wwPDB EM Validation Summary Report

Dec 30, 2024 – 10:12 PM EST

PDB ID	:	8FKV
EMDB ID	:	EMD-29258
Title	:	Human nucleolar pre-60S ribosomal subunit (State D1)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.47 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:

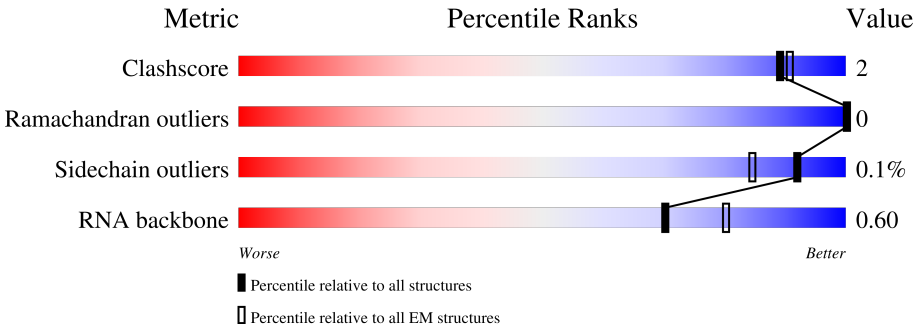
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.47 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	58%, 89%, 8%
2	BB	217	69%, 98%
3	L1	157	6%, 81%, 14%
4	L2	1167	94%
5	L3	5070	36%, 7%, 56%
6	L6	211	50%, 7%, 43%
7	L7	203	94%

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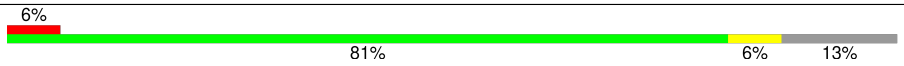
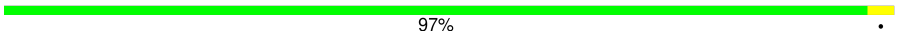
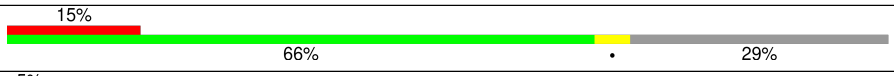
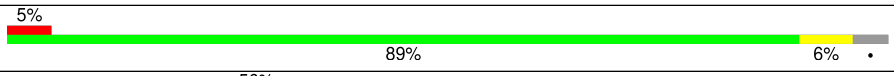
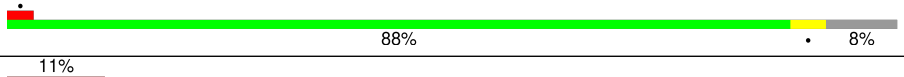
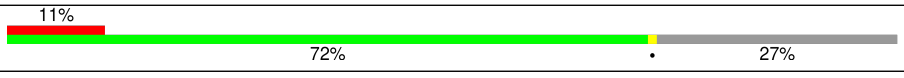
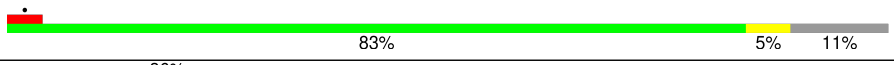
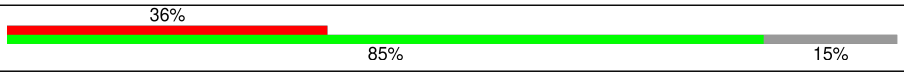
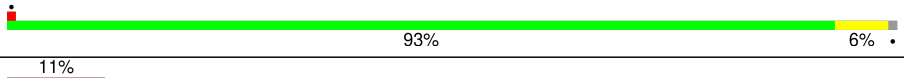
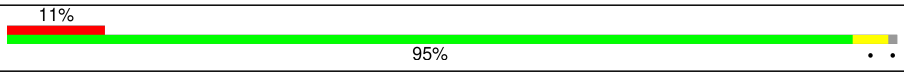
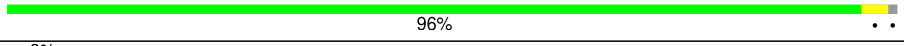
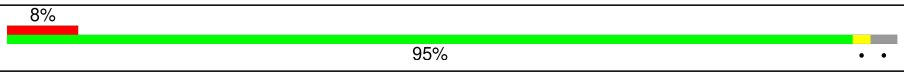
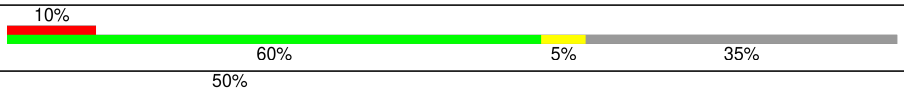
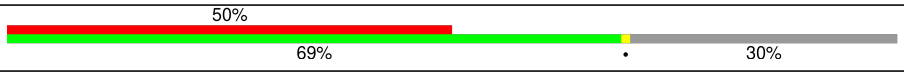
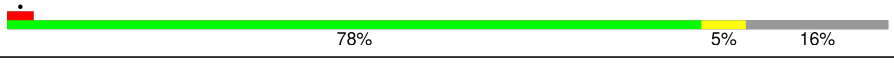
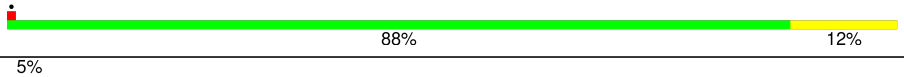
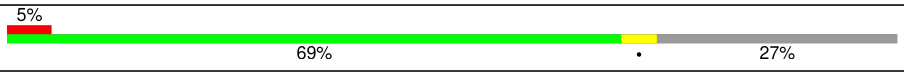
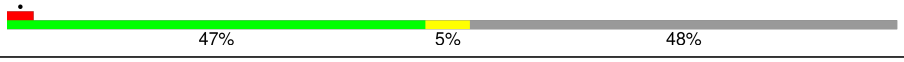
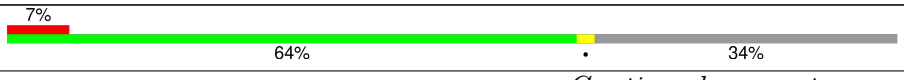
Mol	Chain	Length	Quality of chain
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LE	160	
14	LG	140	
15	LH	156	
16	LI	145	
17	LK	148	
18	LN	403	
19	LP	125	
20	LQ	135	
21	LS	123	
22	LT	110	
23	LU	105	
24	LW	97	
25	NA	749	
26	NB	549	
27	NF	260	
28	NH	180	
29	NI	881	
30	NK	129	
31	NM	300	
32	NO	461	

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Mol	Chain	Length	Quality of chain
33	NQ	385	81% 16%
34	NS	349	84% 13%
35	SA	427	80% 16%
36	SC	288	64% 6% 31%
37	SD	248	92%
38	SE	266	66% 30%
39	SG	192	92% 7%
40	SH	293	51% 49%
41	SI	255	85% 12%
42	SJ	847	8% 36% 60%
43	SK	245	93% 7%
44	SL	490	48% 50%
45	SM	588	11% 74% 23%
46	SN	306	55% 43%
47	SO	353	82% 5% 13%
48	SQ	239	6% 86% 5% 9%
49	SR	634	6% 67% 6% 27%
50	SS	746	30% 67%
51	ST	365	13% 30% 68%
52	SU	800	5% 66% 30%
53	SV	163	17% 74% 9% 16%
54	SW	670	21% 63% 34%
55	SY	812	44% 53%
56	SZ	178	87% 10%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 148975 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 RNA chain called 5.8S rRNA.

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

- Molecule 4 is a RNA chain called ITS2 rRNA.

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

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L3	2213	47439	21130	8683	15413	2213	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

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

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 8 is a protein called 60S ribosomal protein L14.

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

- Molecule 9 is a protein called 60S ribosomal protein L15.

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

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LA	160	Total	C	N	O	S	0	0
			1286	809	240	229	8		

- Molecule 11 is a protein called 60S ribosomal protein L18.

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

- Molecule 12 is a protein called 60S ribosomal protein L18a.

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

- Molecule 13 is a protein called 60S ribosomal protein L21.

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

- Molecule 14 is a protein called 60S ribosomal protein L23.

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

- Molecule 15 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	LH	133	Total 813	C 499	N 172	O 142	0	0

- Molecule 16 is a protein called 60S ribosomal protein L26.

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

- Molecule 17 is a protein called 60S ribosomal protein L27a.

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

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

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

- Molecule 19 is a protein called 60S ribosomal protein L31.

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

- Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	133	Total 1096	C 690	N 225	O 176	S 5	0	0

- Molecule 21 is a protein called 60S ribosomal protein L35.

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

- Molecule 22 is a protein called 60S ribosomal protein L35a.

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

- Molecule 23 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 24 is a protein called 60S ribosomal protein L37.

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

- Molecule 25 is a protein called Nucleolar complex protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NA	484	Total	C	N	O	S	0	0
			3658	2355	644	638	21		

- Molecule 26 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NB	387	Total	C	N	O	S	0	0
			2424	1493	475	450	6		

- Molecule 27 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NF	218	Total	C	N	O	S	0	0
			1783	1136	337	301	9		

- Molecule 28 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

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

- Molecule 29 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NI	647	Total	C	N	O	S	0	0
			5137	3254	934	934	15		

- Molecule 30 is a protein called Protein LLP homolog.

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

- Molecule 31 is a protein called Protein MAK16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NM	182	Total	C	N	O	S	0	0
			1550	983	286	273	8		

- Molecule 32 is a protein called Ribosomal RNA processing protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NO	305	Total	C	N	O	S	0	0
			2487	1577	437	461	12		

- Molecule 33 is a protein called WD repeat-containing protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NQ	324	Total	C	N	O	S	0	0
			2502	1559	471	457	15		

- Molecule 34 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NS	305	Total	C	N	O	S	0	0
			2529	1607	472	444	6		

- Molecule 35 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SA	360	Total	C	N	O	S	0	0
			2864	1803	572	475	14		

- Molecule 36 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SC	199	Total	C	N	O	S	0	0
			1627	1046	305	274	2		

- Molecule 37 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SD	239	Total	C	N	O	S	0	0
			1985	1275	381	320	9		

- Molecule 38 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SE	185	Total	C	N	O	S	0	0
			1491	946	289	252	4		

- Molecule 39 is a protein called 60S ribosomal protein L9.

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

- Molecule 40 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 41 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SI	225	Total	C	N	O	S	1	0
			1864	1207	349	304	4		

- Molecule 42 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SJ	340	Total	C	N	O	S	0	0
			2780	1777	507	489	7		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 44 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 45 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SM	453	Total	C	N	O	S	0	0
			3735	2408	667	648	12		

- Molecule 46 is a protein called Probable rRNA-processing protein EBP2.

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

- Molecule 47 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SO	307	Total	C	N	O	S	0	0
			2544	1637	458	434	15		

- Molecule 48 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 49 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SR	462	Total	C	N	O	S	0	0
			3808	2417	677	696	18		

- Molecule 50 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	SS	243	Total	C	N	O	P	S	0	0
			2011	1271	357	374	2	7		

- Molecule 51 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	ST	116	Total	C	N	O	S	0	0
			838	527	155	154	2		

- Molecule 52 is a protein called Nucleolar complex protein 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SU	561	Total	C	N	O	S	0	0
			4434	2842	761	810	21		

- Molecule 53 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 54 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SW	444	Total	C	N	O	S	0	0
			3549	2282	605	645	17		

- Molecule 55 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

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

- Molecule 56 is a protein called Nucleolar protein 16.

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

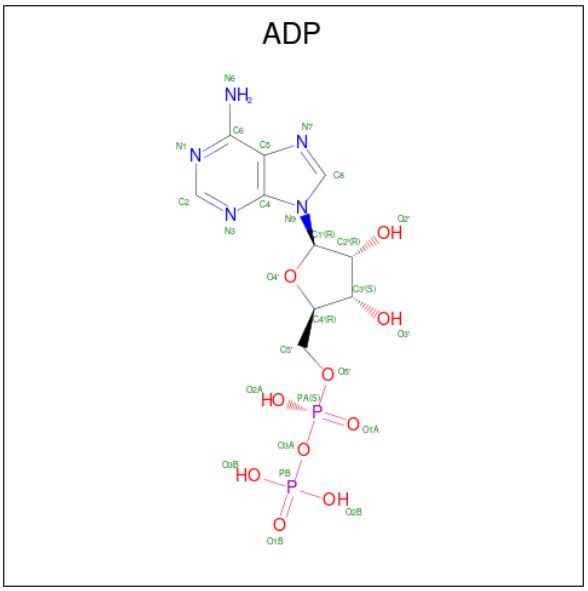
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	L1	4	Total	Mg	0
			4	4	
57	L2	1	Total	Mg	0
			1	1	
57	L3	51	Total	Mg	0
			51	51	
57	L9	1	Total	Mg	0
			1	1	
57	LN	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	1	Total	Mg	0
			1	1	
57	NI	1	Total	Mg	0
			1	1	
57	SA	1	Total	Mg	0
			1	1	
57	SO	1	Total	Mg	0
			1	1	
57	SR	1	Total	Mg	0
			1	1	
57	SU	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

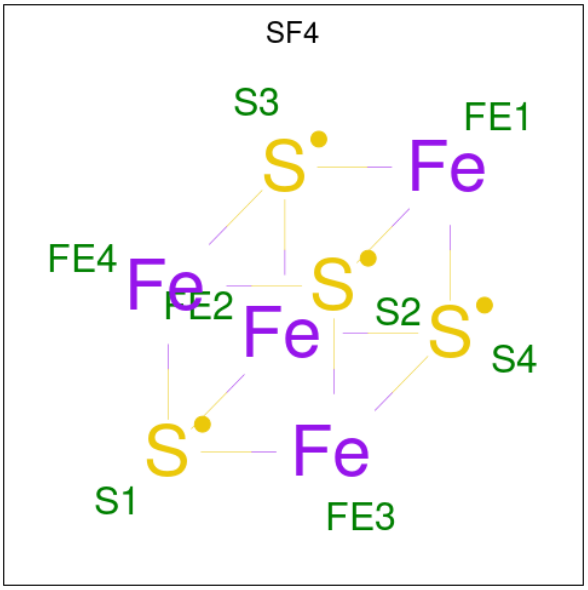
Mol	Chain	Residues	Atoms		AltConf
58	LW	1	Total	Zn	0
			1	1	
58	SV	1	Total	Zn	0
			1	1	

- Molecule 59 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



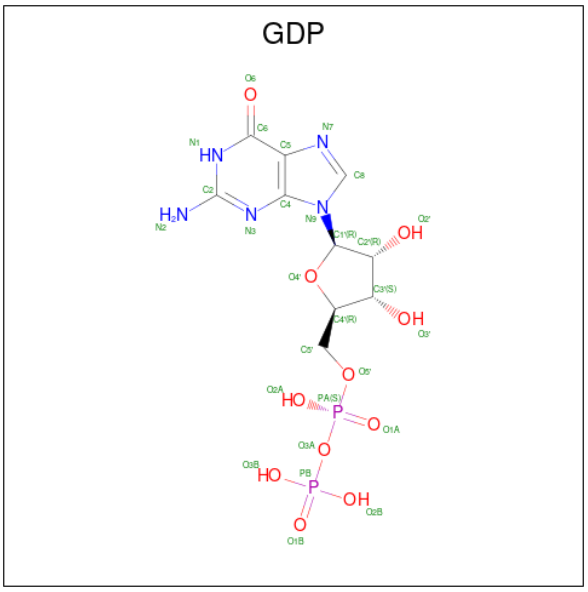
Mol	Chain	Residues	Atoms					AltConf
59	NI	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
60	NM	1	Total	Fe	S	0
			8	4	4	

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

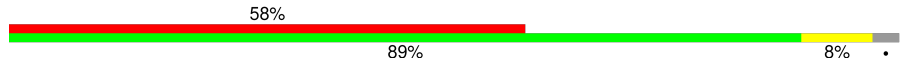
Mol	Chain	Residues	Atoms		AltConf
62	SR	1	Total	K	0
			1	1	

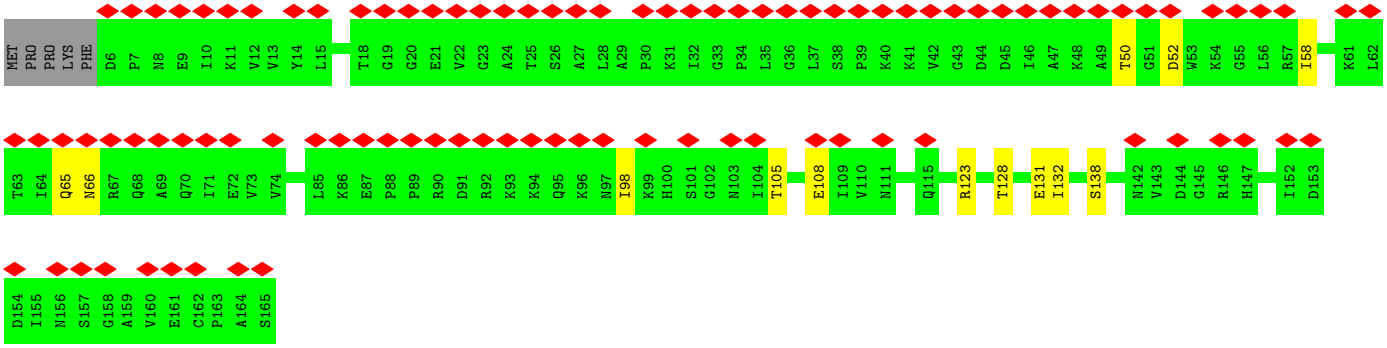
3 Residue-property plots (i)

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

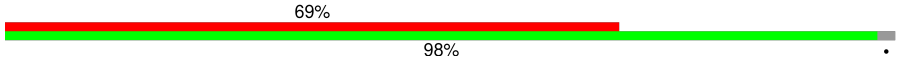
Chain BA:

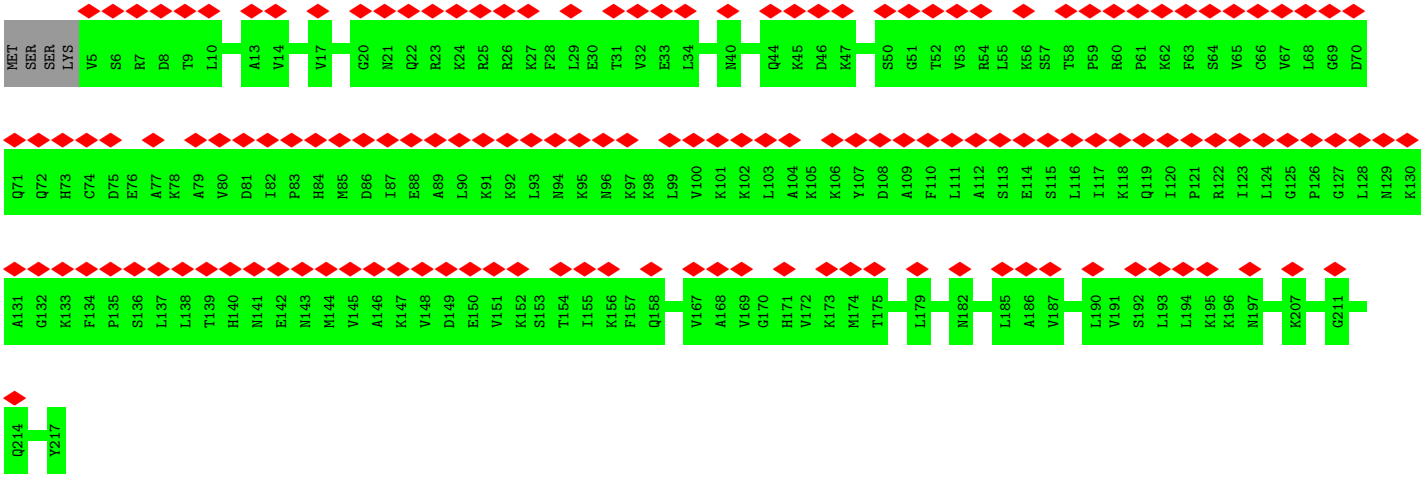




• Molecule 2: 60S ribosomal protein L10a

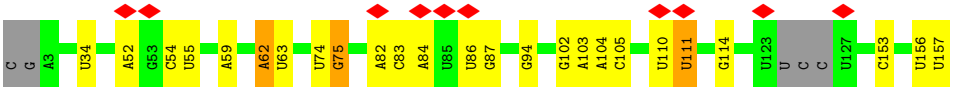
Chain BB:





