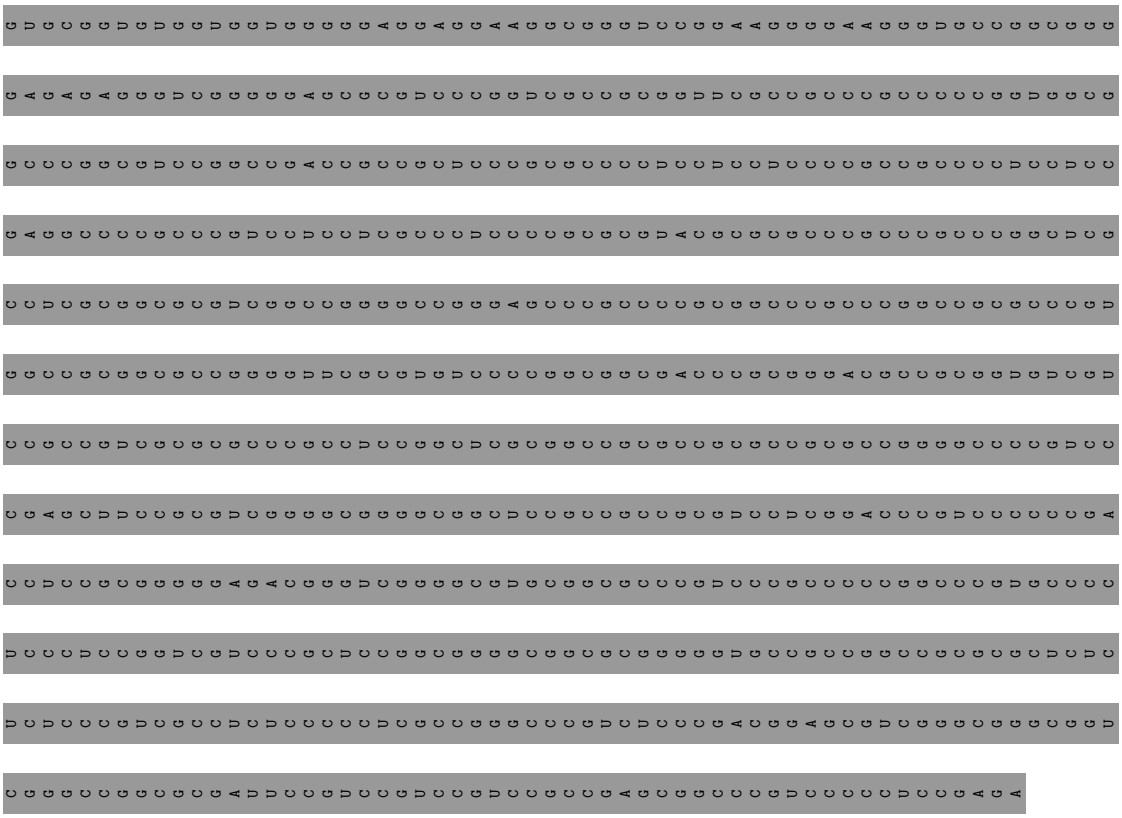
Chain L1:



• Molecule 3: ITS2 rRNA

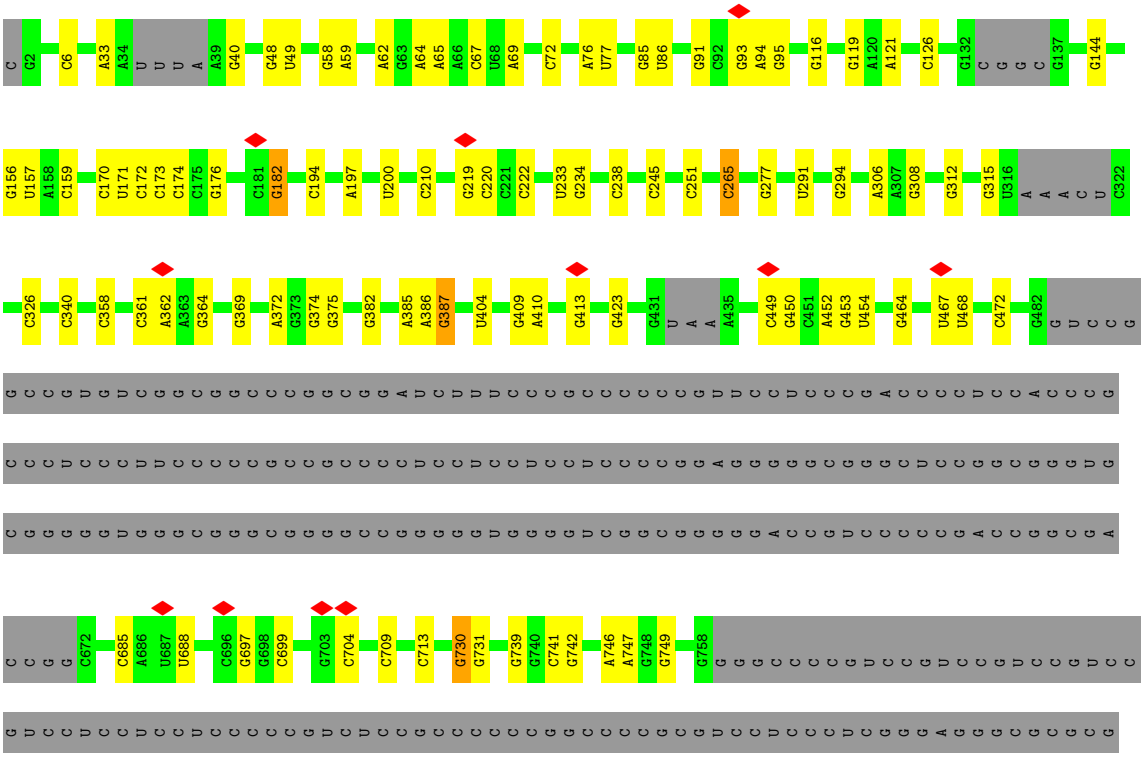
Chain L2:

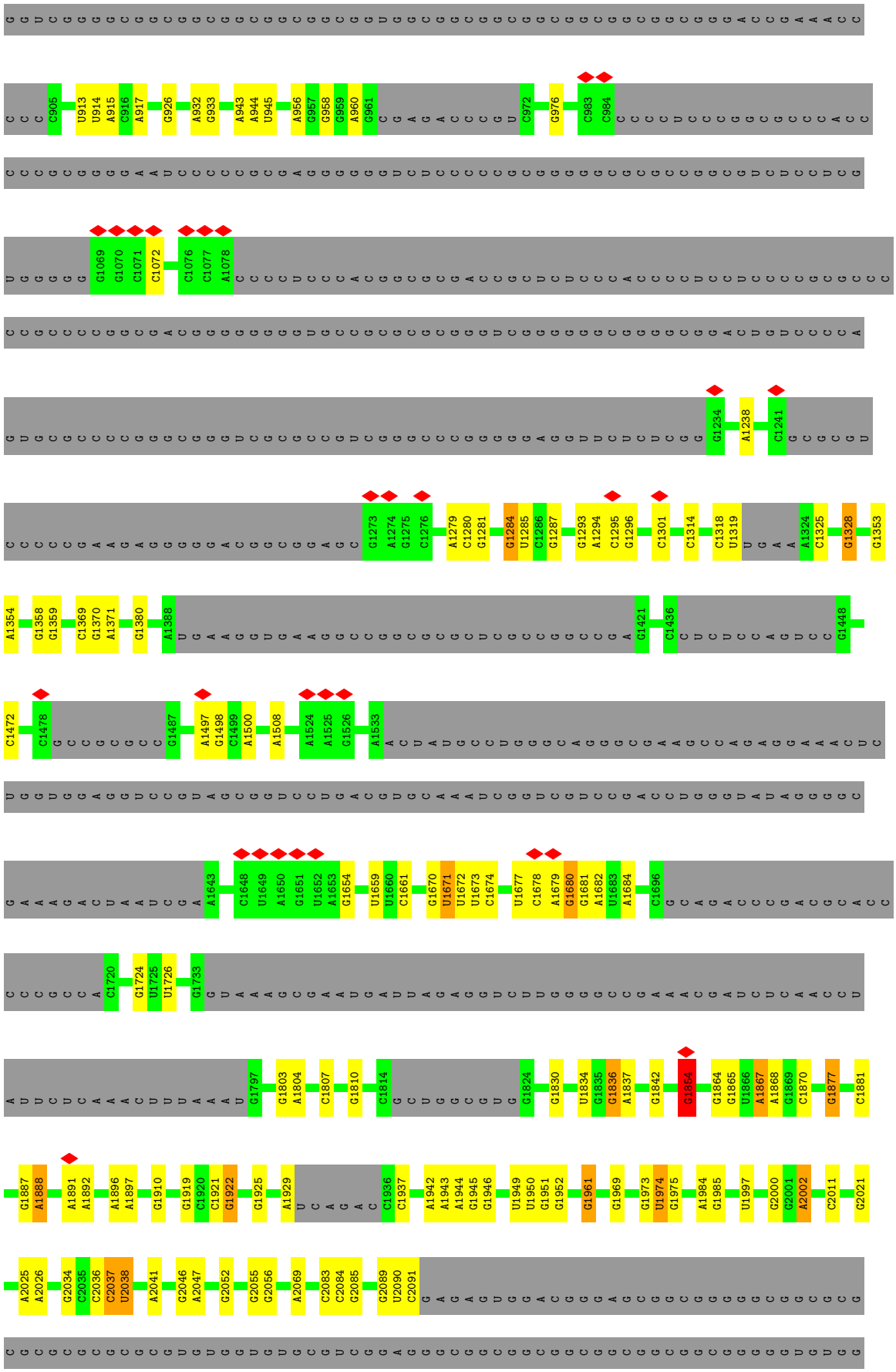


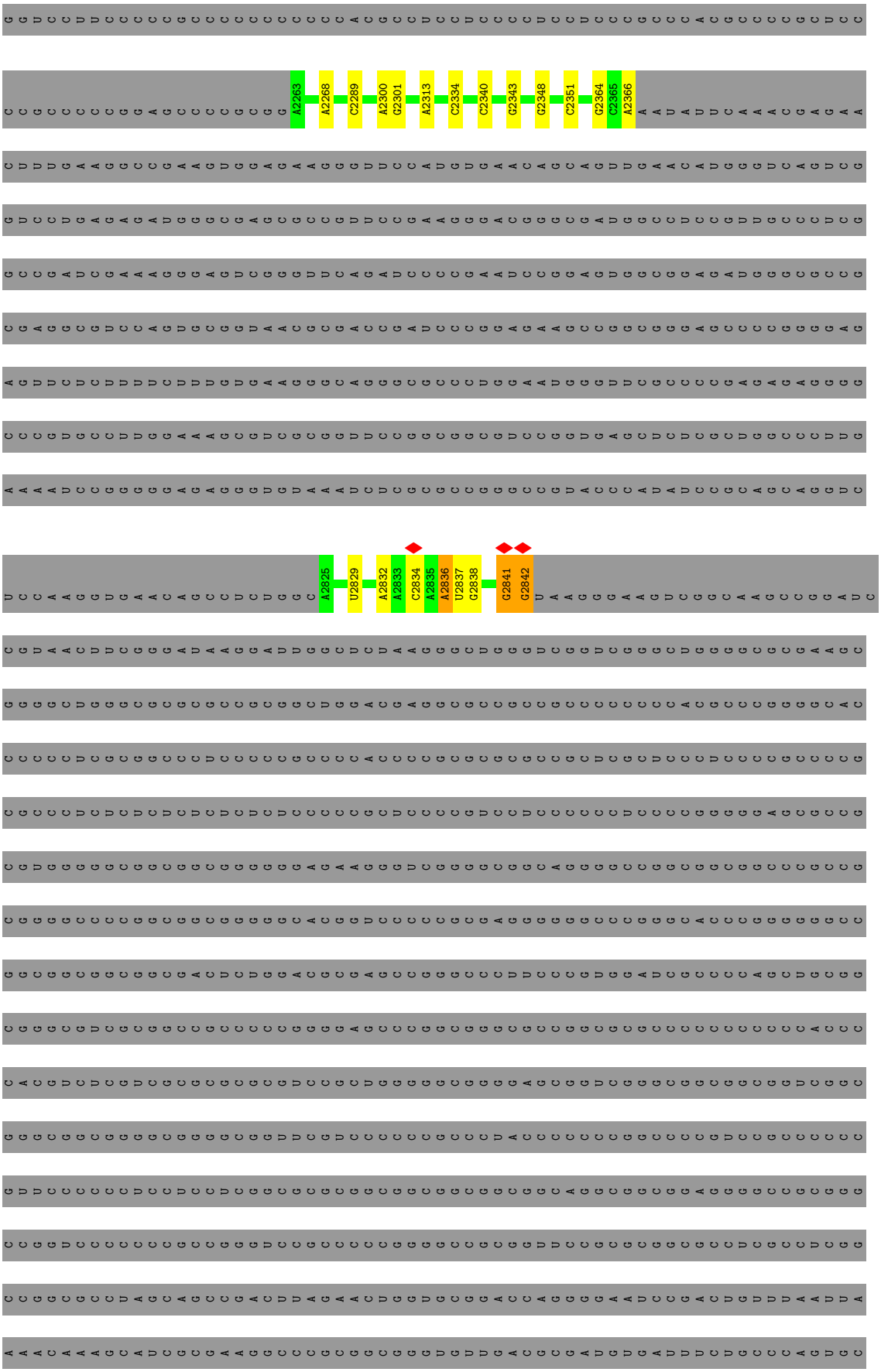


• Molecule 4: 28S rRNA

Chain L3:






A2263
A2268
C2289
A2300
G2301
A2313
C2334
C2340
G2343
G2348
C2351
G2364
C2365
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U2837
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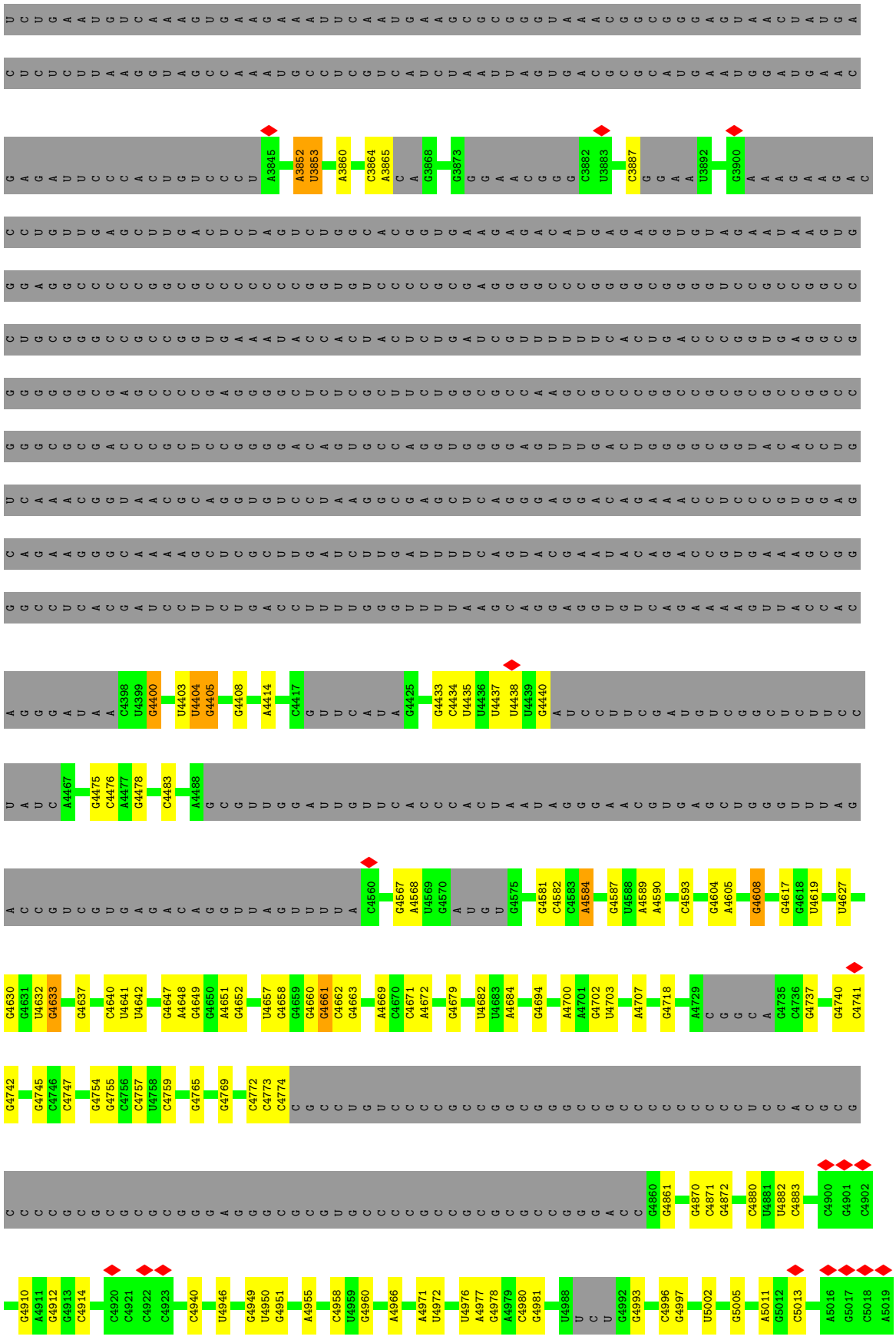
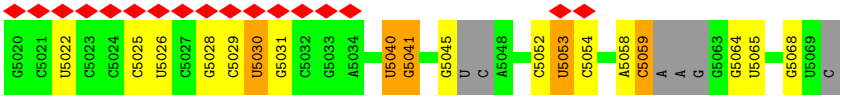
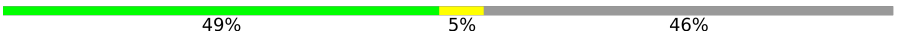
G2842

