wwPDB EM Validation Summary Report

Dec 30, 2024 – 10:16 PM EST

PDB ID	:	8FKY
EMDB ID	:	EMD-29261
Title	:	Human nucleolar pre-60S ribosomal subunit (State F)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.67 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:

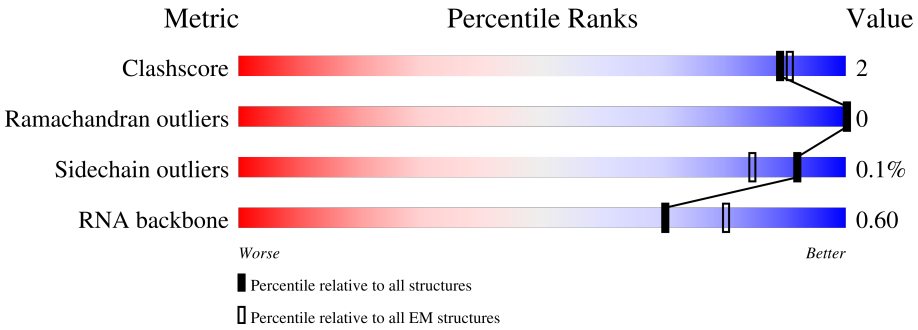
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.67 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	39% 90% 7%
2	BB	217	31% 98%
3	BC	383	7% 80% 9% 12%
4	L1	157	5% 81% 15%
5	L2	1167	5% 94%
6	L3	5070	5% 41% 9% 49%
7	L6	211	53% 43%

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Mol	Chain	Length	Quality of chain
8	L7	203	96%
9	L8	215	61% 37%
10	L9	204	87% 10%
11	LA	184	73% 25%
12	LB	188	74% 6% 20%
13	LC	176	93% 7%
14	LD	196	11% 63% 33%
15	LE	160	28% 67% 29%
16	LG	140	6% 88% 8%
17	LH	156	77% 10% 13%
18	LI	145	86% 6% 8%
19	LJ	136	81% 18%
20	LK	148	16% 70% 27%
21	LL	137	87% 11%
22	LN	403	84% 5% 11%
23	LO	115	72% 10% 17%
24	LP	125	68% 85% 15%
25	LQ	135	88% 7% 5%
26	LR	117	50% 46%
27	LS	123	93% 6%
28	LT	110	92% 7%
29	LU	105	7% 95%
30	LW	97	72% 24%
31	NA	749	14% 62% 35%
32	NB	549	12% 87%

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Mol	Chain	Length	Quality of chain
33	NF	260	78% 20%
34	NH	180	94% 6%
35	NI	881	23% 67% 31%
36	NK	129	5% 50% 48%
37	SA	427	80% 16%
38	SC	288	22% 70% 26%
39	SD	248	5% 86% 5% 9%
40	SE	266	68% 30%
41	SG	192	96%
42	SH	293	5% 49% 49%
43	SI	255	87% 10%
44	SJ	847	9% 29% 70%
45	SK	245	91% 9%
46	SL	490	48% 50%
47	SM	588	6% 81% 15%
48	SN	306	5% 55% 43%
49	SO	353	7% 82% 16%
50	SP	423	23% 90% 6%
51	SQ	239	86% 5% 9%
52	SR	634	5% 70% 26%
53	SS	746	80% 16%
54	ST	365	13% 38% 59%
55	SU	800	10% 64% 5% 31%
56	SV	163	13% 81% 16%
57	SW	670	15% 66% 33%

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Mol	Chain	Length	Quality of chain
58	SY	812	
59	SZ	178	

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 158284 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	160	1208	749	226	229	4	0	0

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	BB	213	1057	631	213	213	0	0

- Molecule 3 is a protein called WD repeat-containing protein 55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BC	338	2580	1616	461	489	14	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L1	155	3294	1470	579	1090	155	0	0

- Molecule 5 is a RNA chain called ITS2 rRNA.

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

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	L3	2585	55445	24687	10158	18015	2585	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	2503	G	U	conflict	GB 86475748
L3	2505	C	G	conflict	GB 86475748

- Molecule 7 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	120	Total	C	N	O	S	0	0
			998	625	218	154	1		

- Molecule 8 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 9 is a protein called 60S ribosomal protein L14.

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

- Molecule 10 is a protein called 60S ribosomal protein L15.

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

- Molecule 11 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	138	Total	C	N	O	S	0	0
			1106	693	208	197	8		

- Molecule 12 is a protein called 60S ribosomal protein L18.

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

- Molecule 13 is a protein called 60S ribosomal protein L18a.

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

- Molecule 14 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LD	132	Total	C	N	O	S	0	0
			1117	704	233	173	7		

- Molecule 15 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LE	113	Total	C	N	O	S	0	0
			926	589	176	159	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LG	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 17 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH	135	Total	C	N	O	S	0	0
			1084	694	203	186	1		

- Molecule 18 is a protein called 60S ribosomal protein L26.

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

- Molecule 19 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 20 is a protein called 60S ribosomal protein L27a.

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

- Molecule 21 is a protein called 60S ribosomal protein L28.

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

- Molecule 22 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	358	Total	C	N	O	S	0	0
			2884	1834	531	506	13		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	LP	106	Total	C	N	O	0	0
			526	314	106	106		

- Molecule 25 is a protein called 60S ribosomal protein L32.

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

- Molecule 26 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	63	Total	C	N	O	S	0	0
			485	303	100	77	5		

- Molecule 27 is a protein called 60S ribosomal protein L35.

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

- Molecule 28 is a protein called 60S ribosomal protein L35a.

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

- Molecule 29 is a protein called 60S ribosomal protein L36.

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

- Molecule 30 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LW	74	Total	C	N	O	S	0	0
			612	379	134	94	5		

- Molecule 31 is a protein called Nucleolar complex protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NA	484	Total	C	N	O	S	0	0
			3389	2157	608	609	15		

- Molecule 32 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NB	71	Total	C	N	O	S	0	0
			603	376	125	99	3		

- Molecule 33 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NF	209	Total	C	N	O	S	0	0
			1696	1078	322	287	9		

- Molecule 34 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NH	180	Total	C	N	O	S	0	0
			1441	925	245	263	8		

- Molecule 35 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NI	612	Total	C	N	O	S	0	0
			4832	3067	866	884	15		

- Molecule 36 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 38 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SC	214	Total	C	N	O	S	0	0
			1721	1107	327	283	4		

- Molecule 39 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 40 is a protein called 60S ribosomal protein L7a.

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

- Molecule 41 is a protein called 60S ribosomal protein L9.

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

- Molecule 42 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 43 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SI	229	Total	C	N	O	S	1	0
			1896	1230	354	308	4		

- Molecule 44 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SJ	255	Total	C	N	O	S	0	0
			1939	1206	381	348	4		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 46 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 47 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SM	500	Total	C	N	O	S	0	0
			4113	2643	738	716	16		

- Molecule 48 is a protein called Probable rRNA-processing protein EBP2.

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

- Molecule 49 is a protein called Ribosome biogenesis protein BRX1 homolog.

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

- Molecule 50 is a protein called Ribosome biogenesis protein WDR12.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SP	397	Total	C	N	O	S	0	0
			2983	1880	507	579	17		

- Molecule 51 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 52 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SR	466	Total	C	N	O	S	0	0
			3841	2437	681	705	18		

- Molecule 53 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	SS	628	Total	C	N	O	P	S	0	0
			5041	3197	915	907	2	20		

- Molecule 54 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ST	148	Total	C	N	O	S	0	0
			1091	675	207	206	3		

- Molecule 55 is a protein called Nucleolar complex protein 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SU	552	Total 4360	C 2795	N 748	O 796	S 21	0	0

- Molecule 56 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 57 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SW	448	Total 3580	C 2299	N 615	O 649	S 17	0	0

- Molecule 58 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SY	378	Total 2985	C 1887	N 533	O 550	S 15	0	0

- Molecule 59 is a protein called Nucleolar protein 16.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	L1	5	Total 5	Mg 5	0
60	L3	56	Total 56	Mg 56	0
60	L9	1	Total 1	Mg 1	0
60	LQ	2	Total 2	Mg 2	0
60	LT	1	Total 1	Mg 1	0
60	NI	1	Total 1	Mg 1	0

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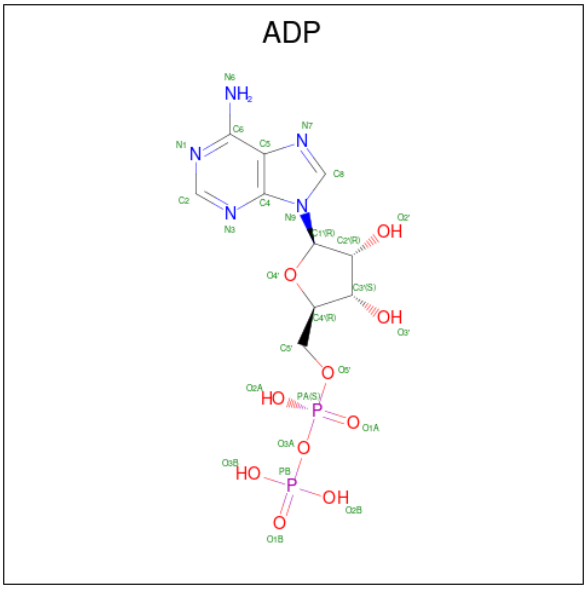
Mol	Chain	Residues	Atoms	AltConf
60	SA	1	Total Mg 1 1	0
60	SO	1	Total Mg 1 1	0
60	SR	1	Total Mg 1 1	0
60	SU	1	Total Mg 1 1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

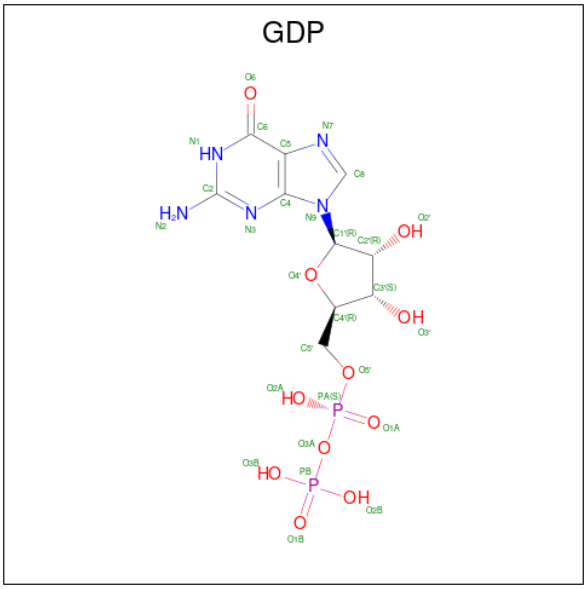
Mol	Chain	Residues	Atoms	AltConf
61	LR	1	Total Zn 1 1	0
61	LW	1	Total Zn 1 1	0
61	SV	1	Total Zn 1 1	0

- Molecule 62 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 64 is POTASSIUM ION (three-letter code: K) (formula: K).

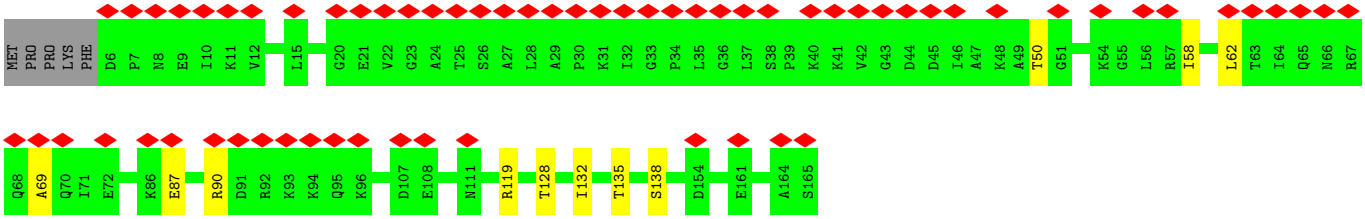
Mol	Chain	Residues	Atoms		AltConf
64	SR	1	Total	K	0
			1	1	

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.

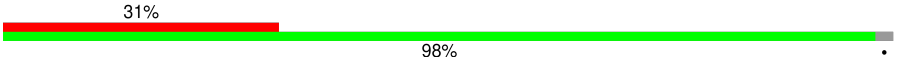
• Molecule 1: 60S ribosomal protein L12

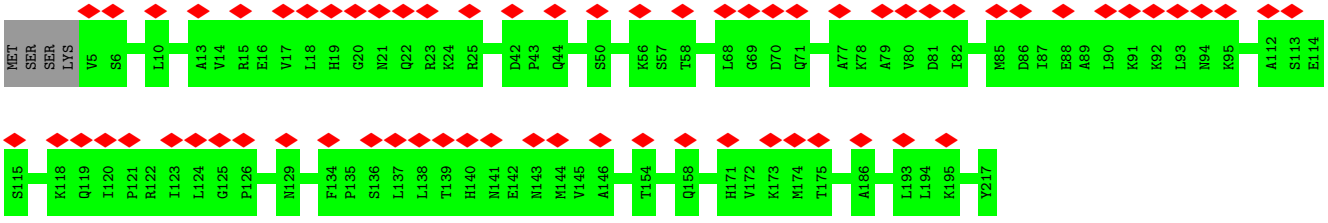
Chain BA:



• Molecule 2: 60S ribosomal protein L10a

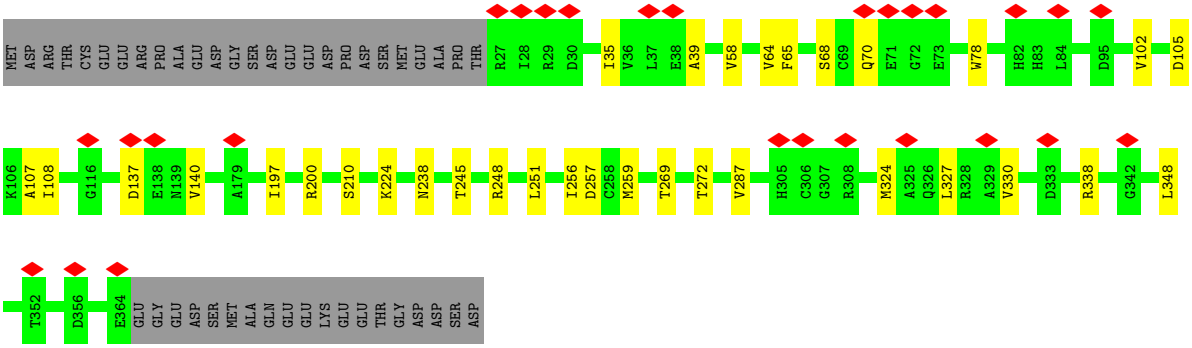
Chain BB:





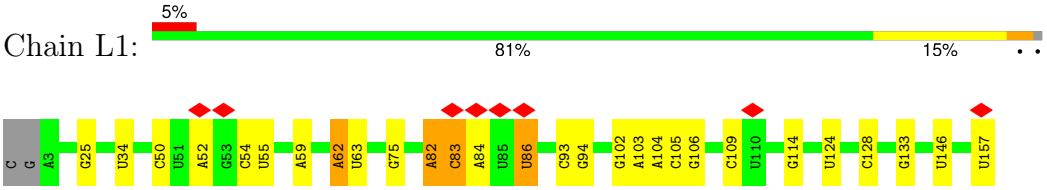
• Molecule 3: WD repeat-containing protein 55

Chain BC:



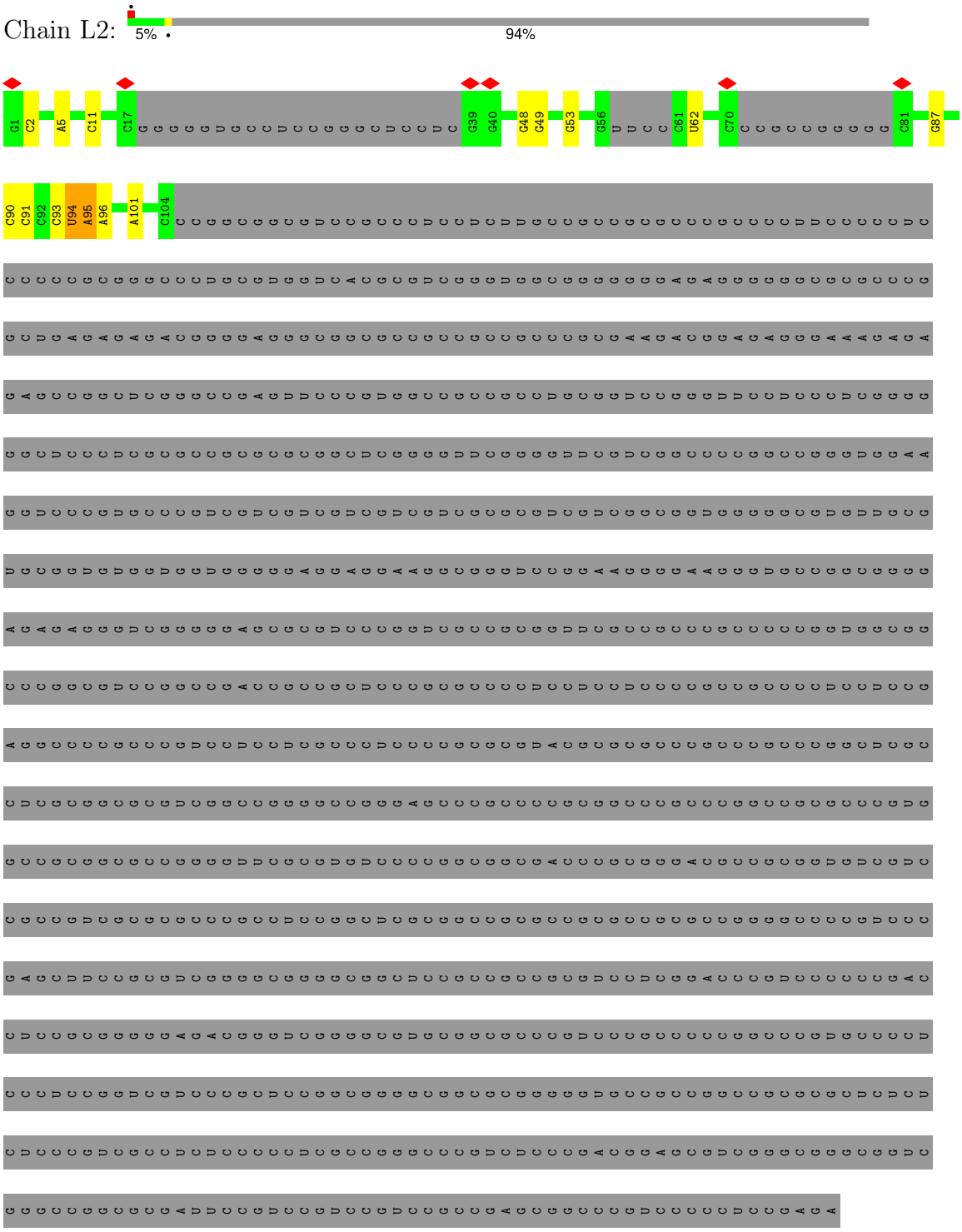
• Molecule 4: 5.8S rRNA

Chain L1:



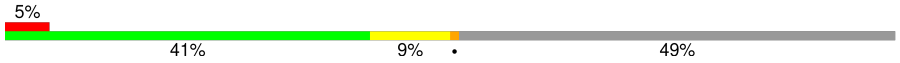
• Molecule 5: ITS2 rRNA

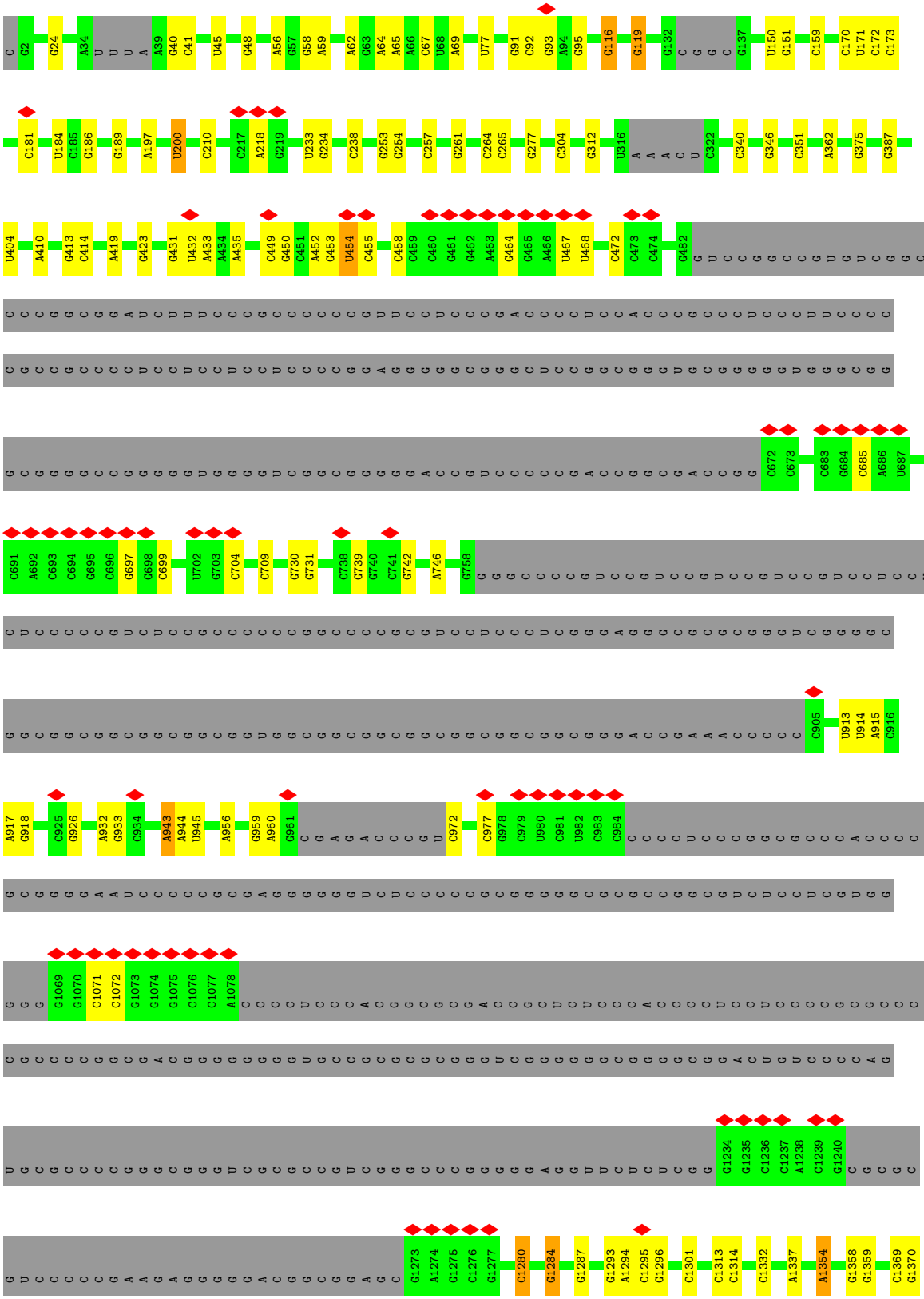
Chain L2:

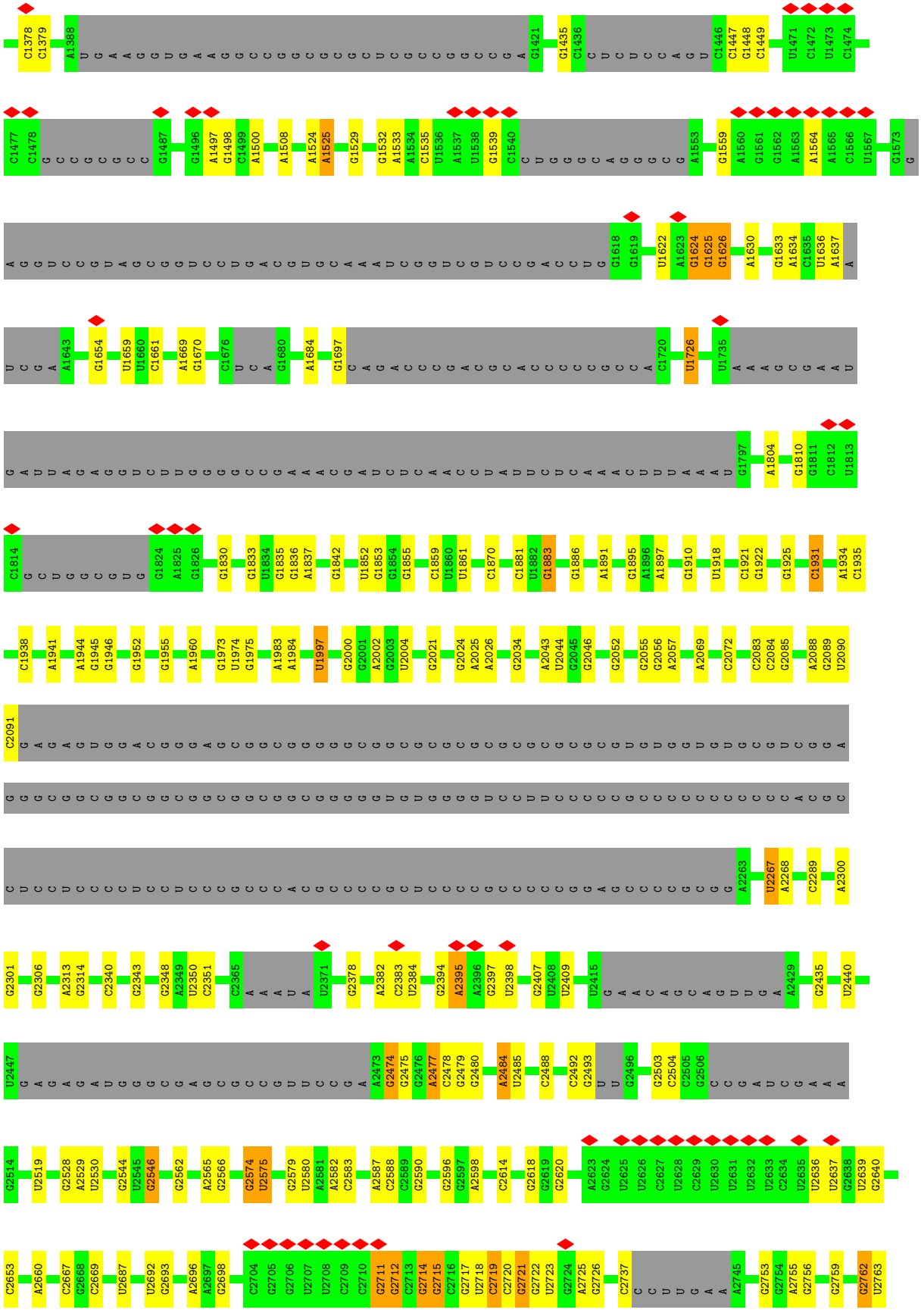


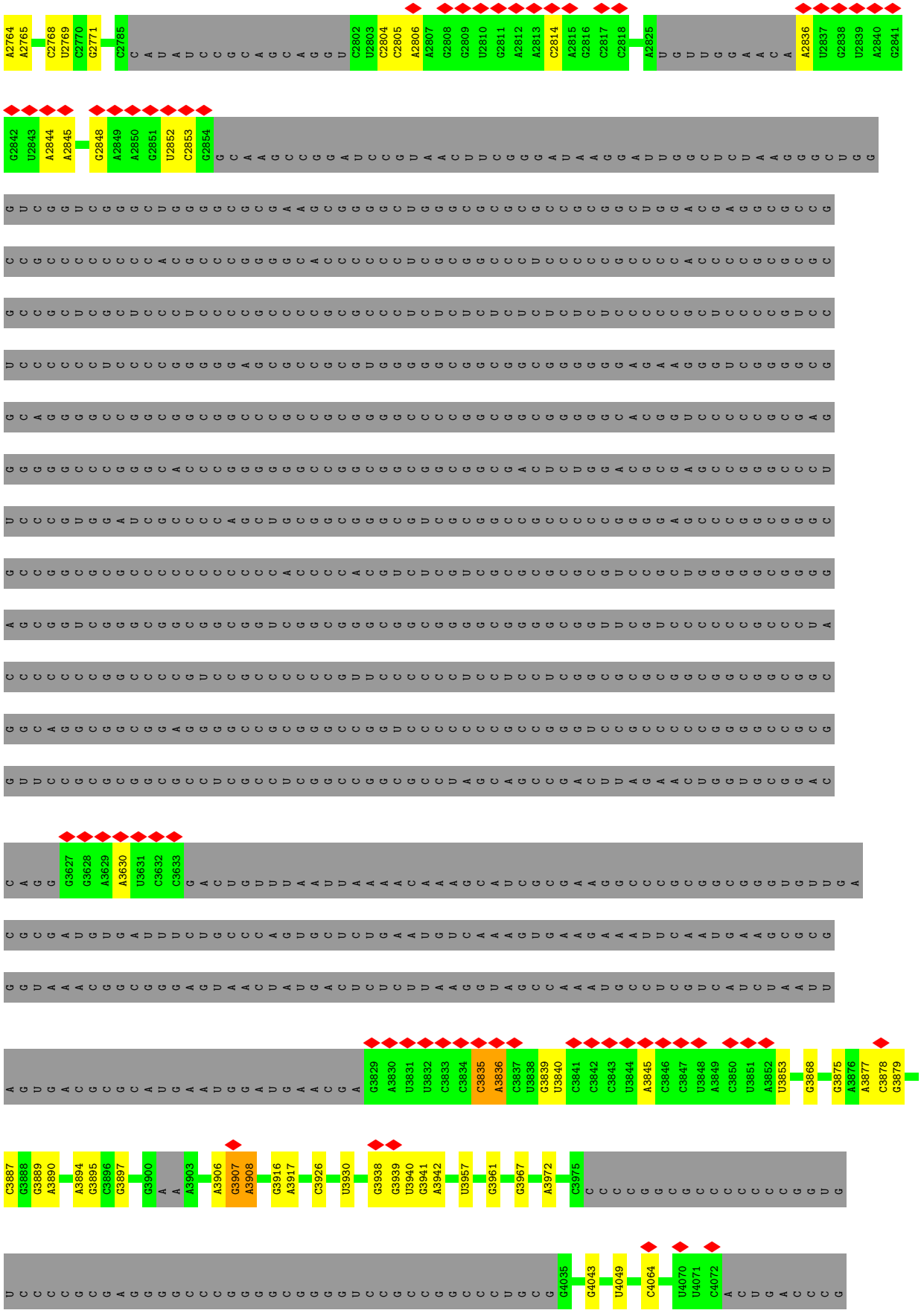
• Molecule 6: 28S rRNA

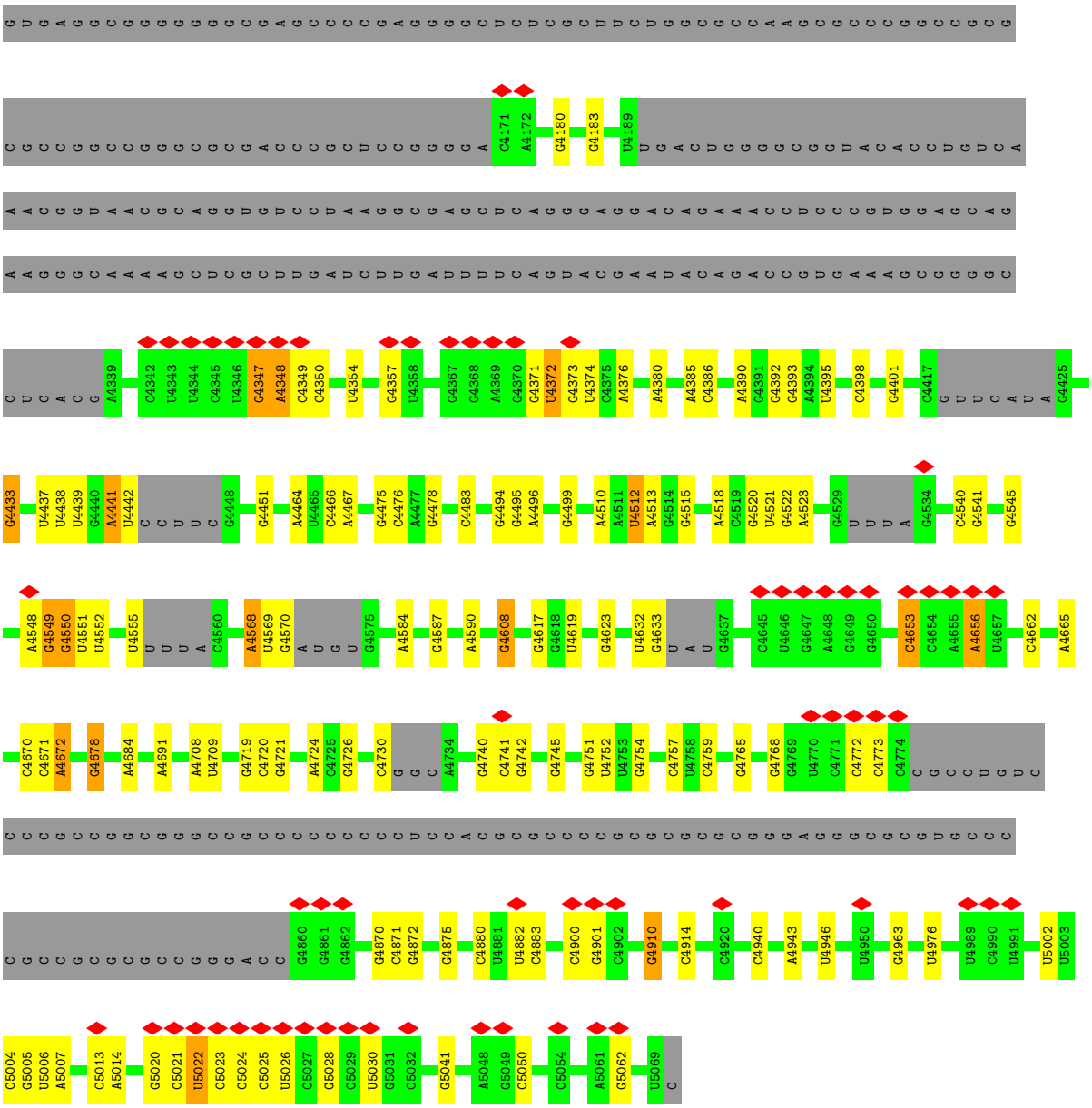
Chain L3:





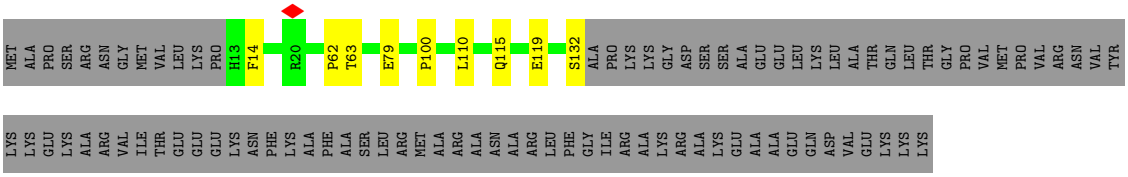






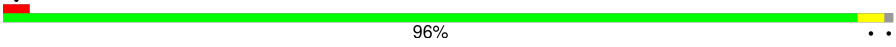
• Molecule 7: 60S ribosomal protein L13

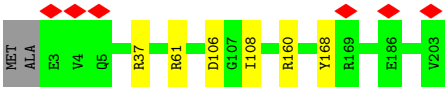
Chain L6:



• Molecule 8: 60S ribosomal protein L13a

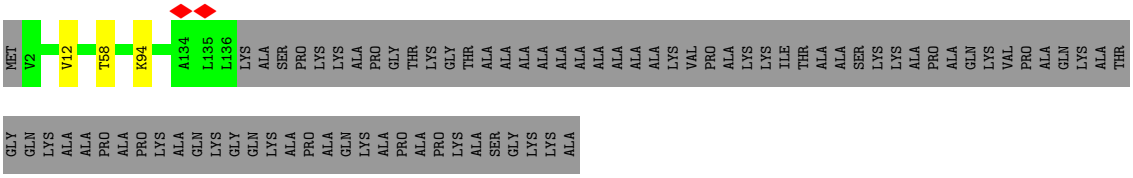
Chain L7:





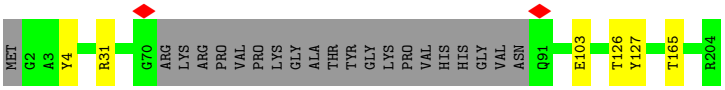
• Molecule 9: 60S ribosomal protein L14

Chain L8:



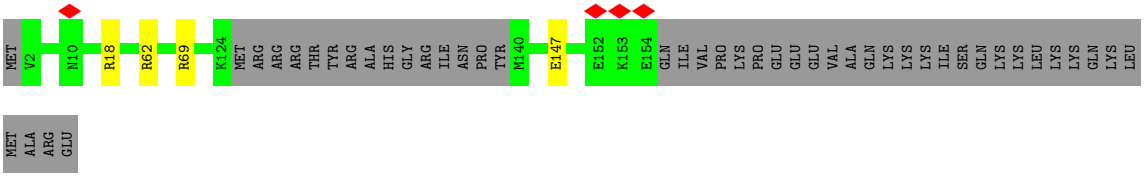
• Molecule 10: 60S ribosomal protein L15

Chain L9:



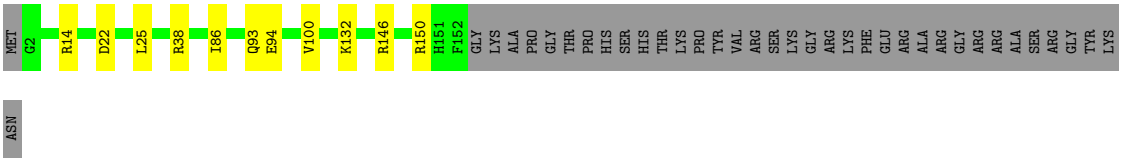
• Molecule 11: 60S ribosomal protein L17

Chain LA:



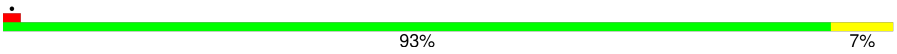
• Molecule 12: 60S ribosomal protein L18

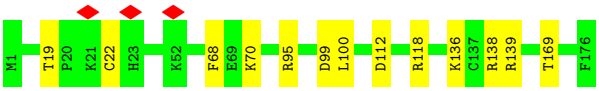
Chain LB:



• Molecule 13: 60S ribosomal protein L18a

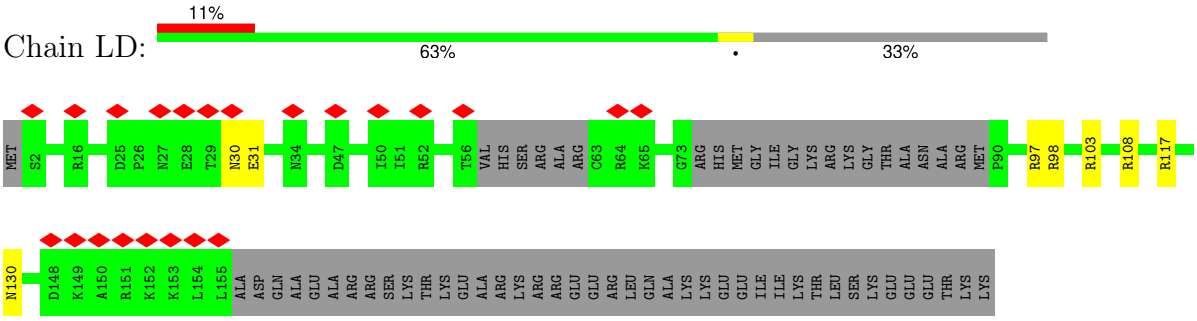
Chain LC:





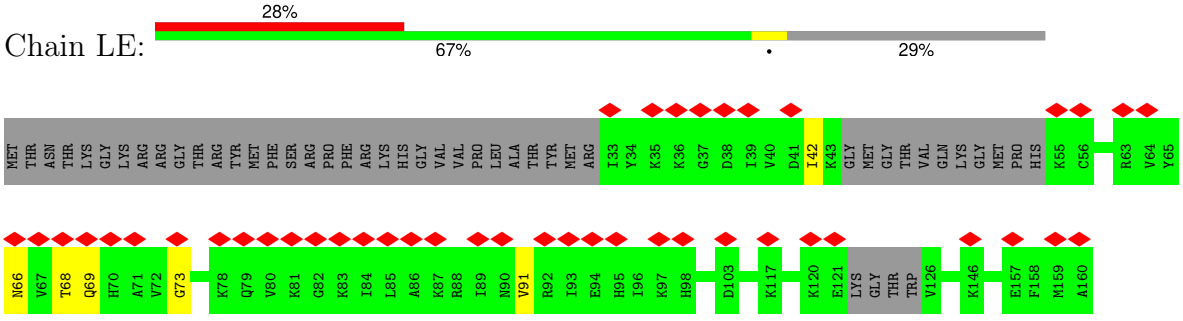
• Molecule 14: 60S ribosomal protein L19

Chain LD:



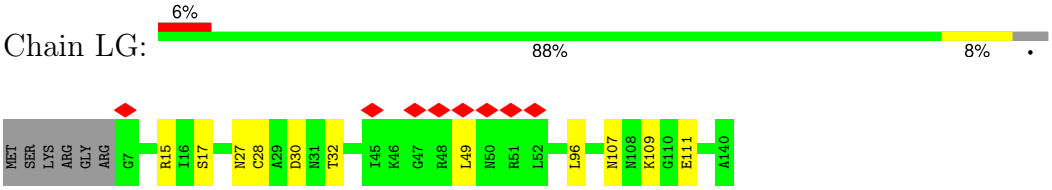
• Molecule 15: 60S ribosomal protein L21

Chain LE:



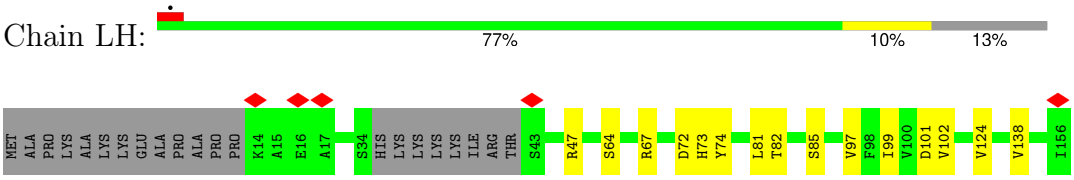
• Molecule 16: 60S ribosomal protein L23

Chain LG:



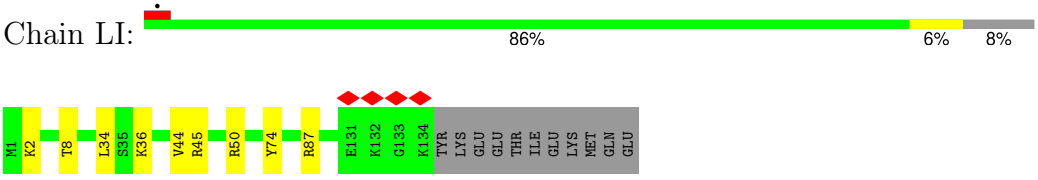
• Molecule 17: 60S ribosomal protein L23a

Chain LH:



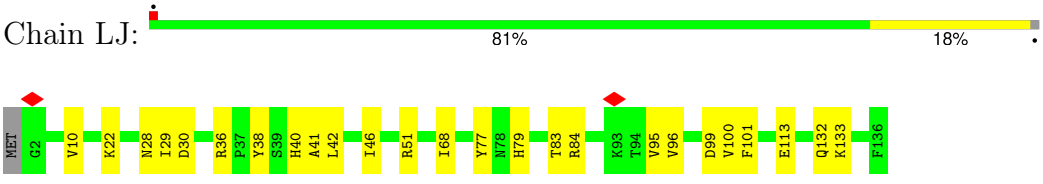
• Molecule 18: 60S ribosomal protein L26

Chain LI:



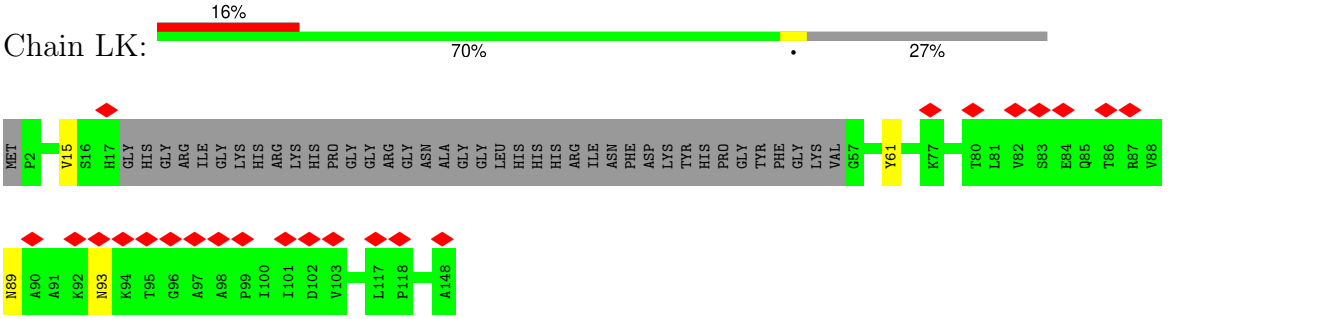
• Molecule 19: 60S ribosomal protein L27

Chain LJ:



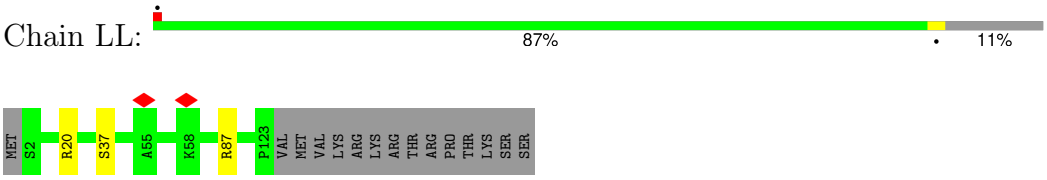
• Molecule 20: 60S ribosomal protein L27a

Chain LK:



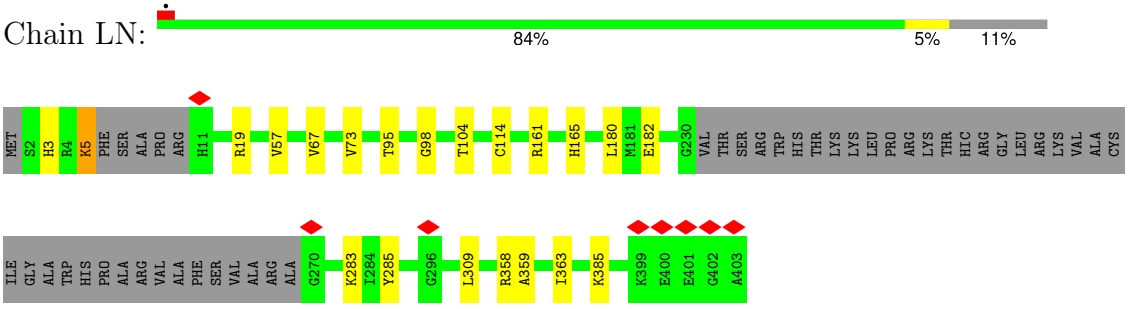
• Molecule 21: 60S ribosomal protein L28

Chain LL:



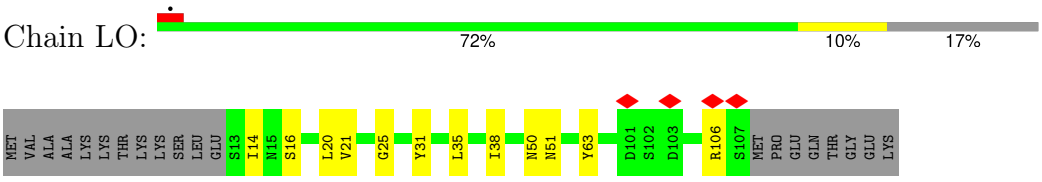
• Molecule 22: 60S ribosomal protein L3

Chain LN:



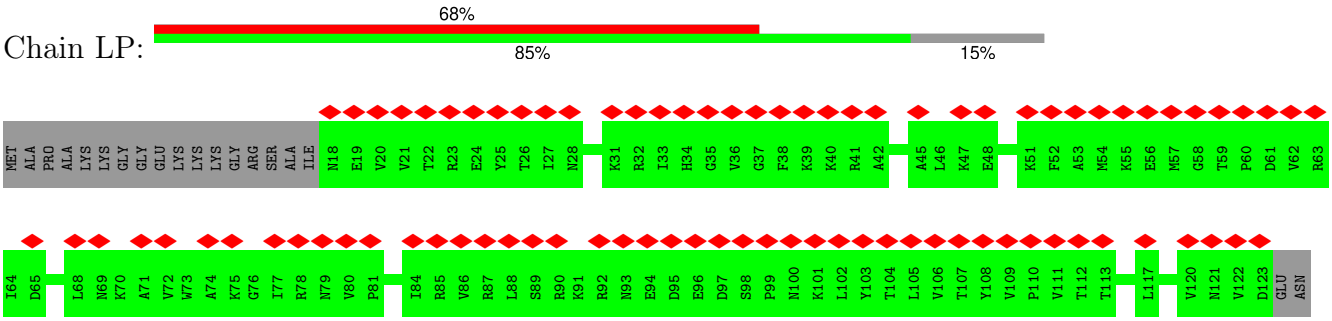
• Molecule 23: 60S ribosomal protein L30

Chain LO:



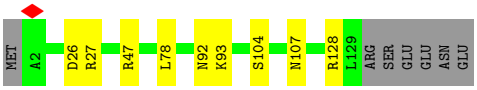
• Molecule 24: 60S ribosomal protein L31

Chain LP:



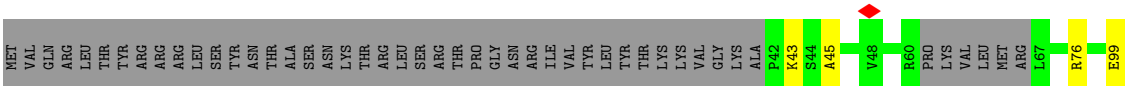
• Molecule 25: 60S ribosomal protein L32

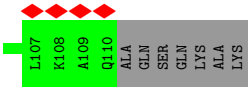
Chain LQ:



• Molecule 26: 60S ribosomal protein L34

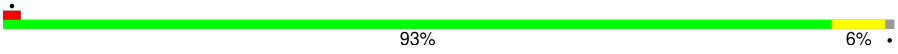
Chain LR:

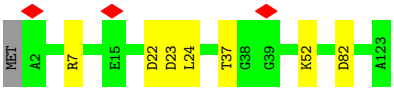




• Molecule 27: 60S ribosomal protein L35

Chain LS:



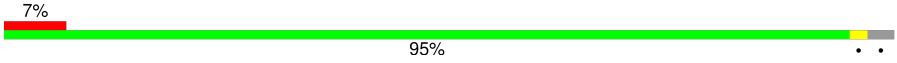


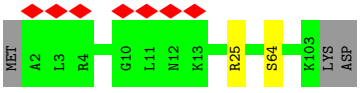
• Molecule 28: 60S ribosomal protein L35a

Chain LT:

• Molecule 29: 60S ribosomal protein L36

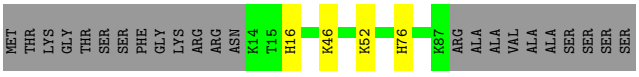
Chain LU:





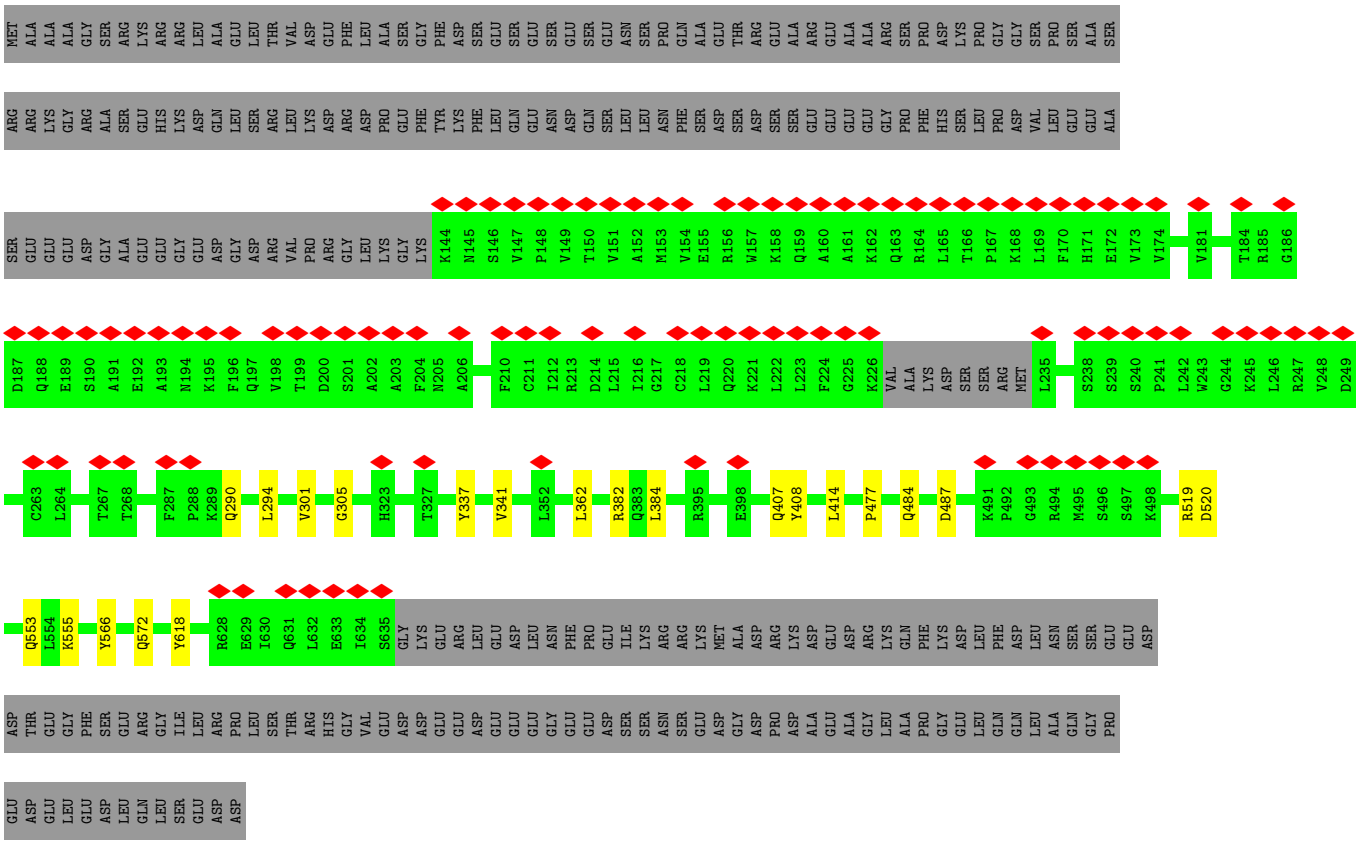
• Molecule 30: 60S ribosomal protein L37

Chain LW:



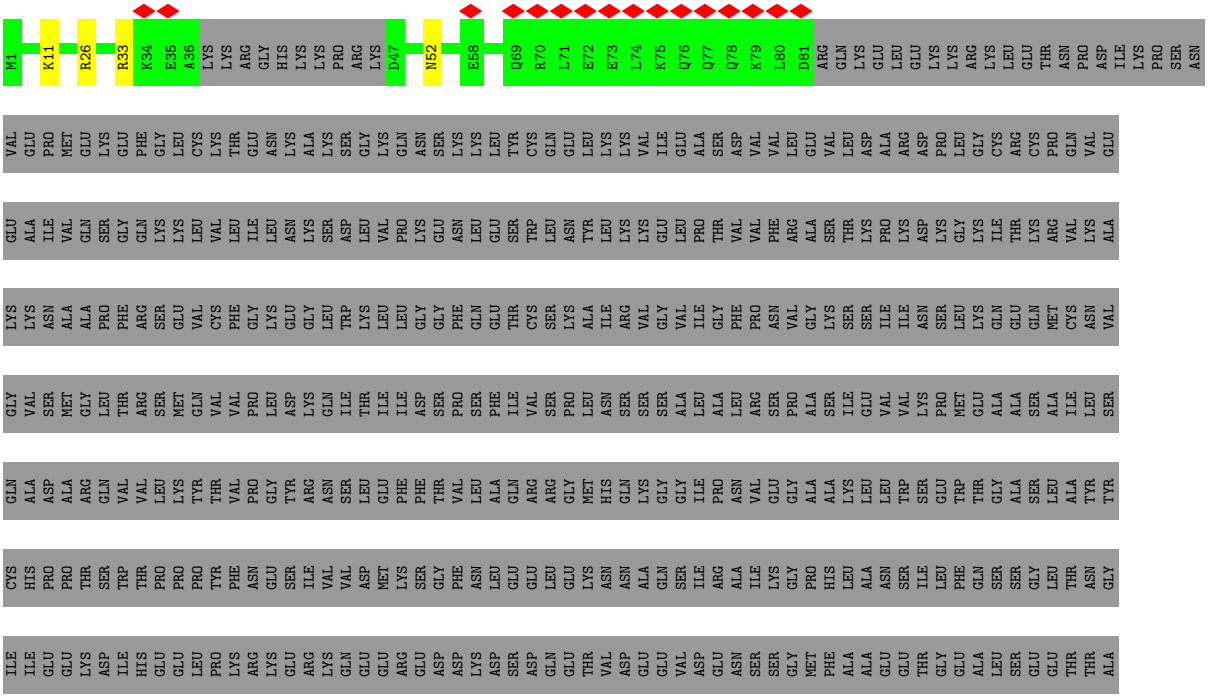
• Molecule 31: Nucleolar complex protein 2 homolog

Chain NA:



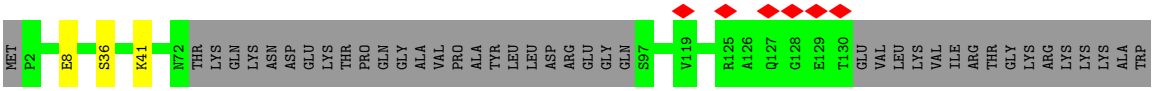
• Molecule 32: Guanine nucleotide-binding protein-like 3

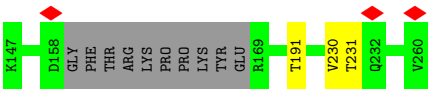
Chain NB:



• Molecule 33: Ribosome biogenesis protein NSA2 homolog

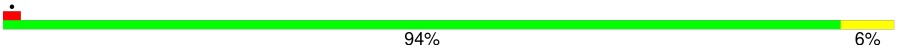
Chain NF:

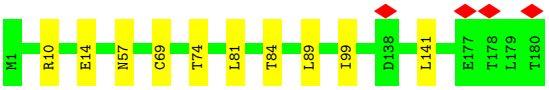




• Molecule 34: 60S ribosome subunit biogenesis protein NIP7 homolog

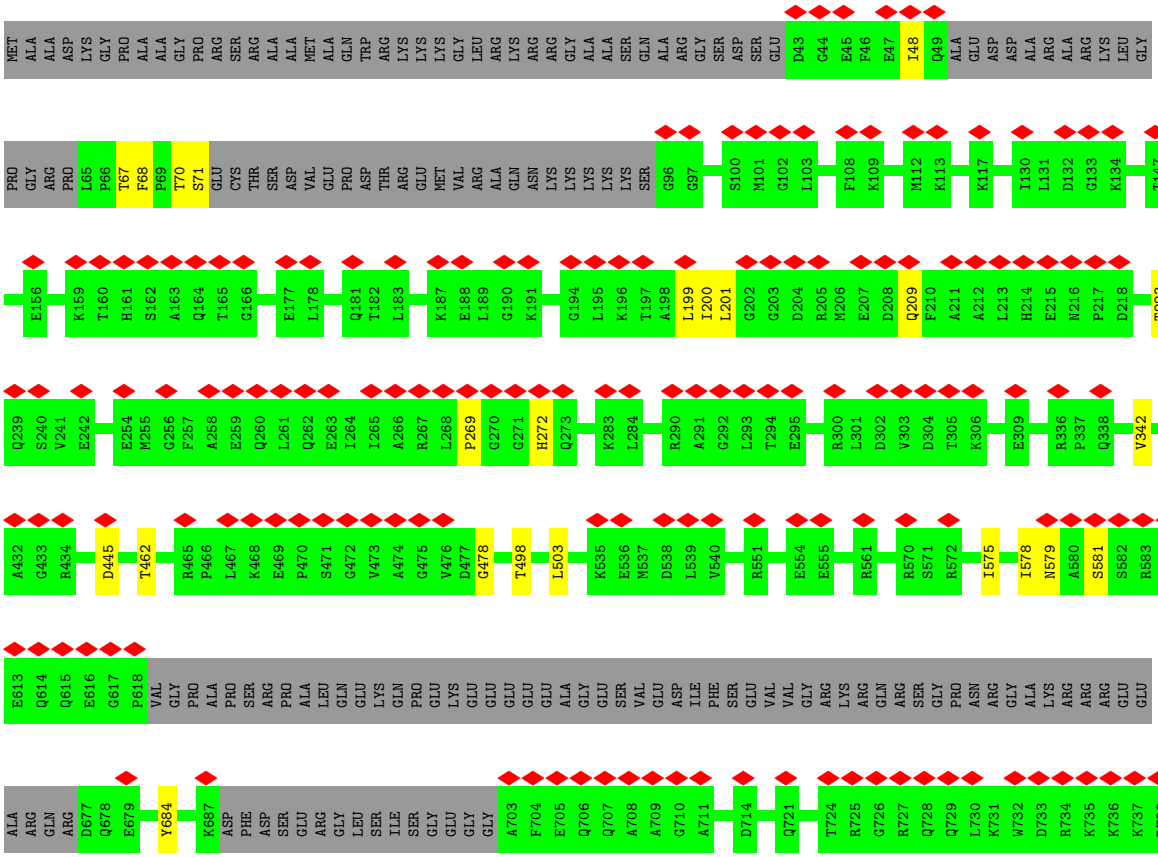
Chain NH:

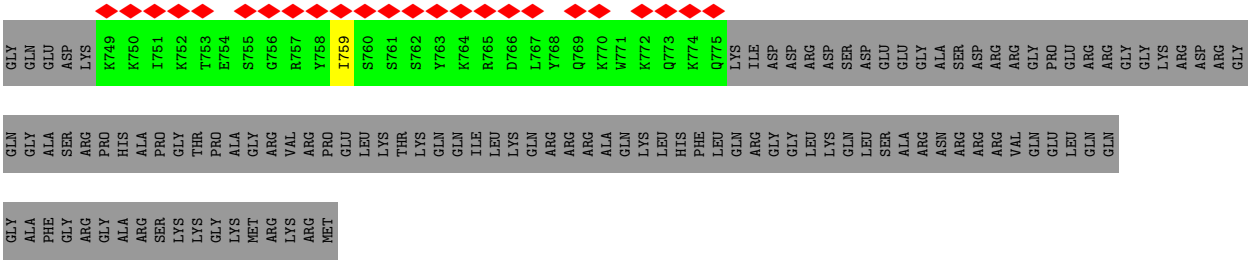




• Molecule 35: ATP-dependent RNA helicase DDX54

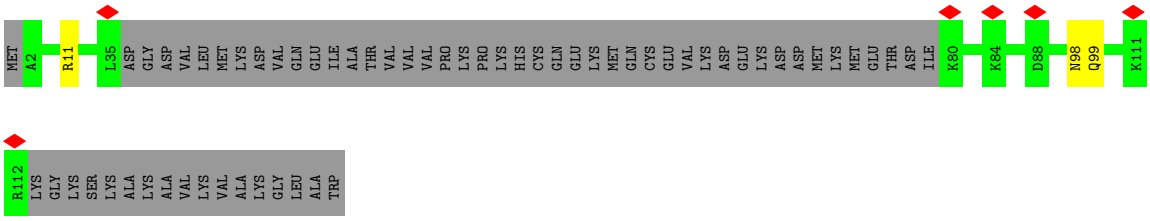
Chain NI:





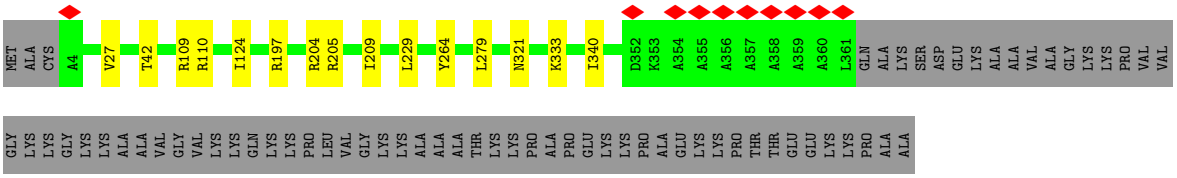
• Molecule 36: Protein LLP homolog

Chain NK:



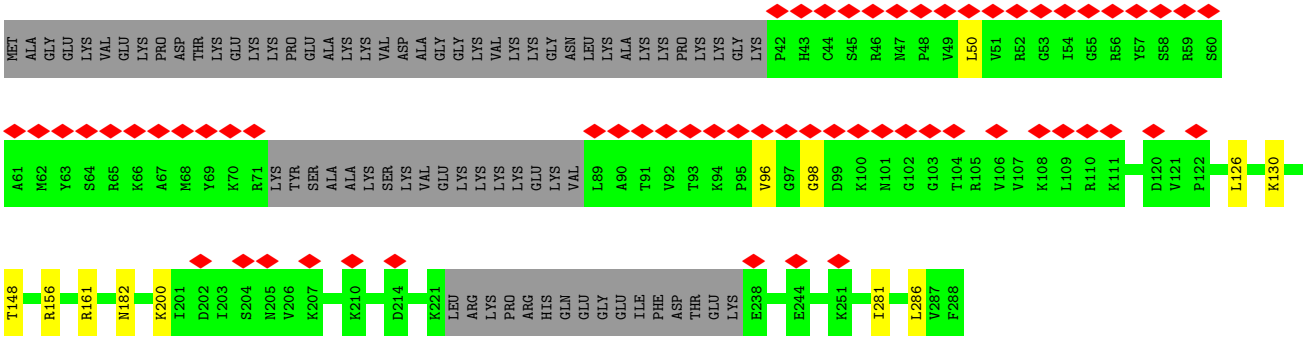
• Molecule 37: 60S ribosomal protein L4

Chain SA:



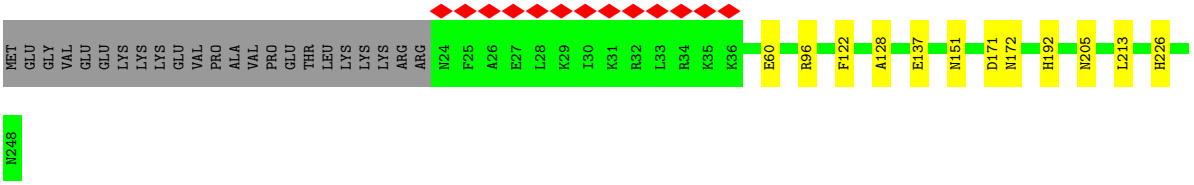
• Molecule 38: 60S ribosomal protein L6

Chain SC:



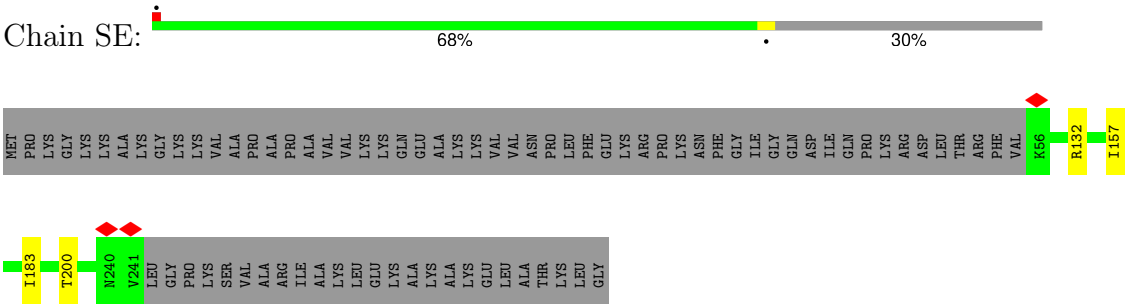
• Molecule 39: 60S ribosomal protein L7

Chain SD:



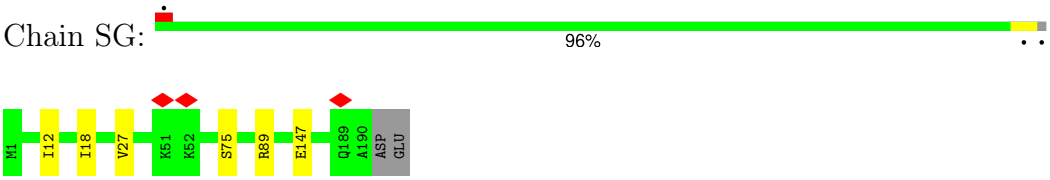
• Molecule 40: 60S ribosomal protein L7a

Chain SE:



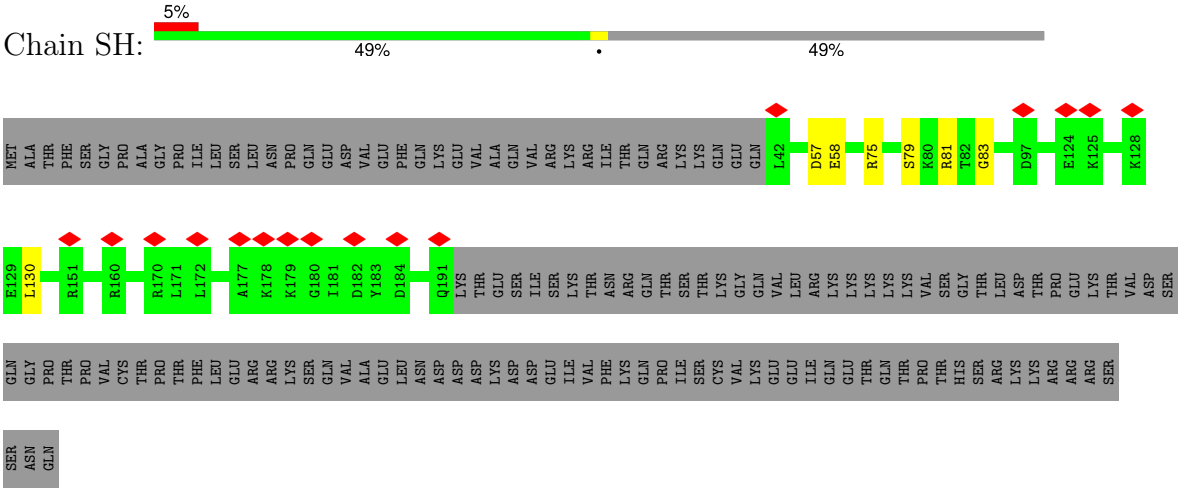
• Molecule 41: 60S ribosomal protein L9

Chain SG:



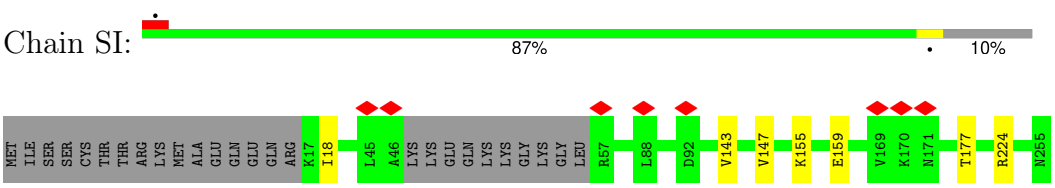
• Molecule 42: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain SH:



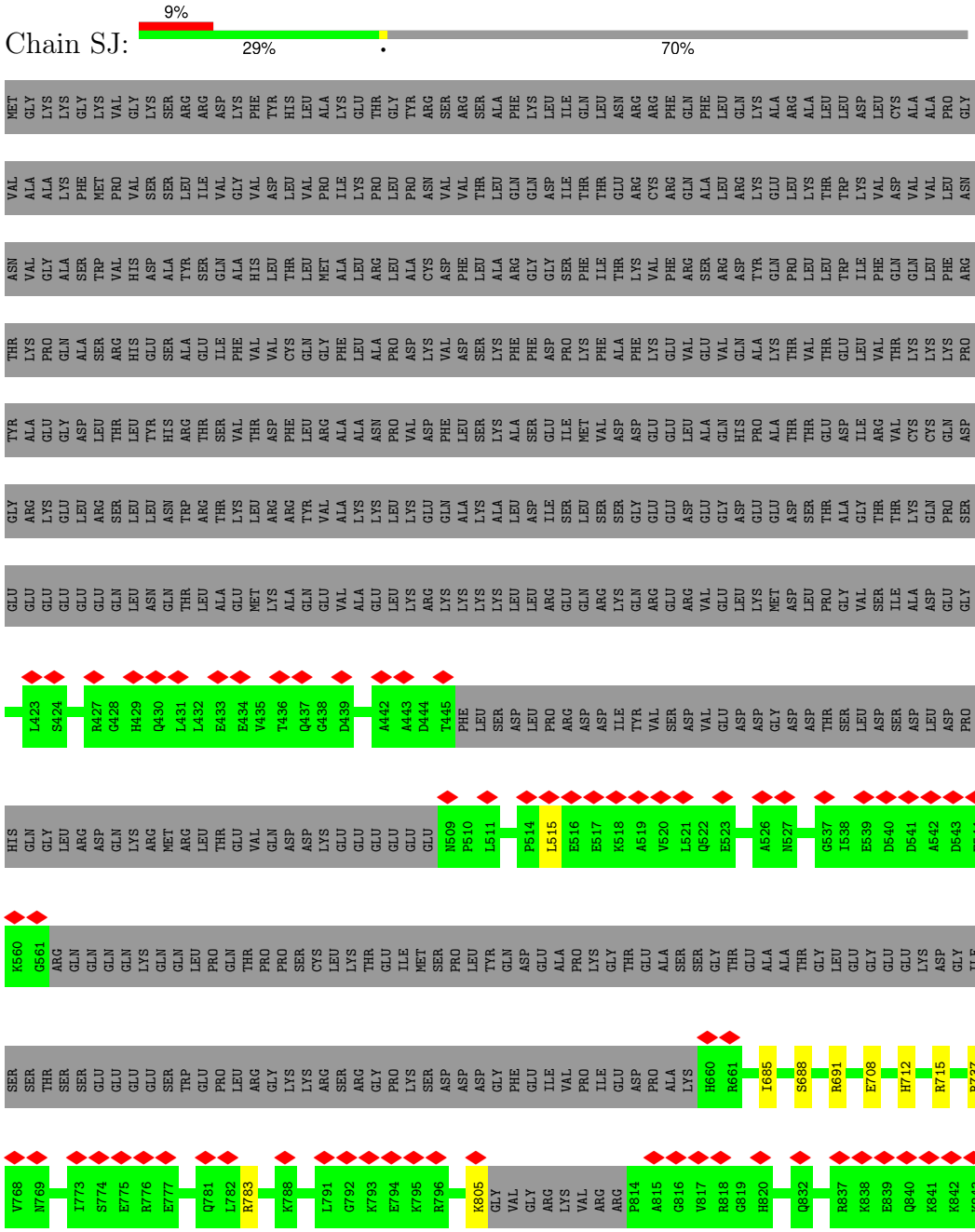
• Molecule 43: 60S ribosomal protein L7-like 1

Chain SI:



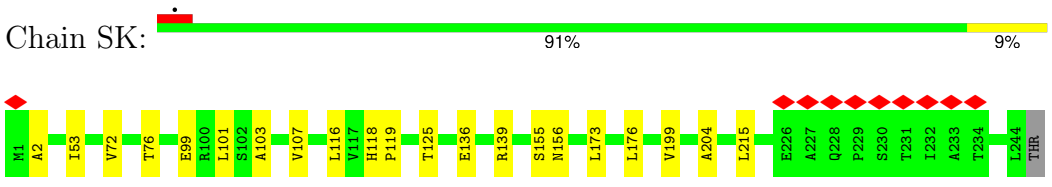
• Molecule 44: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

Chain SJ:



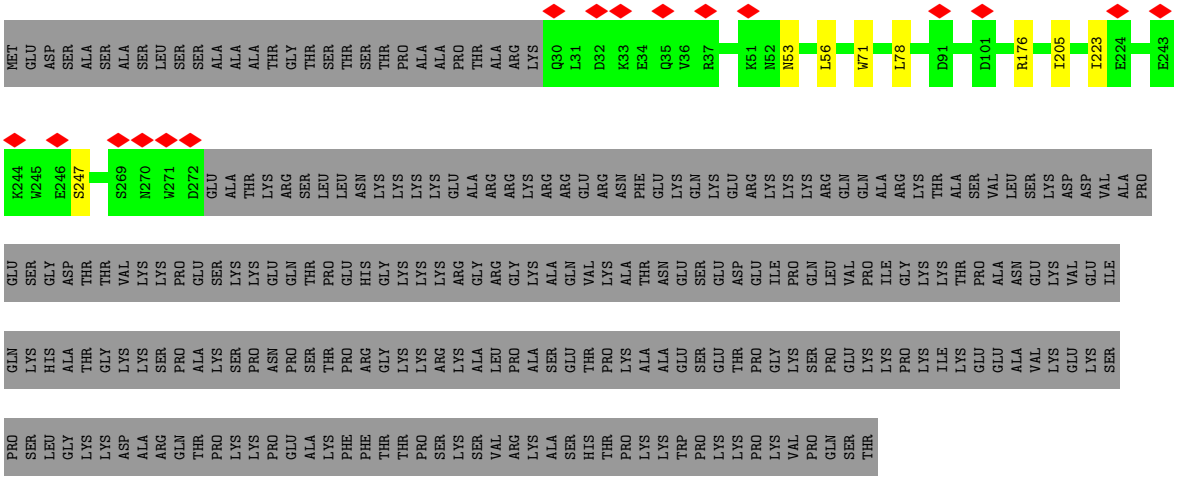
• Molecule 45: Eukaryotic translation initiation factor 6

Chain SK:



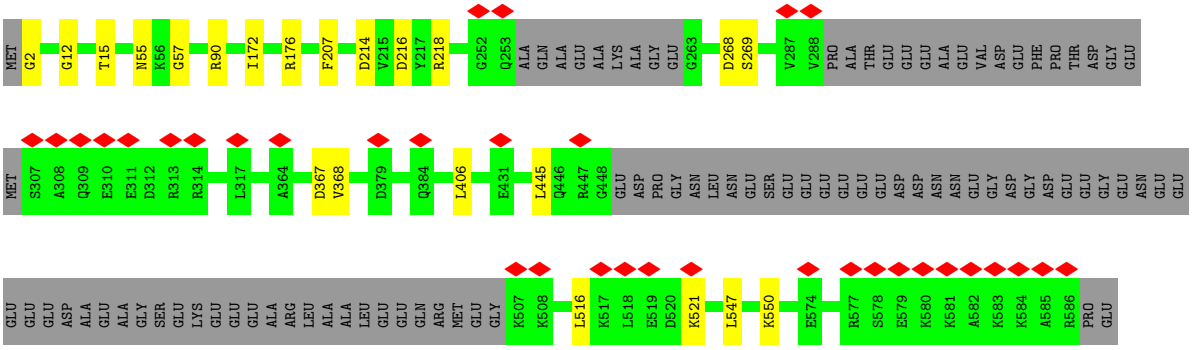
• Molecule 46: Ribosomal L1 domain-containing protein 1

Chain SL:



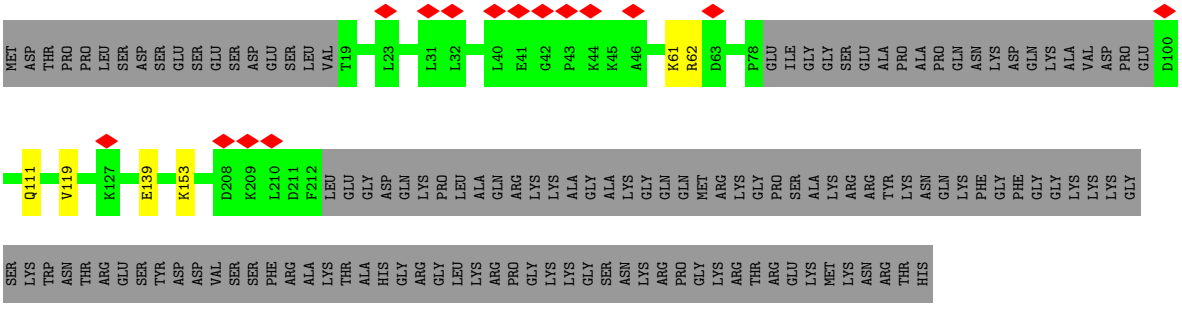
• Molecule 47: Pescadillo homolog

Chain SM:



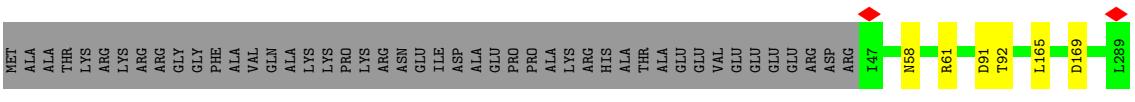
• Molecule 48: Probable rRNA-processing protein EBP2

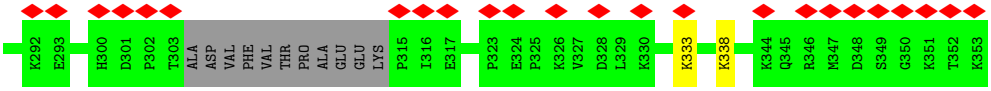
Chain SN:



• Molecule 49: Ribosome biogenesis protein BRX1 homolog

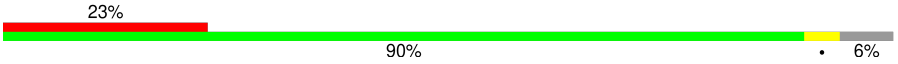
Chain SO:

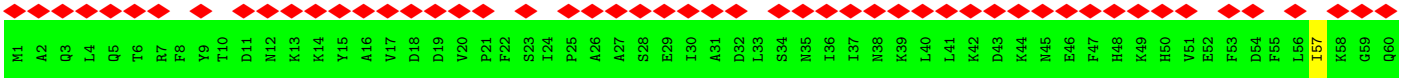


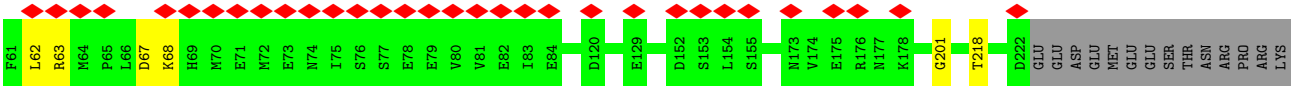


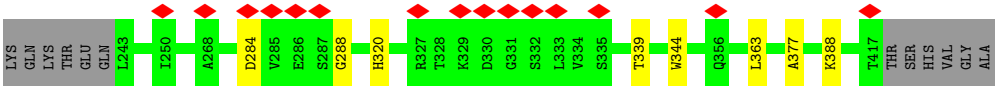
• Molecule 50: Ribosome biogenesis protein WDR12

Chain SP:



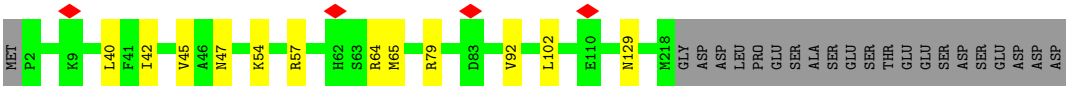






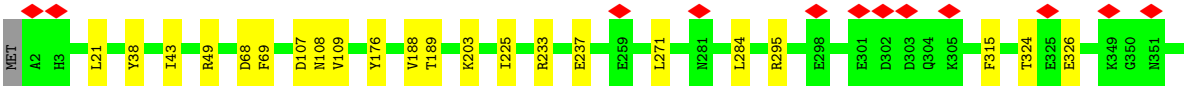
• Molecule 51: mRNA turnover protein 4 homolog

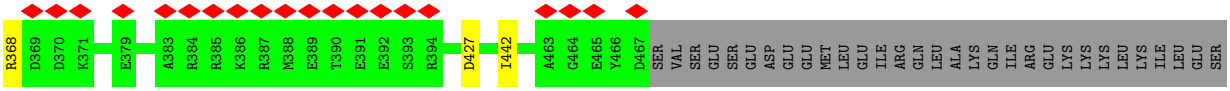
Chain SQ:



• Molecule 52: GTP-binding protein 4

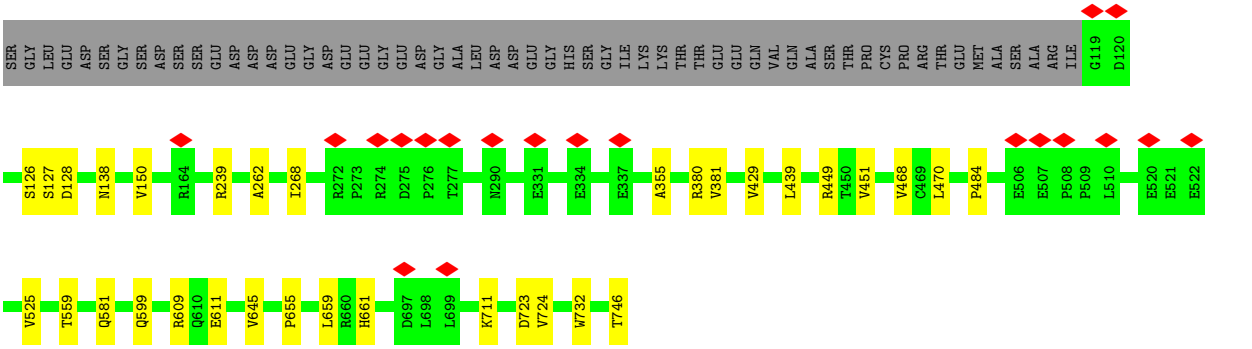
Chain SR:





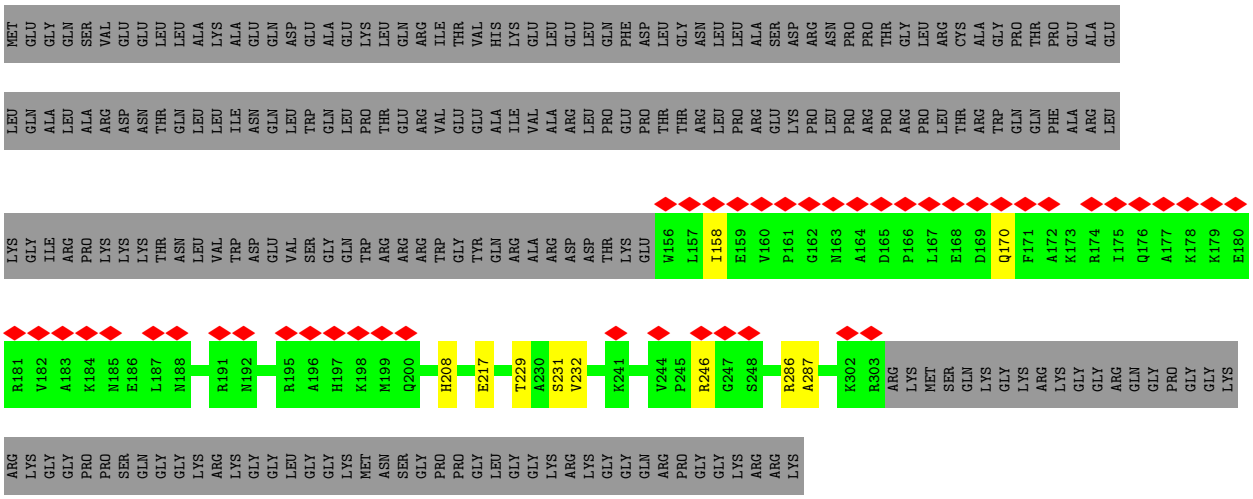
• Molecule 53: Ribosome biogenesis protein BOP1

Chain SS:



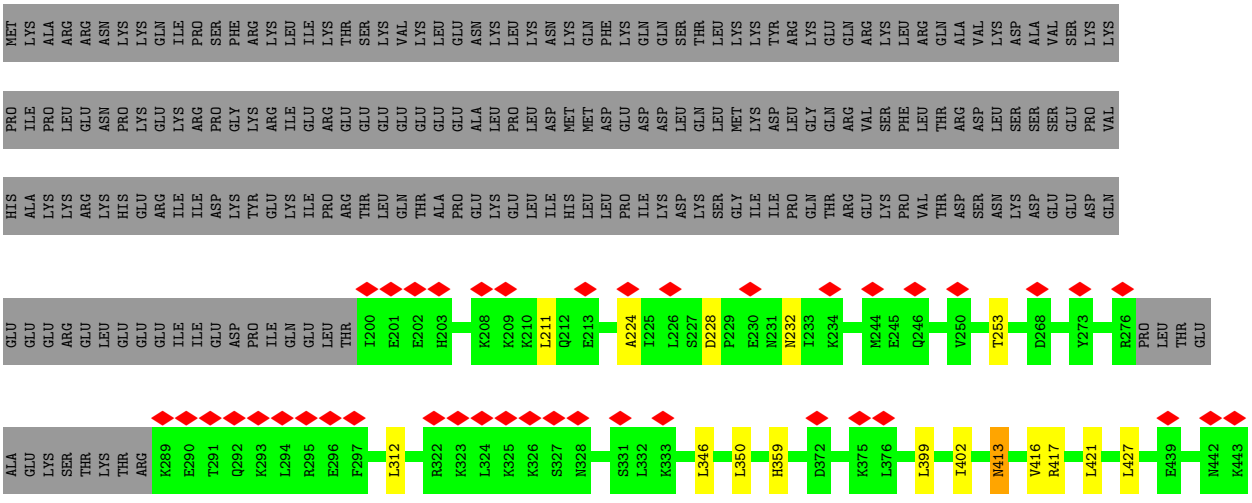
• Molecule 54: Ribosome biogenesis regulatory protein homolog

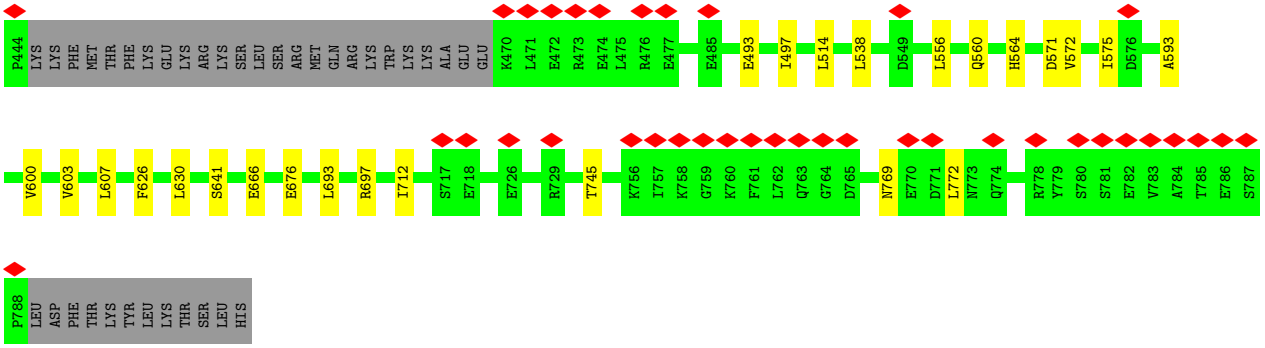
Chain ST:



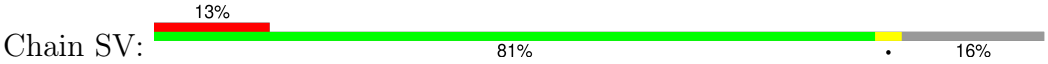
• Molecule 55: Nucleolar complex protein 3 homolog

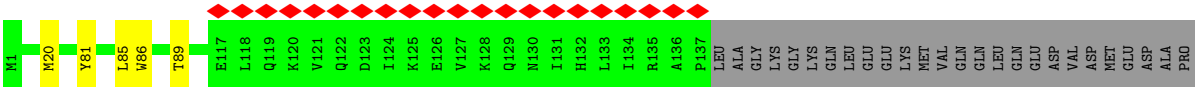
Chain SU:



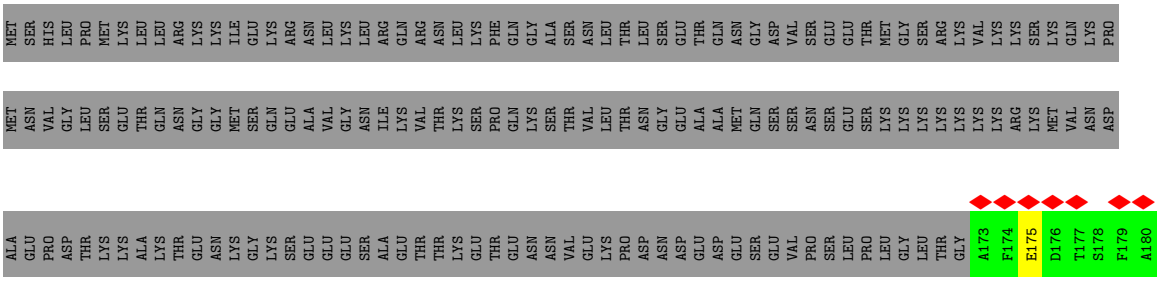


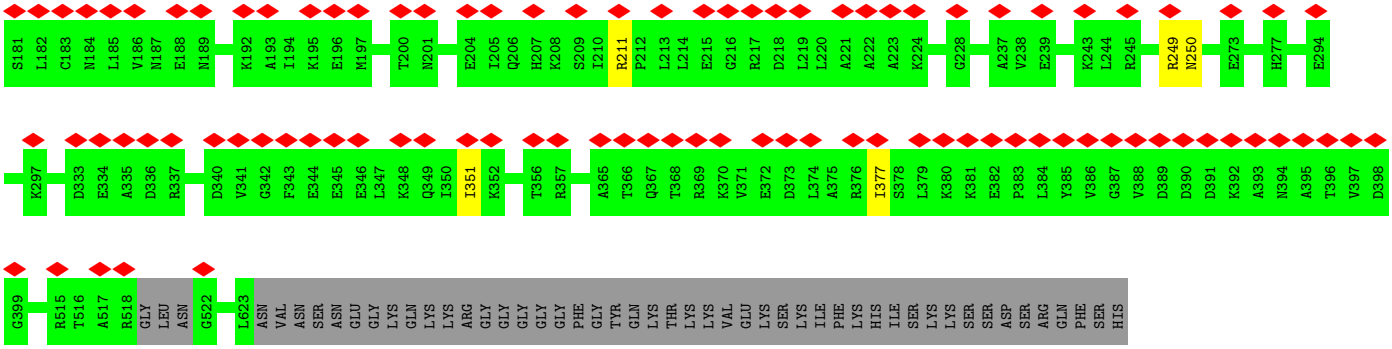
• Molecule 56: Probable ribosome biogenesis protein RLP24



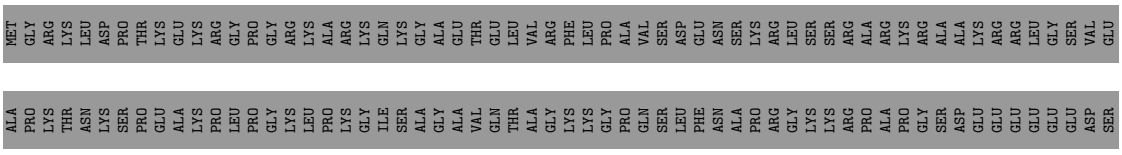


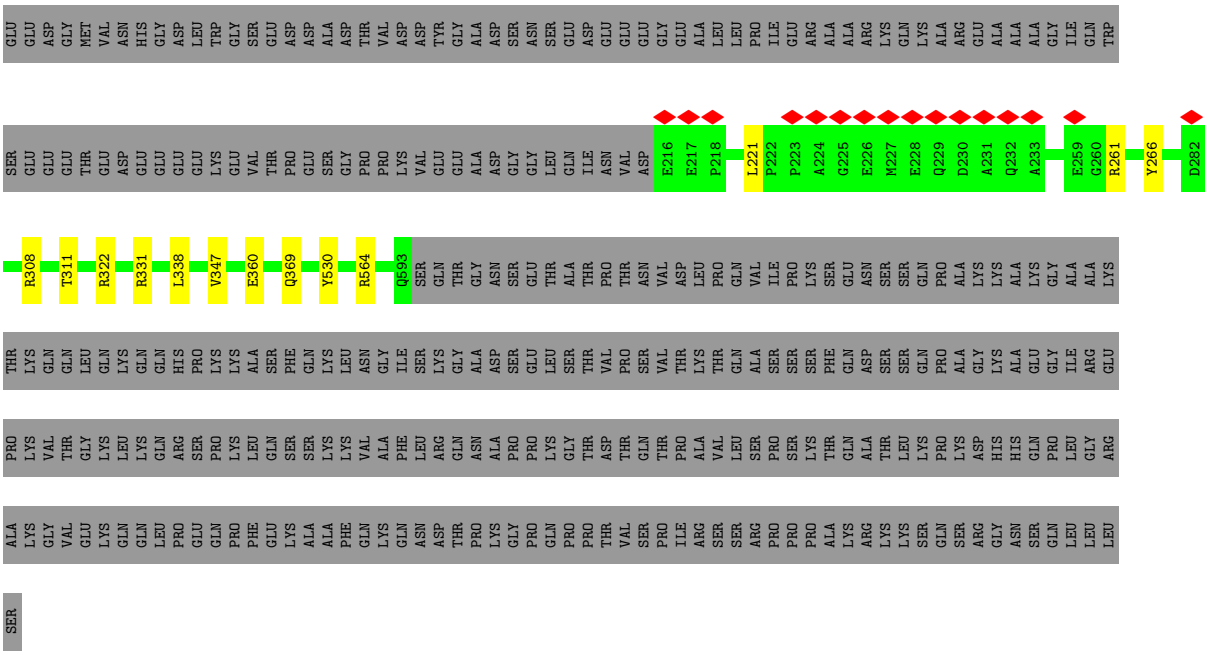
• Molecule 57: ATP-dependent RNA helicase DDX18





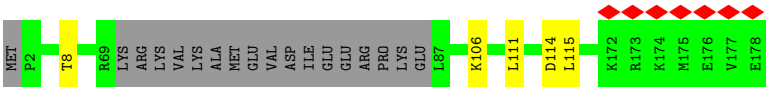
• Molecule 58: Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase





• Molecule 59: 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	76907	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	9.161	Depositor
Minimum map value	0.000	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.192	Depositor
Recommended contour level	0.85	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: ZN, MG, K, ADP, SEP, GDP

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	0.24	0/1224	0.50	0/1651
2	BB	0.24	0/1056	0.45	0/1472
3	BC	0.25	0/2628	0.56	0/3551
4	L1	0.27	0/3678	0.74	1/5729 (0.0%)
5	L2	0.23	0/1634	0.78	0/2538
6	L3	0.26	0/61994	0.77	2/96630 (0.0%)
7	L6	0.25	0/1020	0.65	0/1367
8	L7	0.26	0/1682	0.55	0/2250
9	L8	0.25	0/1133	0.52	0/1516
10	L9	0.25	0/1584	0.63	0/2117
11	LA	0.24	0/1127	0.51	0/1511
12	LB	0.25	0/1239	0.64	0/1658
13	LC	0.26	0/1501	0.57	0/2013
14	LD	0.24	0/1129	0.58	0/1492
15	LE	0.25	0/941	0.50	0/1254
16	LG	0.26	0/1007	0.55	0/1350
17	LH	0.25	0/1101	0.51	0/1475
18	LI	0.26	0/1132	0.61	0/1504
19	LJ	0.27	0/1130	0.56	0/1507
20	LK	0.23	0/648	0.52	0/880
21	LL	0.25	0/995	0.59	0/1334
22	LN	0.25	0/2938	0.53	0/3923
23	LO	0.27	0/748	0.51	0/1004
24	LP	0.23	0/525	0.42	0/731
25	LQ	0.24	0/1071	0.56	0/1429
26	LR	0.25	0/488	0.58	0/644
27	LS	0.25	0/1023	0.56	0/1351
28	LT	0.25	0/895	0.60	0/1198
29	LU	0.25	0/854	0.62	0/1129
30	LW	0.26	0/626	0.64	0/829
31	NA	0.25	0/3451	0.45	0/4714
32	NB	0.25	0/610	0.55	0/802

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	NF	0.25	0/1724	0.52	0/2295
34	NH	0.26	0/1473	0.52	0/1988
35	NI	0.24	0/4914	0.49	0/6619
36	NK	0.25	0/587	0.62	0/767
37	SA	0.25	0/2907	0.57	0/3905
38	SC	0.25	0/1754	0.55	0/2353
39	SD	0.26	0/1905	0.55	0/2539
40	SE	0.25	0/1524	0.55	0/2056
41	SG	0.25	0/1548	0.54	0/2081
42	SH	0.25	0/1298	0.51	0/1742
43	SI	0.25	0/1939	0.52	0/2606
44	SJ	0.25	0/1961	0.52	0/2623
45	SK	0.24	0/1877	0.52	0/2554
46	SL	0.25	0/1994	0.51	0/2684
47	SM	0.25	0/4199	0.50	0/5636
48	SN	0.25	0/1368	0.49	0/1830
49	SO	0.24	0/2521	0.51	0/3384
50	SP	0.24	0/3048	0.49	0/4151
51	SQ	0.25	0/1817	0.51	0/2435
52	SR	0.25	0/3916	0.51	0/5283
53	SS	0.25	0/5162	0.54	0/7027
54	ST	0.24	0/1107	0.50	0/1491
55	SU	0.25	0/4433	0.47	0/5976
56	SV	0.29	0/1194	0.56	0/1582
57	SW	0.25	0/3651	0.48	0/4926
58	SY	0.25	0/3046	0.53	0/4117
59	SZ	0.24	0/1364	0.53	0/1826
All	All	0.25	0/167043	0.65	3/239029 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L3	4653	C	C2-N1-C1'	5.97	125.37	118.80
6	L3	1973	G	N9-C4-C5	5.05	107.42	105.40
4	L1	50	C	N3-C2-O2	-5.05	118.37	121.90