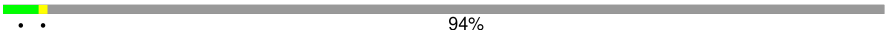
• Molecule 3: 5.8S rRNA

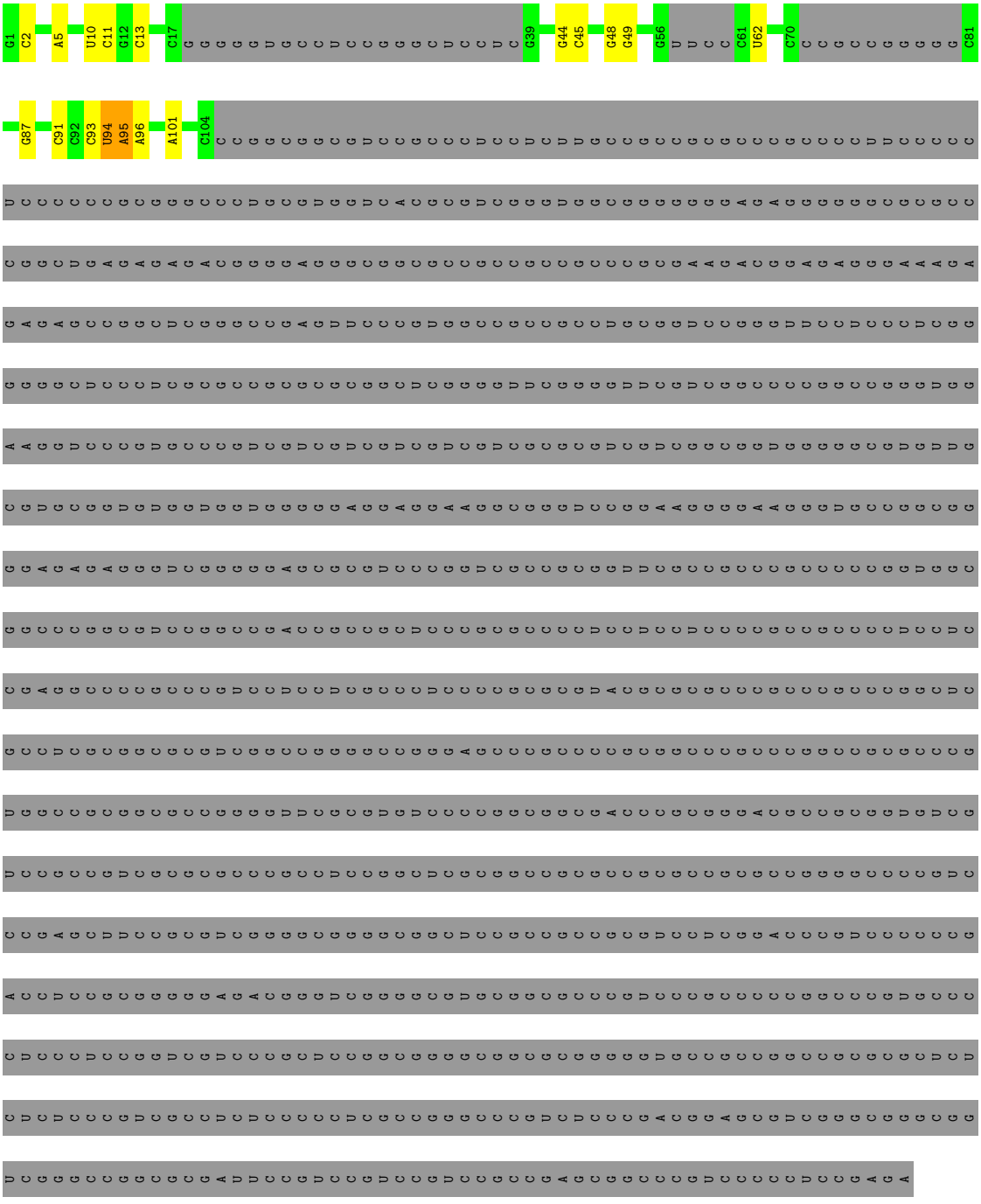
Chain L1:



• Molecule 4: ITS2 rRNA

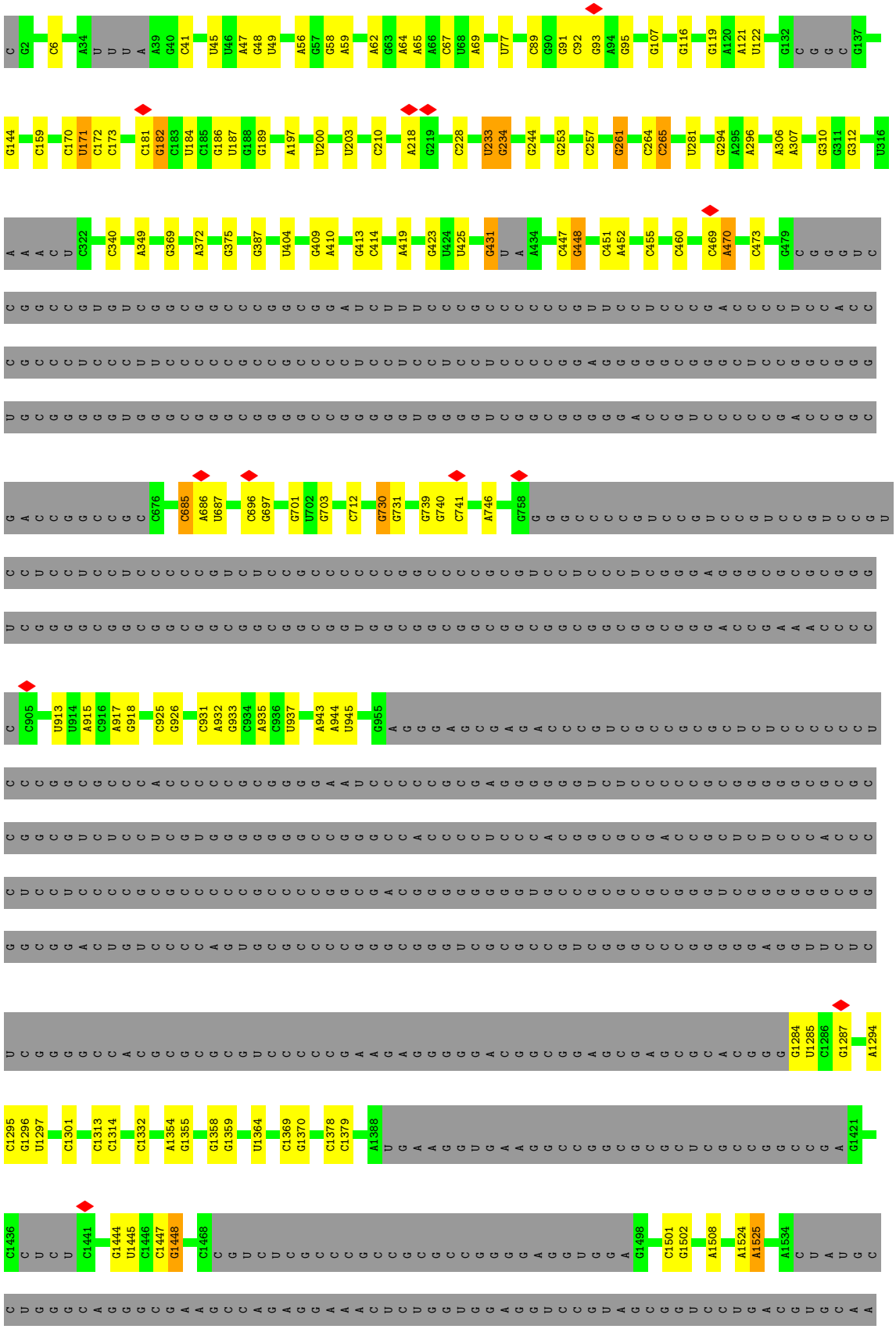
Chain L2:

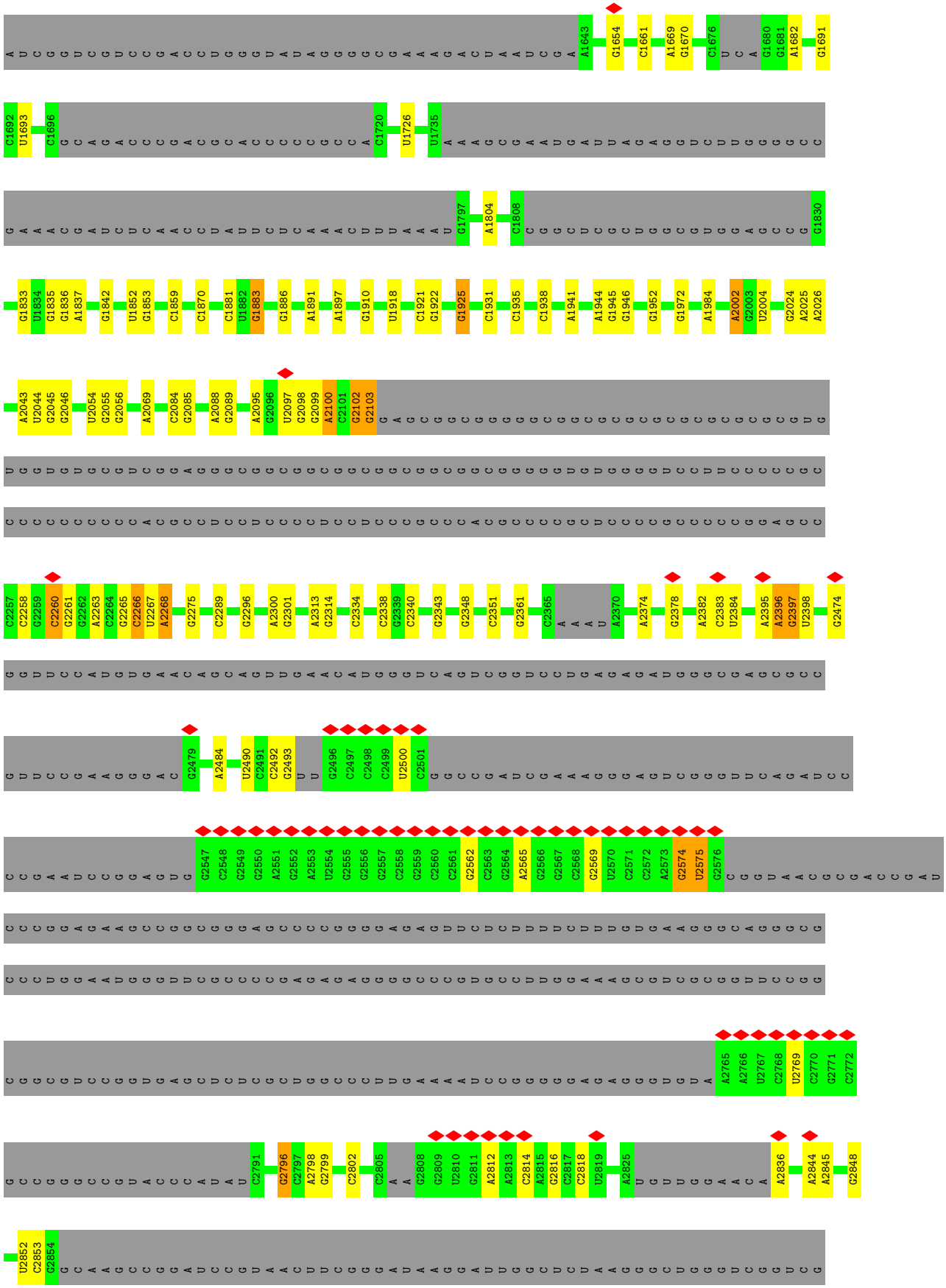


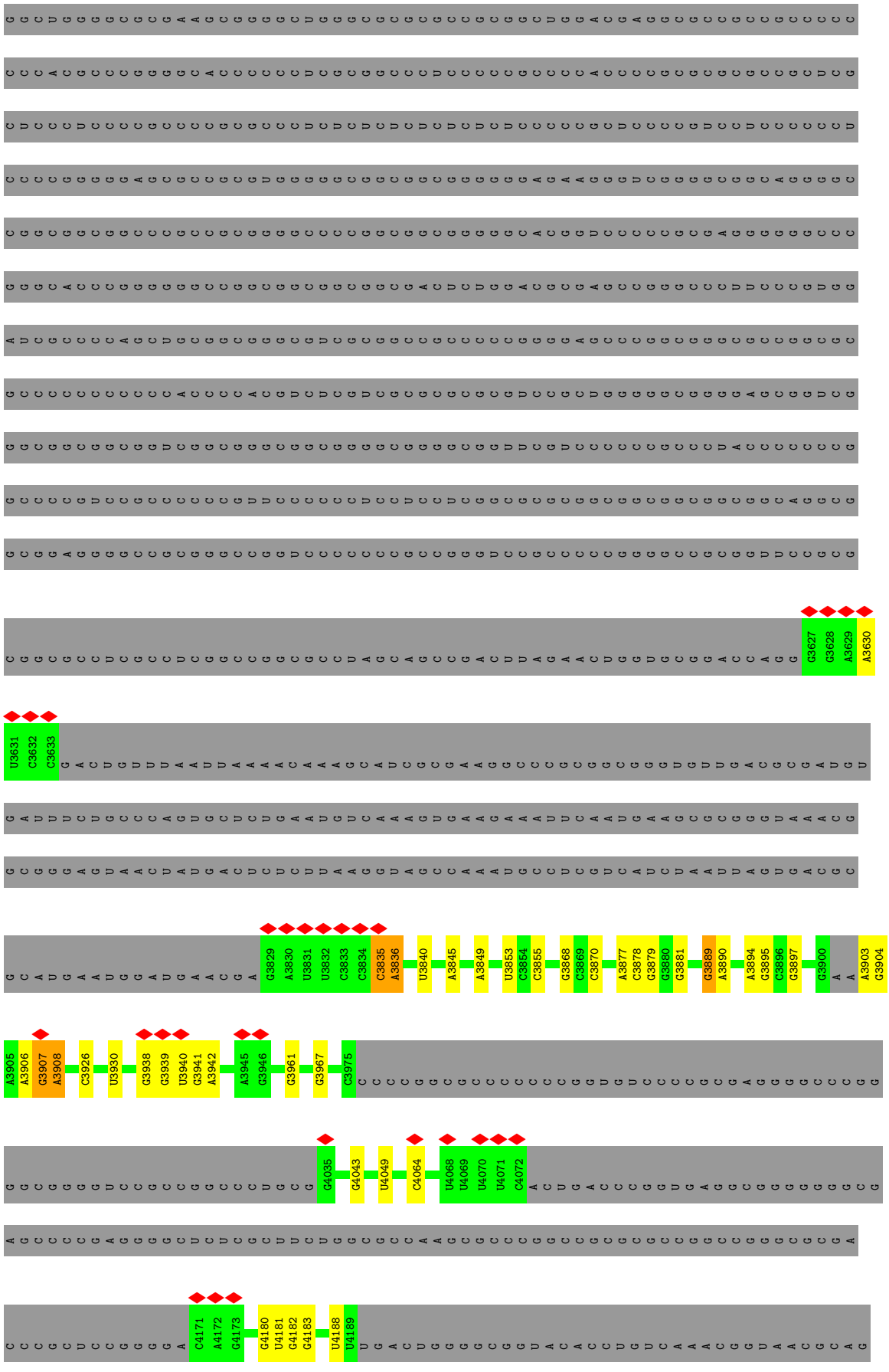


• Molecule 5: 28S rRNA

Chain L3:






G3627
G3628
A3629
A3630
U3631
C3632
C3633
G3829
A3830
U3831
U3832
C3833
C3834
C3835
A3836
U3840
A3845
A3849
U3853
C3854
C3855
G3868
C3869
C3870
A3877
C3878
G3879
G3880
G3881
G3889
A3890
A3894
G3895
C3896
G3897
G3900
A3903
G3904
A3905
A3906
G3907
A3908
C3926
U3930
G3938
G3939
U3940
G3941
A3942
A3945
G3946
G3961
G3967
C3975
G4035
G4043
U4049
C4064
U4068
U4069
U4070
U4071
C4072
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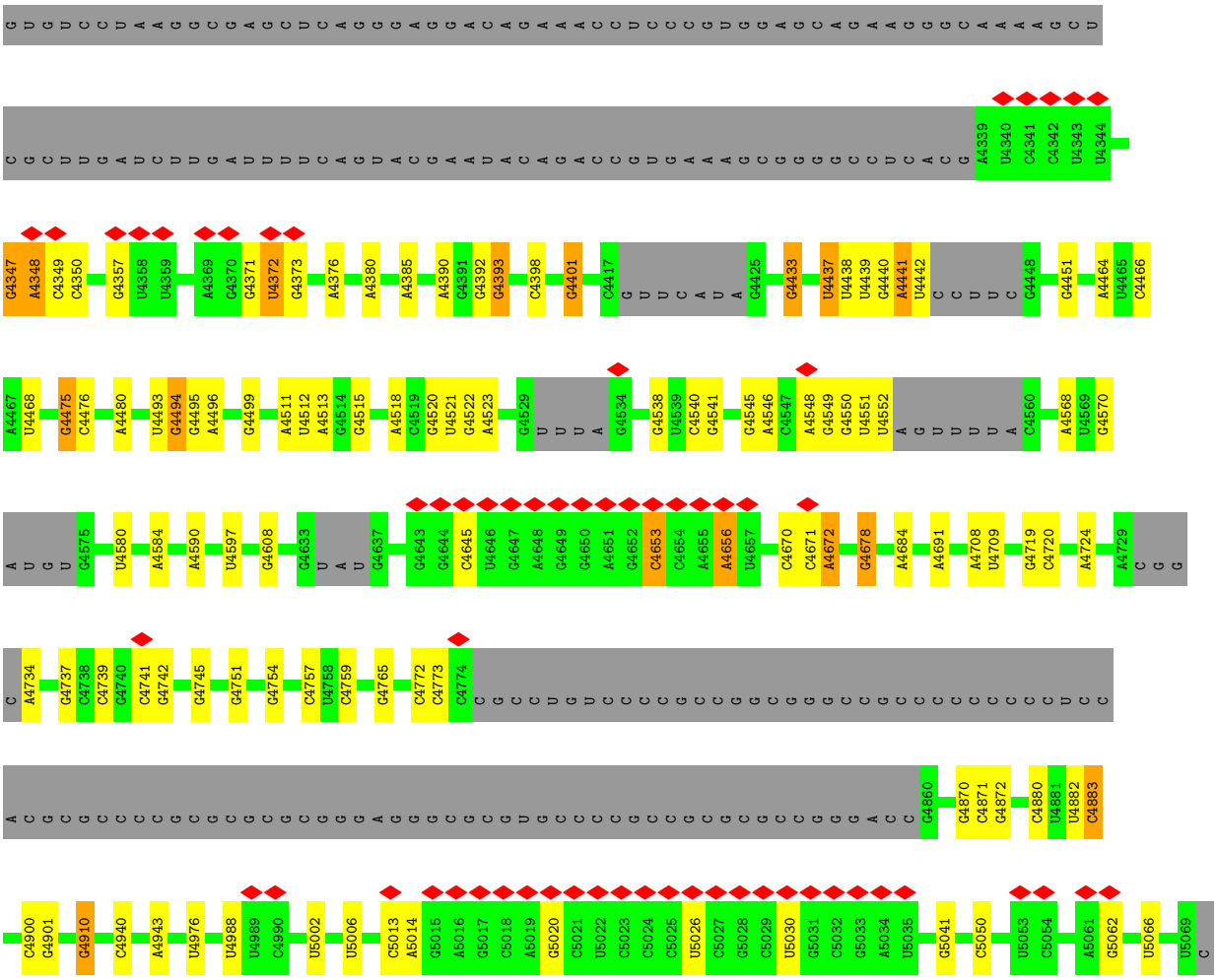
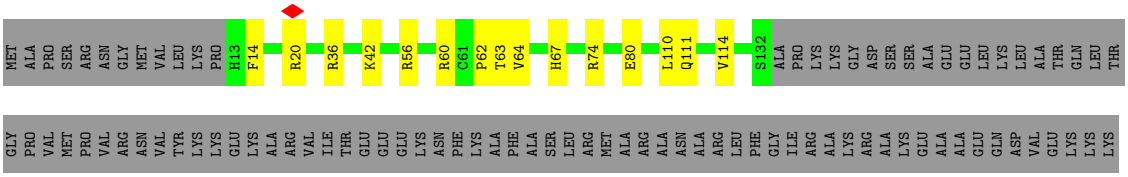
G4173
G4180
U4181
G4182
G4183
U4188
U4189