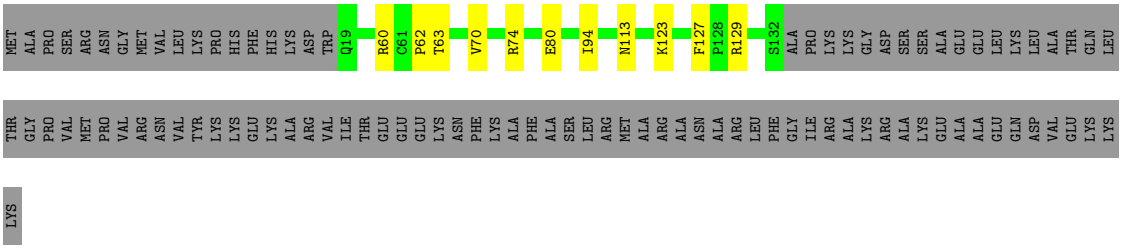




• Molecule 5: 60S ribosomal protein L13

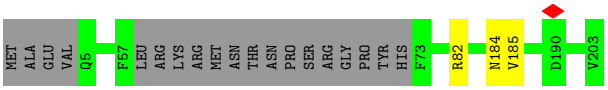
Chain L6:





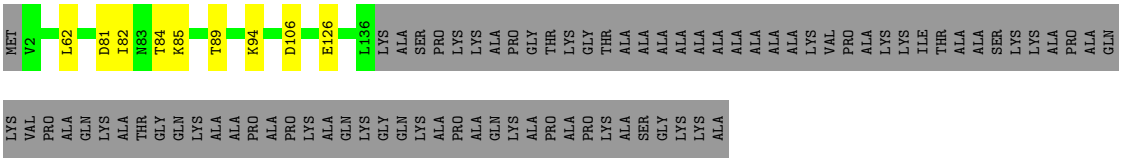
• Molecule 6: 60S ribosomal protein L13a

Chain L7:



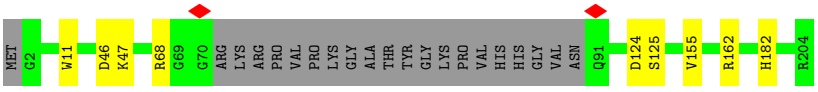
• Molecule 7: 60S ribosomal protein L14

Chain L8:



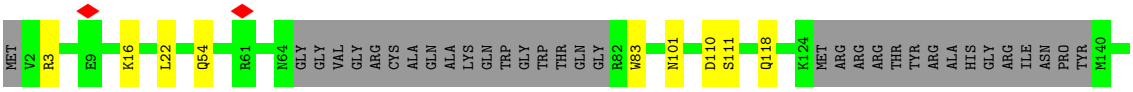
• Molecule 8: 60S ribosomal protein L15

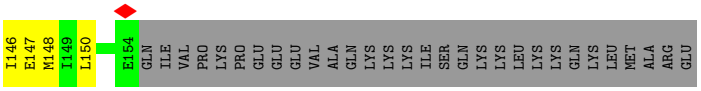
Chain L9:



• Molecule 9: 60S ribosomal protein L17

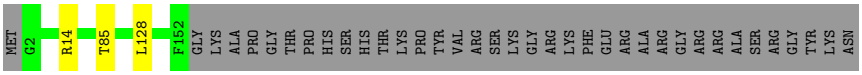
Chain LA:





• Molecule 10: 60S ribosomal protein L18

Chain LB:

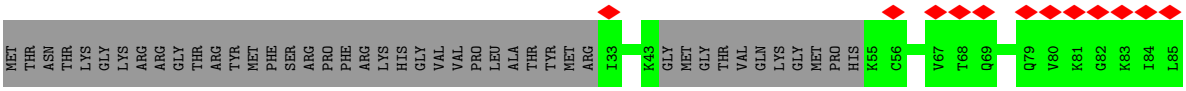


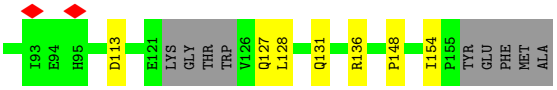
• Molecule 11: 60S ribosomal protein L18a

Chain LC:

• Molecule 12: 60S ribosomal protein L21

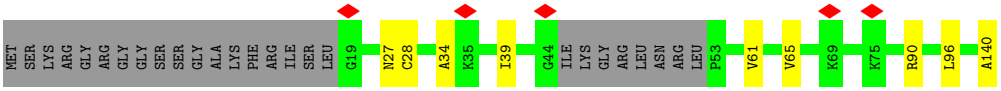
Chain LE:





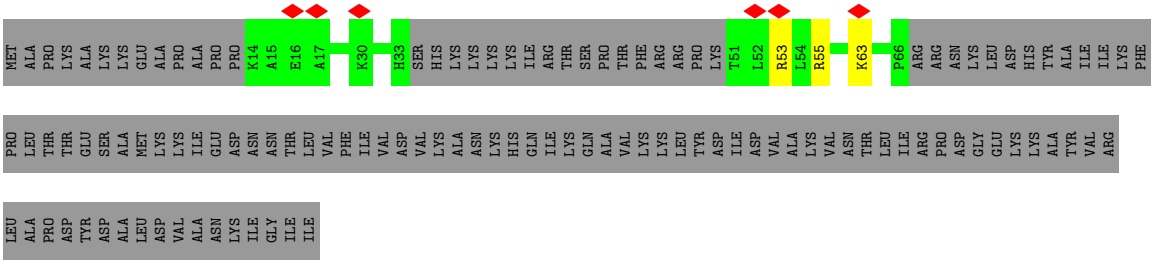
• Molecule 13: 60S ribosomal protein L23

Chain LG:



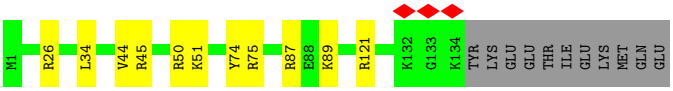
• Molecule 14: 60S ribosomal protein L23a

Chain LH:



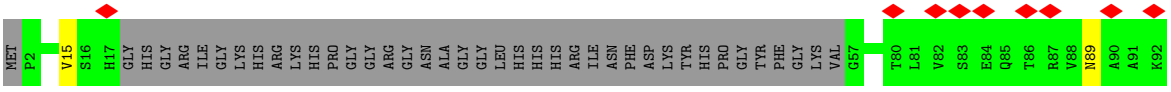
• Molecule 15: 60S ribosomal protein L26

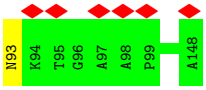
Chain LI:



• Molecule 16: 60S ribosomal protein L27a

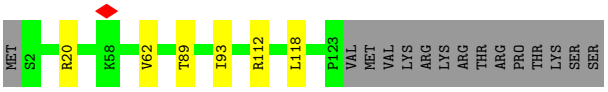
Chain LK:





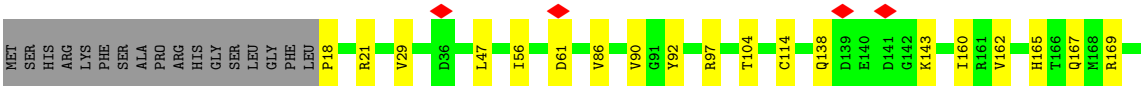
• Molecule 17: 60S ribosomal protein L28

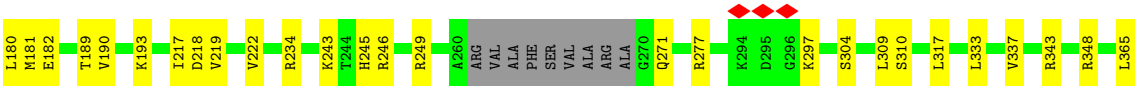
Chain LL:

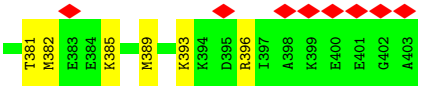


• Molecule 18: 60S ribosomal protein L3

Chain LN:

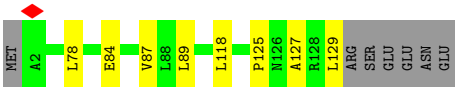






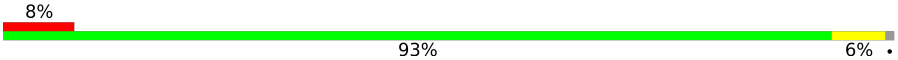
• Molecule 19: 60S ribosomal protein L32

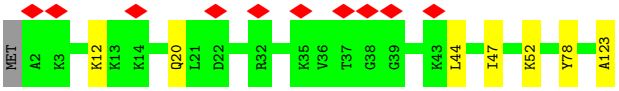
Chain LQ:



• Molecule 20: 60S ribosomal protein L35

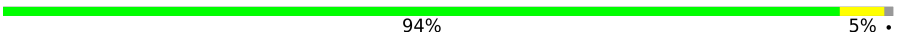
Chain LS:





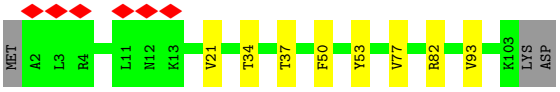
• Molecule 21: 60S ribosomal protein L35a

Chain LT:



• Molecule 22: 60S ribosomal protein L36

Chain LU:

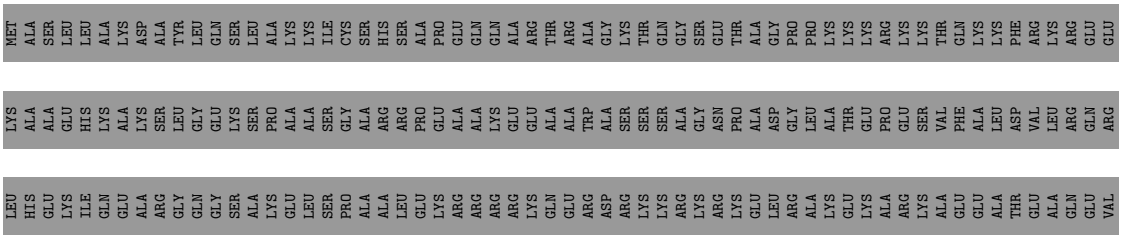


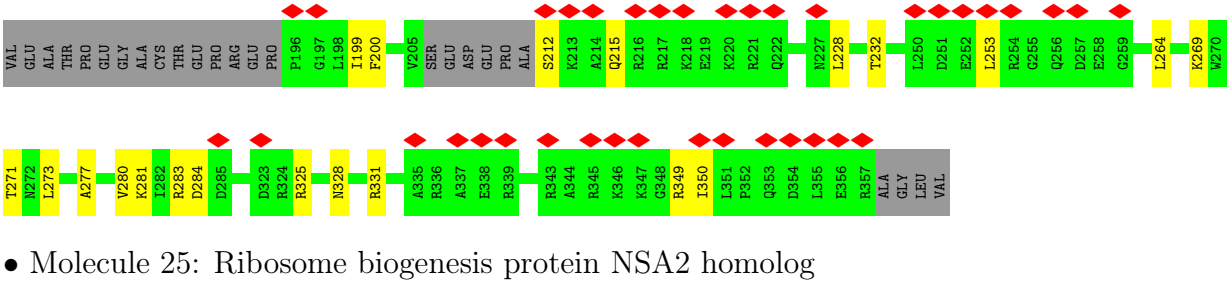
• Molecule 23: 60S ribosomal protein L37

Chain LW:

• Molecule 24: Surfeit locus protein 6

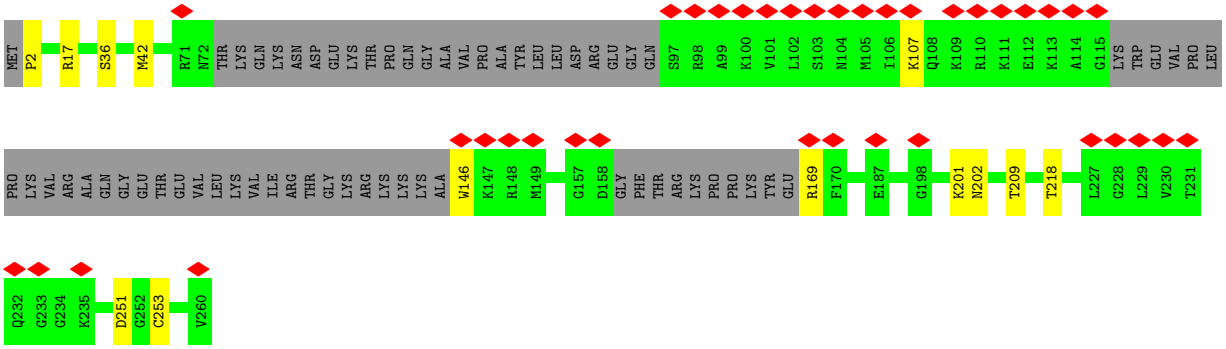
Chain NE:



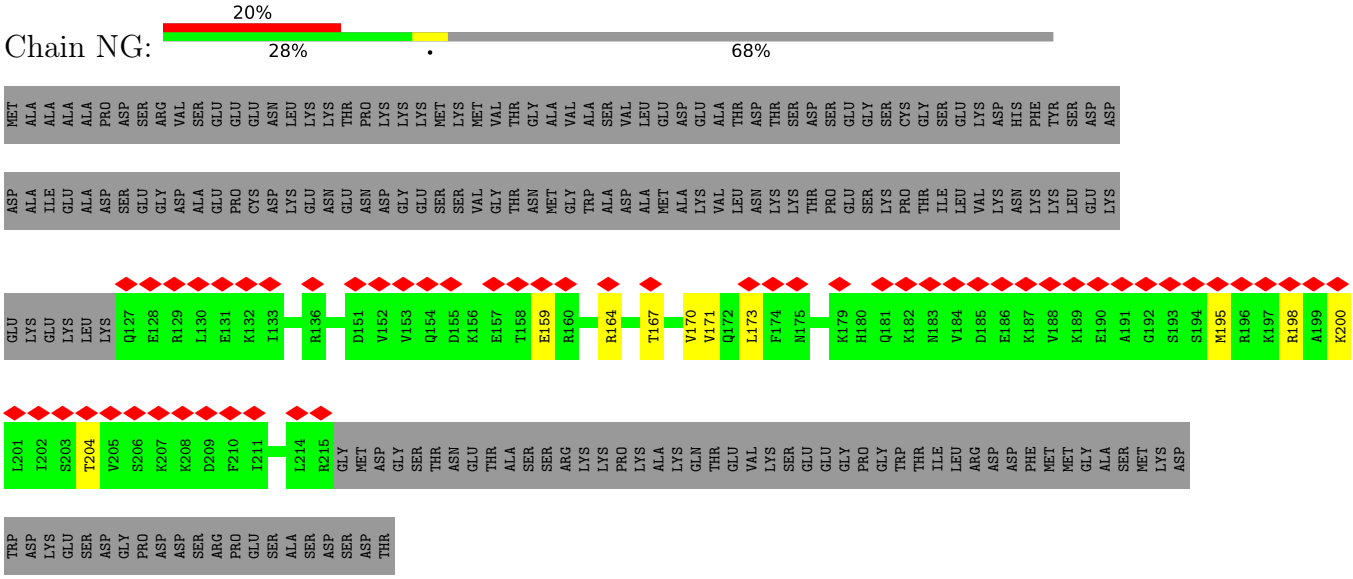


• Molecule 25: Ribosome biogenesis protein NSA2 homolog

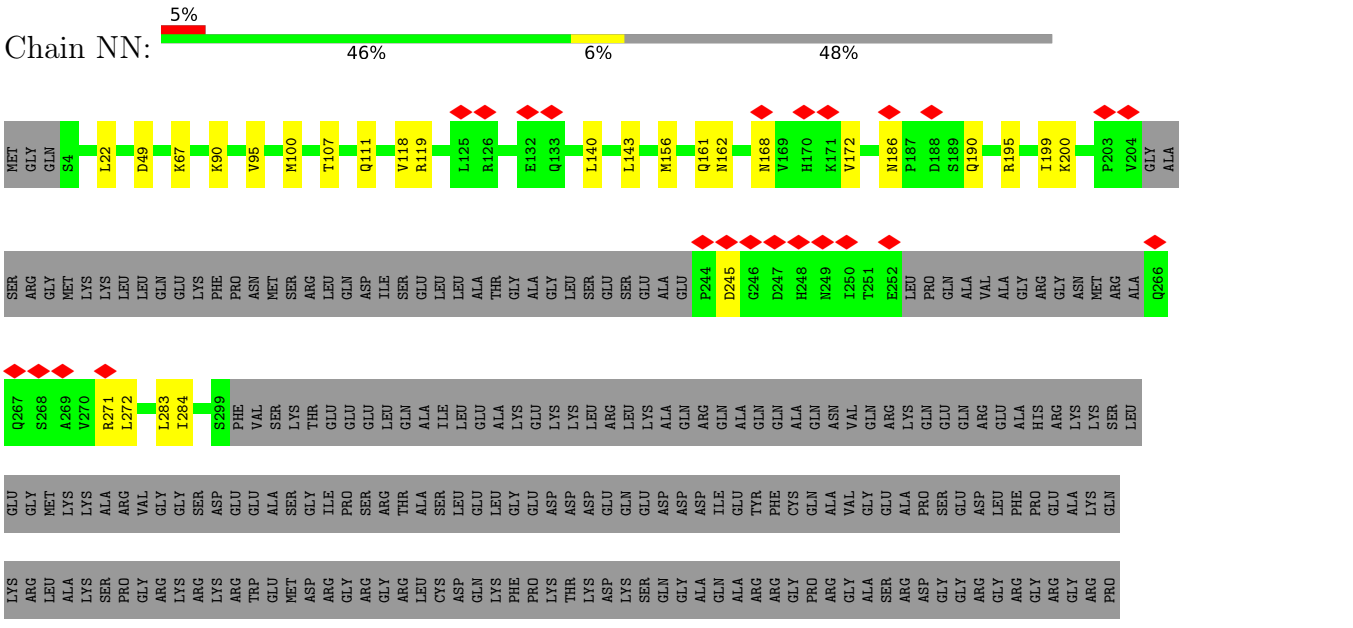
Chain NF:



• Molecule 26: RRP15-like protein

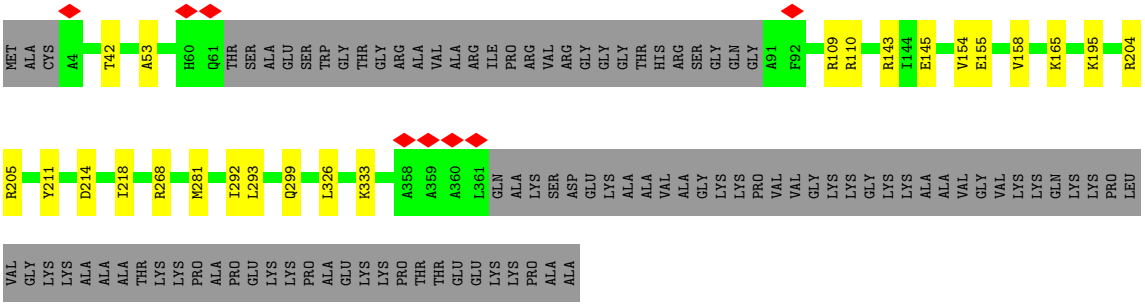


• Molecule 27: Suppressor of SWI4 1 homolog



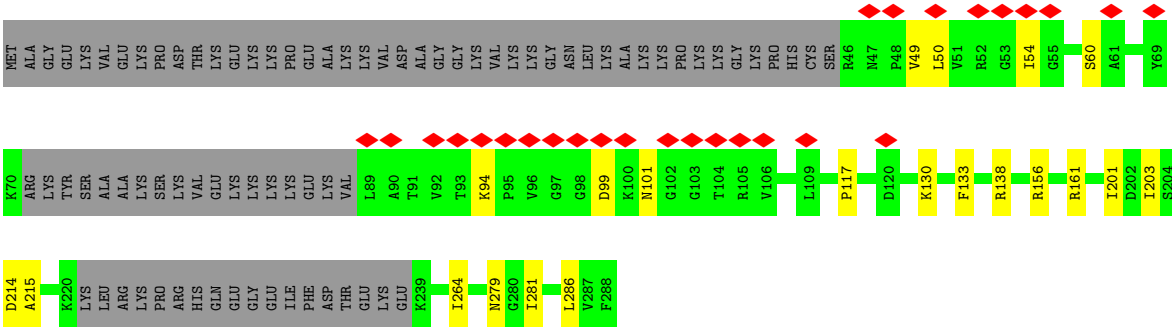
• Molecule 28: 60S ribosomal protein L4

Chain SA:



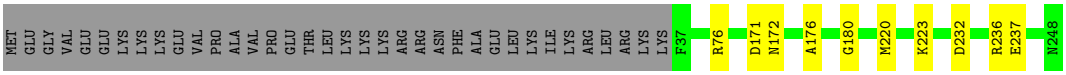
• Molecule 29: 60S ribosomal protein L6

Chain SC:



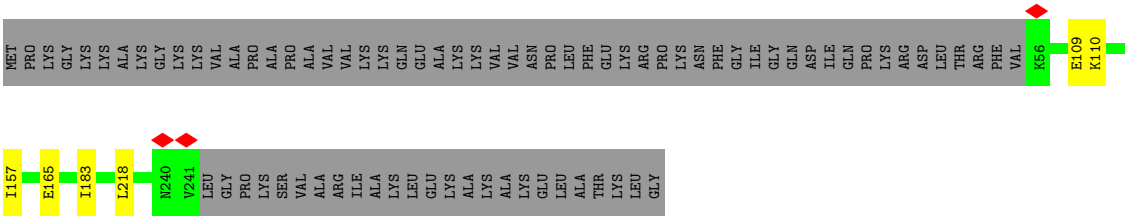
• Molecule 30: 60S ribosomal protein L7

Chain SD:



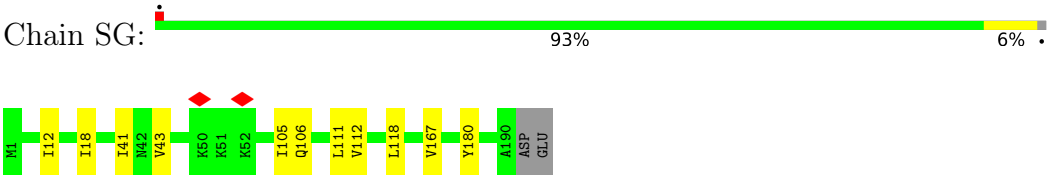
• Molecule 31: 60S ribosomal protein L7a

Chain SE:



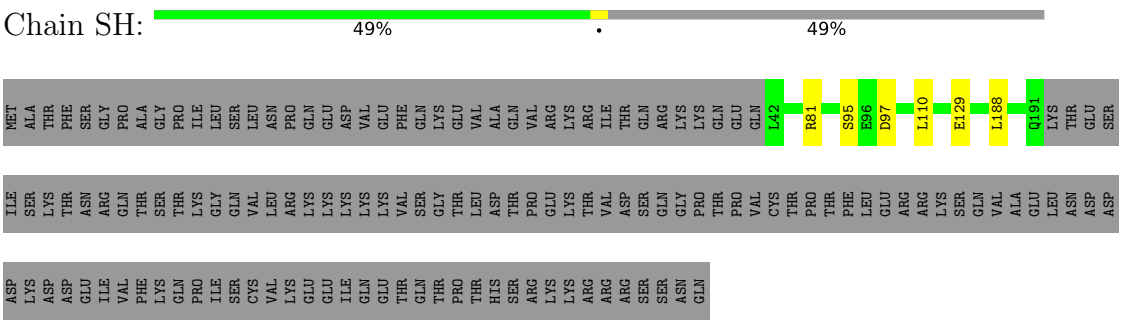
• Molecule 32: 60S ribosomal protein L9

Chain SG:



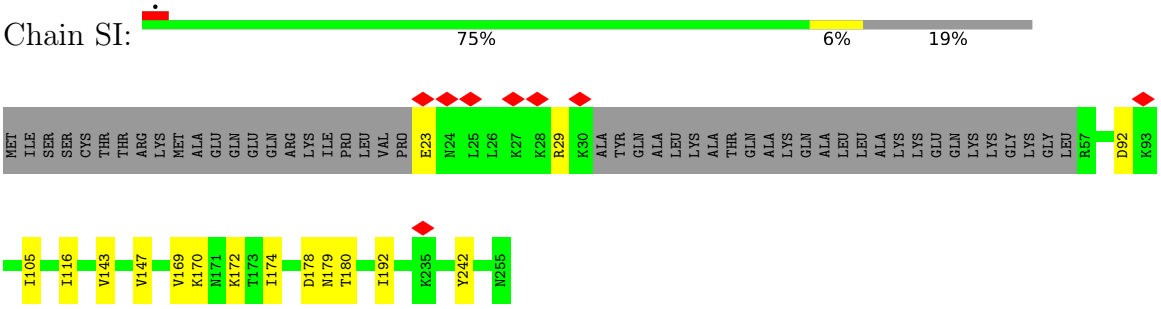
• Molecule 33: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain SH:



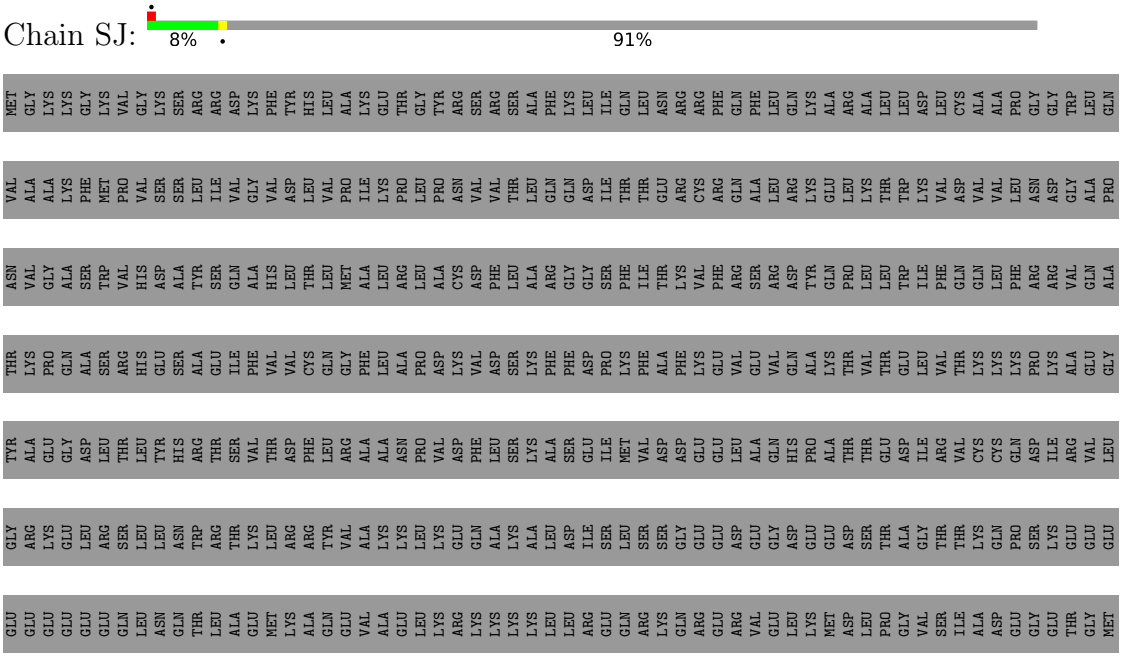
• Molecule 34: 60S ribosomal protein L7-like 1

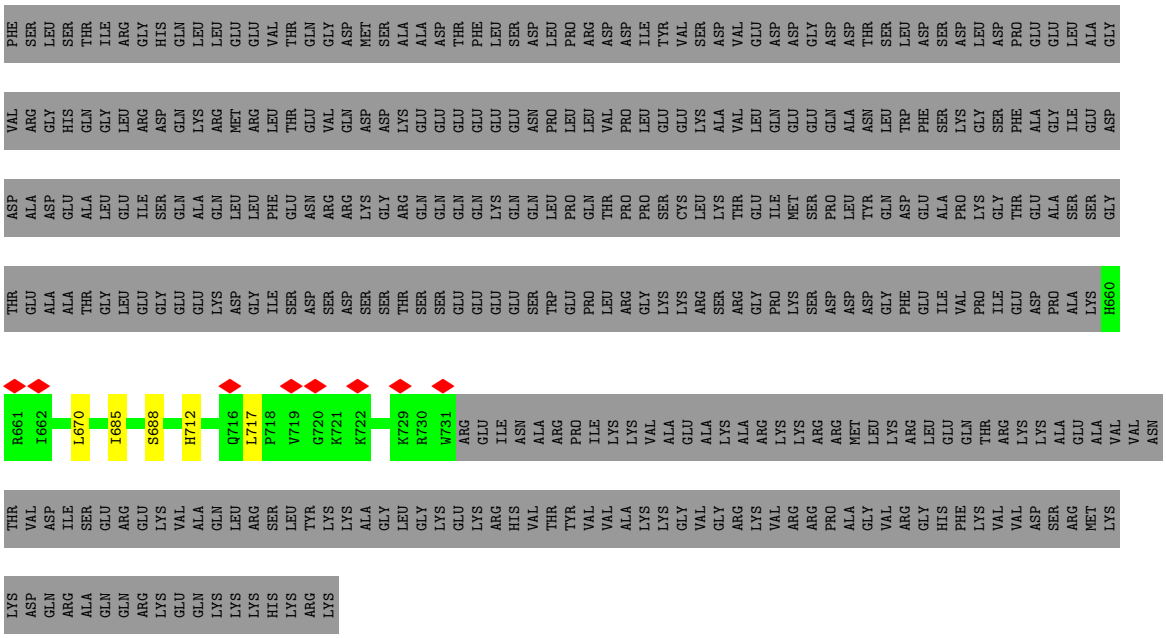
Chain SI:



• Molecule 35: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

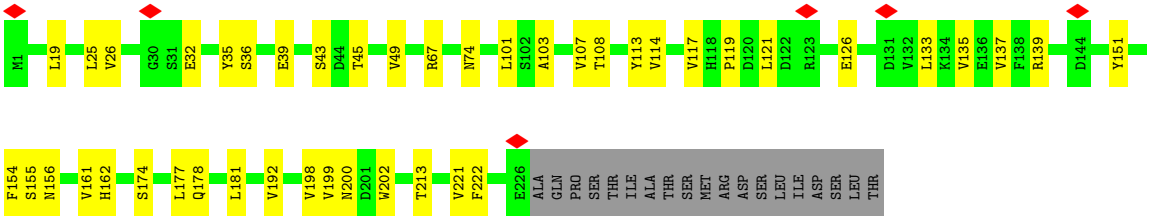
Chain SJ:





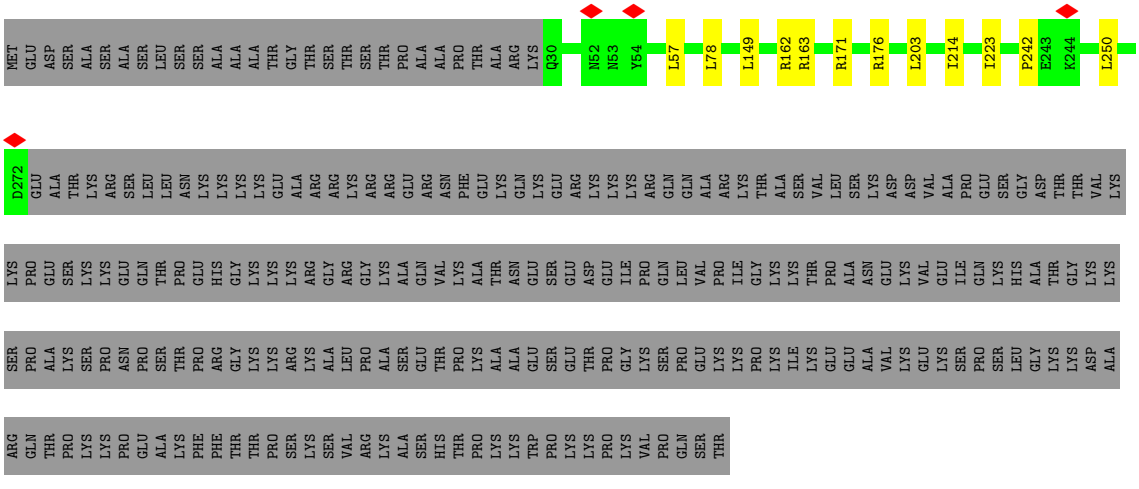
• Molecule 36: Eukaryotic translation initiation factor 6

Chain SK:



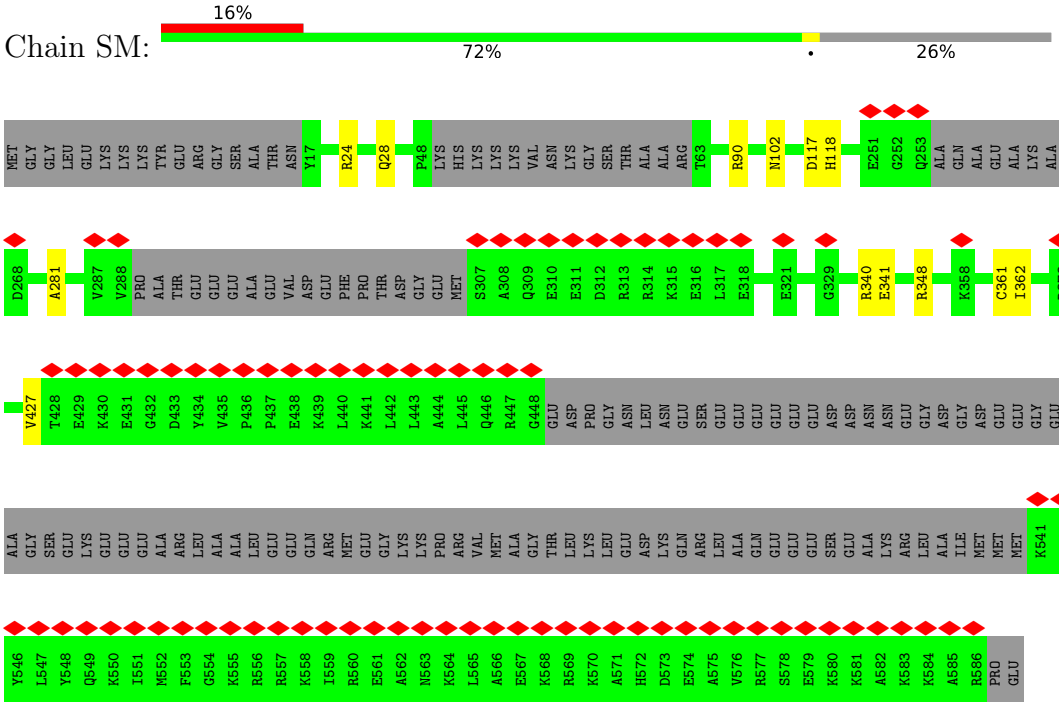
• Molecule 37: Ribosomal L1 domain-containing protein 1

Chain SL:



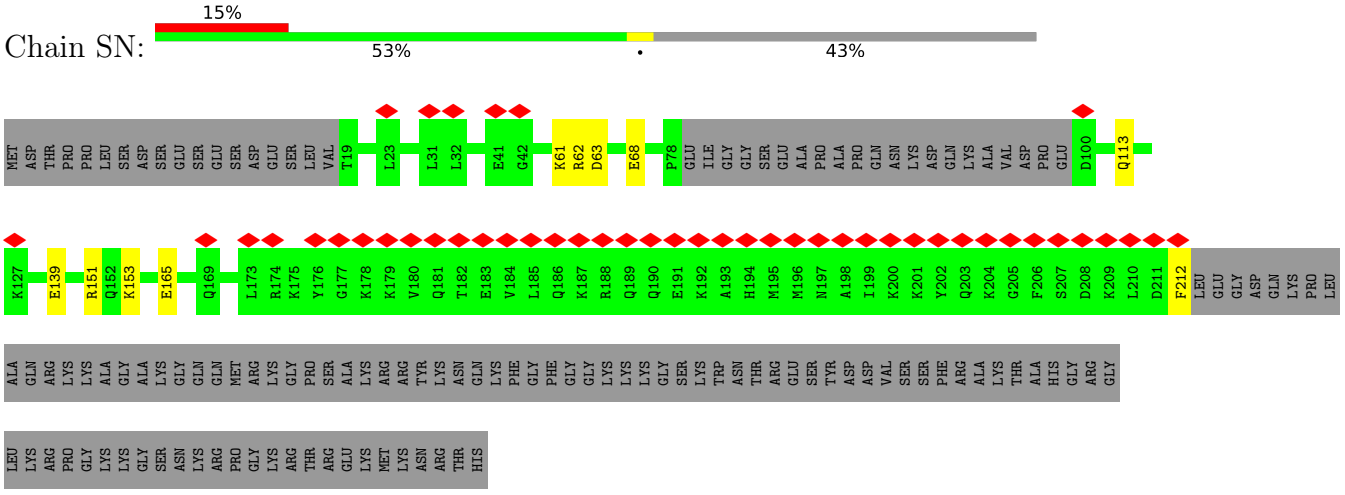
• Molecule 38: Pescadillo homolog

Chain SM:



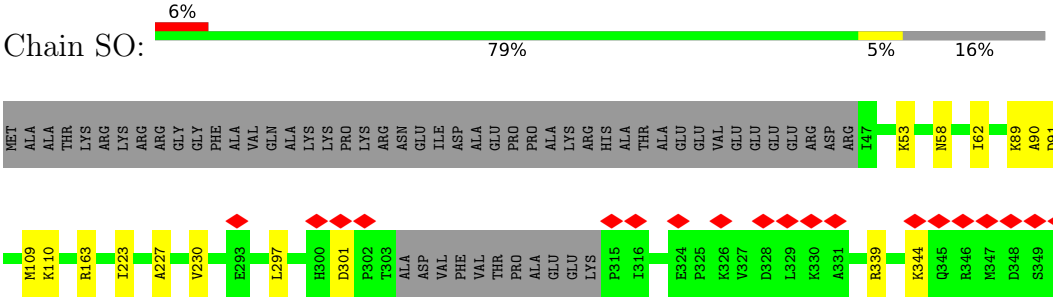
• Molecule 39: Probable rRNA-processing protein EBP2

Chain SN:



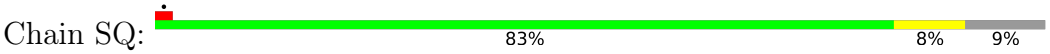
• Molecule 40: Ribosome biogenesis protein BRX1 homolog

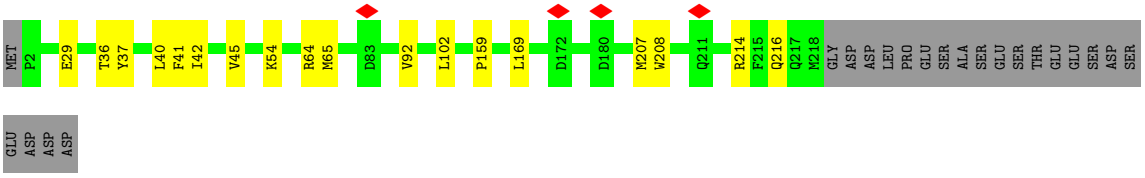
Chain SO:



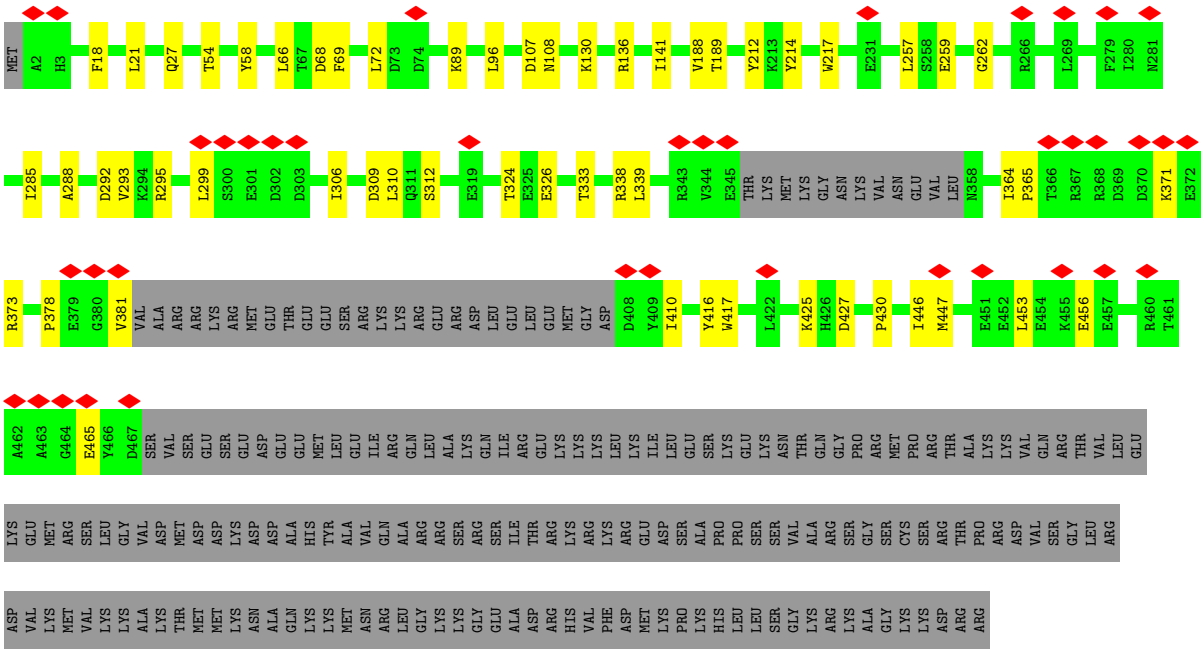
• Molecule 41: mRNA turnover protein 4 homolog

Chain SQ:

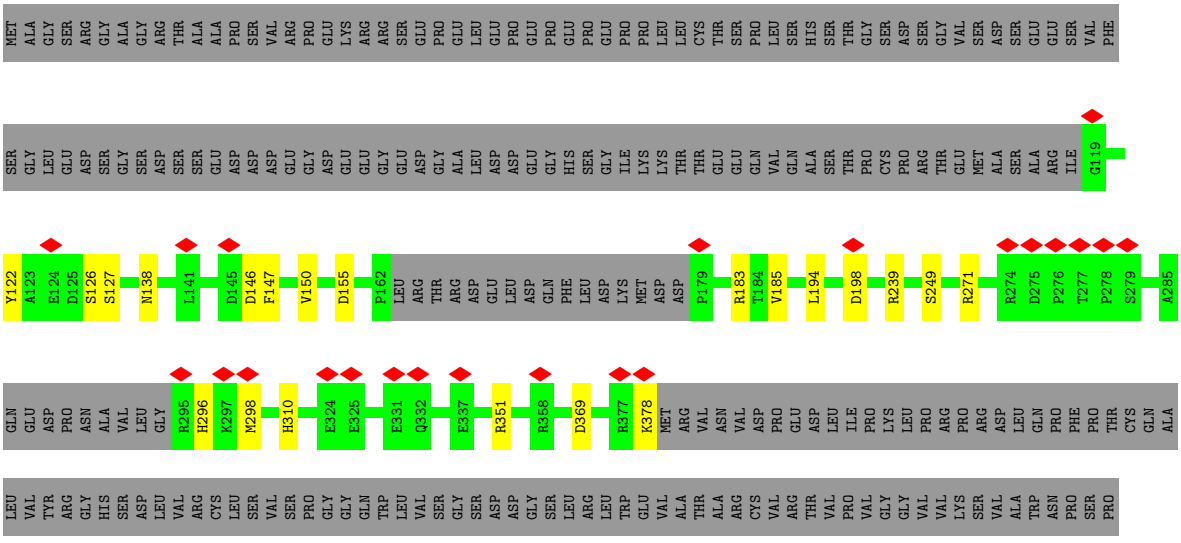


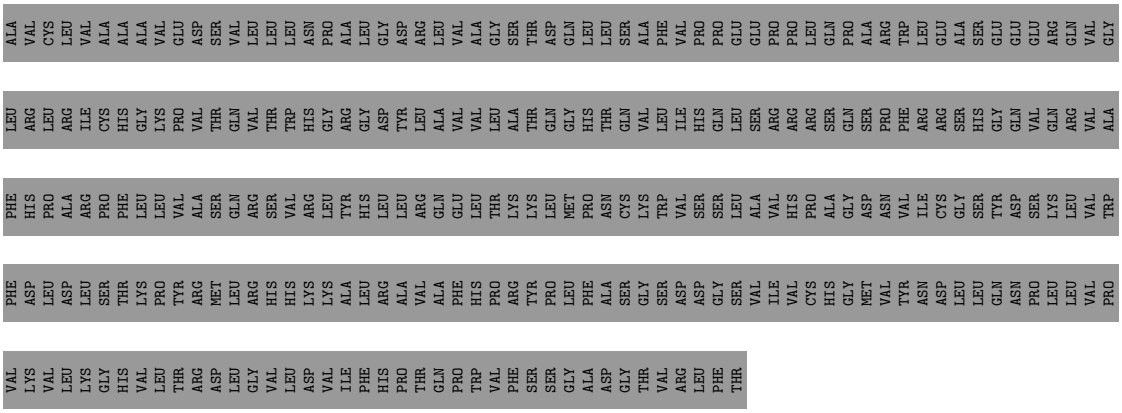


• Molecule 42: GTP-binding protein 4



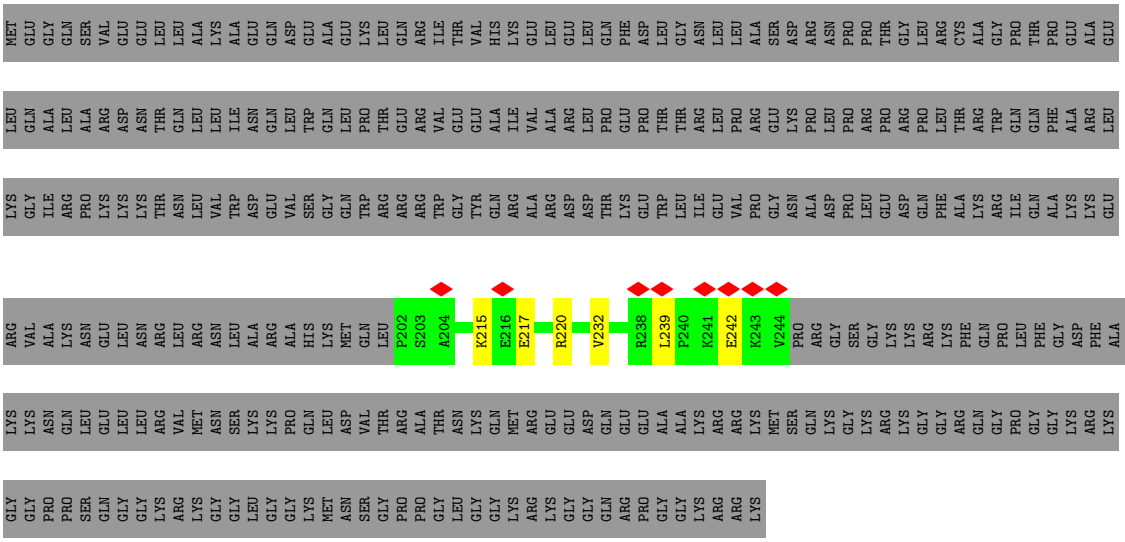
• Molecule 43: Ribosome biogenesis protein BOP1