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	1208	0	1257	8	0
2	BB	1057	0	464	0	0
3	BC	2580	0	2545	22	0
4	L1	3294	0	1670	12	0
5	L2	1468	0	755	5	0
6	L3	55445	0	28037	160	0
7	L6	998	0	1067	6	0
8	L7	1650	0	1794	5	0
9	L8	1111	0	1174	2	0
10	L9	1546	0	1585	7	0
11	LA	1106	0	1130	3	0
12	LB	1223	0	1330	7	0
13	LC	1461	0	1502	8	0
14	LD	1117	0	1243	6	0
15	LE	926	0	979	4	0
16	LG	993	0	1050	9	0
17	LH	1084	0	1177	13	0
18	LI	1115	0	1205	7	0
19	LJ	1107	0	1182	15	0
20	LK	642	0	455	4	0
21	LL	980	0	1041	3	0
22	LN	2884	0	3000	16	0
23	LO	738	0	774	7	0
24	LP	526	0	225	0	0
25	LQ	1053	0	1147	6	0
26	LR	485	0	537	5	0
27	LS	1015	0	1148	6	0
28	LT	876	0	912	7	0
29	LU	840	0	930	2	0
30	LW	612	0	640	4	0
31	NA	3389	0	2971	17	0
32	NB	603	0	661	4	0
33	NF	1696	0	1812	6	0
34	NH	1441	0	1448	7	0
35	NI	4832	0	4965	21	0
36	NK	581	0	656	3	0
37	SA	2853	0	3028	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	SC	1721	0	1871	10	0
39	SD	1870	0	1996	8	0
40	SE	1498	0	1601	3	0
41	SG	1526	0	1614	4	0
42	SH	1267	0	1291	4	0
43	SI	1896	0	2024	6	0
44	SJ	1939	0	1912	14	0
45	SK	1852	0	1828	14	0
46	SL	1960	0	2052	6	0
47	SM	4113	0	4245	16	0
48	SN	1350	0	1345	6	0
49	SO	2460	0	2551	6	0
50	SP	2983	0	2794	10	0
51	SQ	1778	0	1817	8	0
52	SR	3841	0	3895	19	0
53	SS	5041	0	4987	26	0
54	ST	1091	0	1036	6	0
55	SU	4360	0	4474	27	0
56	SV	1171	0	1232	5	0
57	SW	3580	0	3662	3	0
58	SY	2985	0	3004	10	0
59	SZ	1338	0	1352	4	0
60	L1	5	0	0	0	0
60	L3	56	0	0	0	0
60	L9	1	0	0	0	0
60	LQ	2	0	0	0	0
60	LT	1	0	0	0	0
60	NI	1	0	0	0	0
60	SA	1	0	0	0	0
60	SO	1	0	0	0	0
60	SR	1	0	0	0	0
60	SU	1	0	0	0	0
61	LR	1	0	0	0	0
61	LW	1	0	0	0	0
61	SV	1	0	0	0	0
62	NI	27	0	12	0	0
63	SR	28	0	12	0	0
64	SR	1	0	0	0	0
All	All	158284	0	130103	469	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 469 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)
6:L3:2343:G:OP2	37:SA:109:ARG:NH2	2.10	0.84
6:L3:4946:U:HO2'	28:LT:2:SER:N	1.77	0.83
54:ST:229:THR:OG1	54:ST:231:SER:O	1.99	0.80
1:BA:50:THR:HG22	1:BA:58:ILE:HD11	1.63	0.80
12:LB:146:ARG:O	12:LB:150:ARG:NH1	2.15	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	158/165 (96%)	157 (99%)	1 (1%)	0	100	100
2	BB	211/217 (97%)	205 (97%)	6 (3%)	0	100	100
3	BC	336/383 (88%)	333 (99%)	3 (1%)	0	100	100
7	L6	118/211 (56%)	115 (98%)	3 (2%)	0	100	100
8	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
9	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
10	L9	179/204 (88%)	178 (99%)	1 (1%)	0	100	100
11	LA	134/184 (73%)	133 (99%)	1 (1%)	0	100	100
12	LB	149/188 (79%)	149 (100%)	0	0	100	100
13	LC	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
14	LD	126/196 (64%)	125 (99%)	1 (1%)	0	100	100
15	LE	107/160 (67%)	105 (98%)	2 (2%)	0	100	100
16	LG	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
17	LH	131/156 (84%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
19	LJ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
20	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
21	LL	120/137 (88%)	120 (100%)	0	0	100	100
22	LN	352/403 (87%)	349 (99%)	3 (1%)	0	100	100
23	LO	93/115 (81%)	92 (99%)	1 (1%)	0	100	100
24	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
25	LQ	126/135 (93%)	126 (100%)	0	0	100	100
26	LR	59/117 (50%)	58 (98%)	1 (2%)	0	100	100
27	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
28	LT	107/110 (97%)	107 (100%)	0	0	100	100
29	LU	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
30	LW	72/97 (74%)	72 (100%)	0	0	100	100
31	NA	480/749 (64%)	478 (100%)	2 (0%)	0	100	100
32	NB	67/549 (12%)	66 (98%)	1 (2%)	0	100	100
33	NF	201/260 (77%)	200 (100%)	1 (0%)	0	100	100
34	NH	178/180 (99%)	177 (99%)	1 (1%)	0	100	100
35	NI	600/881 (68%)	594 (99%)	6 (1%)	0	100	100
36	NK	63/129 (49%)	63 (100%)	0	0	100	100
37	SA	356/427 (83%)	355 (100%)	1 (0%)	0	100	100
38	SC	208/288 (72%)	205 (99%)	3 (1%)	0	100	100
39	SD	223/248 (90%)	220 (99%)	3 (1%)	0	100	100
40	SE	184/266 (69%)	184 (100%)	0	0	100	100
41	SG	189/192 (98%)	188 (100%)	1 (0%)	0	100	100
42	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
43	SI	226/255 (89%)	223 (99%)	3 (1%)	0	100	100
44	SJ	247/847 (29%)	244 (99%)	3 (1%)	0	100	100
45	SK	242/245 (99%)	236 (98%)	6 (2%)	0	100	100
46	SL	241/490 (49%)	235 (98%)	6 (2%)	0	100	100
47	SM	492/588 (84%)	489 (99%)	3 (1%)	0	100	100
48	SN	169/306 (55%)	169 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	SO	292/353 (83%)	286 (98%)	6 (2%)	0	100	100
50	SP	393/423 (93%)	389 (99%)	4 (1%)	0	100	100
51	SQ	216/239 (90%)	215 (100%)	1 (0%)	0	100	100
52	SR	464/634 (73%)	458 (99%)	6 (1%)	0	100	100
53	SS	624/746 (84%)	615 (99%)	9 (1%)	0	100	100
54	ST	146/365 (40%)	143 (98%)	3 (2%)	0	100	100
55	SU	546/800 (68%)	537 (98%)	9 (2%)	0	100	100
56	SV	135/163 (83%)	135 (100%)	0	0	100	100
57	SW	444/670 (66%)	437 (98%)	7 (2%)	0	100	100
58	SY	376/812 (46%)	372 (99%)	4 (1%)	0	100	100
59	SZ	156/178 (88%)	156 (100%)	0	0	100	100
All	All	12216/17270 (71%)	12083 (99%)	133 (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	132/137 (96%)	132 (100%)	0	100	100
3	BC	273/318 (86%)	273 (100%)	0	100	100
7	L6	104/177 (59%)	104 (100%)	0	100	100
8	L7	173/174 (99%)	173 (100%)	0	100	100
9	L8	115/161 (71%)	115 (100%)	0	100	100
10	L9	155/172 (90%)	155 (100%)	0	100	100
11	LA	121/163 (74%)	121 (100%)	0	100	100
12	LB	136/165 (82%)	136 (100%)	0	100	100
13	LC	157/157 (100%)	157 (100%)	0	100	100
14	LD	122/175 (70%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LE	101/140 (72%)	101 (100%)	0	100	100
16	LG	102/107 (95%)	102 (100%)	0	100	100
17	LH	116/133 (87%)	116 (100%)	0	100	100
18	LI	124/135 (92%)	123 (99%)	1 (1%)	79	91
19	LJ	117/118 (99%)	117 (100%)	0	100	100
20	LK	29/121 (24%)	29 (100%)	0	100	100
21	LL	106/121 (88%)	106 (100%)	0	100	100
22	LN	313/348 (90%)	312 (100%)	1 (0%)	91	97
23	LO	80/97 (82%)	80 (100%)	0	100	100
25	LQ	114/121 (94%)	114 (100%)	0	100	100
26	LR	52/100 (52%)	52 (100%)	0	100	100
27	LS	109/110 (99%)	109 (100%)	0	100	100
28	LT	88/89 (99%)	88 (100%)	0	100	100
29	LU	87/89 (98%)	87 (100%)	0	100	100
30	LW	63/80 (79%)	63 (100%)	0	100	100
31	NA	277/656 (42%)	277 (100%)	0	100	100
32	NB	65/485 (13%)	65 (100%)	0	100	100
33	NF	184/228 (81%)	184 (100%)	0	100	100
34	NH	155/155 (100%)	155 (100%)	0	100	100
35	NI	520/730 (71%)	520 (100%)	0	100	100
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	SA	298/348 (86%)	298 (100%)	0	100	100
38	SC	190/252 (75%)	190 (100%)	0	100	100
39	SD	194/215 (90%)	194 (100%)	0	100	100
40	SE	159/223 (71%)	159 (100%)	0	100	100
41	SG	170/171 (99%)	170 (100%)	0	100	100
42	SH	140/274 (51%)	140 (100%)	0	100	100
43	SI	206/228 (90%)	206 (100%)	0	100	100
44	SJ	182/733 (25%)	182 (100%)	0	100	100
45	SK	212/213 (100%)	212 (100%)	0	100	100
46	SL	226/437 (52%)	226 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	SM	440/509 (86%)	438 (100%)	2 (0%)	86 95
48	SN	133/260 (51%)	133 (100%)	0	100 100
49	SO	274/319 (86%)	273 (100%)	1 (0%)	89 96
50	SP	311/380 (82%)	311 (100%)	0	100 100
51	SQ	195/214 (91%)	195 (100%)	0	100 100
52	SR	425/574 (74%)	425 (100%)	0	100 100
53	SS	550/648 (85%)	550 (100%)	0	100 100
54	ST	101/300 (34%)	100 (99%)	1 (1%)	73 88
55	SU	478/733 (65%)	476 (100%)	2 (0%)	89 96
56	SV	127/149 (85%)	127 (100%)	0	100 100
57	SW	395/591 (67%)	395 (100%)	0	100 100
58	SY	325/685 (47%)	325 (100%)	0	100 100
59	SZ	141/158 (89%)	141 (100%)	0	100 100
All	All	10223/14691 (70%)	10215 (100%)	8 (0%)	92 98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	SU	697	ARG
55	SU	413	ASN
49	SO	333	LYS
47	SM	521	LYS
54	ST	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
53	SS	661	HIS
55	SU	636	HIS
58	SY	430	HIS
57	SW	511	HIS
38	SC	190	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L1	154/157 (98%)	18 (11%)	0
5	L2	65/1167 (5%)	10 (15%)	0
6	L3	2542/5070 (50%)	363 (14%)	10 (0%)
All	All	2761/6394 (43%)	391 (14%)	10 (0%)

5 of 391 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L1	34	U
4	L1	52	A
4	L1	54	C
4	L1	55	U
4	L1	59	A

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L3	4347	G
6	L3	4520	G
6	L3	5013	C
6	L3	2574	G
6	L3	2711	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	SEP	SS	126	53	8,9,10	1.59	1 (12%)	7,12,14	1.26	1 (14%)
53	SEP	SS	127	53	8,9,10	1.58	1 (12%)	7,12,14	1.28	1 (14%)

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
53	SEP	SS	126	53	-	0/6/8/10	-
53	SEP	SS	127	53	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SS	126	SEP	P-O1P	3.50	1.61	1.50
53	SS	127	SEP	P-O1P	3.46	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	SS	126	SEP	OG-CB-CA	2.72	110.79	108.14
53	SS	127	SEP	OG-CB-CA	2.70	110.77	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 76 ligands modelled in this entry, 74 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	GDP	SR	1001	60,64	25,30,30	2.62	9 (36%)	30,47,47	1.54	7 (23%)
62	ADP	NI	901	60	24,29,29	0.90	1 (4%)	29,45,45	1.29	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GDP	SR	1001	60,64	-	0/12/32/32	0/3/3/3
62	ADP	NI	901	60	-	3/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	SR	1001	GDP	O6-C6	7.27	1.40	1.23
63	SR	1001	GDP	PA-O3A	4.98	1.64	1.59
63	SR	1001	GDP	C2-N2	4.80	1.45	1.34
63	SR	1001	GDP	O4'-C1'	4.75	1.47	1.40
63	SR	1001	GDP	C1'-N9	-2.58	1.43	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	NI	901	ADP	N3-C2-N1	-4.24	122.92	128.67
63	SR	1001	GDP	C5-C6-N1	2.93	119.67	114.07
63	SR	1001	GDP	O2B-PB-O3A	2.90	114.36	104.64
63	SR	1001	GDP	C2-N1-C6	-2.86	119.87	125.11
63	SR	1001	GDP	O3B-PB-O3A	2.84	114.16	104.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

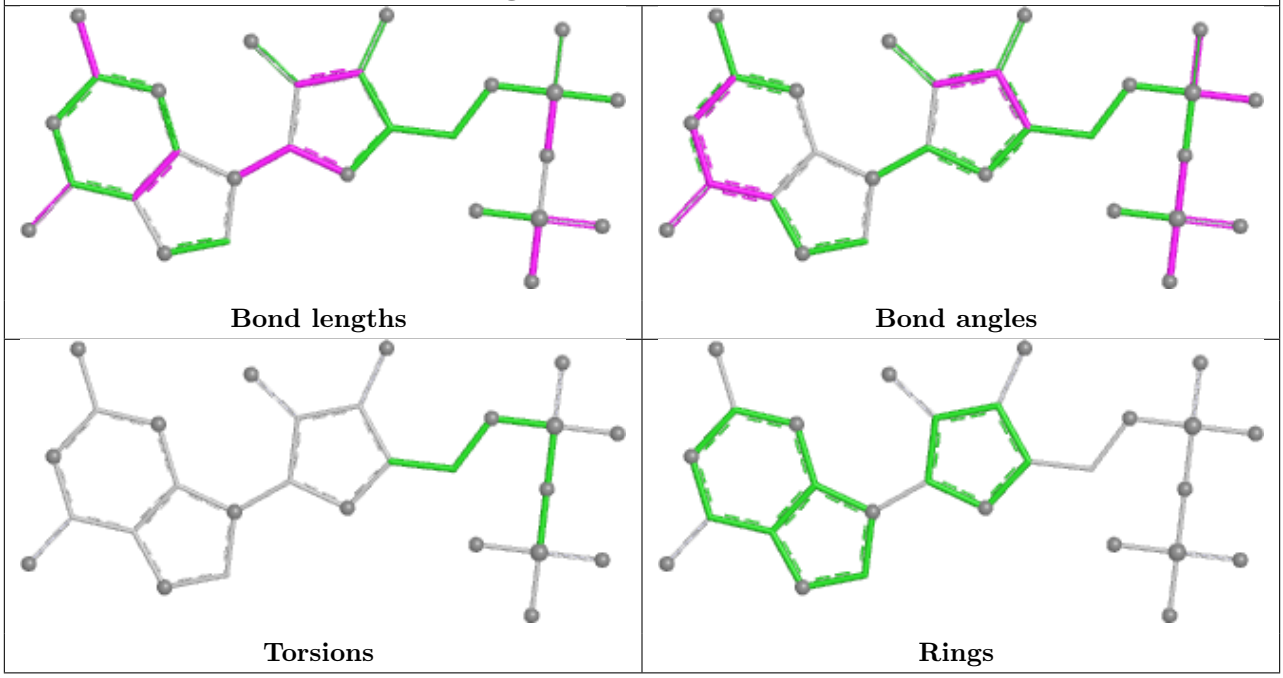
Mol	Chain	Res	Type	Atoms
62	NI	901	ADP	PA-O3A-PB-O3B
62	NI	901	ADP	O4'-C4'-C5'-O5'
62	NI	901	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

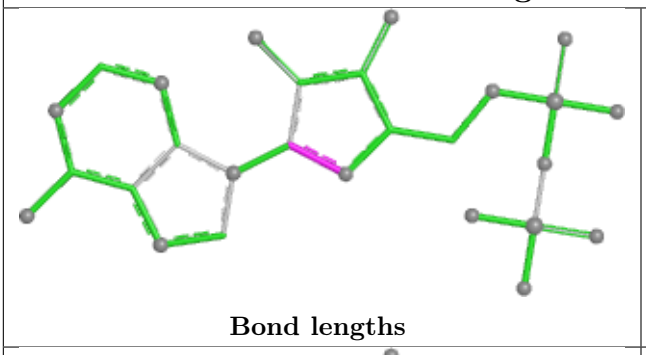
No monomer is involved in short contacts.

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.

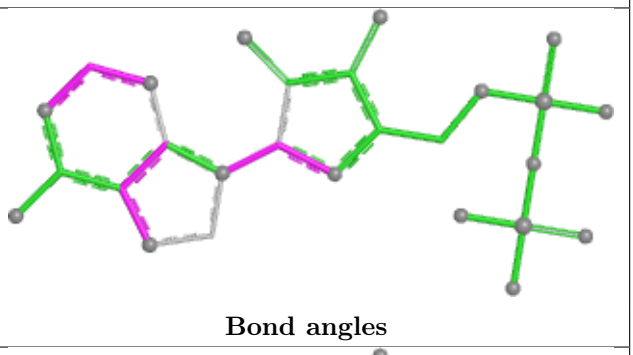
Ligand GDP SR 1001



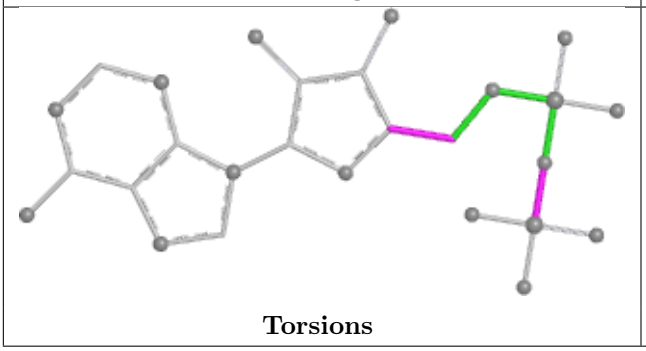
Ligand ADP NI 901



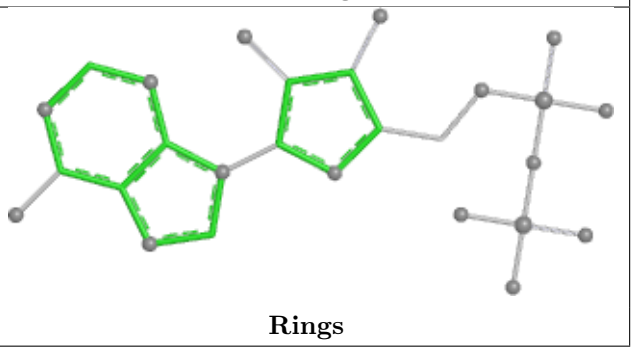
Bond lengths



Bond angles



Torsions



Rings

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.

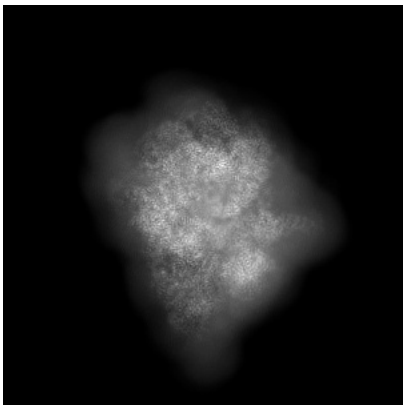
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29261. These allow visual inspection of the internal detail of the map and identification of artifacts.