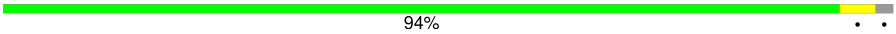
• Molecule 6: 60S ribosomal protein L13

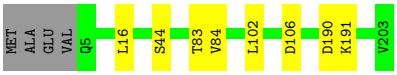
Chain L6:



• Molecule 7: 60S ribosomal protein L13a

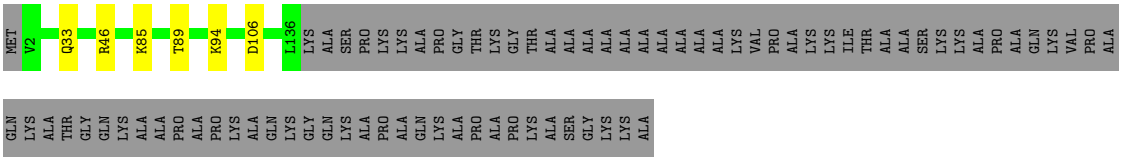
Chain L7:





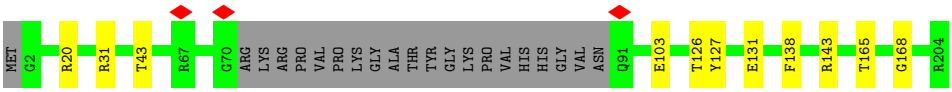
• Molecule 8: 60S ribosomal protein L14

Chain L8:



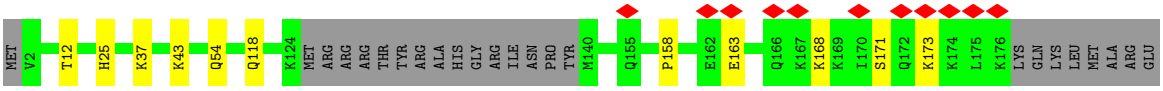
• Molecule 9: 60S ribosomal protein L15

Chain L9:



• Molecule 10: 60S ribosomal protein L17

Chain LA:

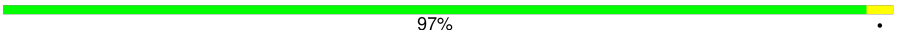


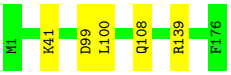
• Molecule 11: 60S ribosomal protein L18

Chain LB:

• Molecule 12: 60S ribosomal protein L18a

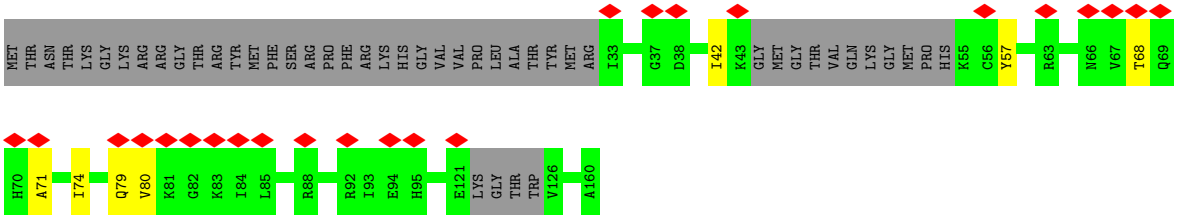
Chain LC:





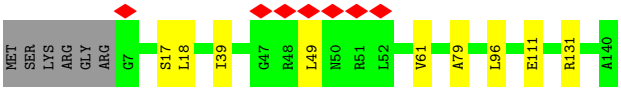
• Molecule 13: 60S ribosomal protein L21

Chain LE:



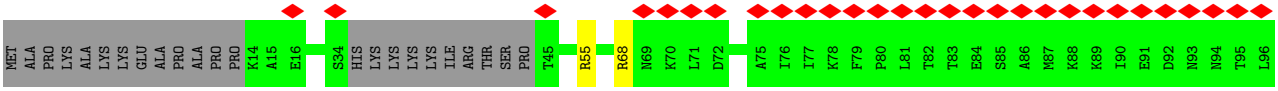
• Molecule 14: 60S ribosomal protein L23

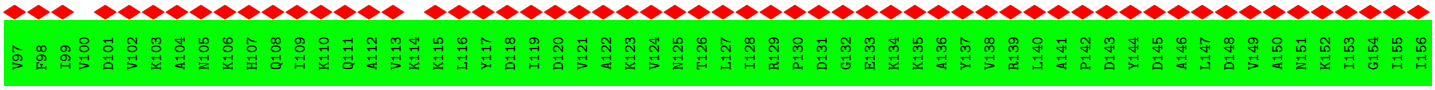
Chain LG:



• Molecule 15: 60S ribosomal protein L23a

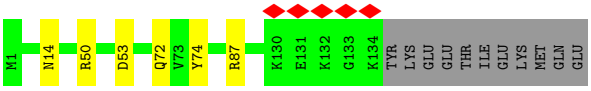
Chain LH:





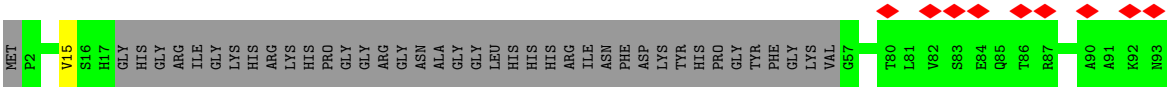
• Molecule 16: 60S ribosomal protein L26

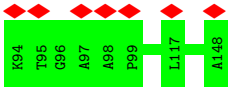
Chain LI:



• Molecule 17: 60S ribosomal protein L27a

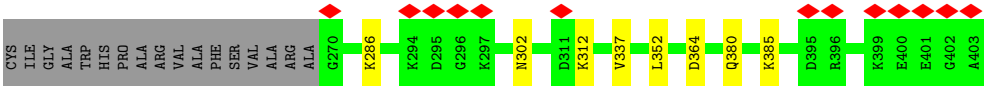
Chain LK:





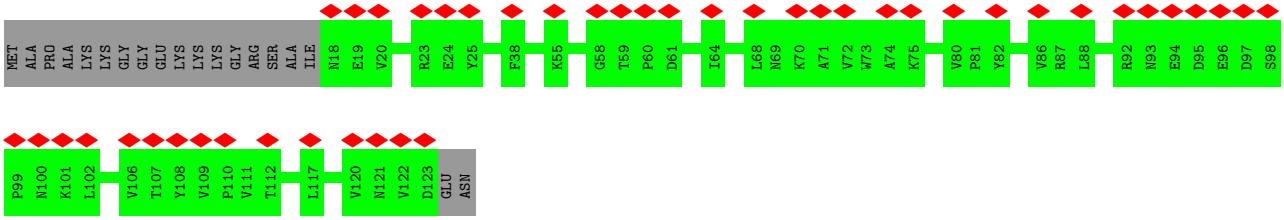
• Molecule 18: 60S ribosomal protein L3

Chain LN:



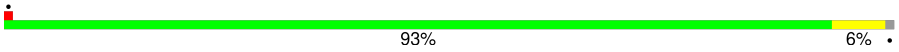
• Molecule 19: 60S ribosomal protein L31

Chain LP:



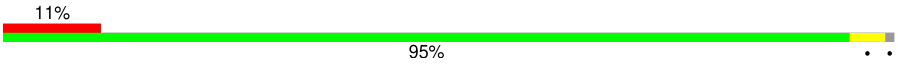
• Molecule 20: 60S ribosomal protein L32

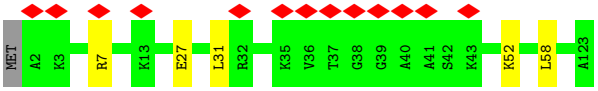
Chain LQ:



• Molecule 21: 60S ribosomal protein L35

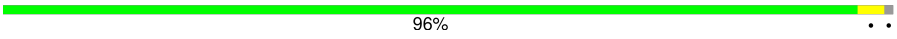
Chain LS:





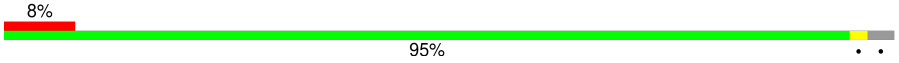
• Molecule 22: 60S ribosomal protein L35a

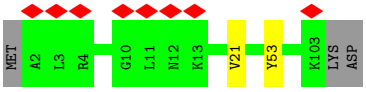
Chain LT:



• Molecule 23: 60S ribosomal protein L36

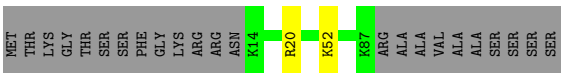
Chain LU:





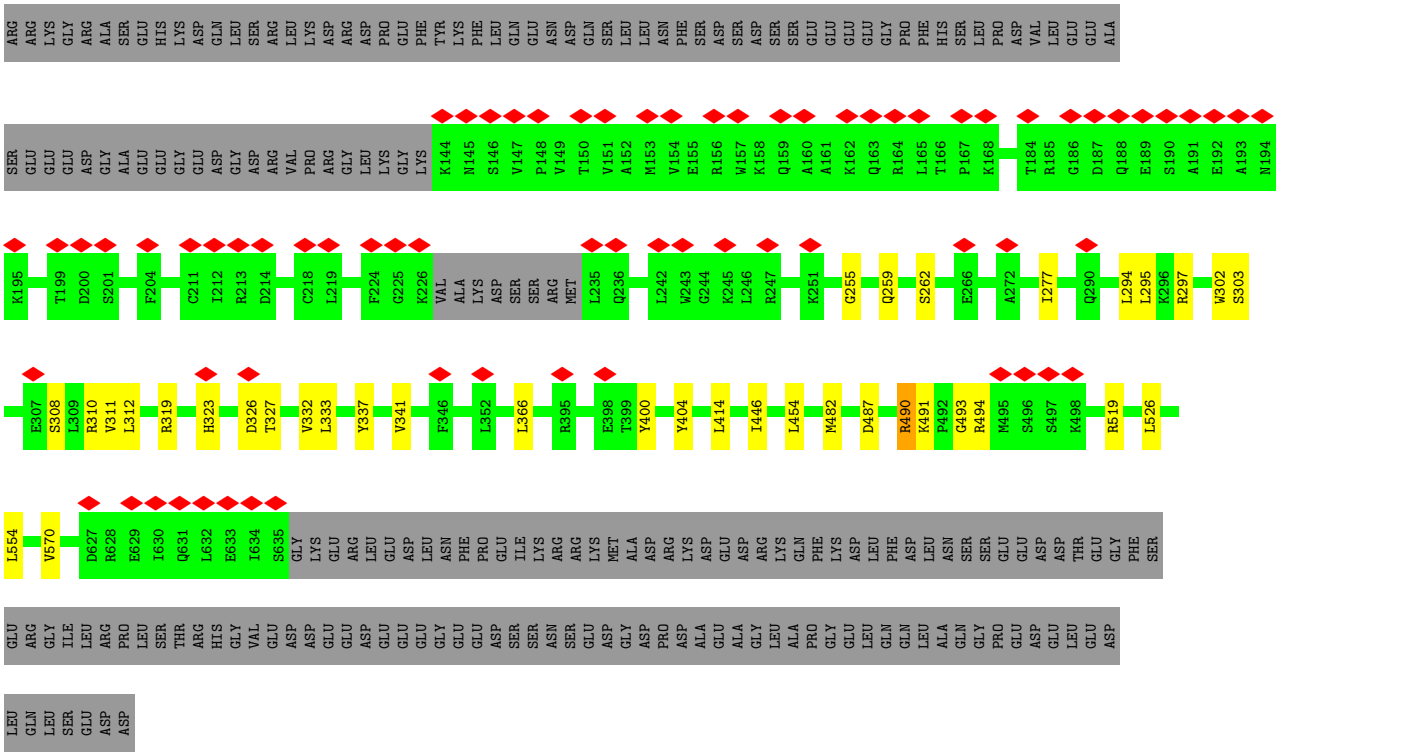
• Molecule 24: 60S ribosomal protein L37

Chain LW:



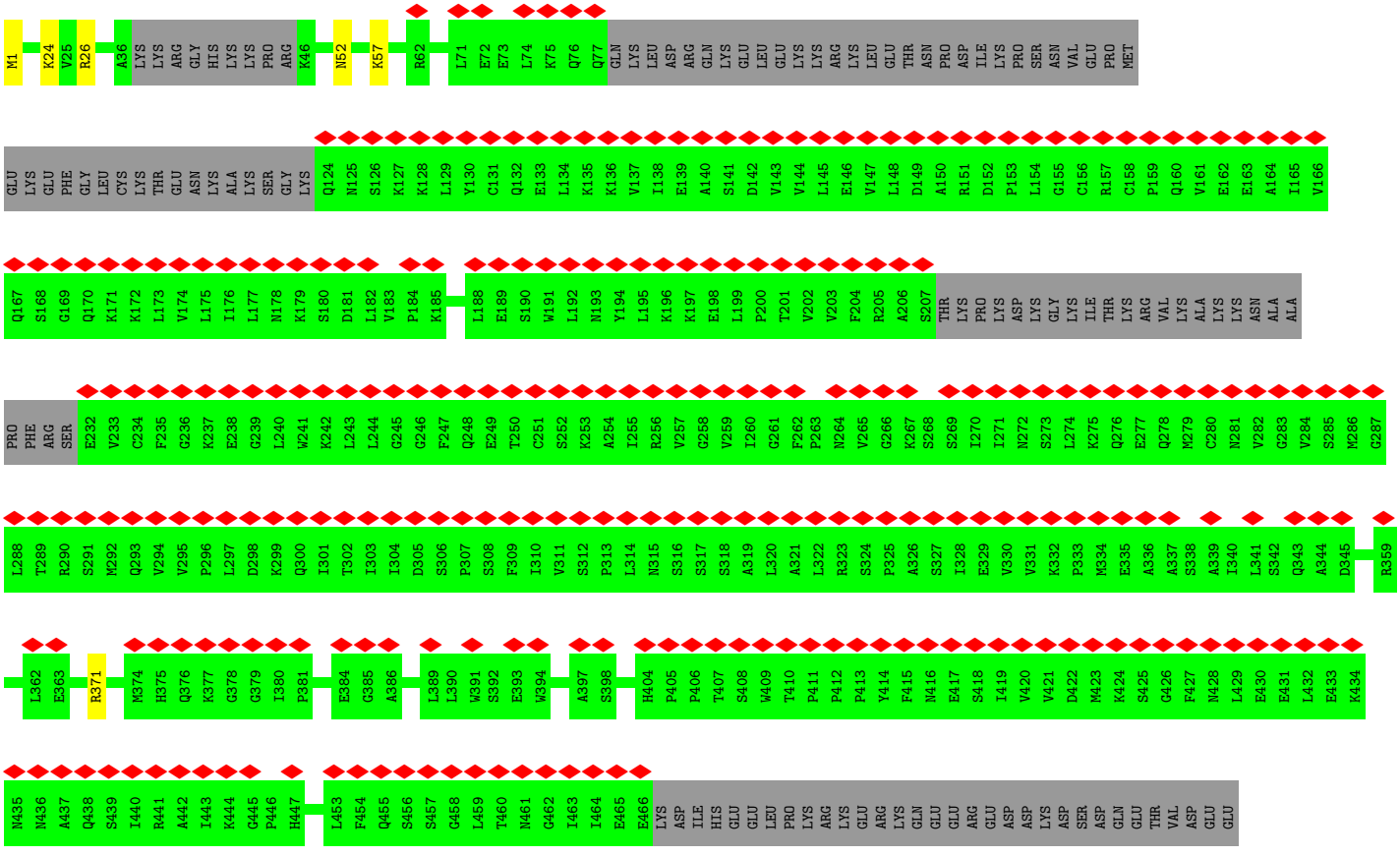
• Molecule 25: Nucleolar complex protein 2 homolog

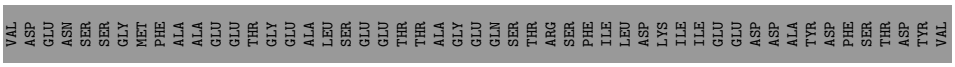
Chain NA:



• Molecule 26: Guanine nucleotide-binding protein-like 3

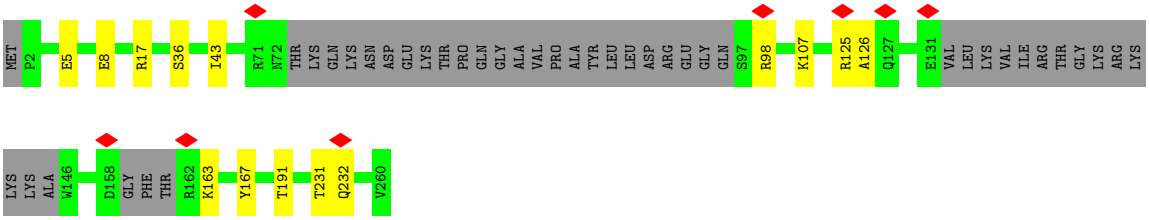
Chain NB:





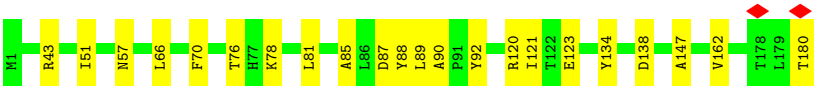
• Molecule 27: Ribosome biogenesis protein NSA2 homolog

Chain NF:



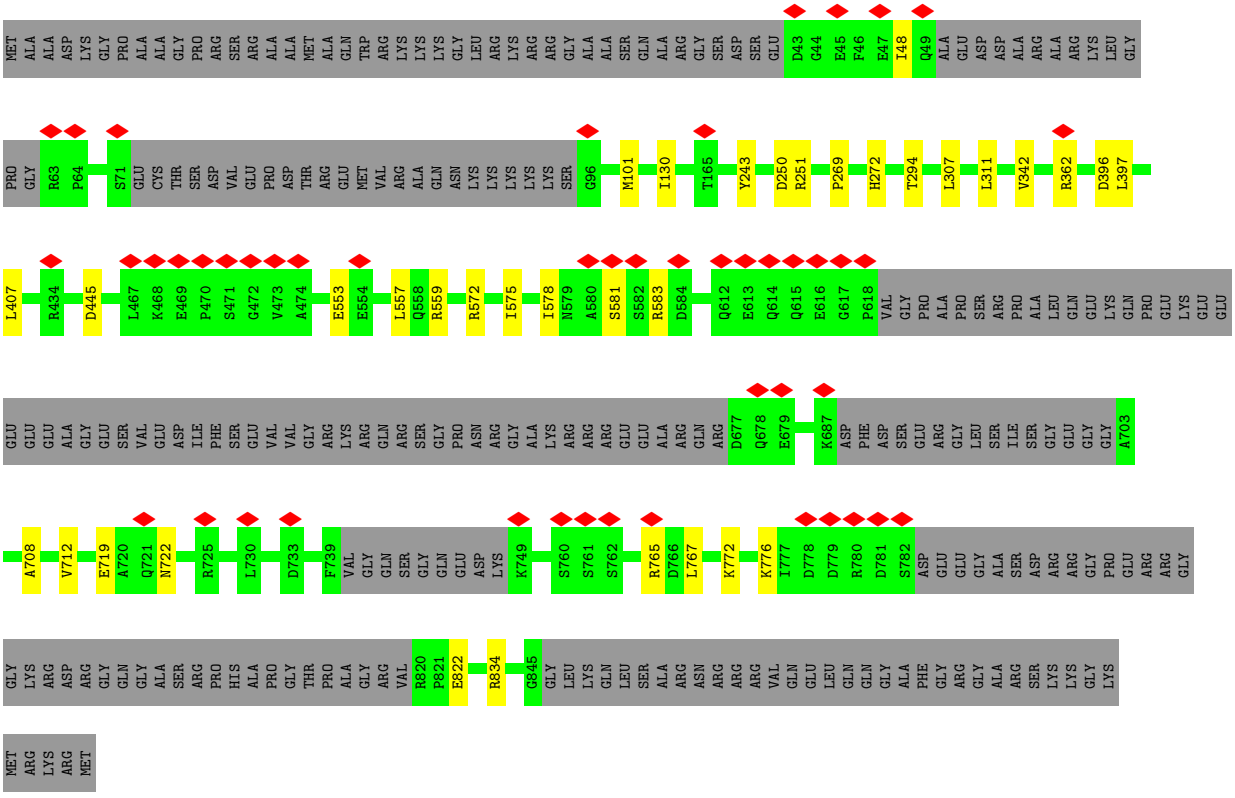
• Molecule 28: 60S ribosome subunit biogenesis protein NIP7 homolog

Chain NH:



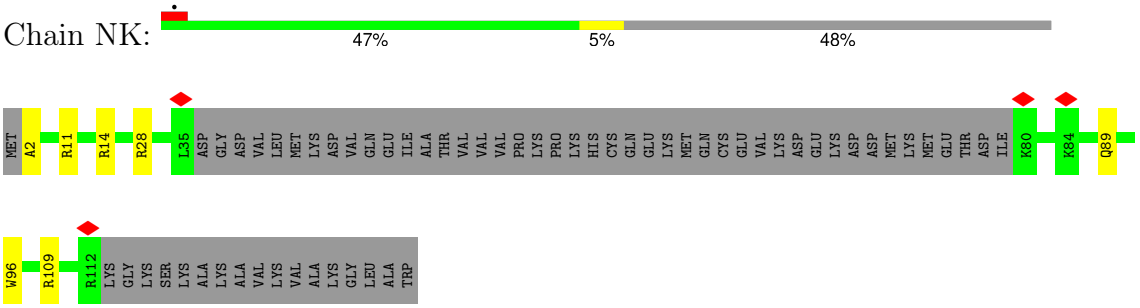
• Molecule 29: ATP-dependent RNA helicase DDX54

Chain NI:



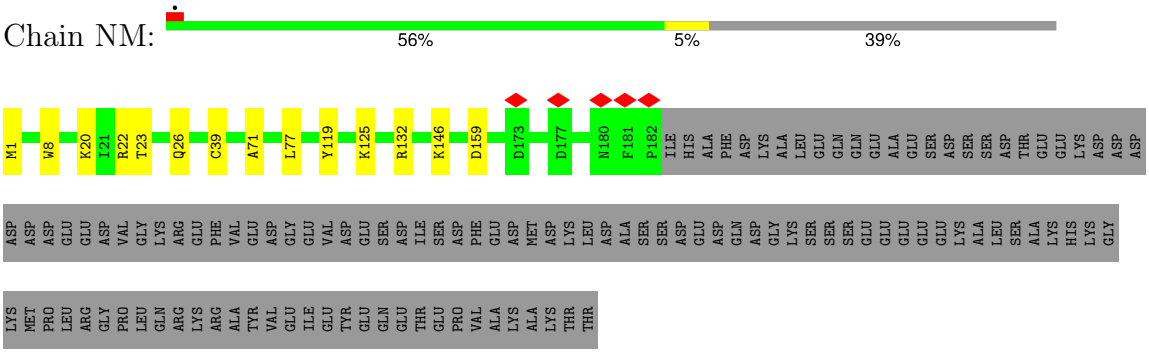
• Molecule 30: Protein LLP homolog

Chain NK:



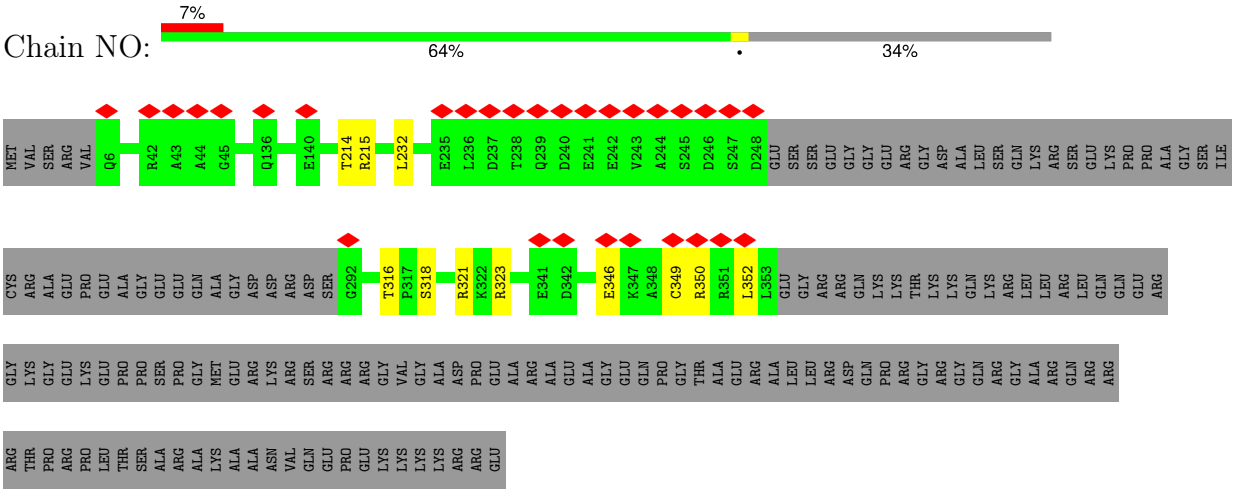
• Molecule 31: Protein MAK16 homolog

Chain NM:



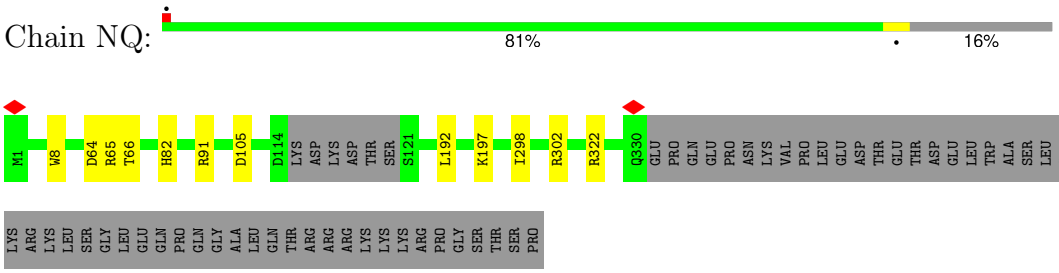
• Molecule 32: Ribosomal RNA processing protein 1 homolog A

Chain NO:



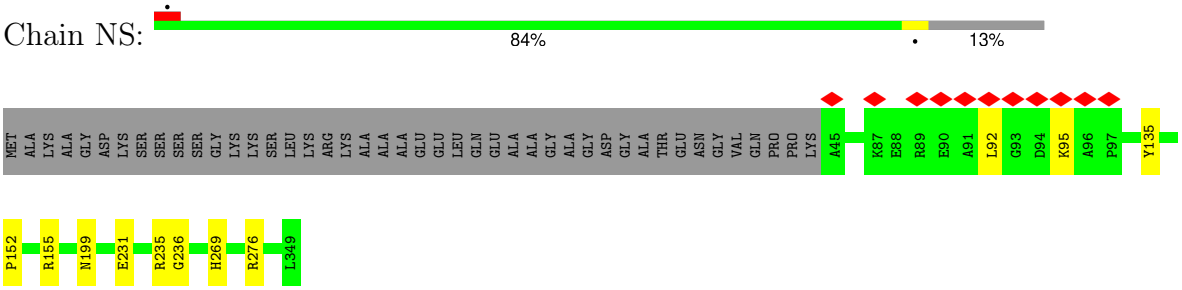
• Molecule 33: WD repeat-containing protein 74

Chain NQ:



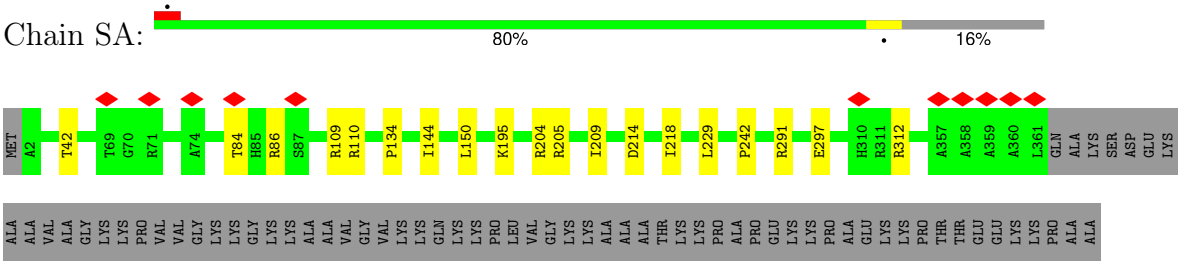
• Molecule 34: Ribosome production factor 1

Chain NS:



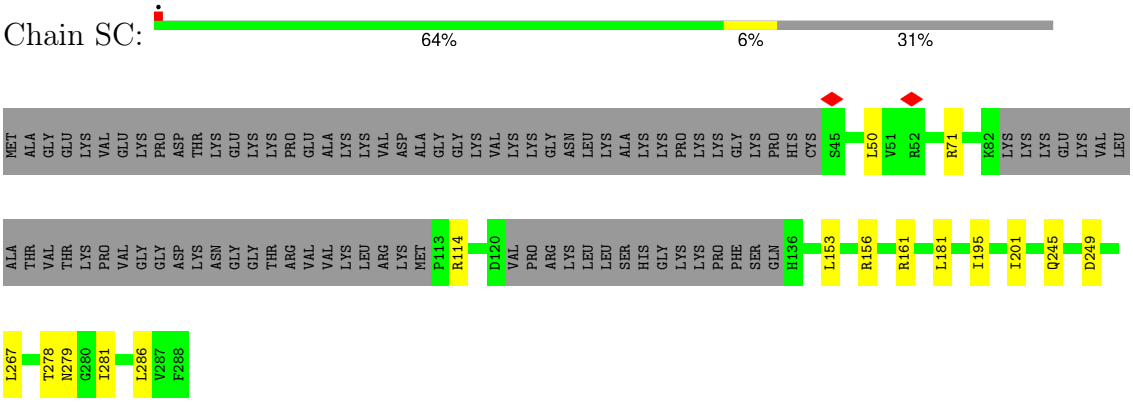
• Molecule 35: 60S ribosomal protein L4

Chain SA:



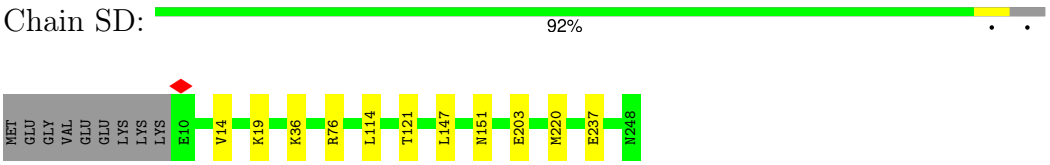
• Molecule 36: 60S ribosomal protein L6

Chain SC:



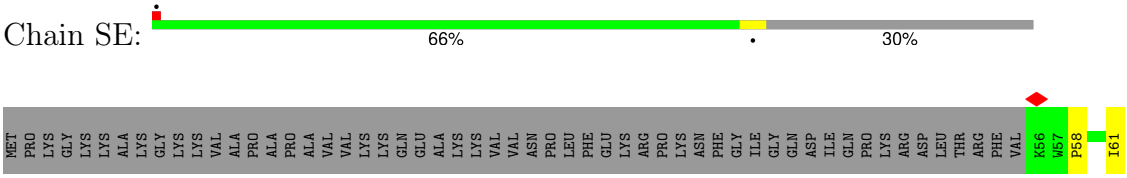
• Molecule 37: 60S ribosomal protein L7

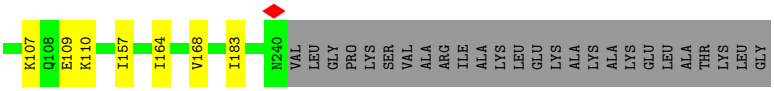
Chain SD:



• Molecule 38: 60S ribosomal protein L7a

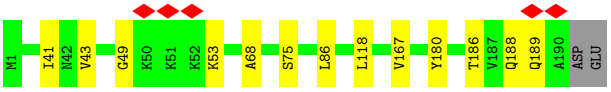
Chain SE:





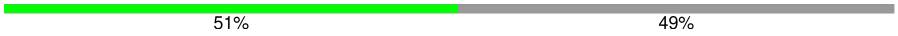
• Molecule 39: 60S ribosomal protein L9

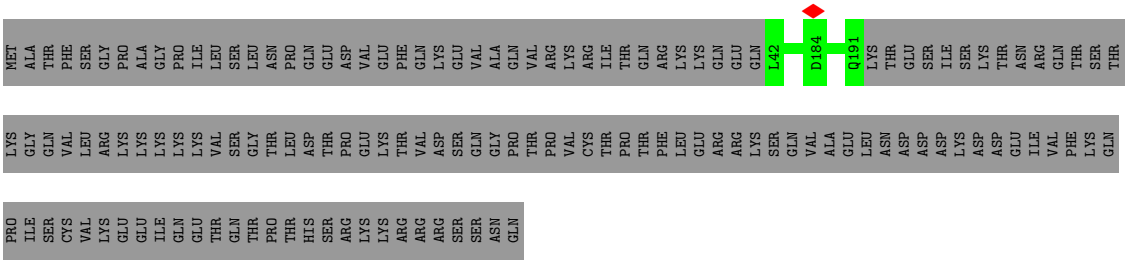
Chain SG:



• Molecule 40: MKI67 FHA domain-interacting nucleolar phosphoprotein

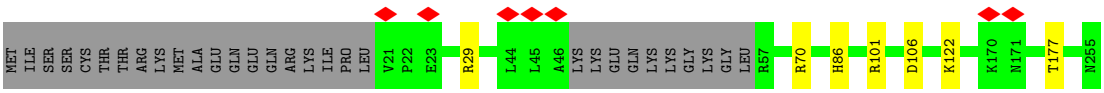
Chain SH:





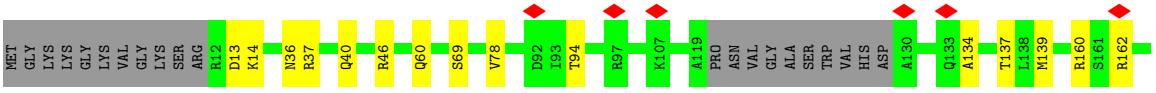
• Molecule 41: 60S ribosomal protein L7-like 1

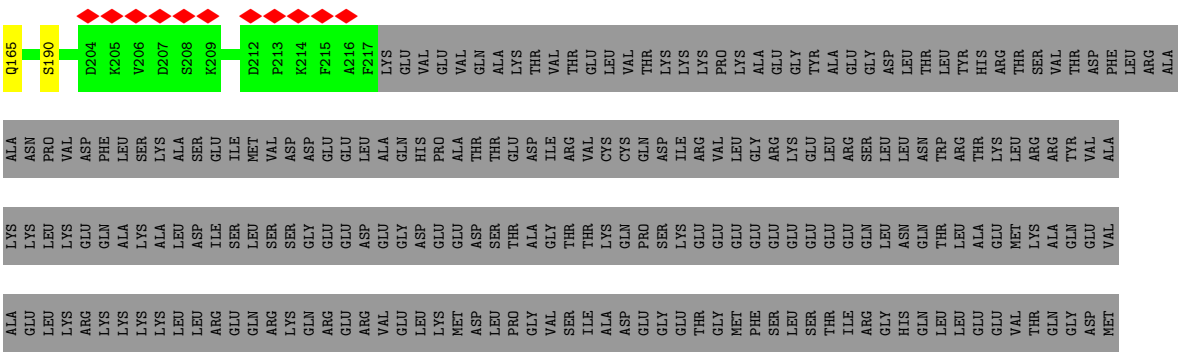
Chain SI:

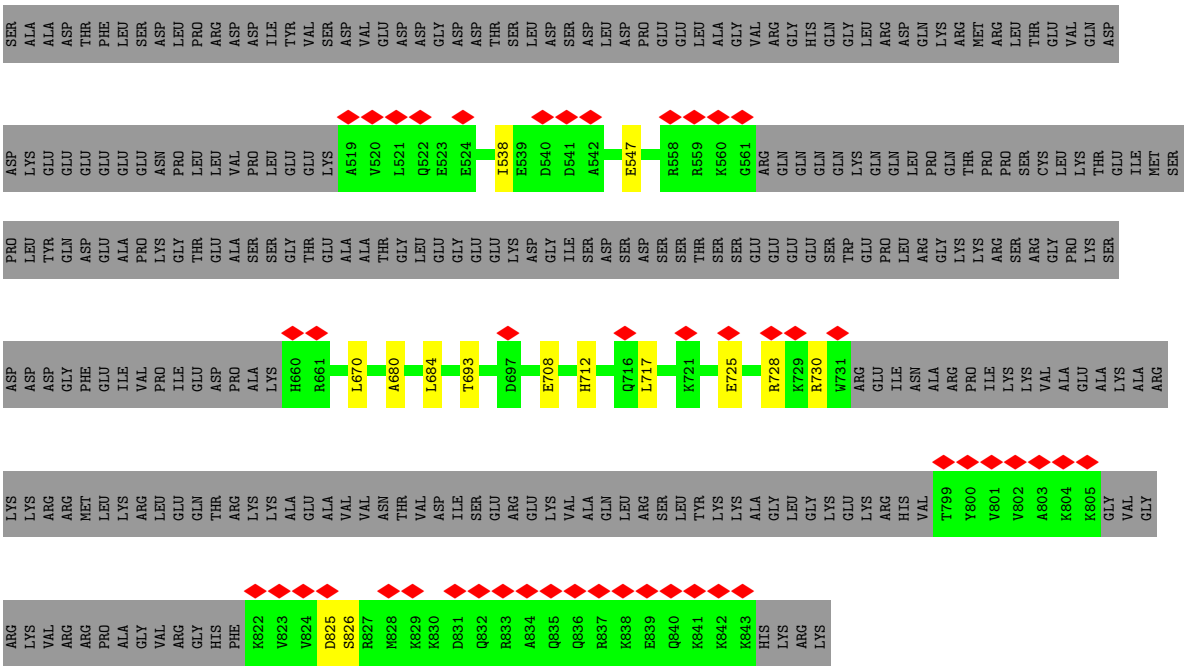


• Molecule 42: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

Chain SJ:

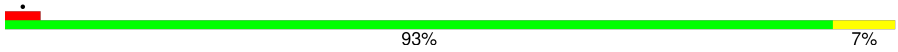






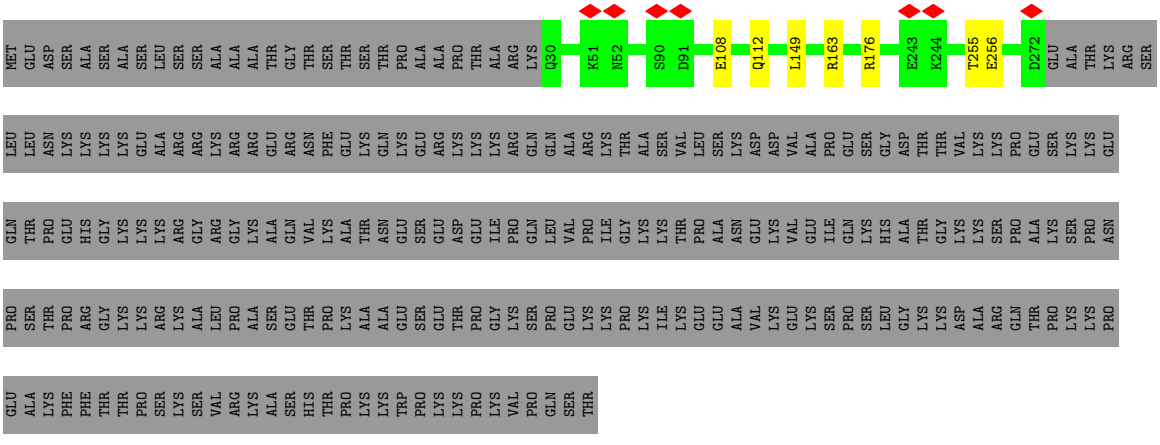
• Molecule 43: Eukaryotic translation initiation factor 6

Chain SK:



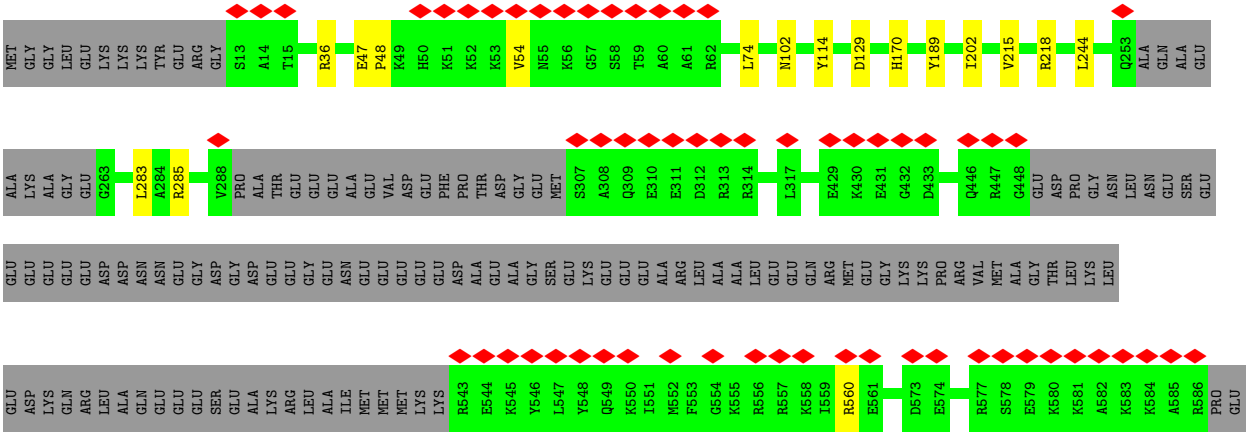
• Molecule 44: Ribosomal L1 domain-containing protein 1