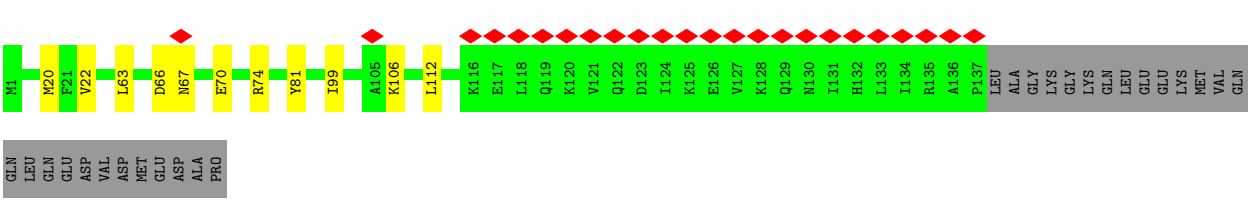
• Molecule 44: Ribosome biogenesis regulatory protein homolog

Chain ST:



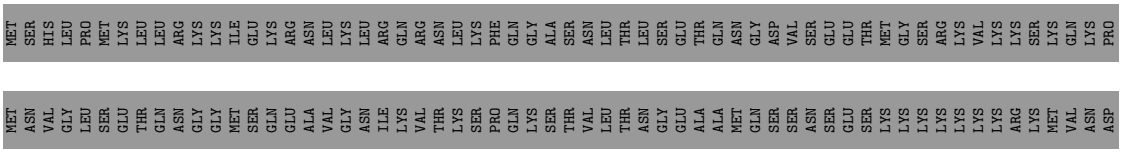
• Molecule 45: Probable ribosome biogenesis protein RLP24

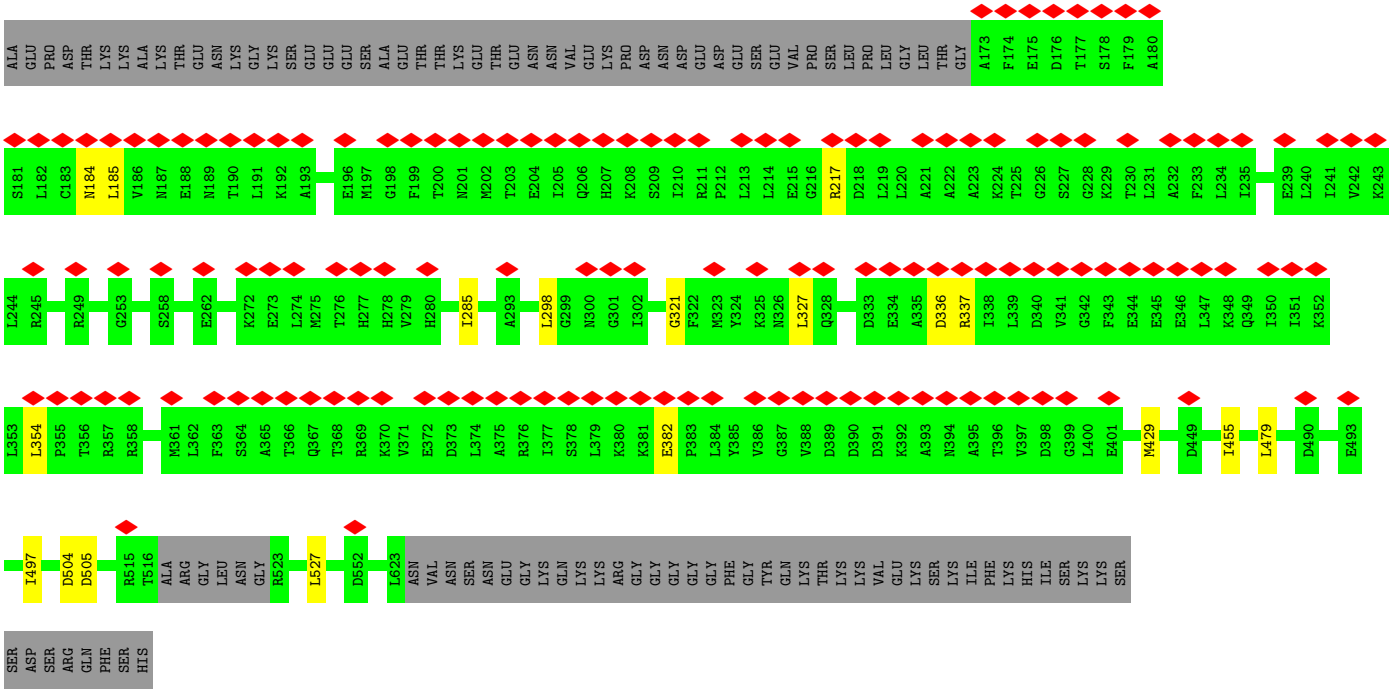
Chain SV:



• Molecule 46: ATP-dependent RNA helicase DDX18

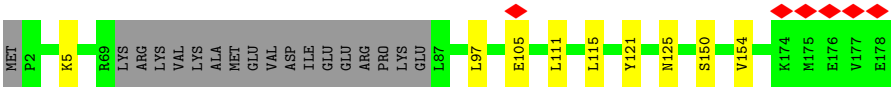
Chain SW:





• Molecule 47: Nucleolar protein 16

Chain SZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39938	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.390	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, SEP, HIC, GDP, 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	BA	0.25	0/1191	0.53	0/1605
2	L1	0.34	0/3611	0.73	0/5623
3	L2	0.36	0/1634	0.80	0/2538
4	L3	0.35	0/43713	0.78	6/68119 (0.0%)
5	L6	0.29	0/953	0.67	0/1276
6	L7	0.27	0/1534	0.56	0/2049
7	L8	0.31	0/1133	0.56	0/1516
8	L9	0.29	0/1584	0.64	0/2117
9	LA	0.25	0/997	0.50	0/1334
10	LB	0.28	0/1239	0.65	0/1658
11	LC	0.29	0/1501	0.58	0/2013
12	LE	0.26	0/708	0.51	0/958
13	LG	0.29	0/856	0.55	0/1149
14	LH	0.25	0/287	0.53	0/378
15	LI	0.28	0/1132	0.60	0/1504
16	LK	0.24	0/648	0.53	0/880
17	LL	0.28	0/995	0.62	0/1334
18	LN	0.28	0/3092	0.53	0/4133
19	LQ	0.26	0/1071	0.58	0/1429
20	LS	0.25	0/1023	0.59	0/1351
21	LT	0.27	0/895	0.61	0/1198
22	LU	0.26	0/854	0.63	0/1129
23	LW	0.27	0/573	0.66	0/755
24	NE	0.25	0/1339	0.64	0/1767
25	NF	0.27	0/1614	0.51	0/2146
26	NG	0.24	0/743	0.52	0/986
27	NN	0.27	0/1988	0.56	0/2678
28	SA	0.27	0/2694	0.57	0/3617
29	SC	0.25	0/1694	0.55	0/2274
30	SD	0.27	0/1789	0.56	0/2388
31	SE	0.28	0/1524	0.56	0/2056
32	SG	0.28	0/1548	0.55	0/2081

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SH	0.29	0/1298	0.52	0/1742
34	SI	0.25	0/1772	0.53	0/2378
35	SJ	0.28	0/623	0.54	0/836
36	SK	0.27	0/1745	0.53	0/2374
37	SL	0.26	0/1994	0.52	0/2684
38	SM	0.26	0/3530	0.48	0/4779
39	SN	0.27	0/1368	0.50	0/1830
40	SO	0.26	0/2521	0.51	0/3384
41	SQ	0.26	0/1817	0.53	0/2435
42	SR	0.27	0/3597	0.51	0/4861
43	SS	0.29	0/1994	0.55	0/2703
44	ST	0.24	0/328	0.50	0/438
45	SV	0.28	0/1194	0.54	0/1582
46	SW	0.26	0/3631	0.48	0/4900
47	SZ	0.25	0/1364	0.53	0/1826
All	All	0.31	0/114933	0.66	6/164791 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L3	2036	C	C2-N1-C1'	5.80	125.18	118.80
4	L3	1854	G	C4-N9-C1'	5.57	133.74	126.50
4	L3	2037	C	C2-N1-C1'	5.41	124.75	118.80
4	L3	2036	C	C6-N1-C2	-5.21	118.22	120.30
4	L3	1961	G	O4'-C1'-N9	5.20	112.36	108.20

There are no chirality outliers.

There are no planarity outliers.

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	BA	1176	0	1234	12	0
2	L1	3234	0	1639	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L2	1468	0	755	7	0
4	L3	39106	0	19811	118	0
5	L6	936	0	1017	9	0
6	L7	1507	0	1649	5	0
7	L8	1111	0	1174	9	0
8	L9	1546	0	1585	6	0
9	LA	981	0	1013	9	0
10	LB	1223	0	1330	4	0
11	LC	1461	0	1502	20	0
12	LE	702	0	561	10	0
13	LG	844	0	883	7	0
14	LH	284	0	330	3	0
15	LI	1115	0	1205	9	0
16	LK	642	0	455	2	0
17	LL	980	0	1041	4	0
18	LN	3044	0	3178	38	0
19	LQ	1053	0	1147	5	0
20	LS	1015	0	1148	5	0
21	LT	876	0	912	5	0
22	LU	840	0	930	5	0
23	LW	563	0	596	6	0
24	NE	1331	0	1430	16	0
25	NF	1588	0	1695	11	0
26	NG	738	0	786	8	0
27	NN	1950	0	2005	21	0
28	SA	2645	0	2823	19	0
29	SC	1663	0	1814	15	0
30	SD	1755	0	1859	7	0
31	SE	1498	0	1601	5	0
32	SG	1526	0	1614	6	0
33	SH	1267	0	1291	5	0
34	SI	1732	0	1837	12	0
35	SJ	609	0	600	3	0
36	SK	1721	0	1695	30	0
37	SL	1960	0	2052	8	0
38	SM	3452	0	3376	10	0
39	SN	1350	0	1345	10	0
40	SO	2460	0	2551	14	0
41	SQ	1778	0	1817	11	0
42	SR	3524	0	3558	39	0
43	SS	1955	0	1871	17	0
44	ST	323	0	332	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	SV	1171	0	1232	11	0
46	SW	3560	0	3641	10	0
47	SZ	1338	0	1352	8	0
48	L1	4	0	0	0	0
48	L2	1	0	0	0	0
48	L3	51	0	0	0	0
48	L9	1	0	0	0	0
48	LN	1	0	0	0	0
48	LQ	1	0	0	0	0
48	LT	1	0	0	0	0
48	SA	1	0	0	0	0
49	LW	1	0	0	0	0
49	SV	1	0	0	0	0
50	SR	28	0	12	0	0
51	SR	1	0	0	0	0
All	All	108693	0	89284	450	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 2.

The worst 5 of 450 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4946:U:HO2'	21:LT:2:SER:N	1.45	1.12
13:LG:39:ILE:HD12	13:LG:61:VAL:HG11	1.58	0.86
4:L3:251:C:O3'	23:LW:85:LYS:NZ	2.11	0.83
18:LN:304:SER:OG	18:LN:310:SER:O	1.99	0.80
47:SZ:111:LEU:HD11	47:SZ:115:LEU:HD23	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
5	L6	112/211 (53%)	111 (99%)	1 (1%)	0	100	100
6	L7	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
7	L8	133/215 (62%)	128 (96%)	5 (4%)	0	100	100
8	L9	179/204 (88%)	179 (100%)	0	0	100	100
9	LA	115/184 (62%)	114 (99%)	1 (1%)	0	100	100
10	LB	149/188 (79%)	149 (100%)	0	0	100	100
11	LC	174/176 (99%)	174 (100%)	0	0	100	100
12	LE	102/160 (64%)	101 (99%)	1 (1%)	0	100	100
13	LG	110/140 (79%)	110 (100%)	0	0	100	100
14	LH	32/156 (20%)	32 (100%)	0	0	100	100
15	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
16	LK	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
17	LL	120/137 (88%)	119 (99%)	1 (1%)	0	100	100
18	LN	372/403 (92%)	365 (98%)	7 (2%)	0	100	100
19	LQ	126/135 (93%)	126 (100%)	0	0	100	100
20	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
21	LT	107/110 (97%)	107 (100%)	0	0	100	100
22	LU	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
23	LW	65/97 (67%)	64 (98%)	1 (2%)	0	100	100
24	NE	152/361 (42%)	148 (97%)	4 (3%)	0	100	100
25	NF	187/260 (72%)	184 (98%)	3 (2%)	0	100	100
26	NG	87/282 (31%)	87 (100%)	0	0	100	100
27	NN	238/473 (50%)	235 (99%)	3 (1%)	0	100	100
28	SA	325/427 (76%)	320 (98%)	5 (2%)	0	100	100
29	SC	201/288 (70%)	198 (98%)	3 (2%)	0	100	100
30	SD	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
31	SE	184/266 (69%)	182 (99%)	2 (1%)	0	100	100
32	SG	189/192 (98%)	187 (99%)	2 (1%)	0	100	100
33	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
34	SI	204/255 (80%)	202 (99%)	2 (1%)	0	100	100
35	SJ	70/847 (8%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	SK	224/245 (91%)	218 (97%)	6 (3%)	0	100	100
37	SL	241/490 (49%)	235 (98%)	6 (2%)	0	100	100
38	SM	427/588 (73%)	426 (100%)	1 (0%)	0	100	100
39	SN	169/306 (55%)	169 (100%)	0	0	100	100
40	SO	292/353 (83%)	288 (99%)	4 (1%)	0	100	100
41	SQ	216/239 (90%)	213 (99%)	3 (1%)	0	100	100
42	SR	422/634 (67%)	417 (99%)	5 (1%)	0	100	100
43	SS	227/746 (30%)	222 (98%)	5 (2%)	0	100	100
44	ST	41/365 (11%)	40 (98%)	1 (2%)	0	100	100
45	SV	135/163 (83%)	135 (100%)	0	0	100	100
46	SW	441/670 (66%)	434 (98%)	7 (2%)	0	100	100
47	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	7873/12574 (63%)	7775 (99%)	98 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	BA	128/137 (93%)	127 (99%)	1 (1%)	81	93
5	L6	98/177 (55%)	98 (100%)	0	100	100
6	L7	157/174 (90%)	157 (100%)	0	100	100
7	L8	115/161 (71%)	115 (100%)	0	100	100
8	L9	155/172 (90%)	155 (100%)	0	100	100
9	LA	111/163 (68%)	111 (100%)	0	100	100
10	LB	136/165 (82%)	136 (100%)	0	100	100
11	LC	157/157 (100%)	157 (100%)	0	100	100
12	LE	47/140 (34%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	LG	87/107 (81%)	87 (100%)	0	100	100
14	LH	28/133 (21%)	28 (100%)	0	100	100
15	LI	124/135 (92%)	124 (100%)	0	100	100
16	LK	29/121 (24%)	29 (100%)	0	100	100
17	LL	106/121 (88%)	106 (100%)	0	100	100
18	LN	328/348 (94%)	326 (99%)	2 (1%)	86	95
19	LQ	114/121 (94%)	114 (100%)	0	100	100
20	LS	109/110 (99%)	109 (100%)	0	100	100
21	LT	88/89 (99%)	88 (100%)	0	100	100
22	LU	87/89 (98%)	87 (100%)	0	100	100
23	LW	58/80 (72%)	58 (100%)	0	100	100
24	NE	136/294 (46%)	136 (100%)	0	100	100
25	NF	172/228 (75%)	172 (100%)	0	100	100
26	NG	83/246 (34%)	83 (100%)	0	100	100
27	NN	218/398 (55%)	218 (100%)	0	100	100
28	SA	279/348 (80%)	279 (100%)	0	100	100
29	SC	183/252 (73%)	183 (100%)	0	100	100
30	SD	182/215 (85%)	182 (100%)	0	100	100
31	SE	159/223 (71%)	159 (100%)	0	100	100
32	SG	170/171 (99%)	170 (100%)	0	100	100
33	SH	140/274 (51%)	140 (100%)	0	100	100
34	SI	190/228 (83%)	190 (100%)	0	100	100
35	SJ	64/733 (9%)	64 (100%)	0	100	100
36	SK	196/213 (92%)	196 (100%)	0	100	100
37	SL	226/437 (52%)	225 (100%)	1 (0%)	91	97
38	SM	350/509 (69%)	350 (100%)	0	100	100
39	SN	133/260 (51%)	133 (100%)	0	100	100
40	SO	274/319 (86%)	274 (100%)	0	100	100
41	SQ	195/214 (91%)	195 (100%)	0	100	100
42	SR	390/574 (68%)	390 (100%)	0	100	100
43	SS	208/648 (32%)	208 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	ST	34/300 (11%)	34 (100%)	0	100 100
45	SV	127/149 (85%)	127 (100%)	0	100 100
46	SW	394/591 (67%)	394 (100%)	0	100 100
47	SZ	141/158 (89%)	141 (100%)	0	100 100
All	All	6906/10882 (64%)	6902 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	54	LYS
18	LN	271	GLN
18	LN	297	LYS
37	SL	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
36	SK	68	HIS
38	SM	211	HIS
46	SW	593	HIS
42	SR	209	HIS
45	SV	17	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	150/157 (95%)	16 (10%)	0
3	L2	65/1167 (5%)	10 (15%)	0
4	L3	1788/5070 (35%)	274 (15%)	1 (0%)
All	All	2003/6394 (31%)	300 (14%)	1 (0%)