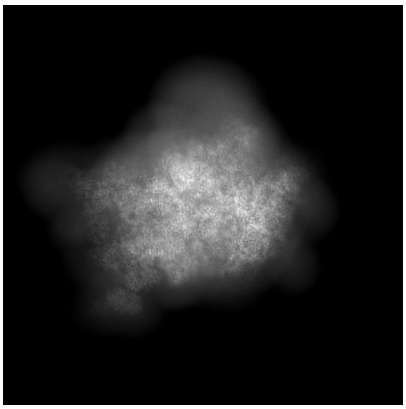
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

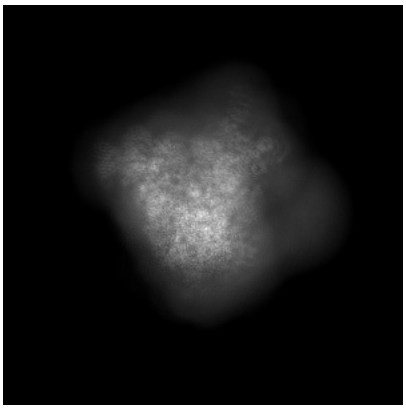
6.1.1 Primary map



X

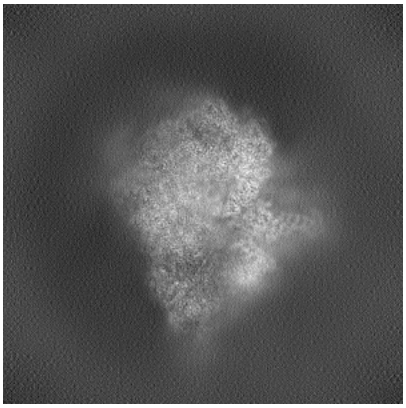


Y

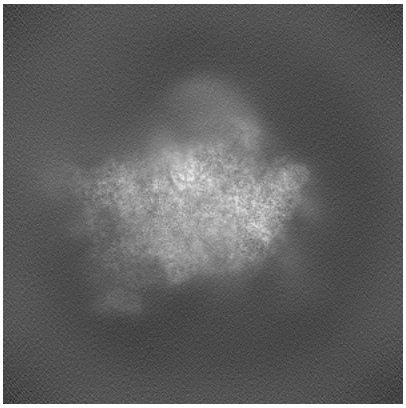


Z

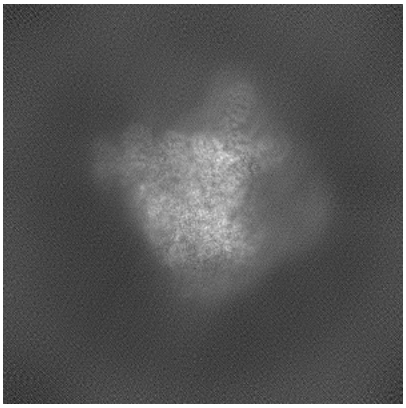
6.1.2 Raw map



X



Y

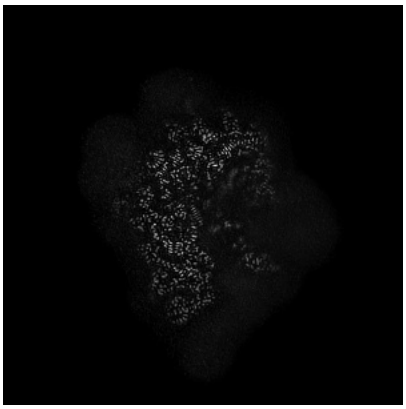


Z

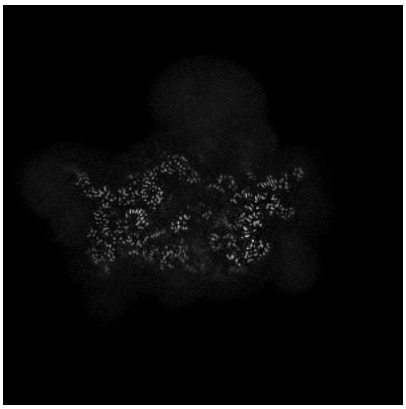
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

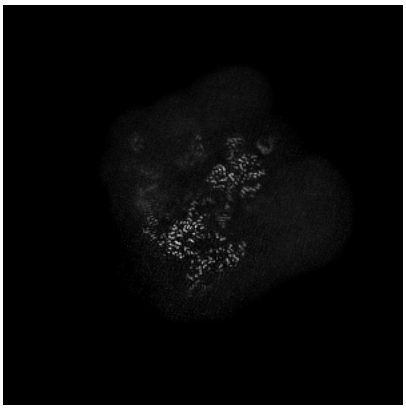
6.2.1 Primary map



X Index: 240

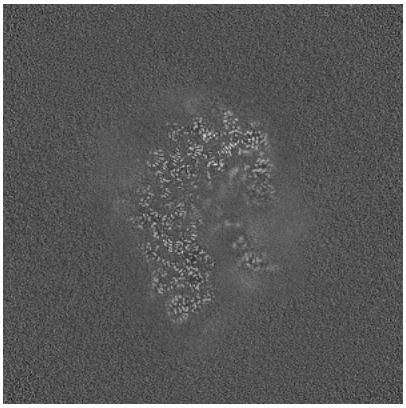


Y Index: 240

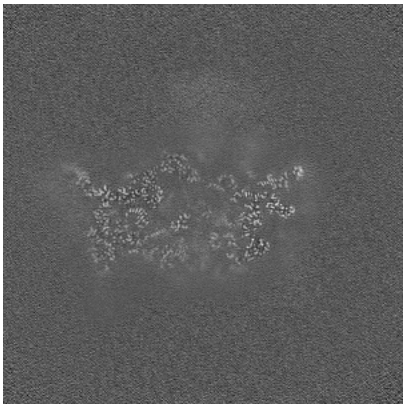


Z Index: 240

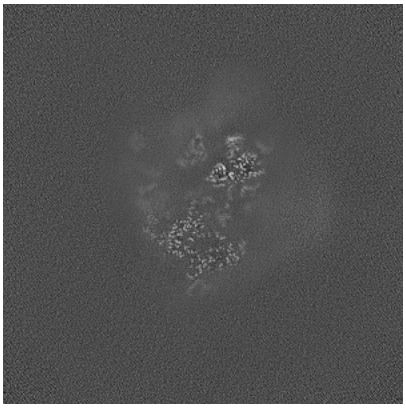
6.2.2 Raw map



X Index: 240



Y Index: 240

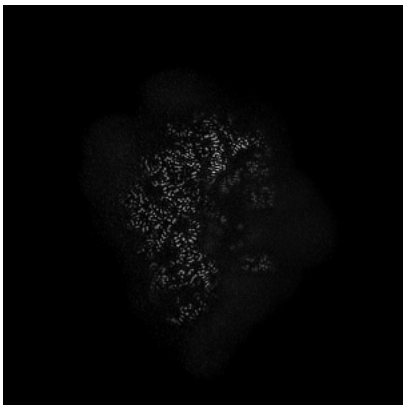


Z Index: 240

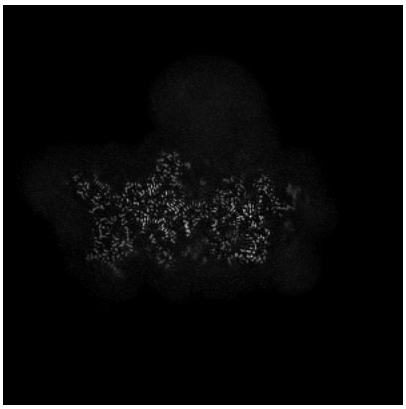
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

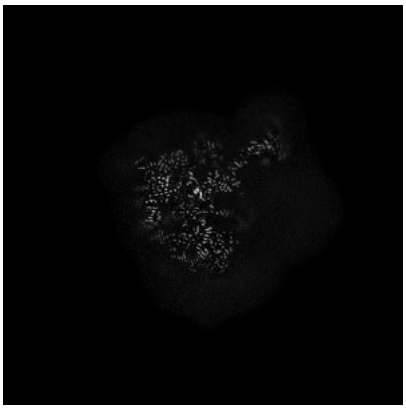
6.3.1 Primary map



X Index: 233

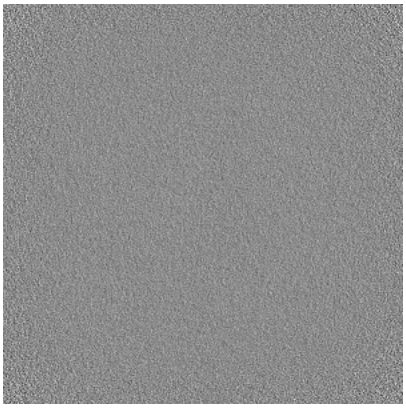


Y Index: 228

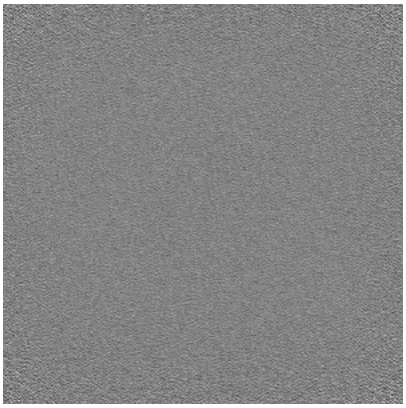


Z Index: 285

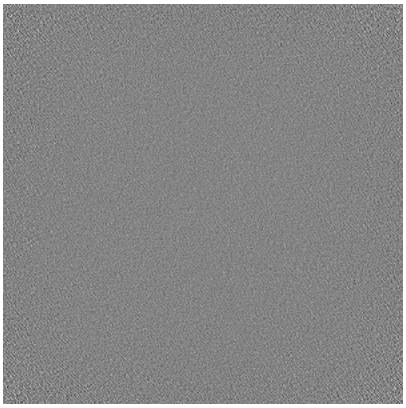
6.3.2 Raw map



X Index: 0



Y Index: 0

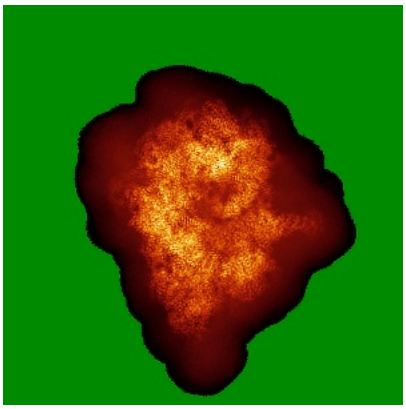


Z Index: 0

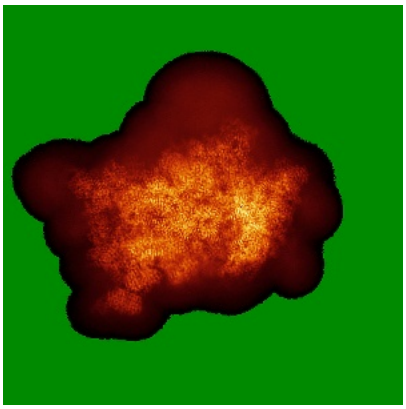
The images above show the largest variance slices of the map in three orthogonal directions.

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

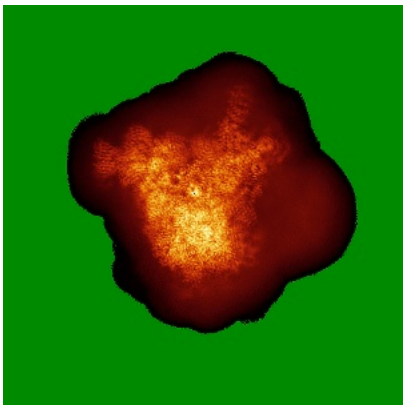
6.4.1 Primary map



X

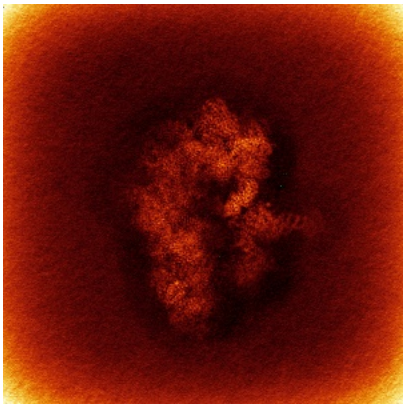


Y

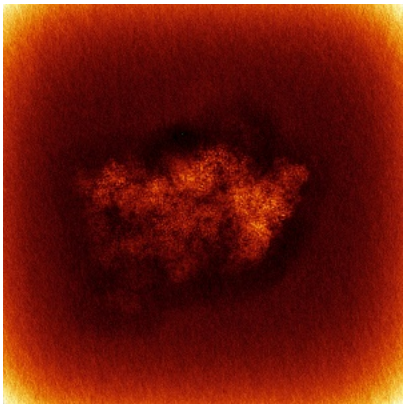


Z

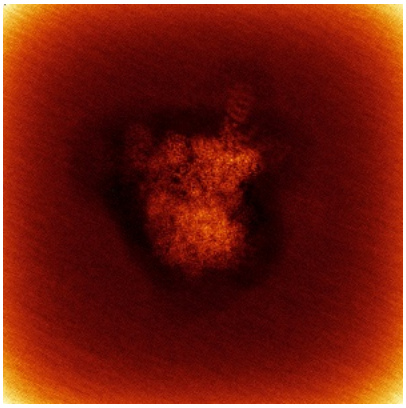
6.4.2 Raw map



X



Y

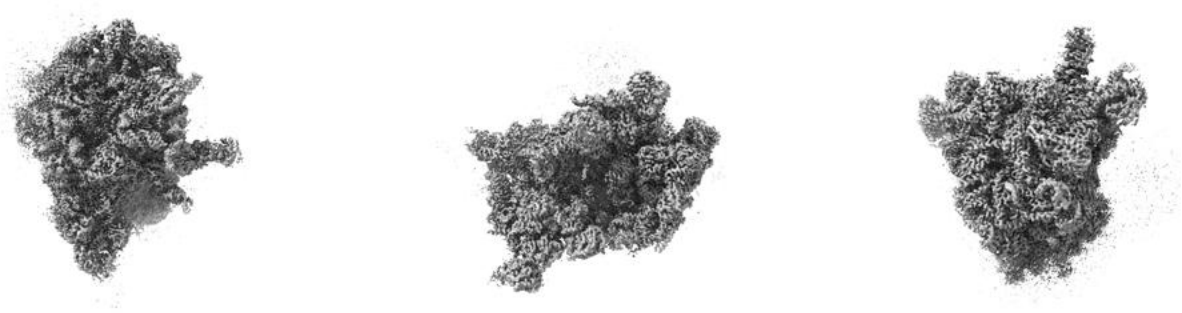


Z

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)

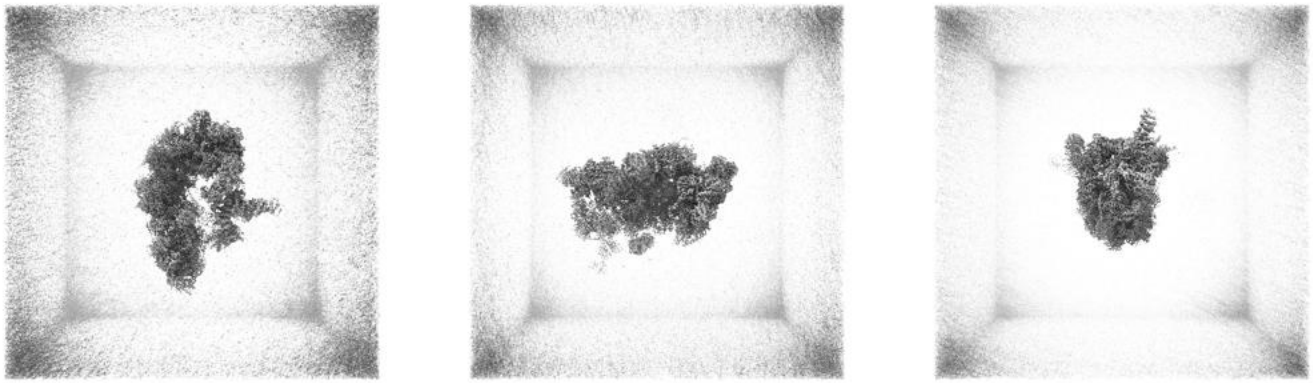
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

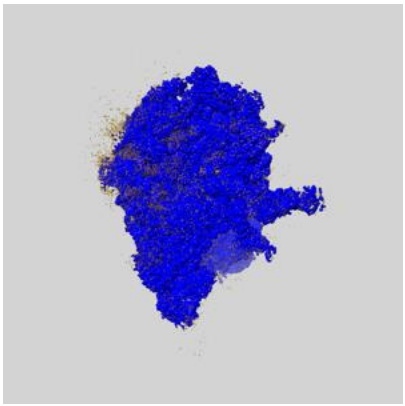
6.6 Mask visualisation (i)

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

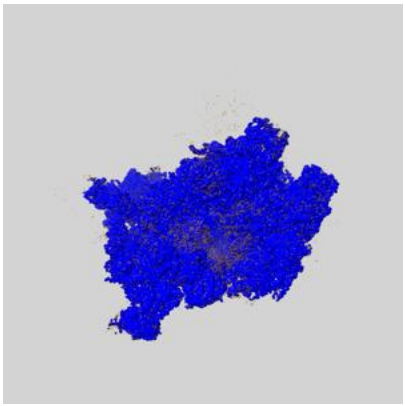
A mask typically either:

- 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_29261_msk_1.map (i)



X



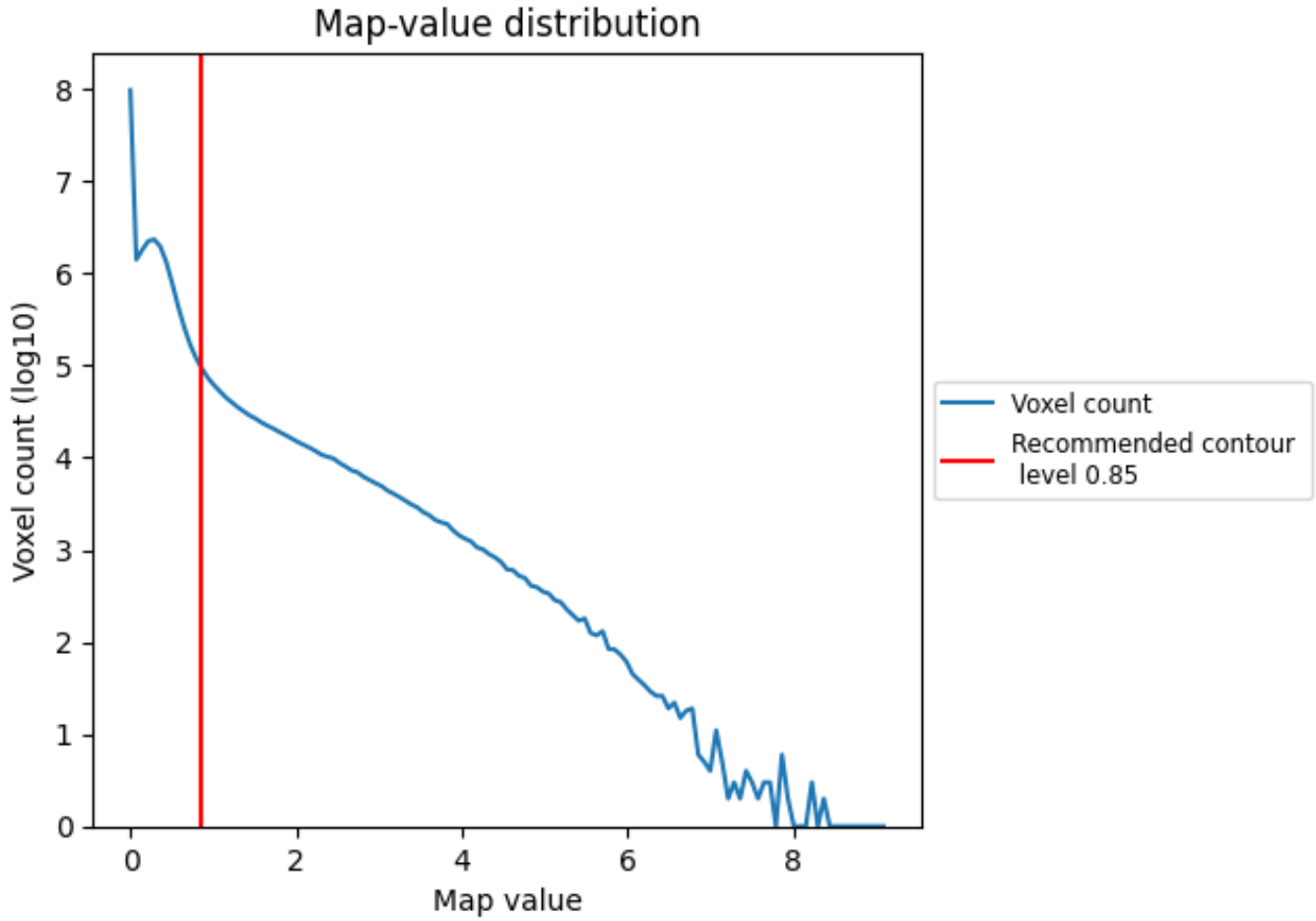
Y

Z

7 Map analysis

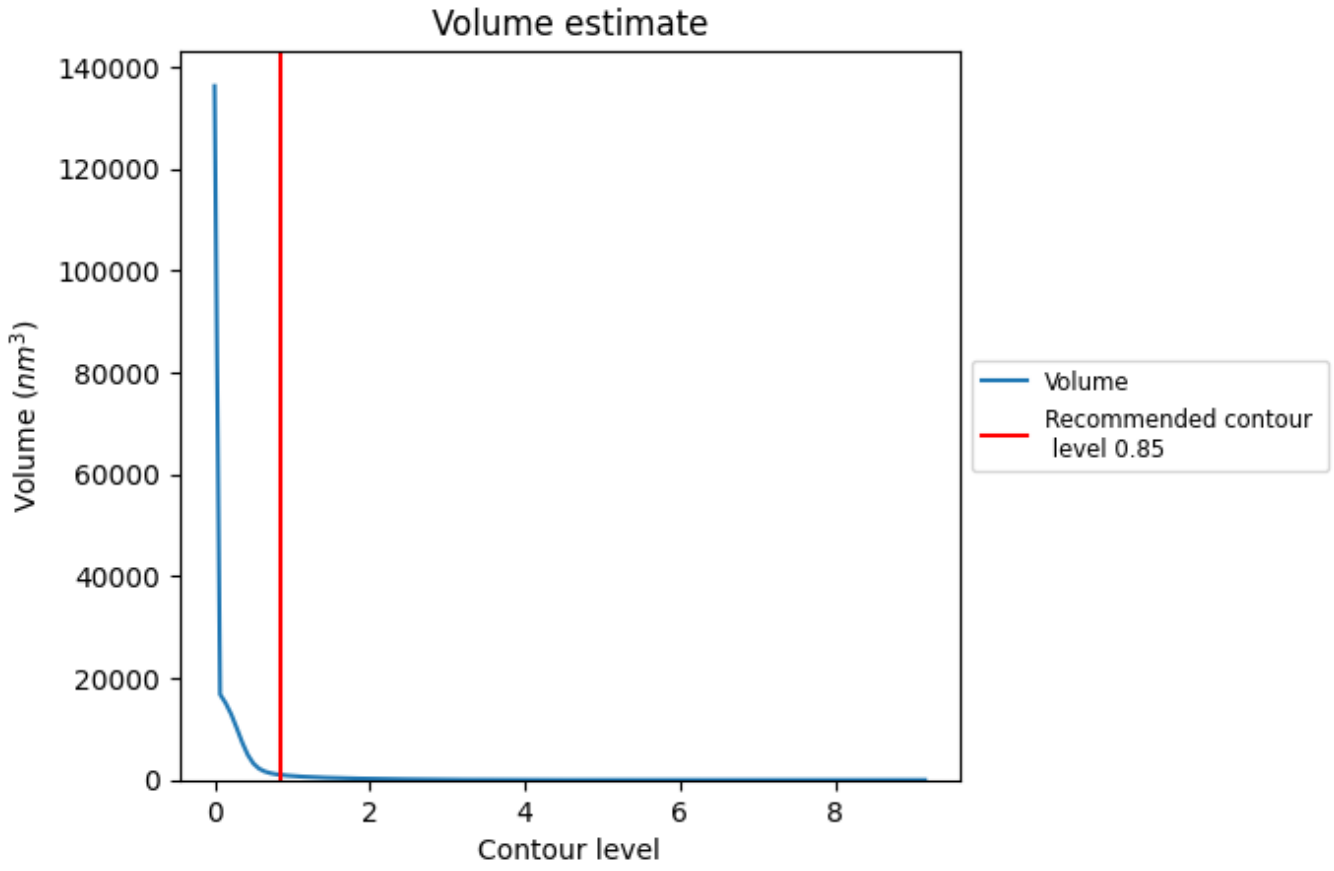
This section contains the results of statistical analysis of the map.