Chain SL:



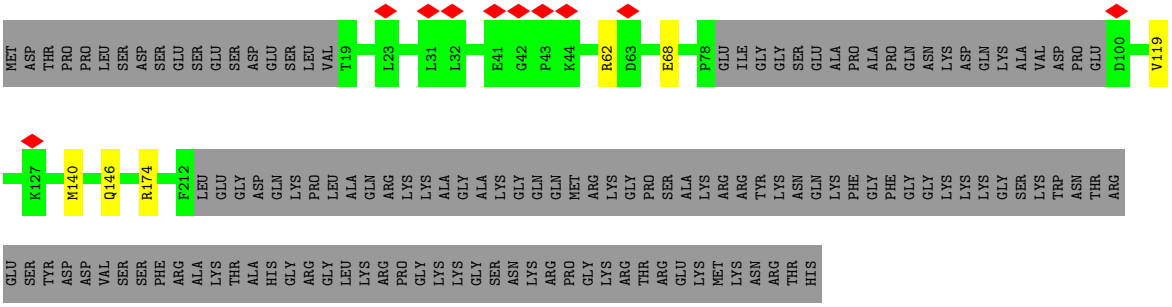
• Molecule 45: Pescadillo homolog

Chain SM:



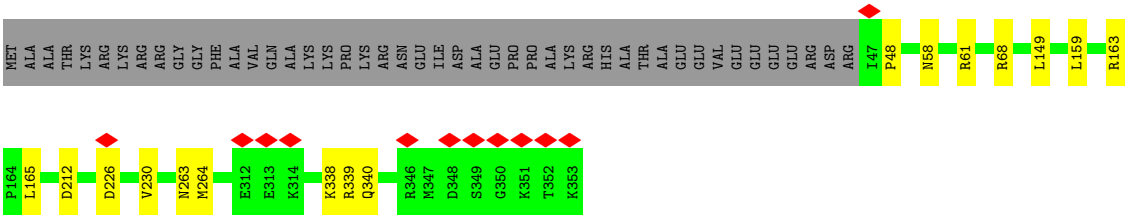
• Molecule 46: Probable rRNA-processing protein EBP2

Chain SN:



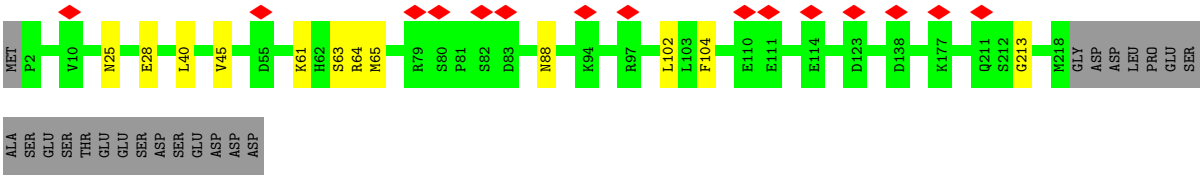
• Molecule 47: Ribosome biogenesis protein BRX1 homolog

Chain SO:



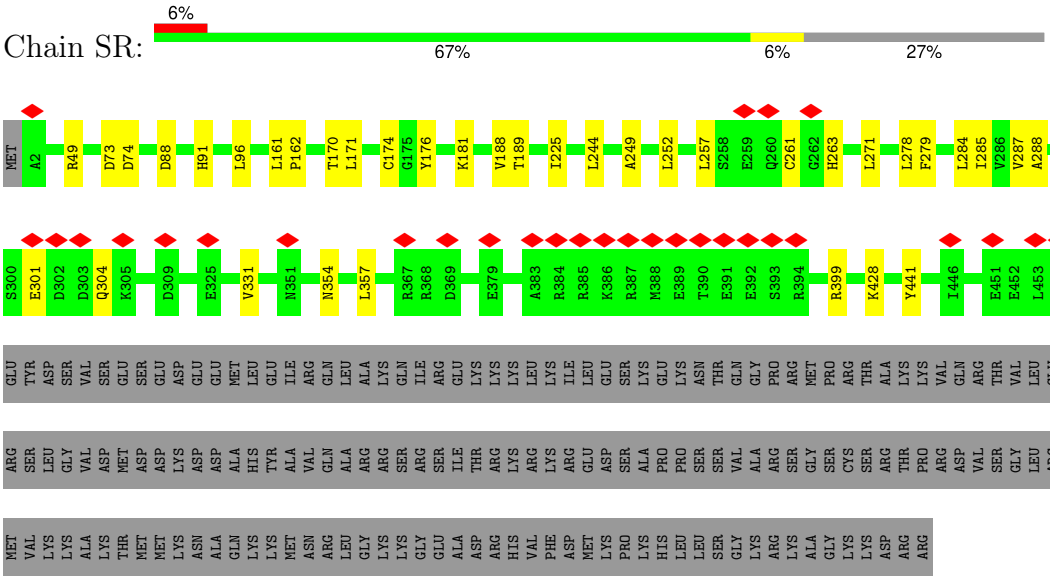
• Molecule 48: mRNA turnover protein 4 homolog

Chain SQ:



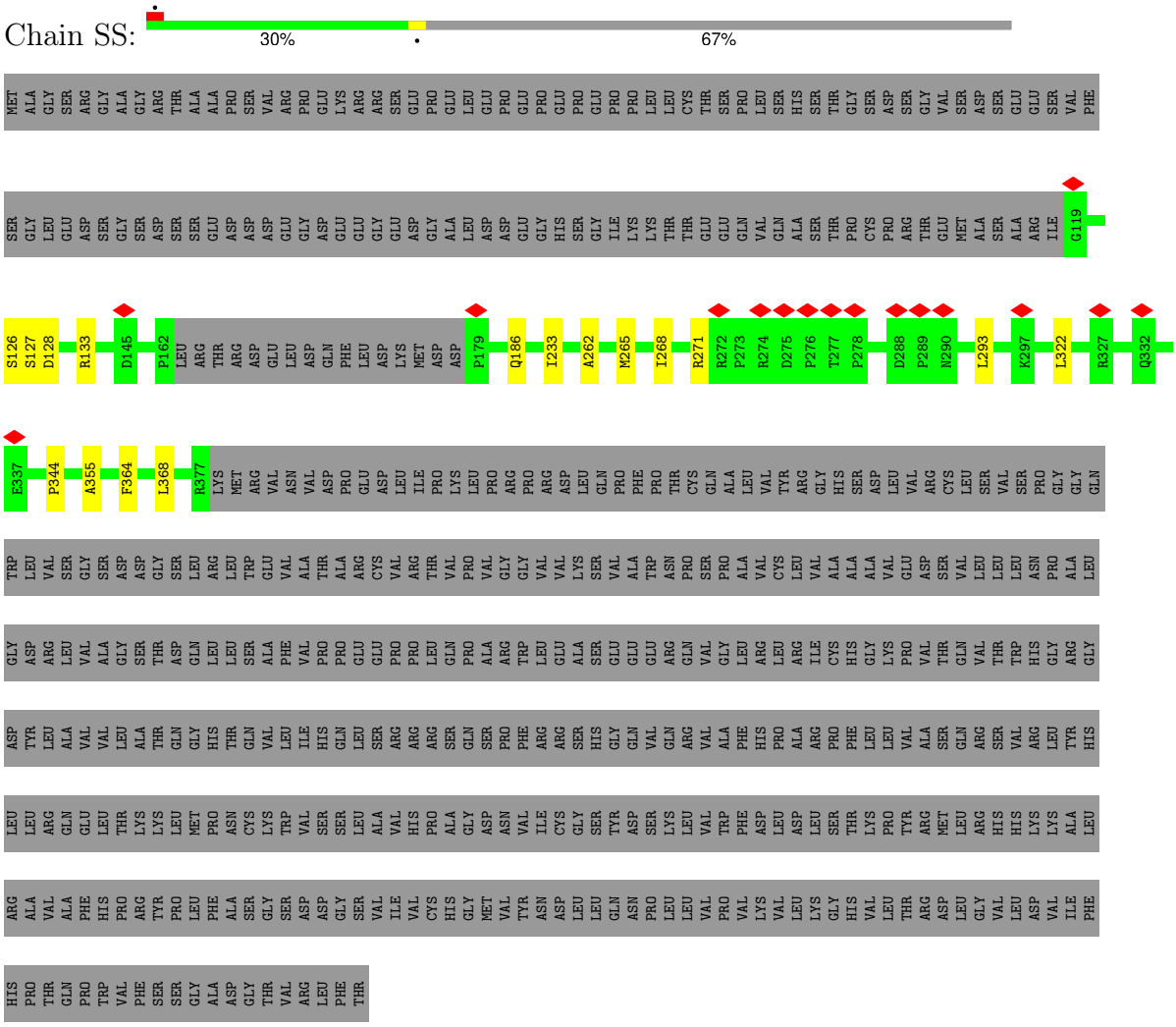
• Molecule 49: GTP-binding protein 4

Chain SR:



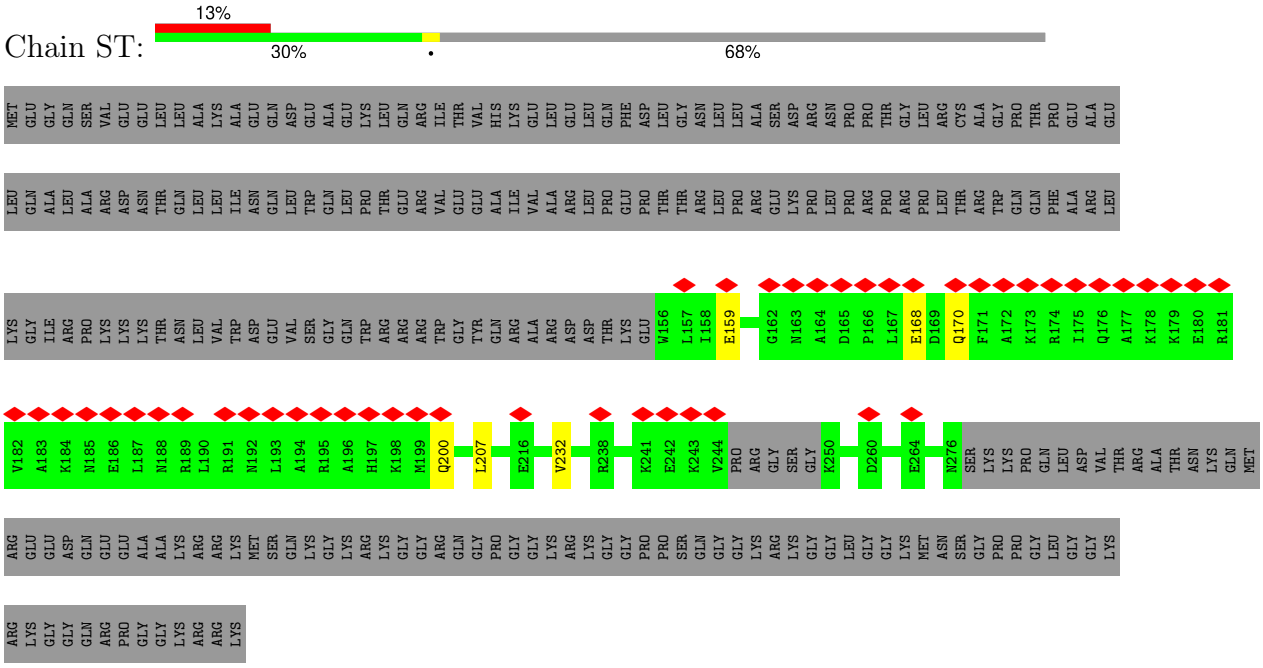
• Molecule 50: Ribosome biogenesis protein BOP1

Chain SS:



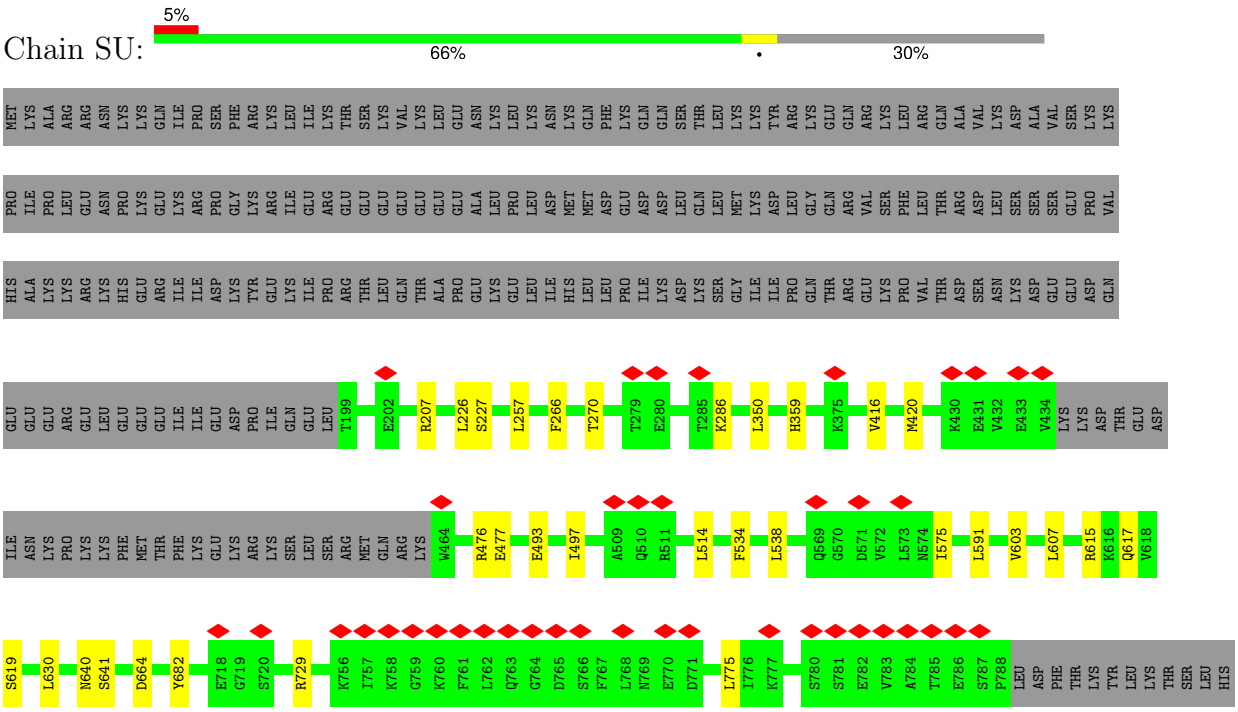
• Molecule 51: Ribosome biogenesis regulatory protein homolog

Chain ST:



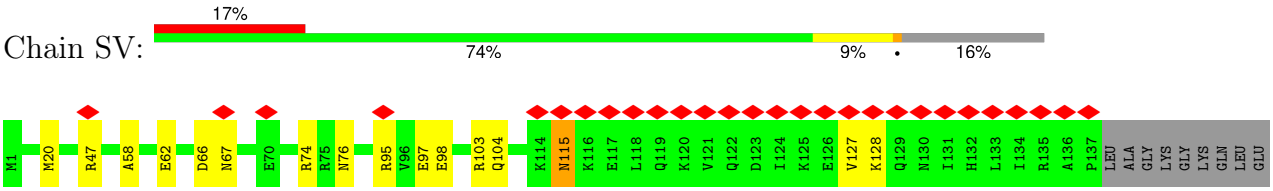
• Molecule 52: Nucleolar complex protein 3 homolog

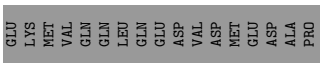
Chain SU:



• Molecule 53: Probable ribosome biogenesis protein RLP24

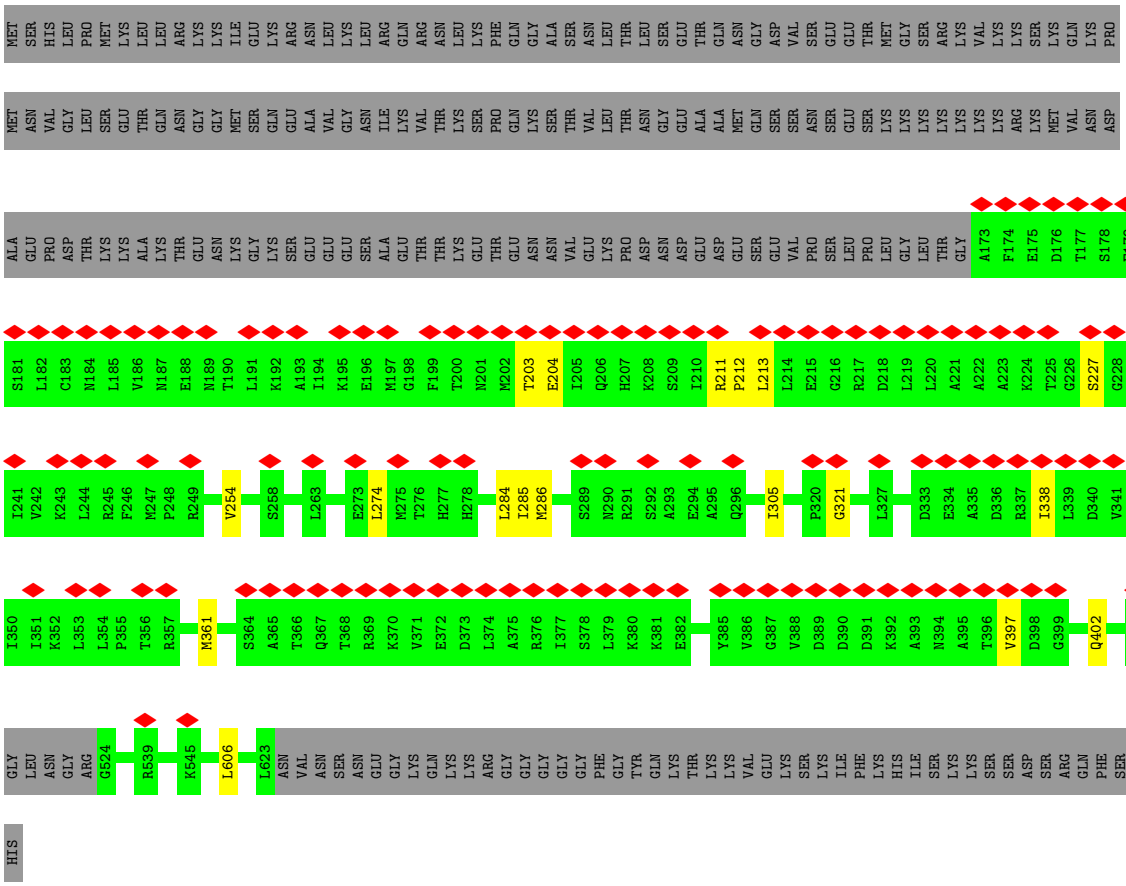
Chain SV:





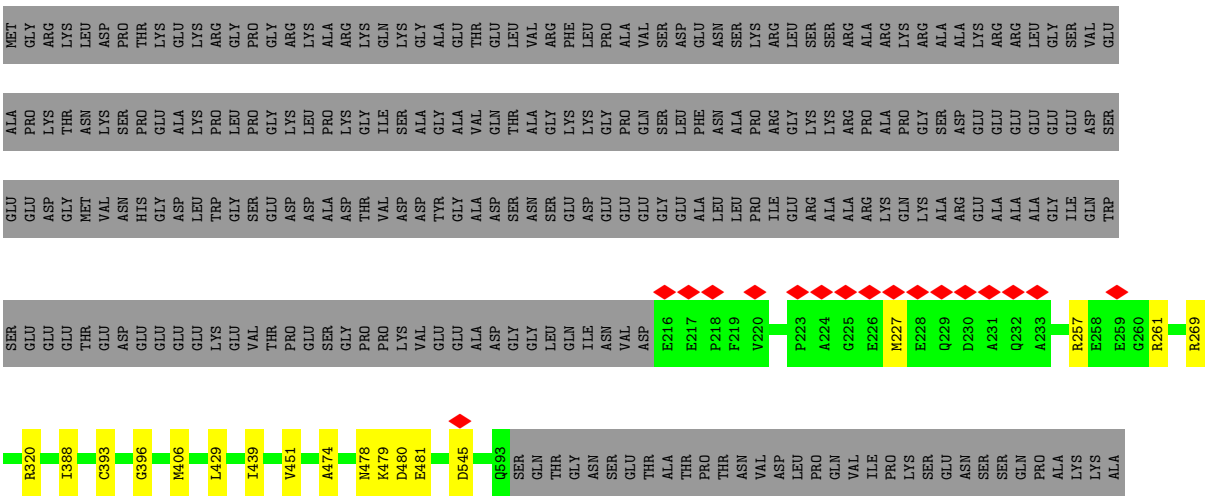
• Molecule 54: ATP-dependent RNA helicase DDX18