5 of 300 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	34	U
2	L1	52	A
2	L1	59	A
2	L1	62	A

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Mol	Chain	Res	Type
2	L1	63	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	3852	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	HIC	LN	245	18	8,11,12	1.63	2 (25%)	6,14,16	1.22	1 (16%)
43	SEP	SS	127	43	8,9,10	1.57	1 (12%)	8,12,14	1.18	1 (12%)
43	SEP	SS	126	43	8,9,10	1.51	1 (12%)	8,12,14	1.65	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HIC	LN	245	18	-	0/5/6/8	0/1/1/1
43	SEP	SS	127	43	-	3/5/8/10	-
43	SEP	SS	126	43	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	LN	245	HIC	CD2-CG	3.48	1.41	1.36
43	SS	127	SEP	P-O1P	3.39	1.61	1.50
43	SS	126	SEP	P-O1P	3.25	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	LN	245	HIC	CZ-NE2	-2.13	1.42	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	SS	126	SEP	OG-CB-CA	3.04	111.11	108.14
43	SS	126	SEP	P-OG-CB	-2.86	110.40	118.30
18	LN	245	HIC	CB-CA-C	-2.19	107.36	111.47
43	SS	127	SEP	OG-CB-CA	2.14	110.23	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	SS	127	SEP	CB-OG-P-O2P
43	SS	127	SEP	CB-OG-P-O3P
43	SS	126	SEP	CA-CB-OG-P
43	SS	127	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 64 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	$\#\|Z\|>2$
50	GDP	SR	1001	51	24,30,30	2.55	8 (33%)	30,47,47	1.76	9 (30%)

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
50	GDP	SR	1001	51	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	SR	1001	GDP	O6-C6	8.31	1.40	1.23
50	SR	1001	GDP	C2-N2	4.72	1.45	1.34
50	SR	1001	GDP	O4'-C1'	4.27	1.47	1.41
50	SR	1001	GDP	C2'-C1'	-2.49	1.50	1.53
50	SR	1001	GDP	C5-C4	2.31	1.49	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	SR	1001	GDP	C3'-C2'-C1'	4.14	107.21	100.98
50	SR	1001	GDP	C5-C6-N1	3.42	120.00	113.95
50	SR	1001	GDP	O2B-PB-O3A	3.04	114.81	104.64
50	SR	1001	GDP	C2-N1-C6	-2.97	119.64	125.10
50	SR	1001	GDP	O3B-PB-O3A	2.82	114.10	104.64

There are no chirality outliers.

There are no torsion outliers.

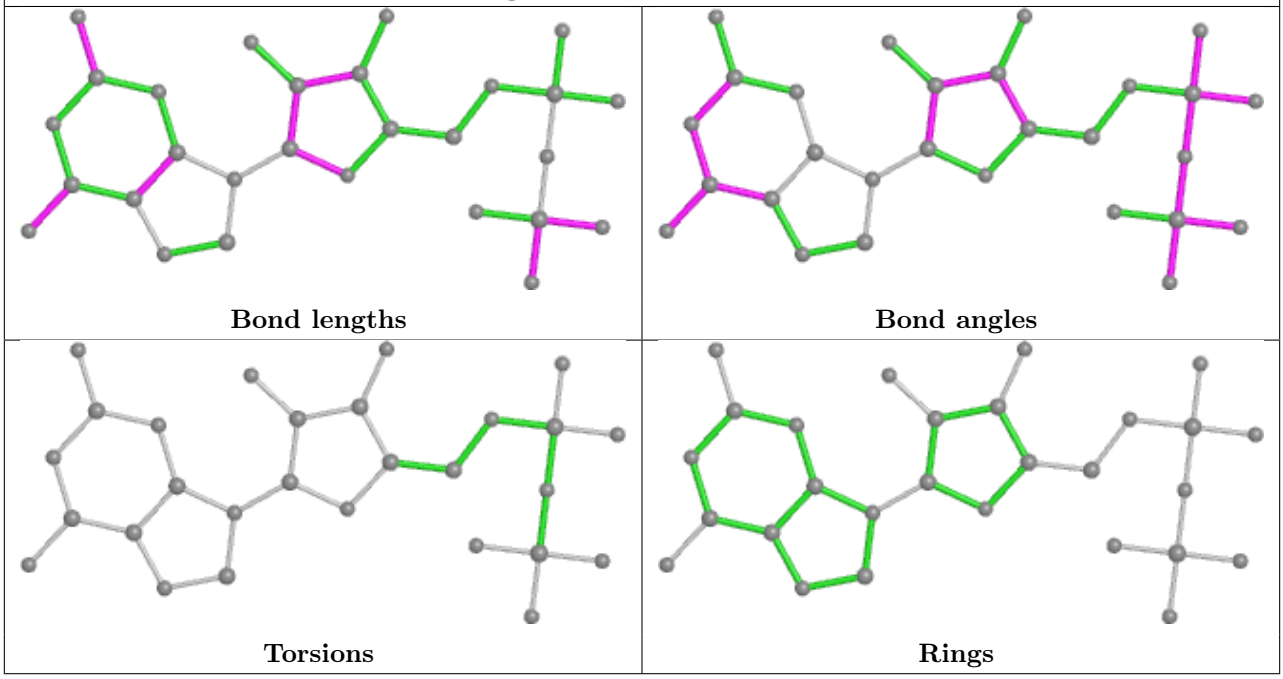
There are no ring outliers.

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 then 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.

Ligand GDP SR 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

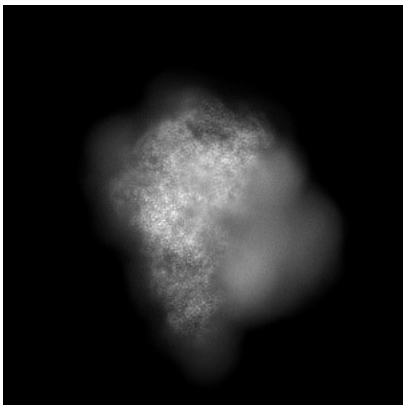
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29255. These allow visual inspection of the internal detail of the map and identification of artifacts.

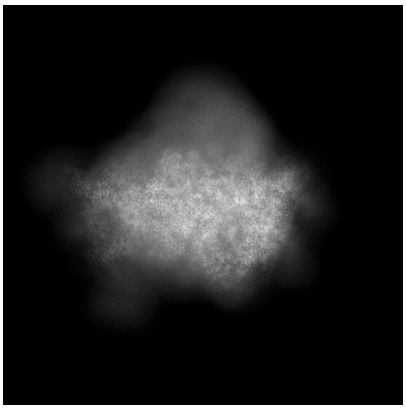
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

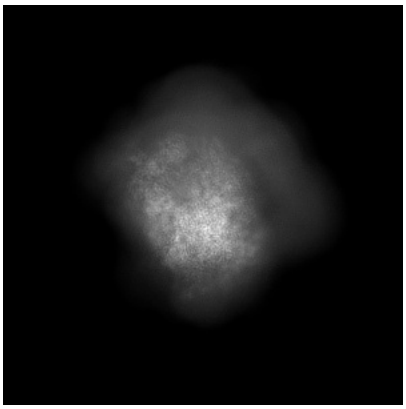
6.1.1 Primary map



X

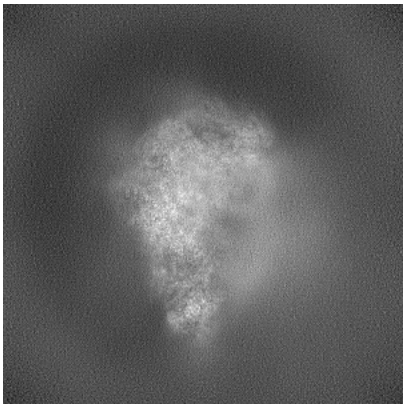


Y

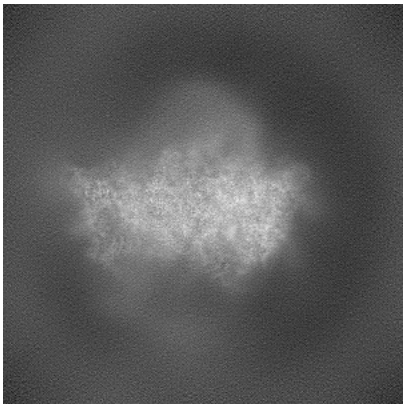


Z

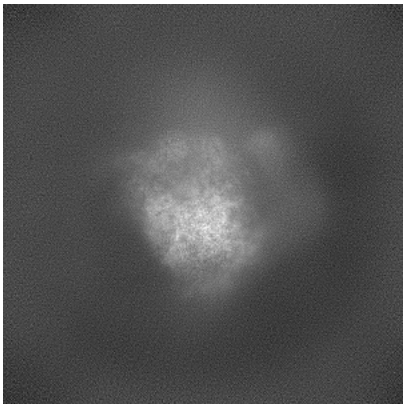
6.1.2 Raw map



X



Y

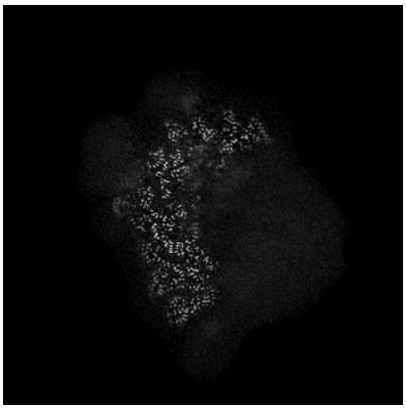


Z

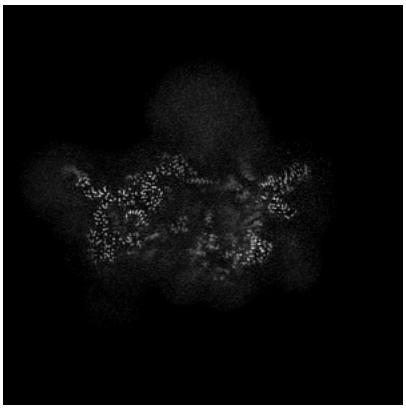
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

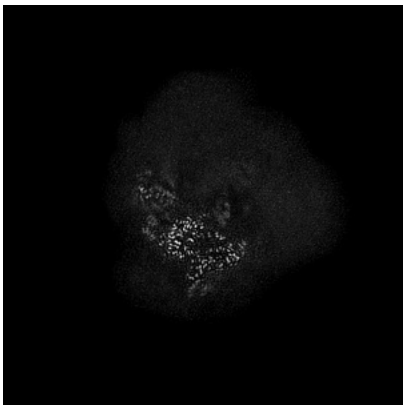
6.2.1 Primary map



X Index: 240

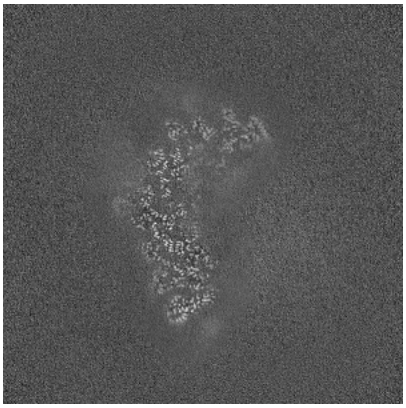


Y Index: 240

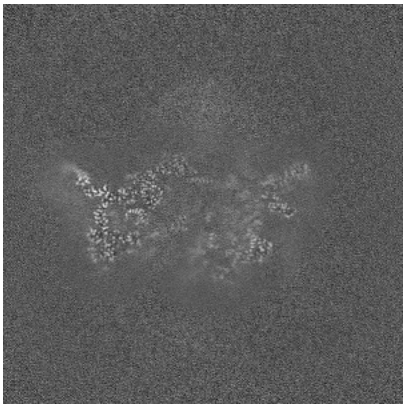


Z Index: 240

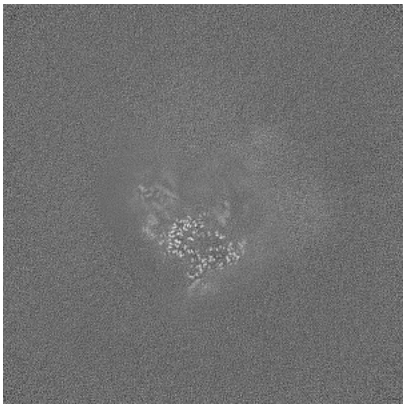
6.2.2 Raw map



X Index: 240



Y Index: 240

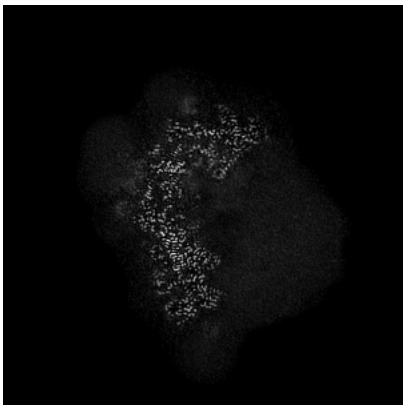


Z Index: 240

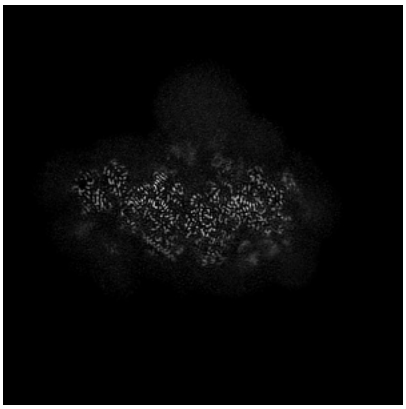
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

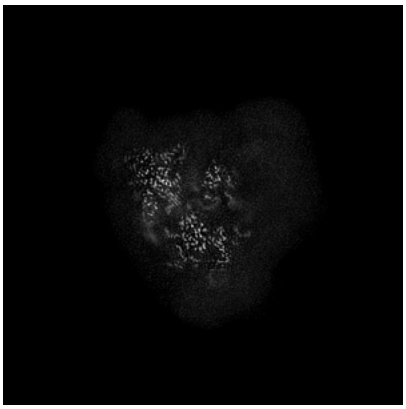
6.3.1 Primary map



X Index: 244

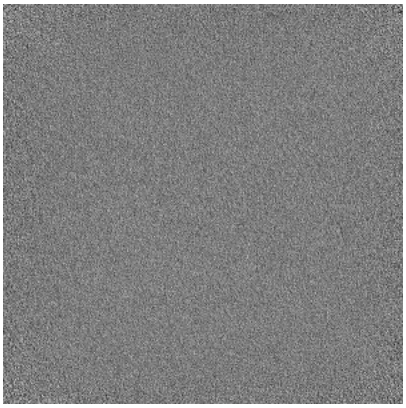


Y Index: 211

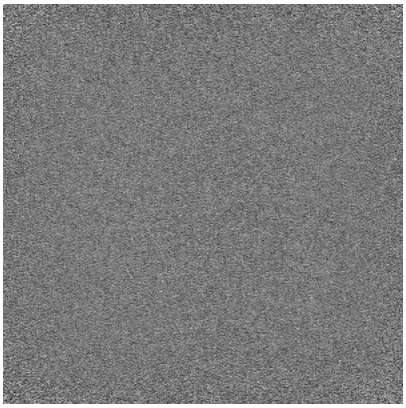


Z Index: 294

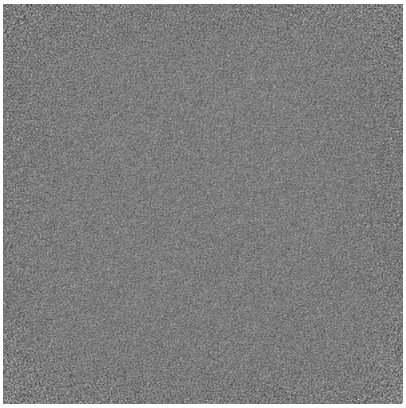
6.3.2 Raw map



X Index: 0



Y Index: 0

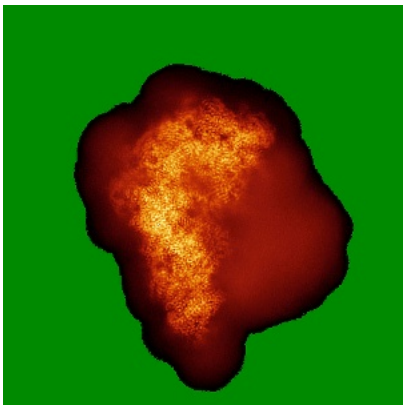


Z Index: 0

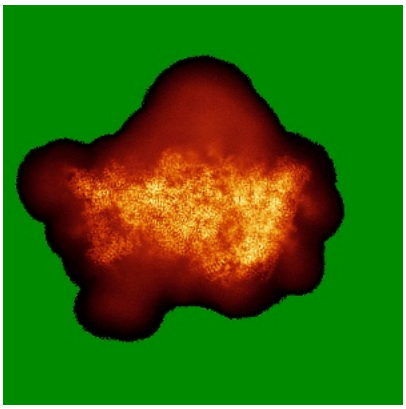
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