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.

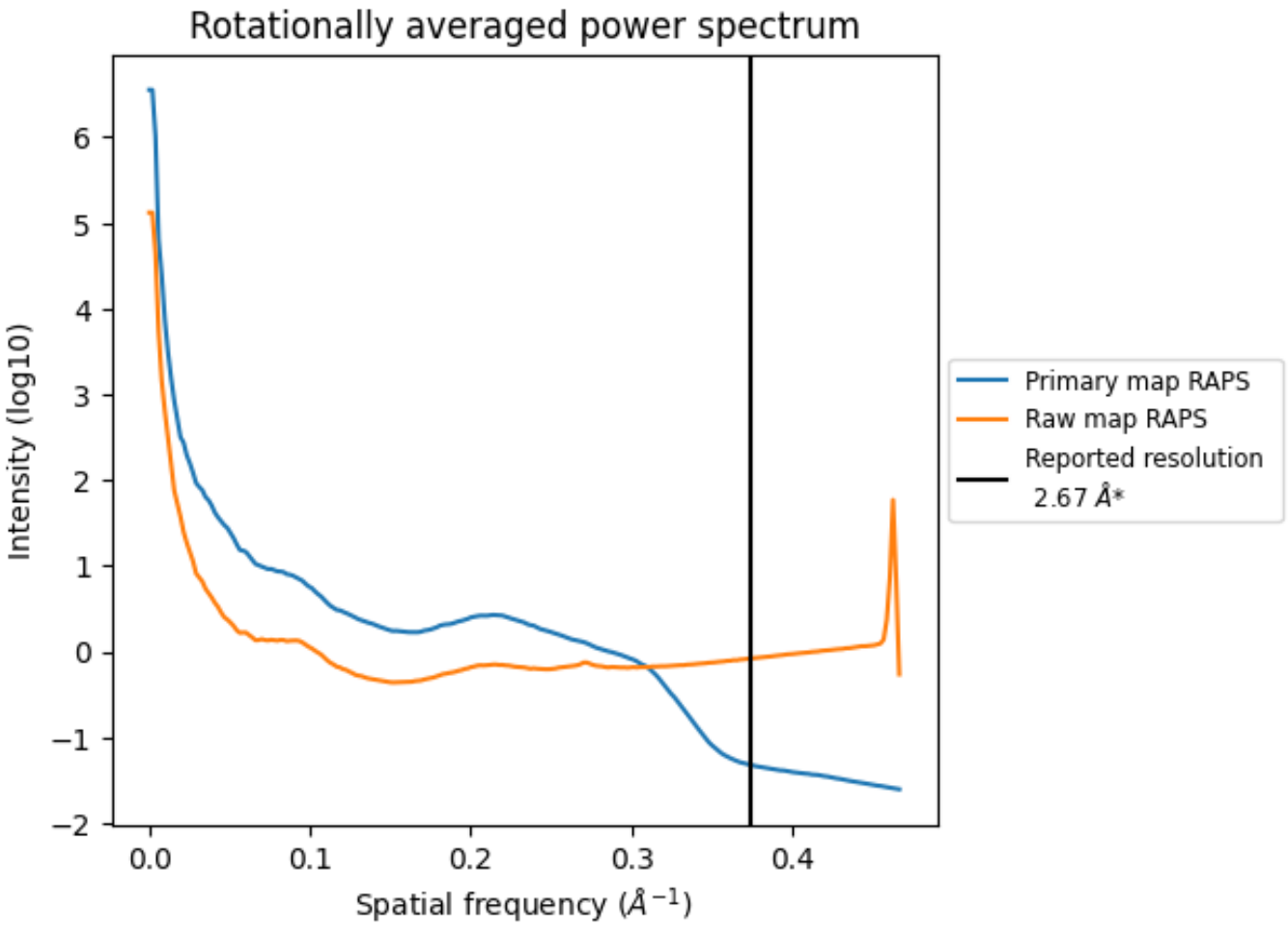
7.2 Volume estimate (i)



The volume at the recommended contour level is 1004 nm^3; this corresponds to an approximate mass of 907 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)

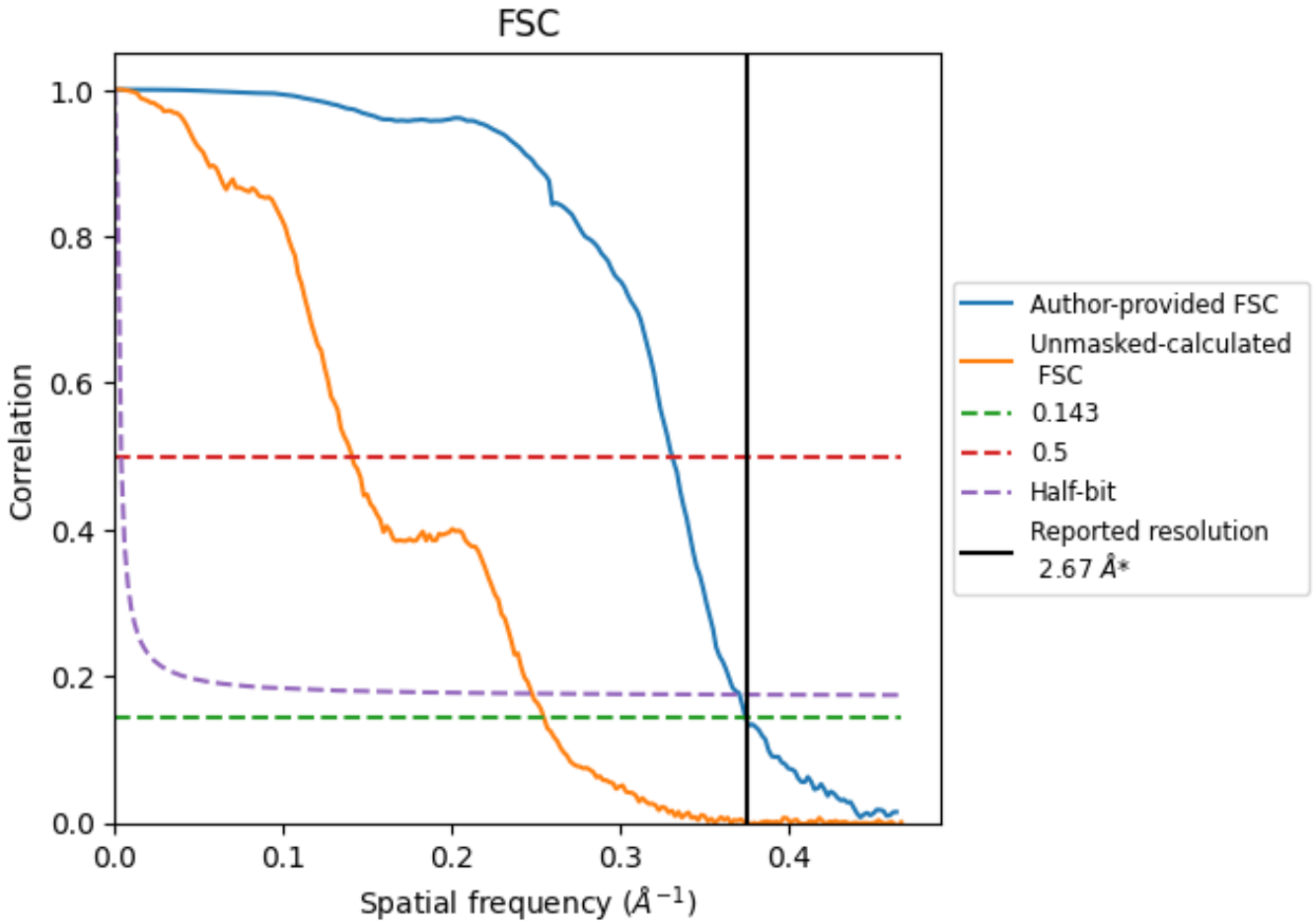


*Reported resolution corresponds to spatial frequency of 0.375 Å^{-1}

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 0.375 Å^{-1}

8.2 Resolution estimates (i)

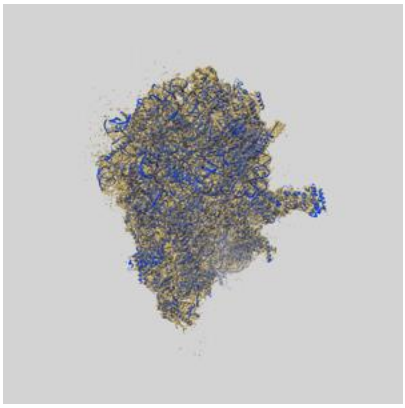
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.03	2.70
Unmasked-calculated*	3.93	7.11	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 2.67 by more than 10 %

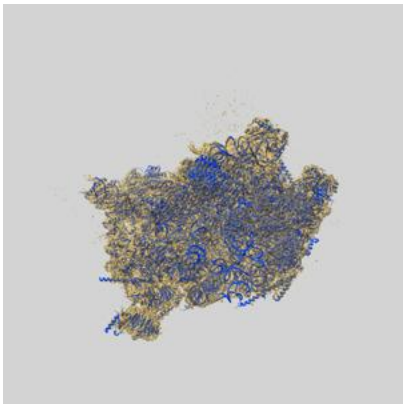
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29261 and PDB model 8FKY. Per-residue inclusion information can be found in section 3 on page 17.

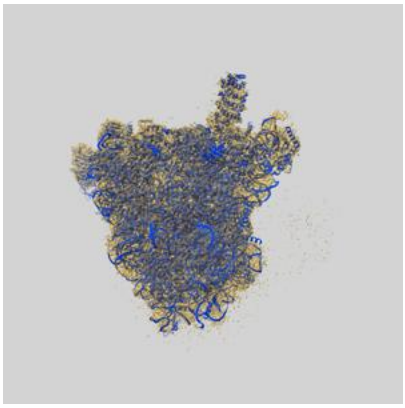
9.1 Map-model overlay



X



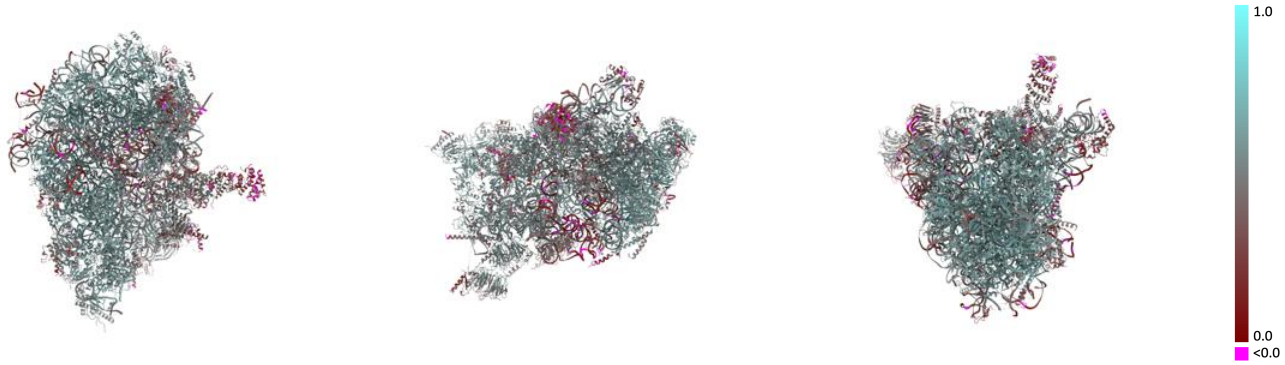
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85 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.

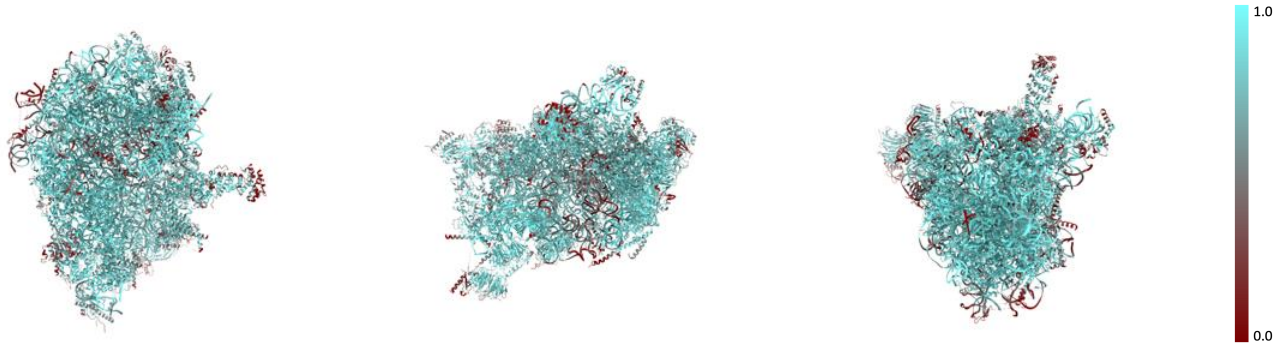
9.2 Q-score mapped to coordinate model (i)



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.

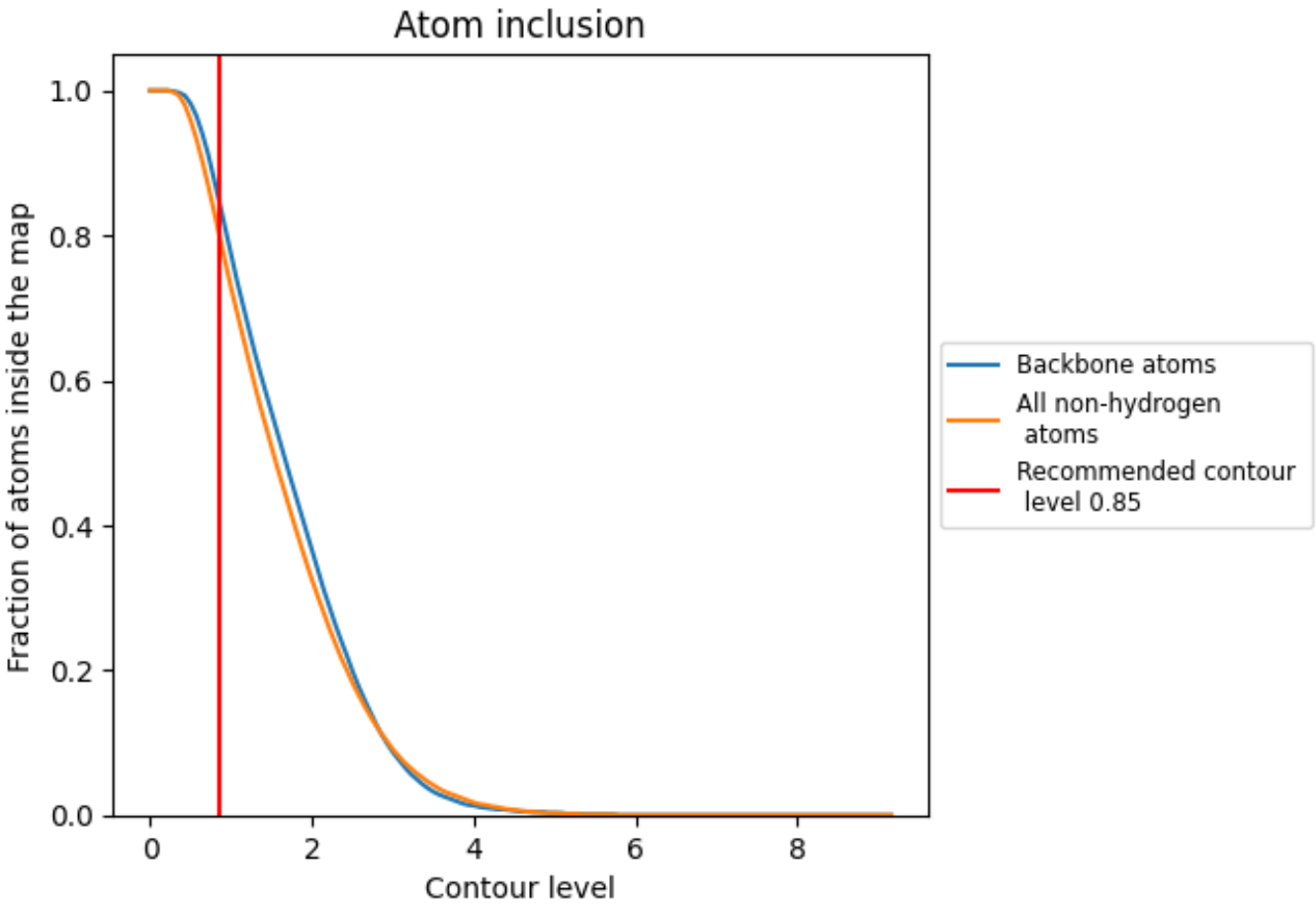
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.85).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.5190
BA	0.4420	0.4340
BB	0.6010	0.3170
BC	0.7330	0.4050
L1	0.9340	0.5760
L2	0.8130	0.5490
L3	0.8430	0.5110
L6	0.9330	0.6060
L7	0.9020	0.6130
L8	0.8620	0.6050
L9	0.9690	0.6290
LA	0.8080	0.5590
LB	0.9380	0.6140
LC	0.8790	0.6200
LD	0.6660	0.3870
LE	0.4810	0.4200
LG	0.8330	0.5550
LH	0.8110	0.5360
LI	0.8790	0.6020
LJ	0.8820	0.5040
LK	0.6990	0.4340
LL	0.9120	0.6030
LN	0.9090	0.6100
LO	0.8410	0.4810
LP	0.2800	0.2770
LQ	0.9420	0.6280
LR	0.8380	0.4760
LS	0.8820	0.5770
LT	0.9510	0.6310
LU	0.8310	0.5830
LW	0.9490	0.6110
NA	0.7250	0.3810
NB	0.6680	0.5320
NF	0.8440	0.5740
NH	0.8950	0.5450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NI	0.5420	0.4370
NK	0.7860	0.5560
SA	0.9220	0.6140
SC	0.5950	0.4930
SD	0.8660	0.5870
SE	0.9060	0.5940
SG	0.8860	0.6090
SH	0.7130	0.5480
SI	0.7840	0.5610
SJ	0.6090	0.4250
SK	0.8560	0.5630
SL	0.7300	0.5450
SM	0.8170	0.5310
SN	0.7080	0.4910
SO	0.7850	0.5440
SP	0.6430	0.4300
SQ	0.7750	0.5660
SR	0.8090	0.5520
SS	0.8490	0.5220
ST	0.5830	0.4000
SU	0.7210	0.4380
SV	0.7510	0.5140
SW	0.6480	0.5030
SY	0.8740	0.5460
SZ	0.8460	0.5580