Chain SW:



• Molecule 55: Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase

Chain SY:



LYS GLY ALA ALA LYS THR LYS GLN GLN LEU GLN LYS GLN GLN HIS PRO LYS LYS ALA SER PHE GLN LYS LEU ASN GLY ILE SER LYS GLY ALA ASP SER GLU LEU SER THR VAL PRO SER VAL THR LYS THR GLN ALA SER SER SER PHE GLN ASP SER SER GLN PRO ALA GLY LYS ALA

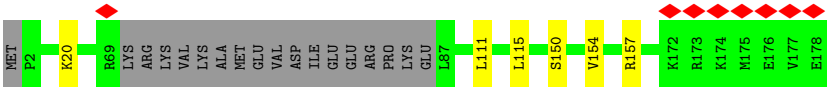
GLU GLY ILE ARG GLU PRO LYS VAL THR GLY LYS LEU LYS GLN ARG SER PRO LYS LEU GLN SER SER LYS LYS VAL ALA PHE LEU ARG GLN ASN ALA PRO PRO LYS GLY THR ASP THR GLN THR PRO ALA VAL LEU SER PRO SER LYS THR GLN ALA SER PRO SER LYS ASP HIS HIS

GLN PRO LEU GLY ARG ALA LYS GLY VAL GLU LYS GLN GLN LEU PRO GLU GLN PRO PHE GLU LYS ALA ALA PHE GLN LYS GLN ASN ASP THR PRO LYS GLY PRO GLN PRO PRO THR VAL SER PRO ILE ARG SER SER ARG PRO PRO PRO ALA LYS ARG LYS LYS SER GLN SER ARG GLY ASN

SER GLN LEU LEU LEU SER

- Molecule 56: 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	209464	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	8.435	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.039	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.8	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, ZN, SF4, K, AME, ADP, GDP, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	BA	0.24	0/1224	0.50	0/1651
2	BB	0.24	0/1056	0.45	0/1472
3	L1	0.24	0/3611	0.74	0/5623
4	L2	0.24	0/1634	0.78	0/2538
5	L3	0.25	0/53038	0.78	2/82653 (0.0%)
6	L6	0.25	0/1020	0.64	0/1367
7	L7	0.26	0/1666	0.55	0/2228
8	L8	0.26	0/1133	0.53	0/1516
9	L9	0.25	0/1584	0.63	0/2117
10	LA	0.24	0/1309	0.47	0/1752
11	LB	0.24	0/1239	0.62	0/1658
12	LC	0.25	0/1501	0.57	0/2013
13	LE	0.25	0/941	0.52	0/1254
14	LG	0.26	0/1007	0.55	0/1350
15	LH	0.23	0/818	0.51	0/1111
16	LI	0.26	0/1132	0.61	1/1504 (0.1%)
17	LK	0.23	0/648	0.52	0/880
18	LN	0.25	0/2938	0.52	0/3923
19	LP	0.22	0/525	0.43	0/731
20	LQ	0.24	0/1114	0.58	0/1486
21	LS	0.25	0/1023	0.56	0/1351
22	LT	0.25	0/895	0.61	0/1198
23	LU	0.25	0/843	0.62	0/1115
24	LW	0.25	0/626	0.64	0/829
25	NA	0.26	0/3734	0.47	0/5079
26	NB	0.24	0/2449	0.46	0/3335
27	NF	0.25	0/1816	0.52	0/2420
28	NH	0.26	0/1473	0.50	0/1988
29	NI	0.24	0/5222	0.52	0/7025
30	NK	0.23	0/587	0.58	0/767
31	NM	0.25	0/1566	0.54	0/2097
32	NO	0.24	0/2530	0.49	0/3412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	NQ	0.24	0/2556	0.54	0/3466
34	NS	0.25	0/2592	0.53	0/3487
35	SA	0.24	0/2918	0.57	0/3920
36	SC	0.25	0/1657	0.55	0/2219
37	SD	0.25	0/2022	0.56	0/2696
38	SE	0.24	0/1517	0.54	0/2046
39	SG	0.25	0/1548	0.54	0/2081
40	SH	0.26	0/1298	0.50	0/1742
41	SI	0.24	0/1906	0.51	0/2561
42	SJ	0.24	0/2833	0.49	0/3801
43	SK	0.24	0/1877	0.52	0/2554
44	SL	0.24	0/1994	0.50	0/2684
45	SM	0.25	0/3819	0.49	0/5139
46	SN	0.24	0/1368	0.48	0/1830
47	SO	0.25	0/2608	0.51	0/3506
48	SQ	0.25	0/1817	0.51	0/2435
49	SR	0.25	0/3882	0.51	0/5237
50	SS	0.25	0/2052	0.52	0/2786
51	ST	0.24	0/851	0.45	0/1149
52	SU	0.25	0/4510	0.45	0/6082
53	SV	0.26	0/1194	0.53	0/1582
54	SW	0.24	0/3620	0.47	0/4886
55	SY	0.24	0/3046	0.52	0/4117
56	SZ	0.24	0/1364	0.53	0/1826
All	All	0.25	0/156751	0.64	3/223275 (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})
5	L3	4653	C	C2-N1-C1'	5.44	124.78	118.80
16	LI	53	ASP	CB-CG-OD1	5.15	122.94	118.30
5	L3	2266	C	C2-N1-C1'	5.01	124.31	118.80

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	10	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	6	0
4	L2	1468	0	755	6	0
5	L3	47439	0	24001	139	0
6	L6	998	0	1067	11	0
7	L7	1634	0	1779	5	0
8	L8	1111	0	1174	6	0
9	L9	1546	0	1585	9	0
10	LA	1286	0	1338	10	0
11	LB	1223	0	1330	6	0
12	LC	1461	0	1502	4	0
13	LE	926	0	979	4	0
14	LG	993	0	1050	9	0
15	LH	813	0	640	2	0
16	LI	1115	0	1205	4	0
17	LK	642	0	455	1	0
18	LN	2884	0	3000	19	0
19	LP	526	0	225	0	0
20	LQ	1096	0	1183	7	0
21	LS	1015	0	1148	4	0
22	LT	876	0	912	2	0
23	LU	832	0	917	2	0
24	LW	612	0	640	2	0
25	NA	3658	0	3564	23	0
26	NB	2424	0	1868	5	0
27	NF	1783	0	1896	11	0
28	NH	1441	0	1448	16	0
29	NI	5137	0	5294	22	0
30	NK	581	0	656	7	0
31	NM	1550	0	1599	12	0
32	NO	2487	0	2506	8	0
33	NQ	2502	0	2481	7	0
34	NS	2529	0	2563	9	0
35	SA	2864	0	3038	13	0
36	SC	1627	0	1751	11	0
37	SD	1985	0	2128	8	0
38	SE	1491	0	1592	6	0
39	SG	1526	0	1614	8	0
40	SH	1267	0	1291	0	0
41	SI	1864	0	1982	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	SJ	2780	0	2826	25	0
43	SK	1852	0	1828	9	0
44	SL	1960	0	2052	5	0
45	SM	3735	0	3830	11	0
46	SN	1350	0	1345	6	0
47	SO	2544	0	2631	15	0
48	SQ	1778	0	1817	8	0
49	SR	3808	0	3873	24	0
50	SS	2011	0	1919	14	0
51	ST	838	0	781	5	0
52	SU	4434	0	4551	31	0
53	SV	1171	0	1232	12	0
54	SW	3549	0	3628	15	0
55	SY	2985	0	3004	11	0
56	SZ	1338	0	1352	5	0
57	L1	4	0	0	0	0
57	L2	1	0	0	0	0
57	L3	51	0	0	0	0
57	L9	1	0	0	0	0
57	LN	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	1	0	0	0	0
57	NI	1	0	0	0	0
57	SA	1	0	0	0	0
57	SO	1	0	0	0	0
57	SR	1	0	0	0	0
57	SU	1	0	0	0	0
58	LW	1	0	0	0	0
58	SV	1	0	0	0	0
59	NI	27	0	12	0	0
60	NM	8	0	0	0	0
61	SR	28	0	12	0	0
62	SR	1	0	0	0	0
All	All	148975	0	124209	466	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 466 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)
5:L3:712:C:O2	5:L3:1284:G:N2	2.01	0.93
25:NA:302:TRP:O	25:NA:310:ARG:NH1	2.11	0.84
1:BA:105:THR:OG1	1:BA:108:GLU:OE1	1.97	0.82
5:L3:2338:C:OP1	31:NM:22:ARG:NH1	2.13	0.82
54:SW:238:VAL:HG21	54:SW:274:LEU:HD22	1.61	0.82

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%)	158 (100%)	0	0	100	100
2	BB	211/217 (97%)	205 (97%)	6 (3%)	0	100	100
6	L6	118/211 (56%)	116 (98%)	2 (2%)	0	100	100
7	L7	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
8	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
9	L9	179/204 (88%)	179 (100%)	0	0	100	100
10	LA	156/184 (85%)	155 (99%)	1 (1%)	0	100	100
11	LB	149/188 (79%)	149 (100%)	0	0	100	100
12	LC	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
13	LE	107/160 (67%)	104 (97%)	3 (3%)	0	100	100
14	LG	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
15	LH	129/156 (83%)	129 (100%)	0	0	100	100
16	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
17	LK	104/148 (70%)	101 (97%)	3 (3%)	0	100	100
18	LN	352/403 (87%)	350 (99%)	2 (1%)	0	100	100
19	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LQ	131/135 (97%)	131 (100%)	0	0	100	100
21	LS	120/123 (98%)	120 (100%)	0	0	100	100
22	LT	107/110 (97%)	107 (100%)	0	0	100	100
23	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
24	LW	72/97 (74%)	72 (100%)	0	0	100	100
25	NA	480/749 (64%)	480 (100%)	0	0	100	100
26	NB	379/549 (69%)	375 (99%)	4 (1%)	0	100	100
27	NF	210/260 (81%)	208 (99%)	2 (1%)	0	100	100
28	NH	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
29	NI	633/881 (72%)	626 (99%)	7 (1%)	0	100	100
30	NK	63/129 (49%)	63 (100%)	0	0	100	100
31	NM	180/300 (60%)	178 (99%)	2 (1%)	0	100	100
32	NO	301/461 (65%)	300 (100%)	1 (0%)	0	100	100
33	NQ	320/385 (83%)	318 (99%)	2 (1%)	0	100	100
34	NS	303/349 (87%)	300 (99%)	3 (1%)	0	100	100
35	SA	358/427 (84%)	352 (98%)	6 (2%)	0	100	100
36	SC	193/288 (67%)	191 (99%)	2 (1%)	0	100	100
37	SD	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
38	SE	183/266 (69%)	181 (99%)	2 (1%)	0	100	100
39	SG	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
40	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
41	SI	222/255 (87%)	217 (98%)	5 (2%)	0	100	100
42	SJ	328/847 (39%)	323 (98%)	5 (2%)	0	100	100
43	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100
44	SL	241/490 (49%)	236 (98%)	5 (2%)	0	100	100
45	SM	445/588 (76%)	444 (100%)	1 (0%)	0	100	100
46	SN	169/306 (55%)	169 (100%)	0	0	100	100
47	SO	305/353 (86%)	302 (99%)	3 (1%)	0	100	100
48	SQ	216/239 (90%)	214 (99%)	2 (1%)	0	100	100
49	SR	460/634 (73%)	453 (98%)	7 (2%)	0	100	100
50	SS	237/746 (32%)	233 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	ST	112/365 (31%)	110 (98%)	2 (2%)	0	100	100
52	SU	557/800 (70%)	549 (99%)	8 (1%)	0	100	100
53	SV	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
54	SW	440/670 (66%)	434 (99%)	6 (1%)	0	100	100
55	SY	376/812 (46%)	373 (99%)	3 (1%)	0	100	100
56	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	12061/17258 (70%)	11931 (99%)	130 (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
6	L6	104/177 (59%)	104 (100%)	0	100	100
7	L7	171/174 (98%)	171 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	155/172 (90%)	155 (100%)	0	100	100
10	LA	142/163 (87%)	142 (100%)	0	100	100
11	LB	136/165 (82%)	136 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LE	101/140 (72%)	101 (100%)	0	100	100
14	LG	102/107 (95%)	102 (100%)	0	100	100
15	LH	39/133 (29%)	39 (100%)	0	100	100
16	LI	124/135 (92%)	123 (99%)	1 (1%)	79	90
17	LK	29/121 (24%)	29 (100%)	0	100	100
18	LN	313/348 (90%)	313 (100%)	0	100	100
20	LQ	119/121 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	LS	109/110 (99%)	109 (100%)	0	100	100
22	LT	88/89 (99%)	88 (100%)	0	100	100
23	LU	86/89 (97%)	86 (100%)	0	100	100
24	LW	63/80 (79%)	63 (100%)	0	100	100
25	NA	362/656 (55%)	361 (100%)	1 (0%)	91	96
26	NB	142/485 (29%)	142 (100%)	0	100	100
27	NF	193/228 (85%)	192 (100%)	1 (0%)	86	94
28	NH	155/155 (100%)	155 (100%)	0	100	100
29	NI	553/730 (76%)	551 (100%)	2 (0%)	89	95
30	NK	61/115 (53%)	61 (100%)	0	100	100
31	NM	168/272 (62%)	168 (100%)	0	100	100
32	NO	269/392 (69%)	269 (100%)	0	100	100
33	NQ	265/318 (83%)	265 (100%)	0	100	100
34	NS	276/305 (90%)	276 (100%)	0	100	100
35	SA	299/348 (86%)	298 (100%)	1 (0%)	91	96
36	SC	178/252 (71%)	177 (99%)	1 (1%)	84	93
37	SD	207/215 (96%)	207 (100%)	0	100	100
38	SE	158/223 (71%)	158 (100%)	0	100	100
39	SG	170/171 (99%)	170 (100%)	0	100	100
40	SH	140/274 (51%)	140 (100%)	0	100	100
41	SI	202/228 (89%)	202 (100%)	0	100	100
42	SJ	293/733 (40%)	293 (100%)	0	100	100
43	SK	212/213 (100%)	212 (100%)	0	100	100
44	SL	226/437 (52%)	226 (100%)	0	100	100
45	SM	401/509 (79%)	400 (100%)	1 (0%)	92	97
46	SN	133/260 (51%)	133 (100%)	0	100	100
47	SO	283/319 (89%)	283 (100%)	0	100	100
48	SQ	195/214 (91%)	195 (100%)	0	100	100
49	SR	422/574 (74%)	422 (100%)	0	100	100
50	SS	214/648 (33%)	214 (100%)	0	100	100
51	ST	74/300 (25%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	SU	485/733 (66%)	485 (100%)	0	100 100
53	SV	127/149 (85%)	126 (99%)	1 (1%)	79 90
54	SW	393/591 (66%)	393 (100%)	0	100 100
55	SY	325/685 (47%)	325 (100%)	0	100 100
56	SZ	141/158 (89%)	141 (100%)	0	100 100
All	All	10007/14669 (68%)	9998 (100%)	9 (0%)	92 97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	SM	218	ARG
53	SV	115	ASN
29	NI	362	ARG
29	NI	572	ARG
35	SA	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
49	SR	157	HIS
50	SS	310	HIS
49	SR	304	GLN
52	SU	359	HIS
35	SA	60	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	21 (14%)	0
4	L2	65/1167 (5%)	10 (15%)	0
5	L3	2173/5070 (42%)	300 (13%)	7 (0%)
All	All	2388/6394 (37%)	331 (13%)	7 (0%)

5 of 331 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L1	34	U
3	L1	52	A

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Mol	Chain	Res	Type
3	L1	54	C
3	L1	55	U
3	L1	59	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	3835	C
5	L3	4347	G
5	L3	5013	C
5	L3	4520	G
5	L3	2798	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	$\#\|Z\| > 2$
50	SEP	SS	127	50	8,9,10	1.59	1 (12%)	7,12,14	1.14	1 (14%)
31	AME	NM	1	31	9,10,11	1.53	1 (11%)	9,11,13	1.31	1 (11%)
50	SEP	SS	126	50	8,9,10	1.60	1 (12%)	7,12,14	1.45	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
50	SEP	SS	127	50	-	1/6/8/10	-
31	AME	NM	1	31	-	2/9/10/12	-
50	SEP	SS	126	50	-	1/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	NM	1	AME	CT1-N	3.52	1.45	1.34
50	SS	126	SEP	P-O1P	3.52	1.61	1.50
50	SS	127	SEP	P-O1P	3.49	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	SS	126	SEP	OG-CB-CA	3.21	111.26	108.14
31	NM	1	AME	CT2-CT1-N	2.24	119.83	116.12
50	SS	127	SEP	OG-CB-CA	2.05	110.14	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	NM	1	AME	C-CA-CB-CG
31	NM	1	AME	N-CA-CB-CG
50	SS	127	SEP	N-CA-CB-OG
50	SS	126	SEP	CA-CB-OG-P

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 71 ligands modelled in this entry, 68 are monoatomic - leaving 3 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	$\#\|Z\|>2$
59	ADP	NI	1001	57	24,29,29	0.88	0	29,45,45	1.28	2 (6%)
61	GDP	SR	1001	57,62	25,30,30	2.63	9 (36%)	30,47,47	1.56	8 (26%)
60	SF4	NM	401	31	0,12,12	-	-	-		

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
59	ADP	NI	1001	57	-	2/12/32/32	0/3/3/3
61	GDP	SR	1001	57,62	-	0/12/32/32	0/3/3/3
60	SF4	NM	401	31	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	SR	1001	GDP	O6-C6	7.26	1.40	1.23
61	SR	1001	GDP	PA-O3A	5.11	1.65	1.59
61	SR	1001	GDP	C2-N2	4.84	1.45	1.34
61	SR	1001	GDP	O4'-C1'	4.77	1.47	1.40
61	SR	1001	GDP	C1'-N9	-2.64	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})
59	NI	1001	ADP	N3-C2-N1	-4.28	122.86	128.67
61	SR	1001	GDP	C5-C6-N1	3.01	119.81	114.07
61	SR	1001	GDP	O2B-PB-O3A	2.92	114.41	104.64
61	SR	1001	GDP	C2-N1-C6	-2.88	119.84	125.11
61	SR	1001	GDP	O3B-PB-O3A	2.78	113.95	104.64

There are no chirality outliers.