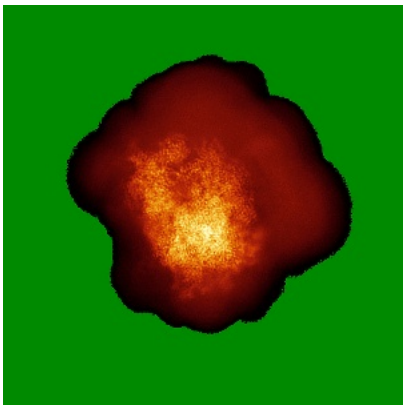
6.4.1 Primary map



X

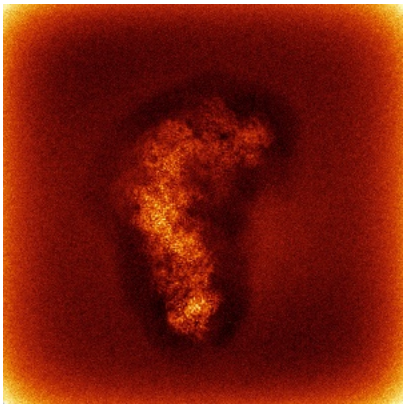


Y

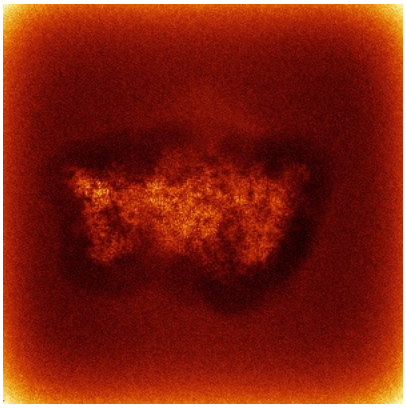


Z

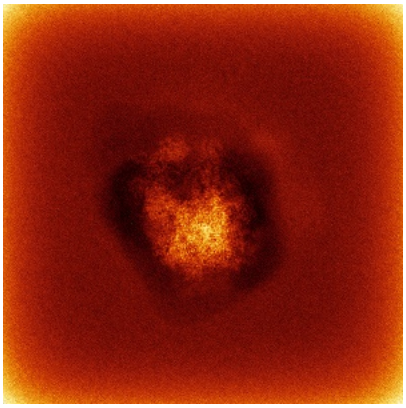
6.4.2 Raw map



X



Y



Z

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

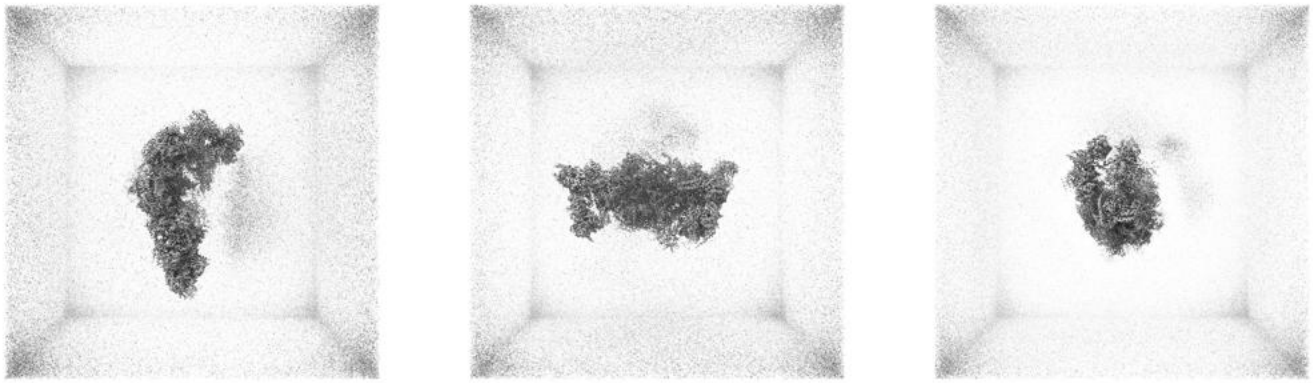
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

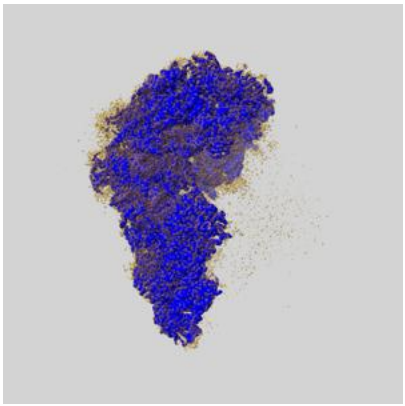
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

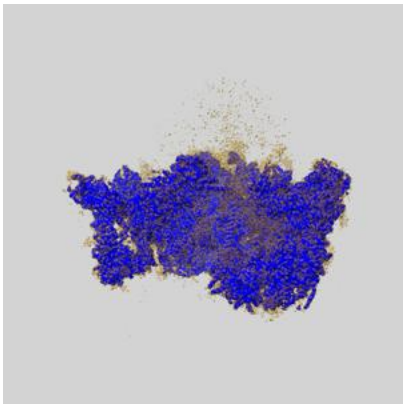
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

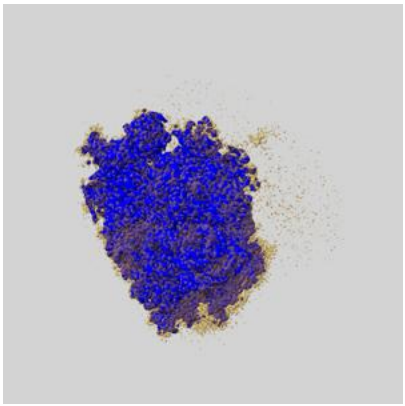
6.6.1 emd_29255_msk_1.map



X



Y

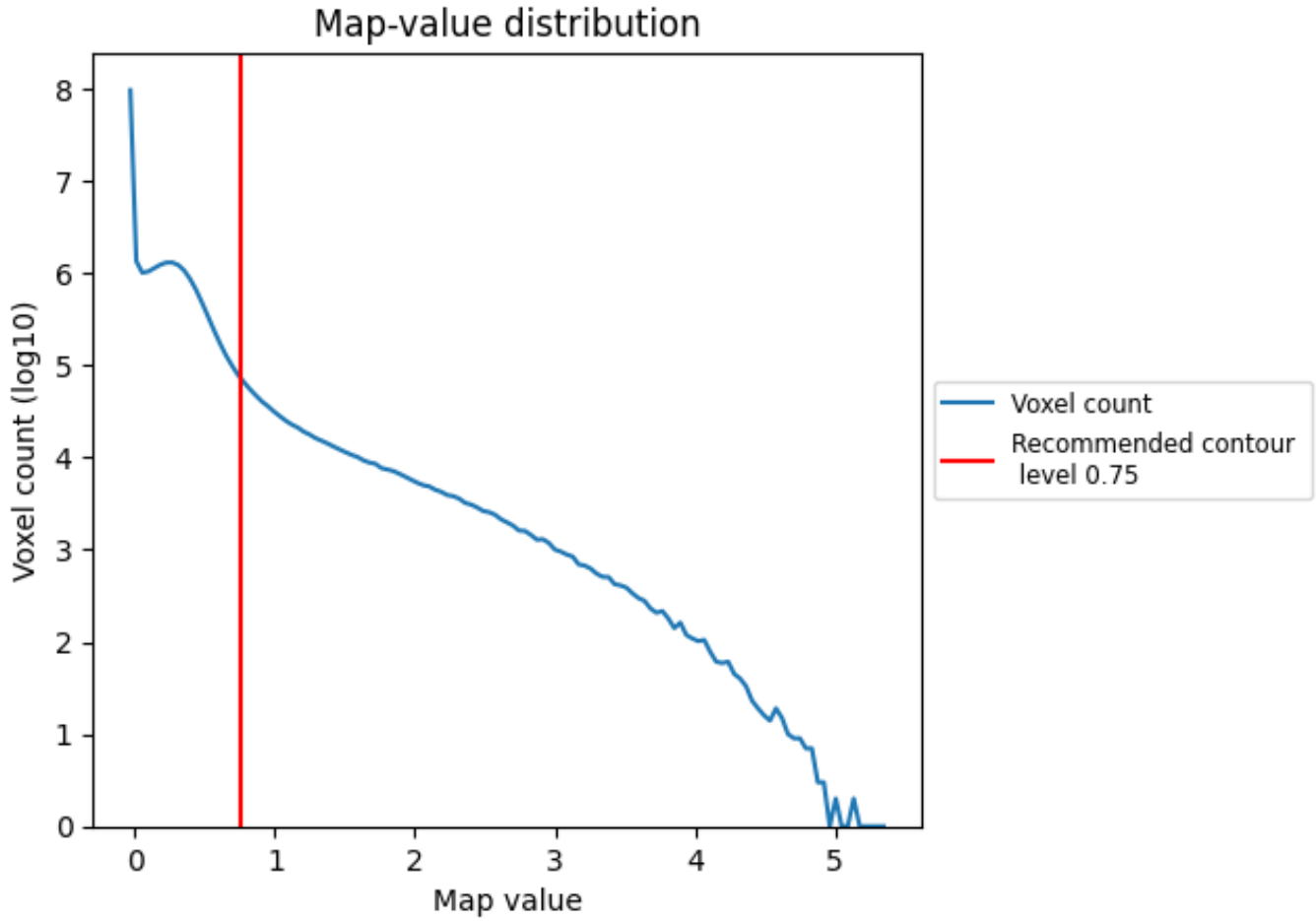


Z

7 Map analysis

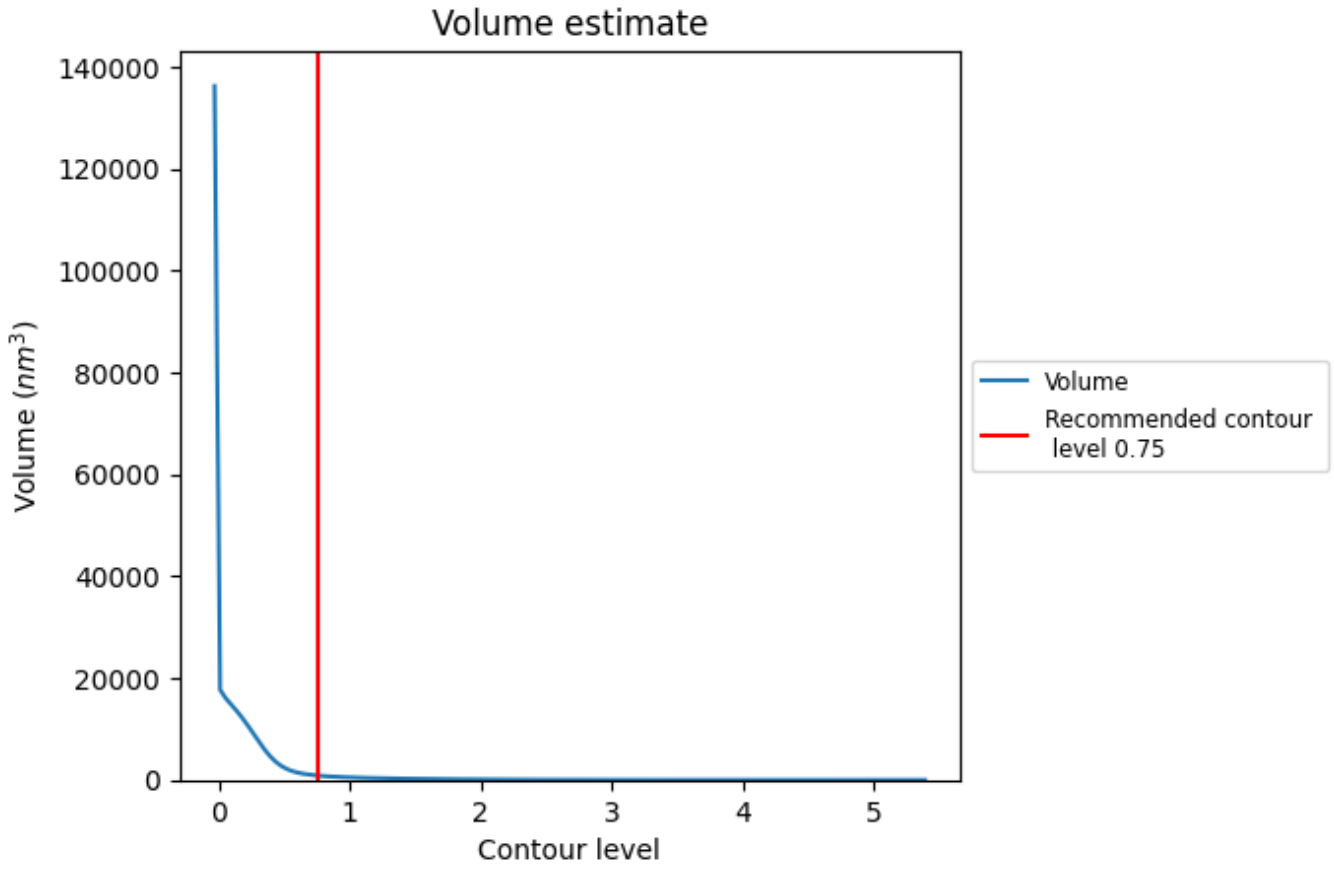
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

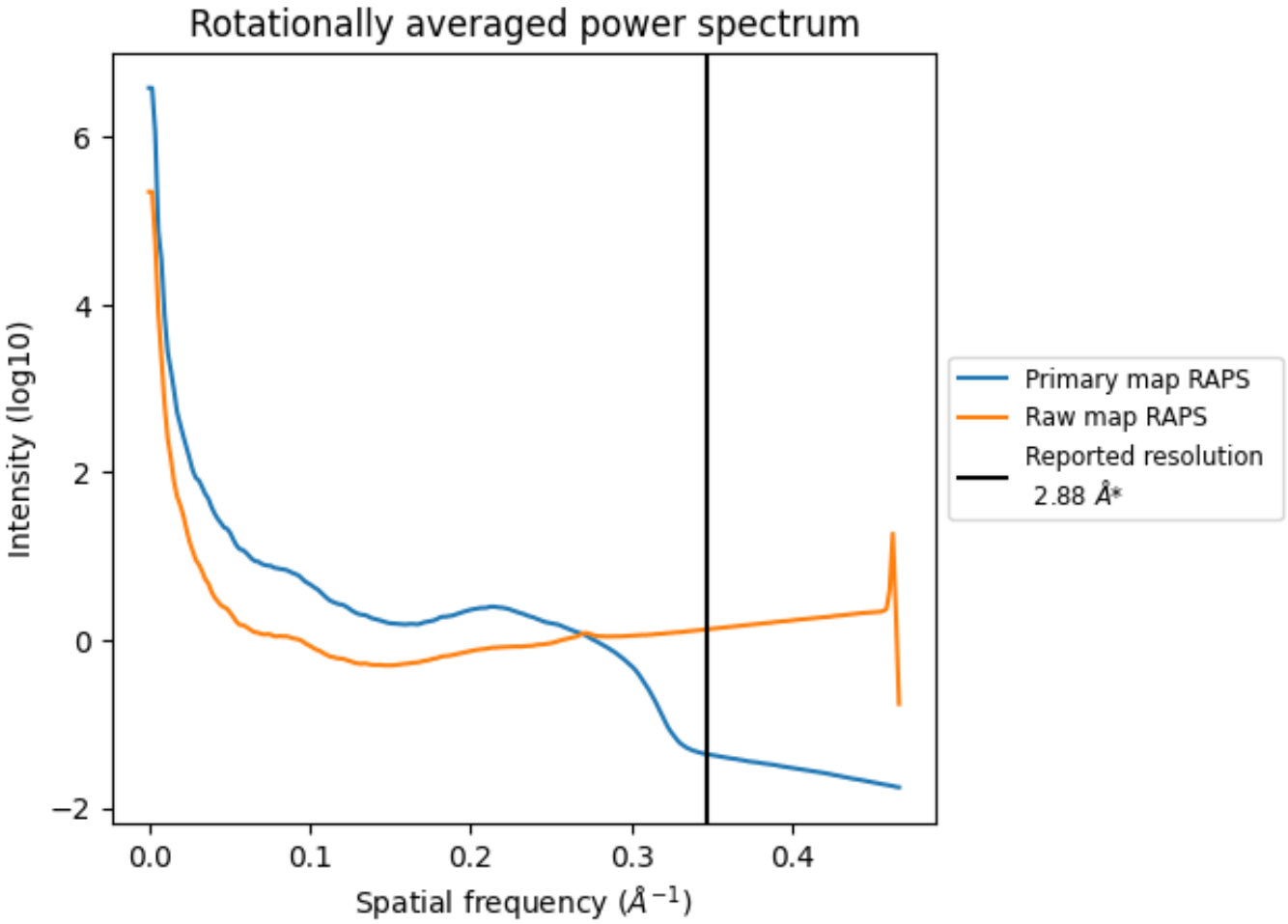
7.2 Volume estimate



The volume at the recommended contour level is 877 nm^3; this corresponds to an approximate mass of 792 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)

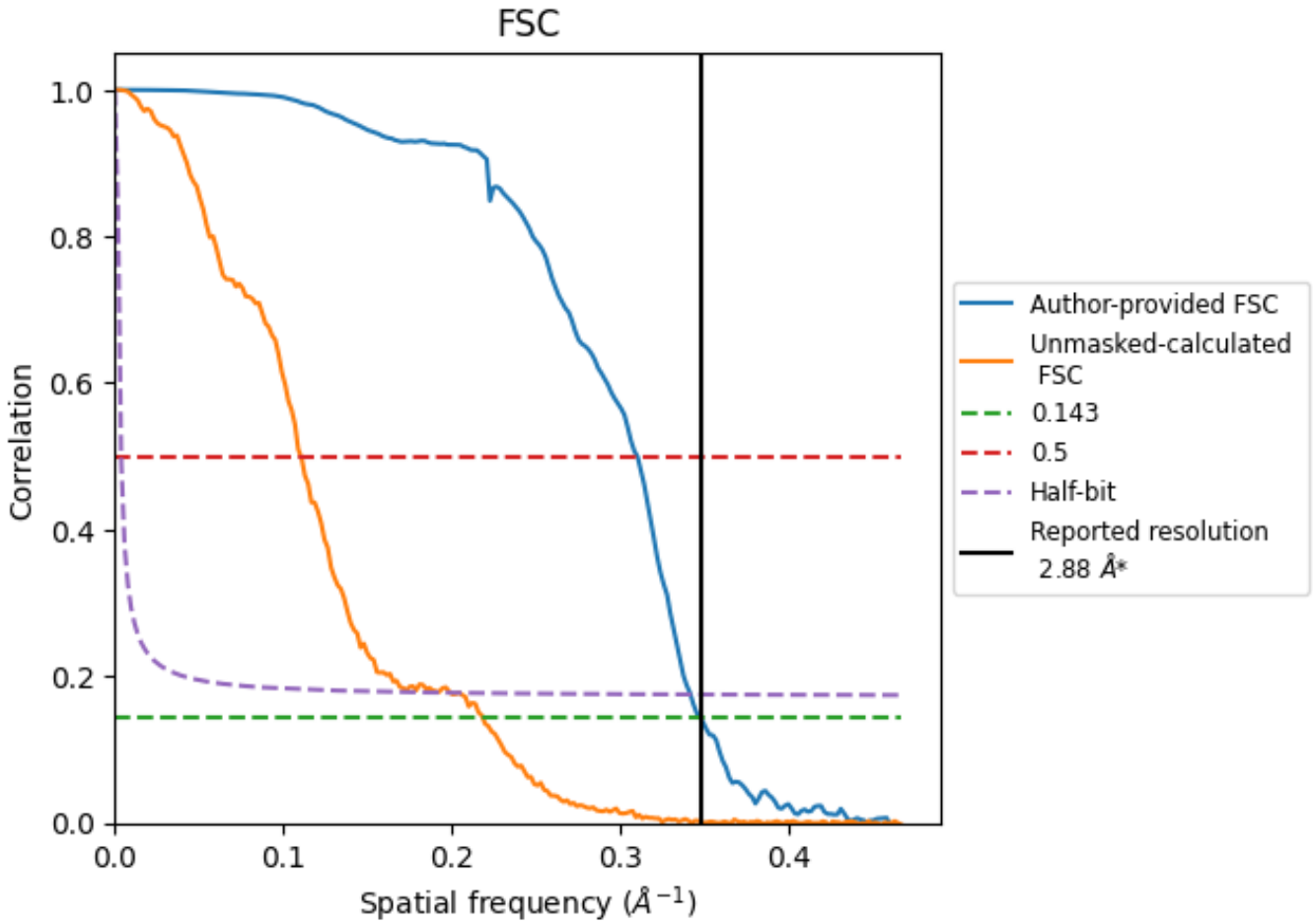


*Reported resolution corresponds to spatial frequency of 0.347 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8.2 Resolution estimates (i)

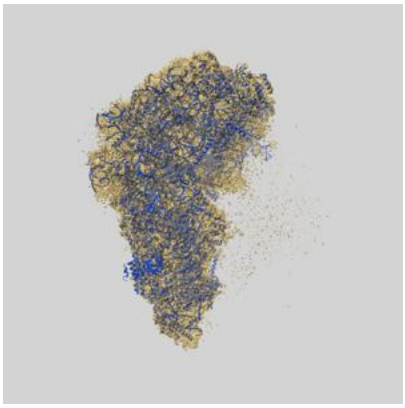
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.23	2.93
Unmasked-calculated*	4.58	9.06	5.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.58 differs from the reported value 2.88 by more than 10 %

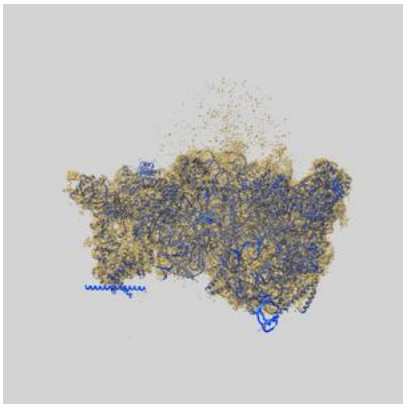
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29255 and PDB model 8FKS. Per-residue inclusion information can be found in section 3 on page 14.

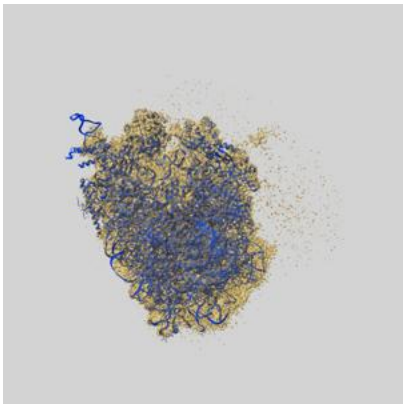
9.1 Map-model overlay



X



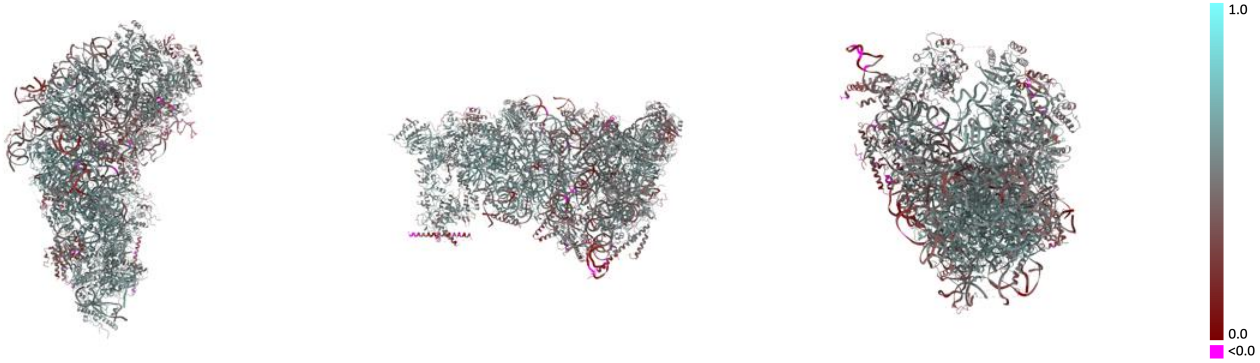
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.75 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.

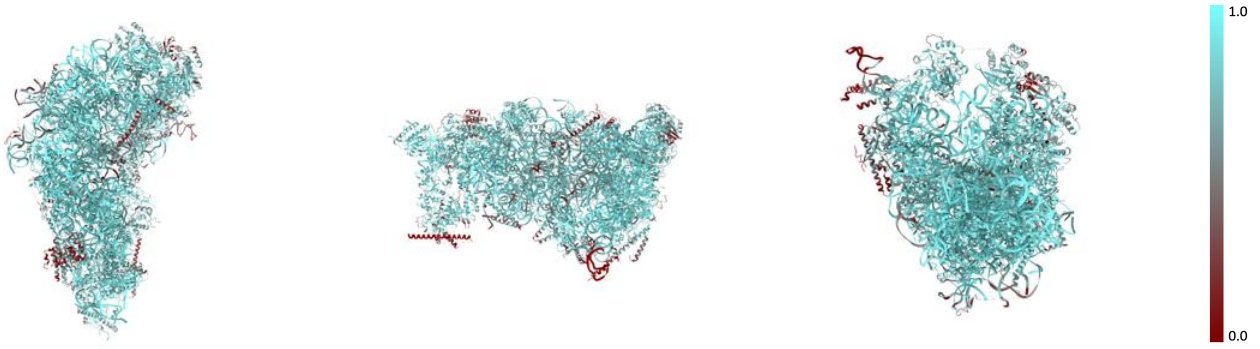
9.2 Q-score mapped to coordinate model



X Y Z

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

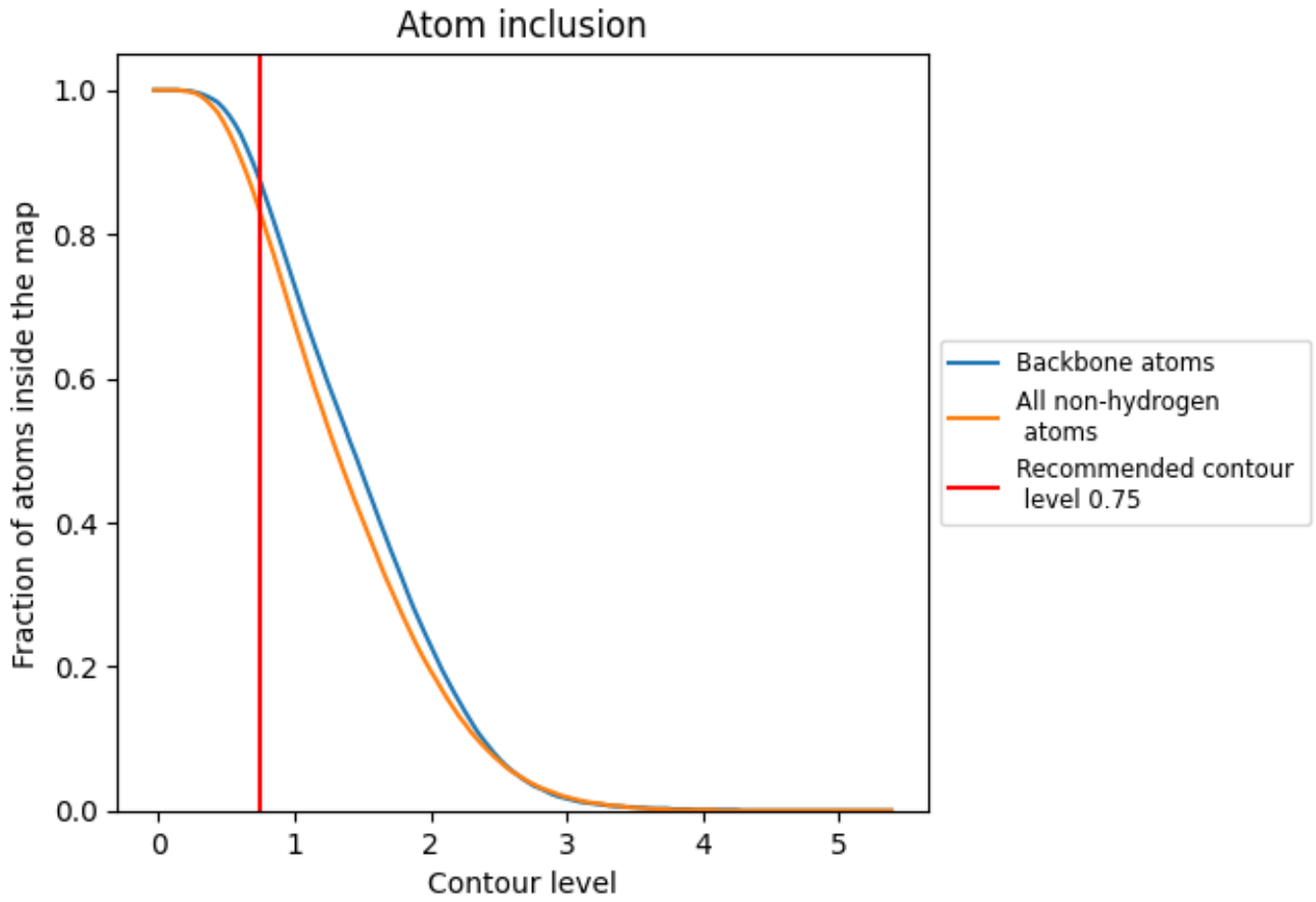
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.75).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.4980
BA	0.5410	0.3930
L1	0.8690	0.5050
L2	0.9130	0.5310
L3	0.8930	0.4880
L6	0.9560	0.5890
L7	0.9300	0.4890
L8	0.9180	0.5190
L9	0.9500	0.6070
LA	0.7650	0.4740
LB	0.9580	0.6000
LC	0.9240	0.5410
LE	0.7330	0.4060
LG	0.7750	0.4410
LH	0.6000	0.4890
LI	0.8780	0.5750
LK	0.7970	0.4290
LL	0.9240	0.5860
LN	0.8690	0.5090
LQ	0.9150	0.5950
LS	0.7650	0.5170
LT	0.9590	0.5830
LU	0.8260	0.5570
LW	0.8310	0.5640
NE	0.5940	0.3490
NF	0.6540	0.4370
NG	0.3150	0.2450
NN	0.7670	0.4480
SA	0.9270	0.5900
SC	0.7410	0.4660
SD	0.9400	0.5810
SE	0.9170	0.5670
SG	0.8630	0.5550
SH	0.8350	0.5500
SI	0.7700	0.5310

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SJ	0.6770	0.4860
SK	0.8190	0.4670
SL	0.7980	0.5350
SM	0.6930	0.4710
SN	0.5920	0.4250
SO	0.7940	0.5360
SQ	0.7560	0.5010
SR	0.7420	0.4790
SS	0.7490	0.4880
ST	0.6120	0.4590
SV	0.6610	0.4260
SW	0.5670	0.4430
SZ	0.8420	0.5280