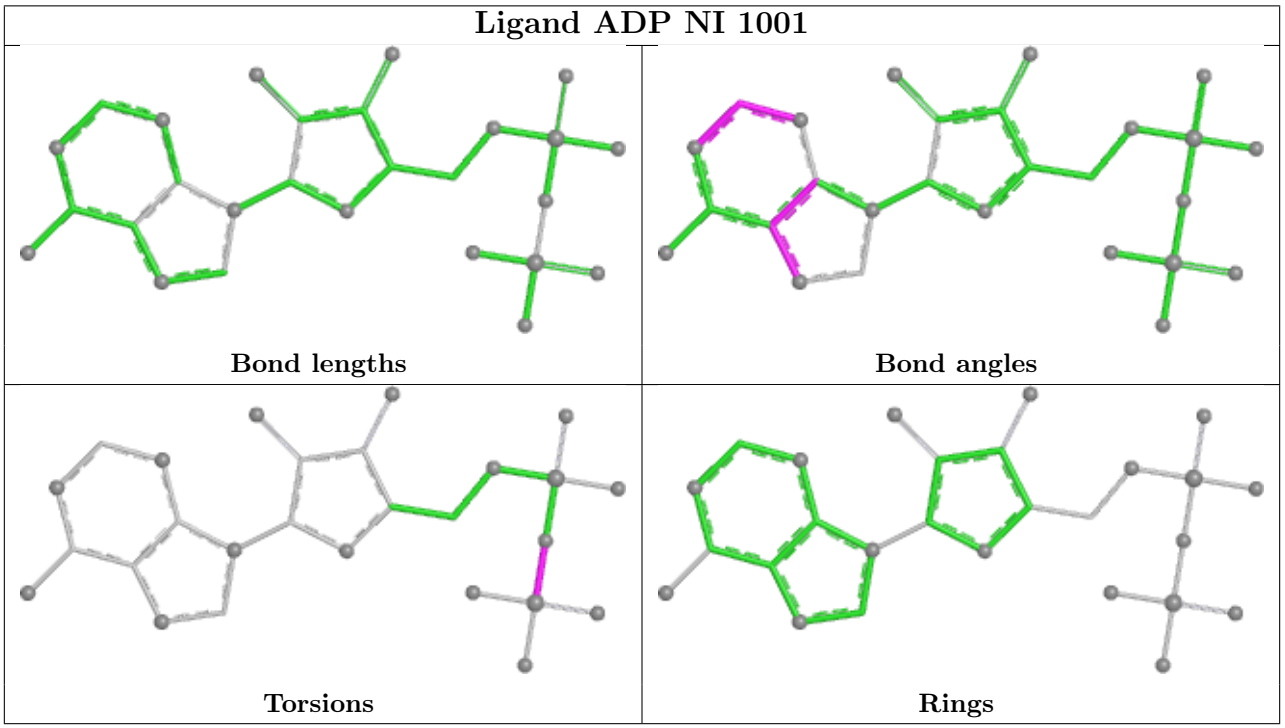
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	NI	1001	ADP	PA-O3A-PB-O3B
59	NI	1001	ADP	PA-O3A-PB-O1B

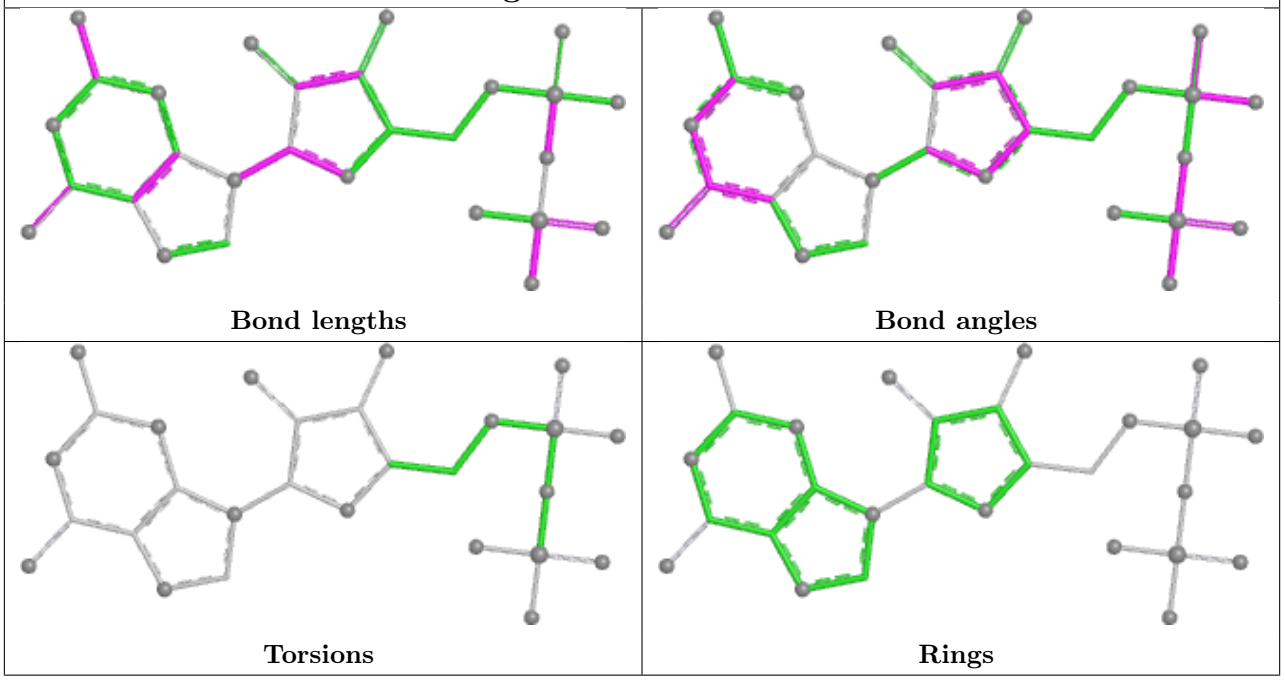
There are no ring outliers.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L3	2403:A	O3'	2473:A	P	61.11

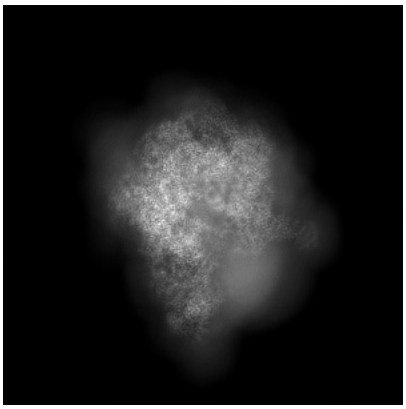
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29258. These allow visual inspection of the internal detail of the map and identification of artifacts.

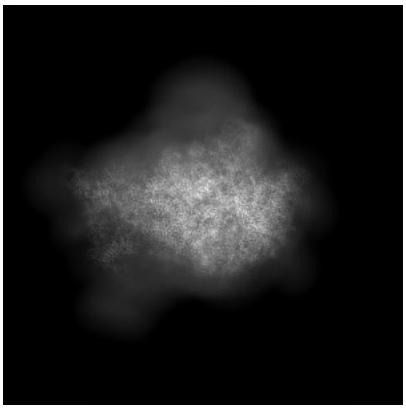
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

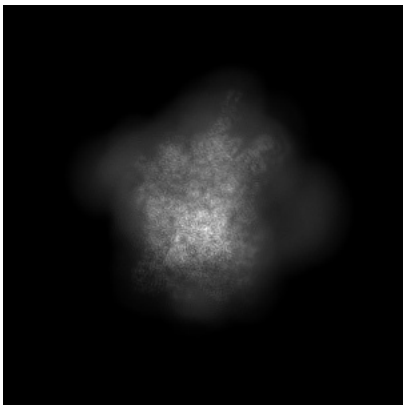
6.1.1 Primary map



X

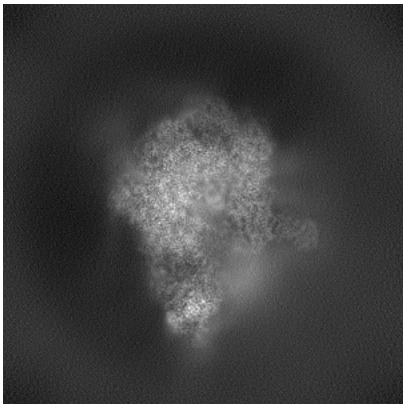


Y

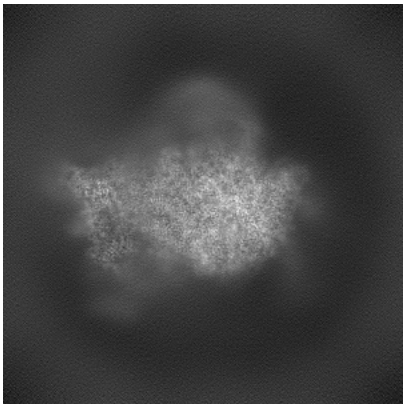


Z

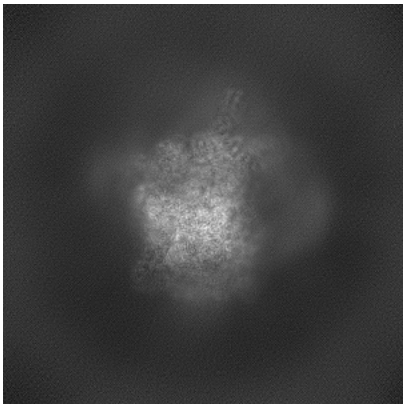
6.1.2 Raw map



X



Y

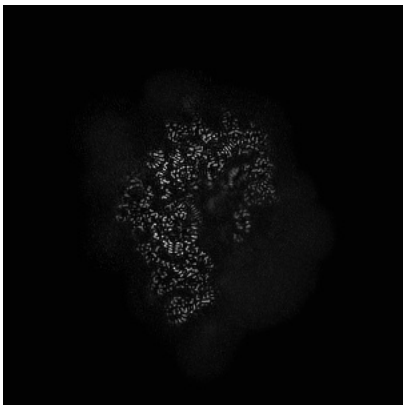


Z

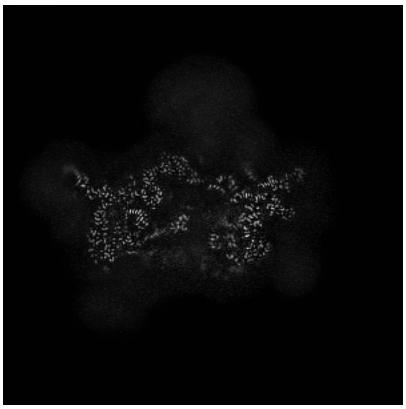
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

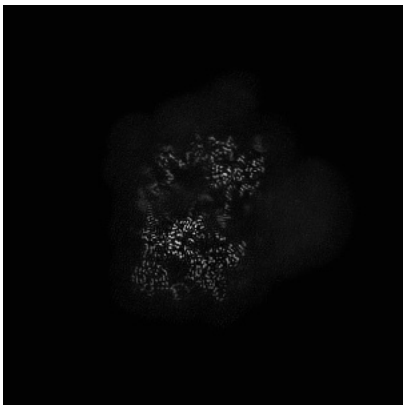
6.2.1 Primary map



X Index: 240

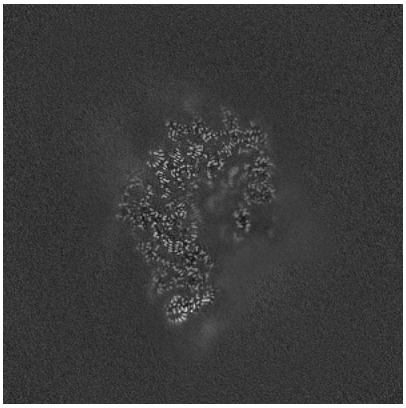


Y Index: 240

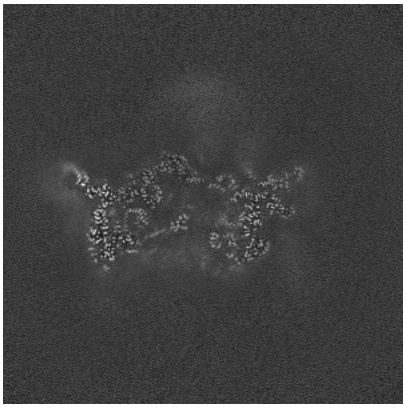


Z Index: 240

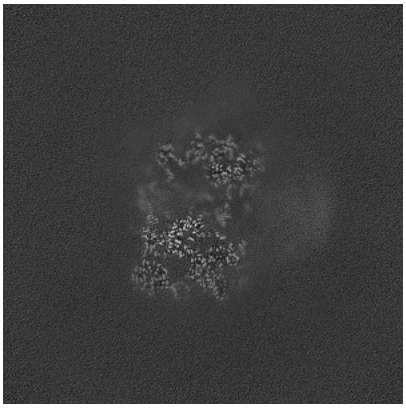
6.2.2 Raw map



X Index: 240



Y Index: 240

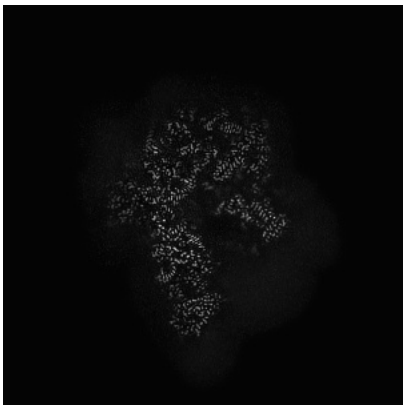


Z Index: 240

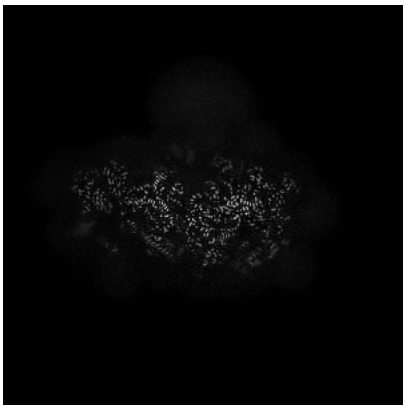
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

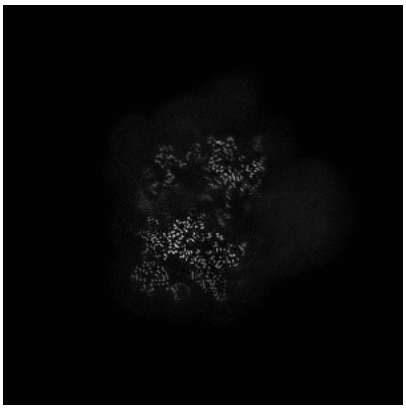
6.3.1 Primary map



X Index: 255

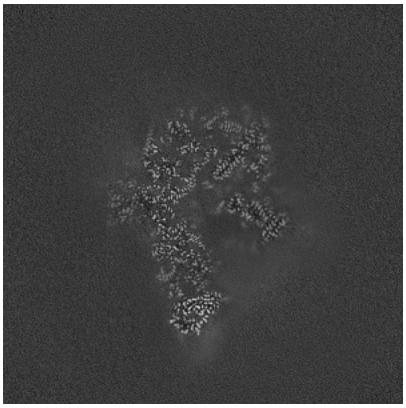


Y Index: 210

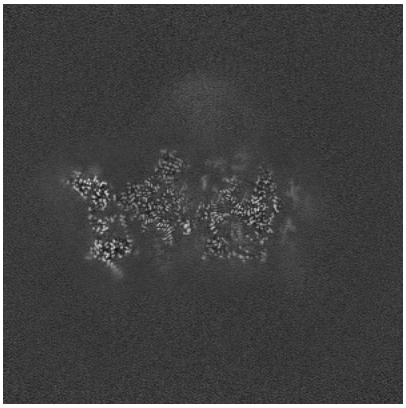


Z Index: 239

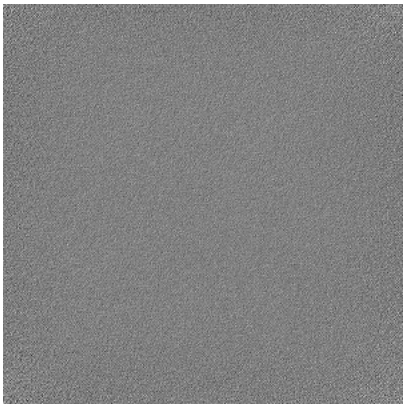
6.3.2 Raw map



X Index: 255



Y Index: 225

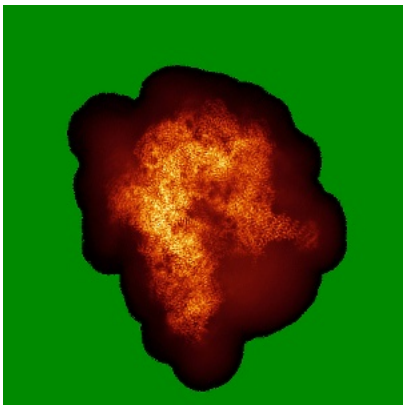


Z Index: 0

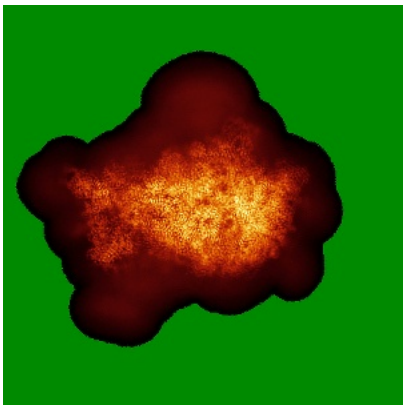
The images above show the largest variance slices of the map in three orthogonal directions.

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

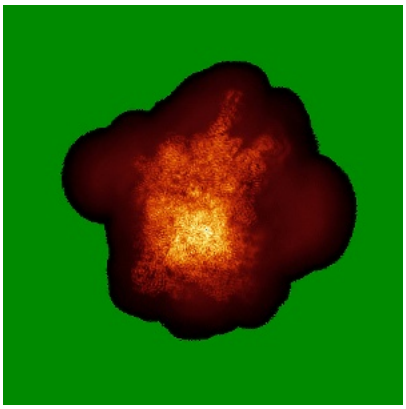
6.4.1 Primary map



X

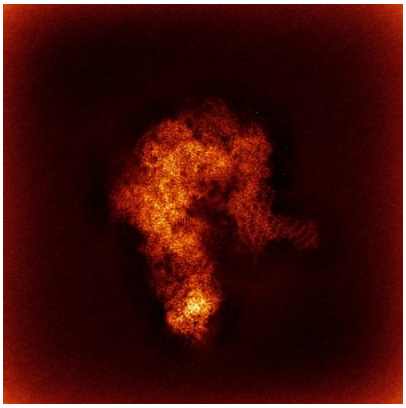


Y

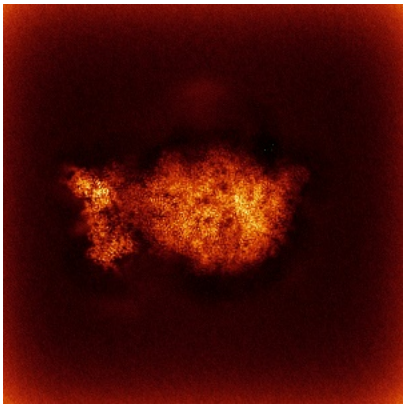


Z

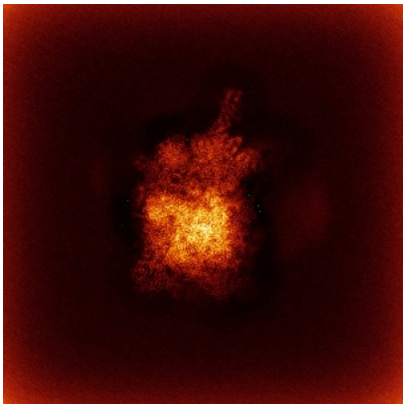
6.4.2 Raw map



X



Y



Z

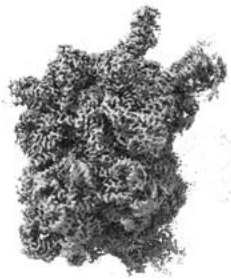
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

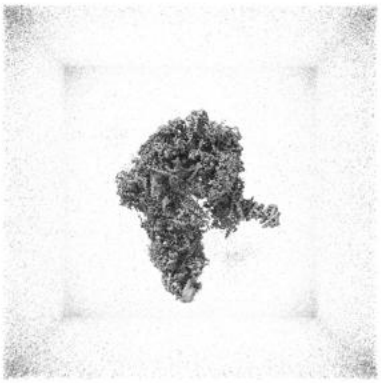
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

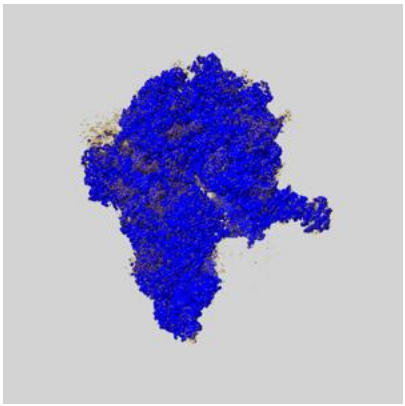
6.6 Mask visualisation (i)

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

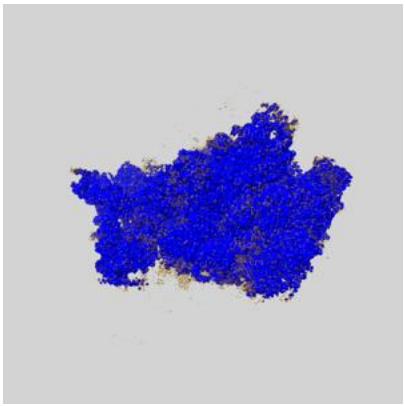
A mask typically either:

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

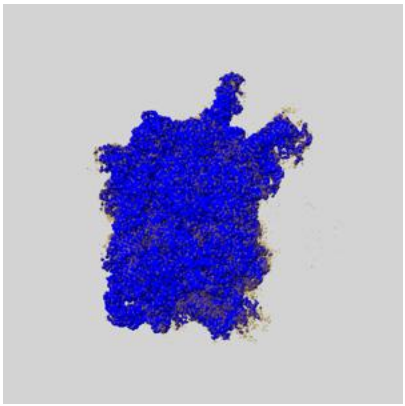
6.6.1 emd_29258_msk_1.map (i)



X



Y

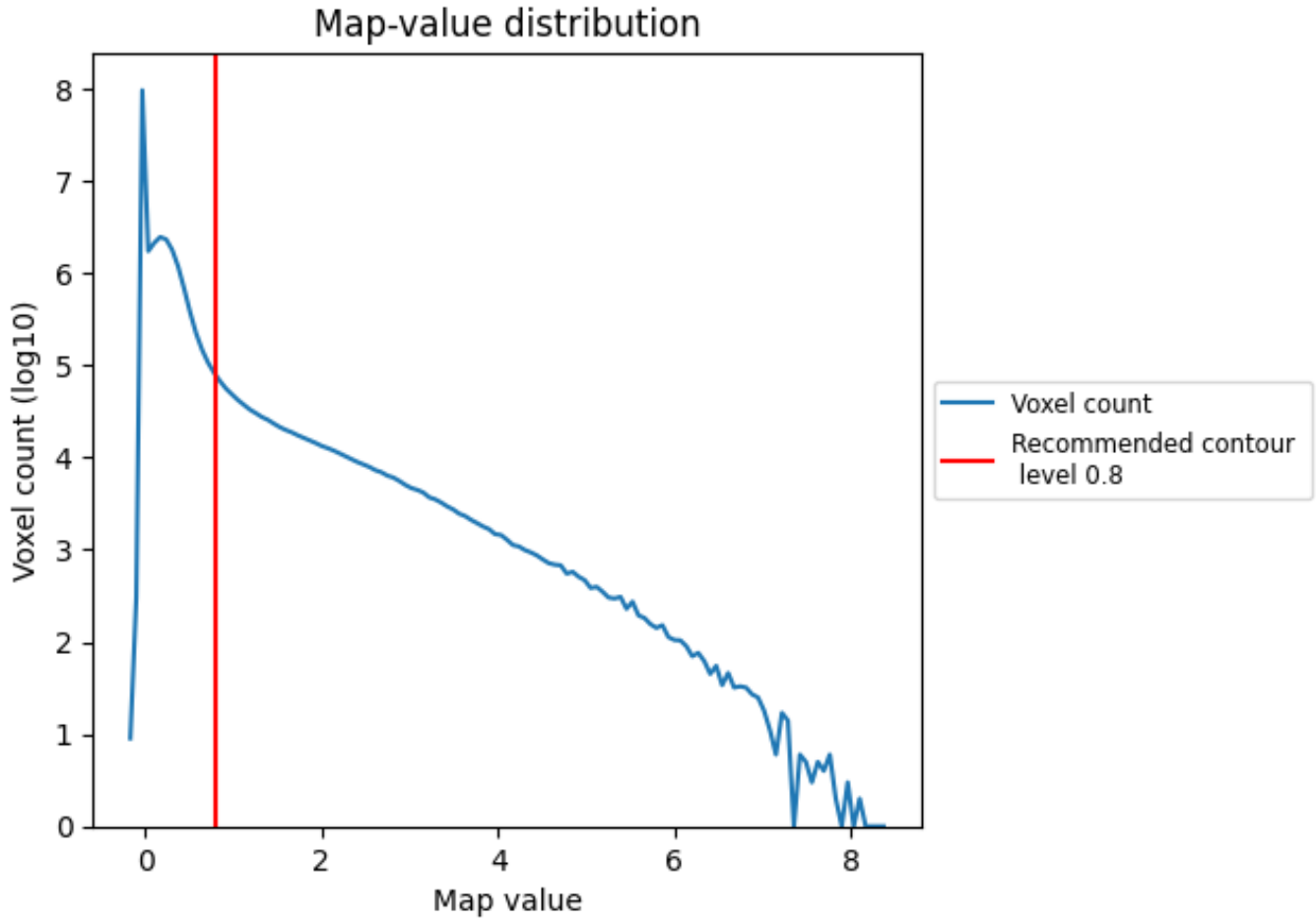


Z

7 Map analysis

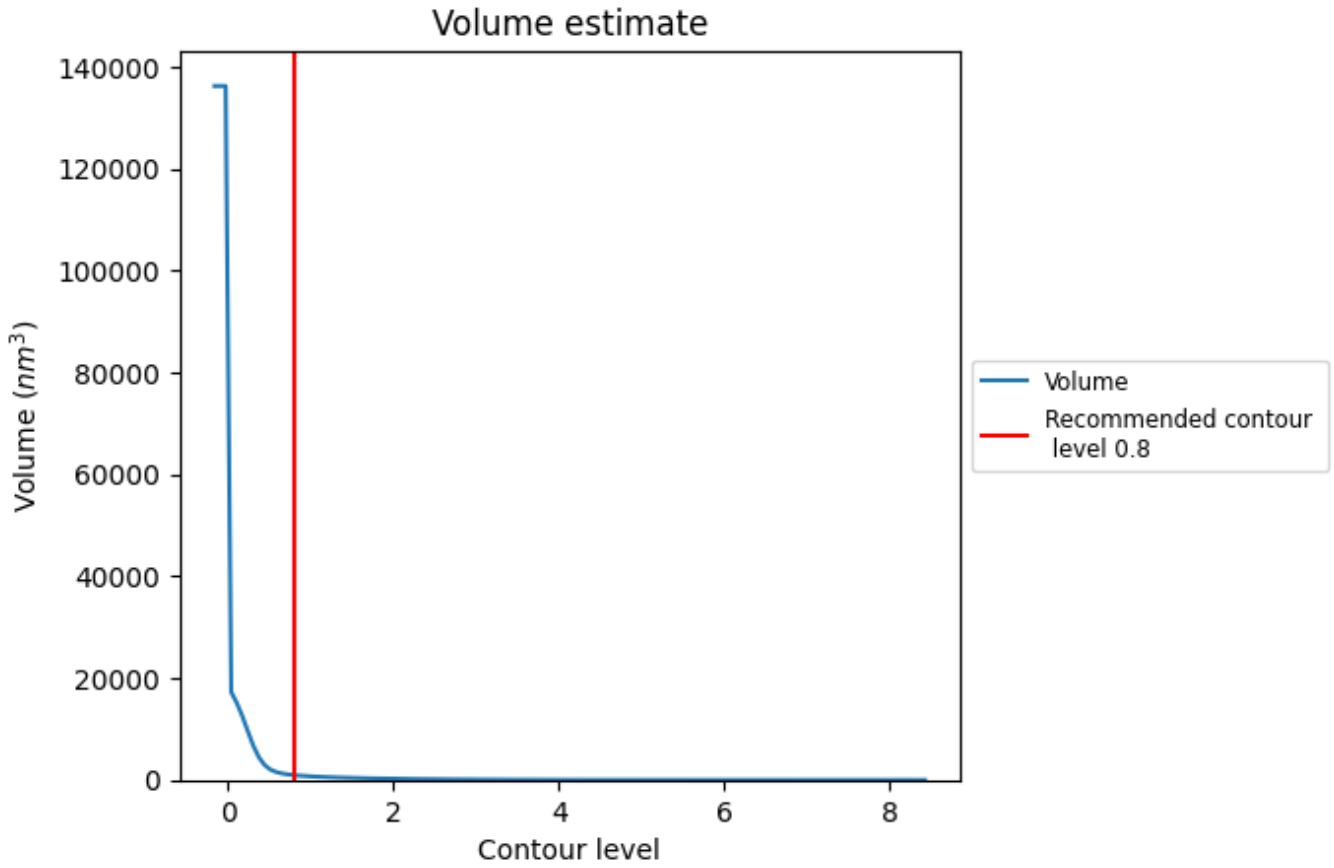
This section contains the results of statistical analysis of the map.

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.

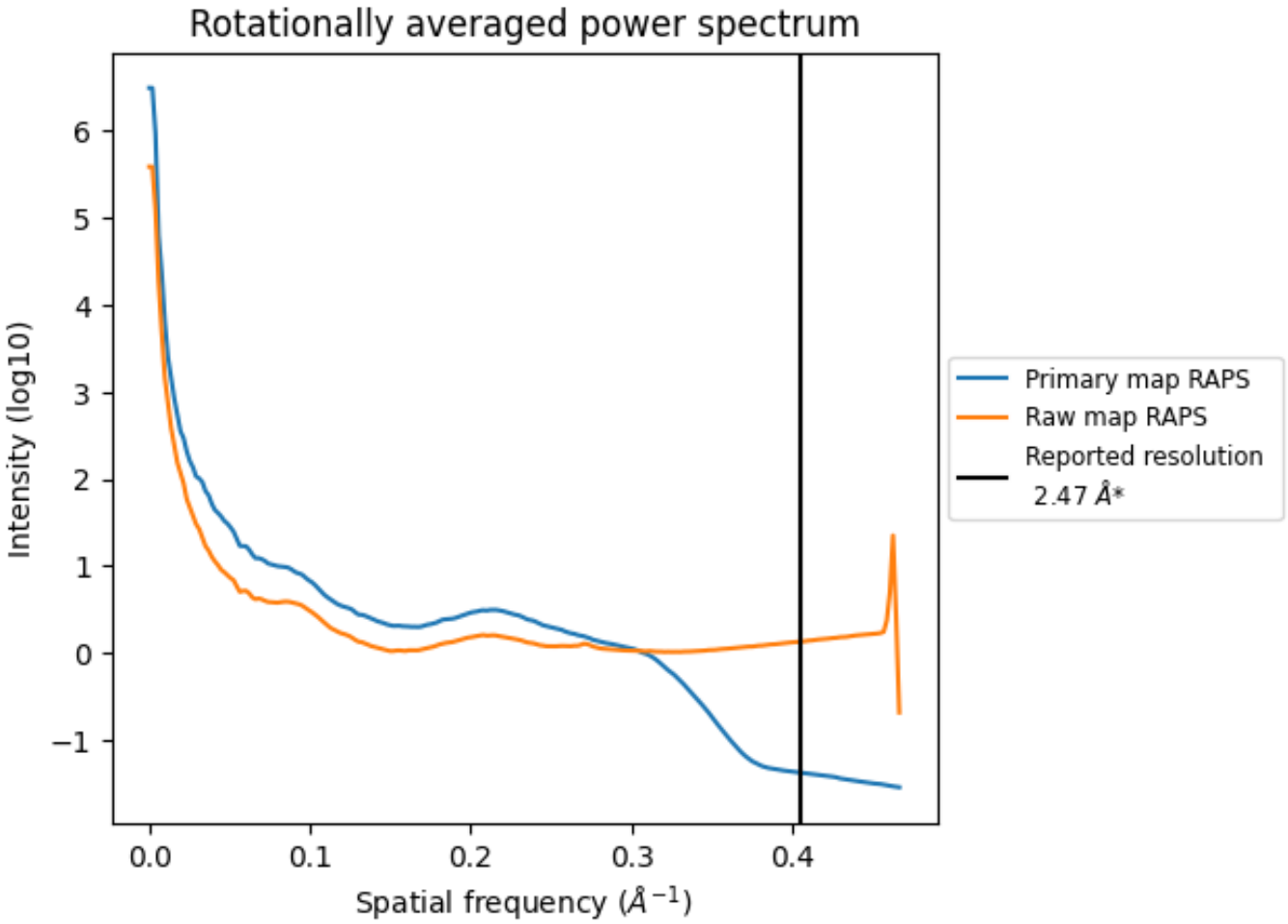
7.2 Volume estimate (i)



The volume at the recommended contour level is 950 nm^3; this corresponds to an approximate mass of 859 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)

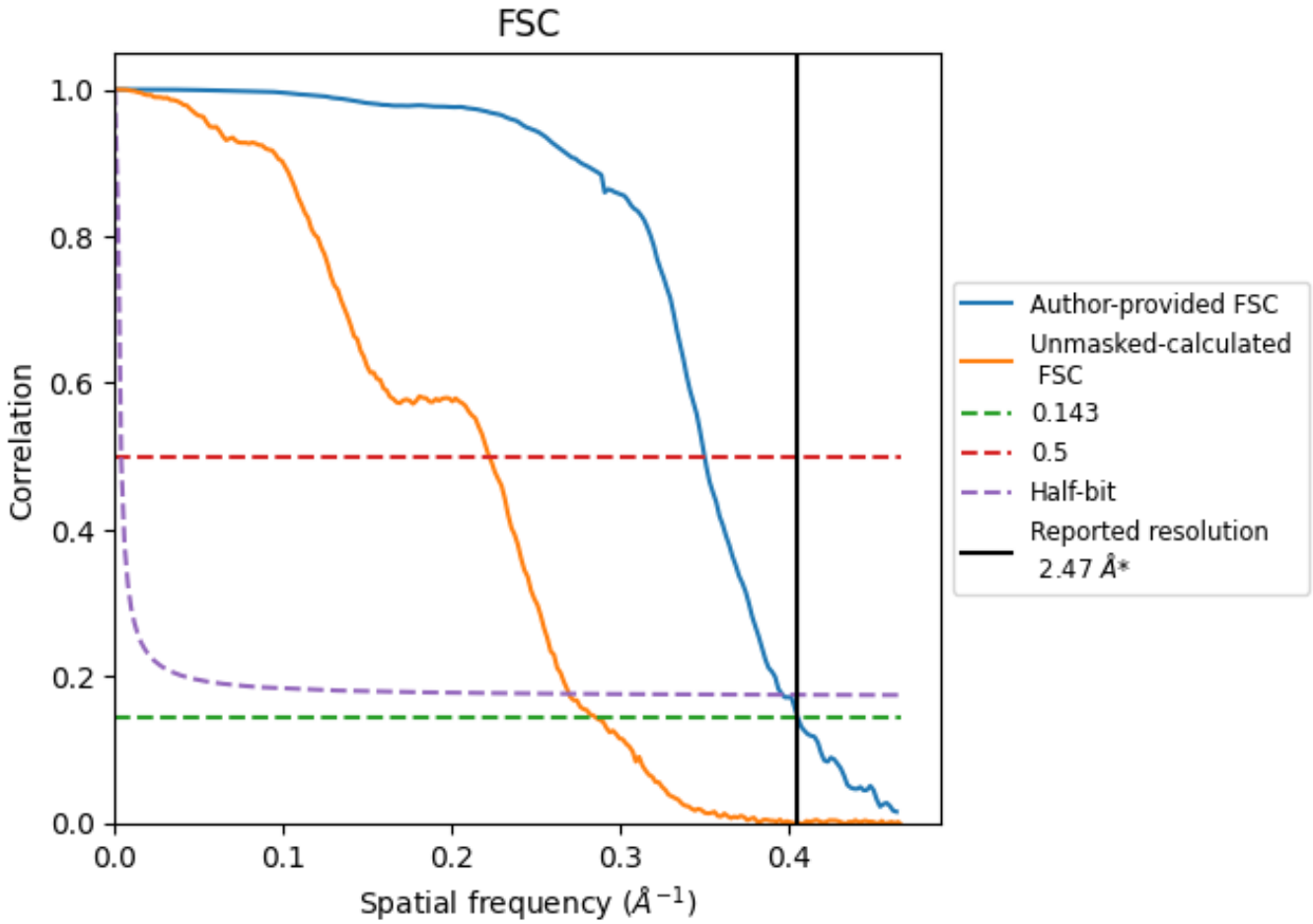


*Reported resolution corresponds to spatial frequency of 0.405 $Å^{-1}$

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 0.405 Å^{-1}

8.2 Resolution estimates (i)

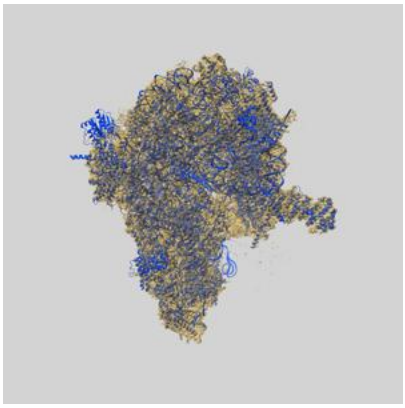
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.86	2.52
Unmasked-calculated*	3.50	4.50	3.71

*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 3.50 differs from the reported value 2.47 by more than 10 %

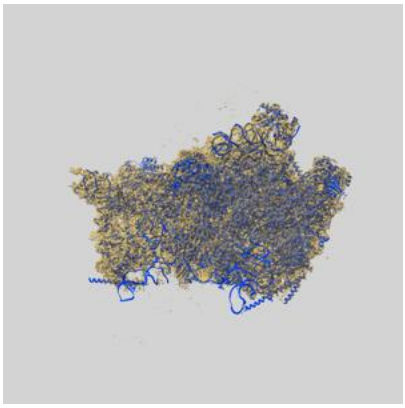
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29258 and PDB model 8FKV. Per-residue inclusion information can be found in section 3 on page 16.

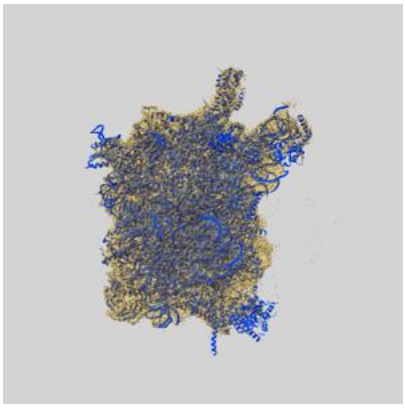
9.1 Map-model overlay



X



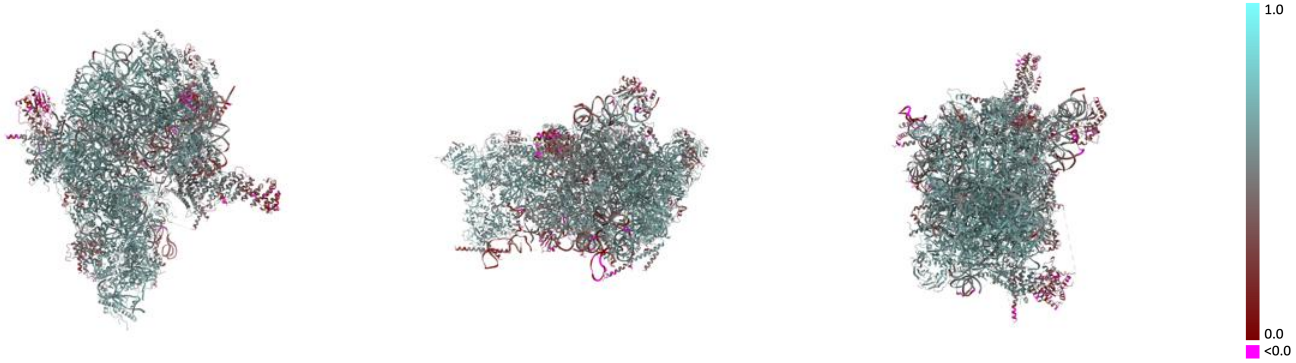
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

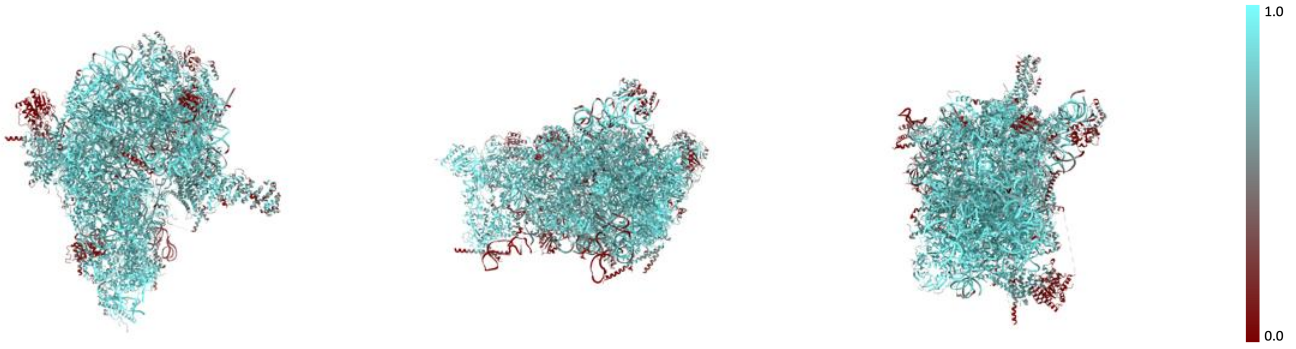
9.2 Q-score mapped to coordinate model (i)



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.

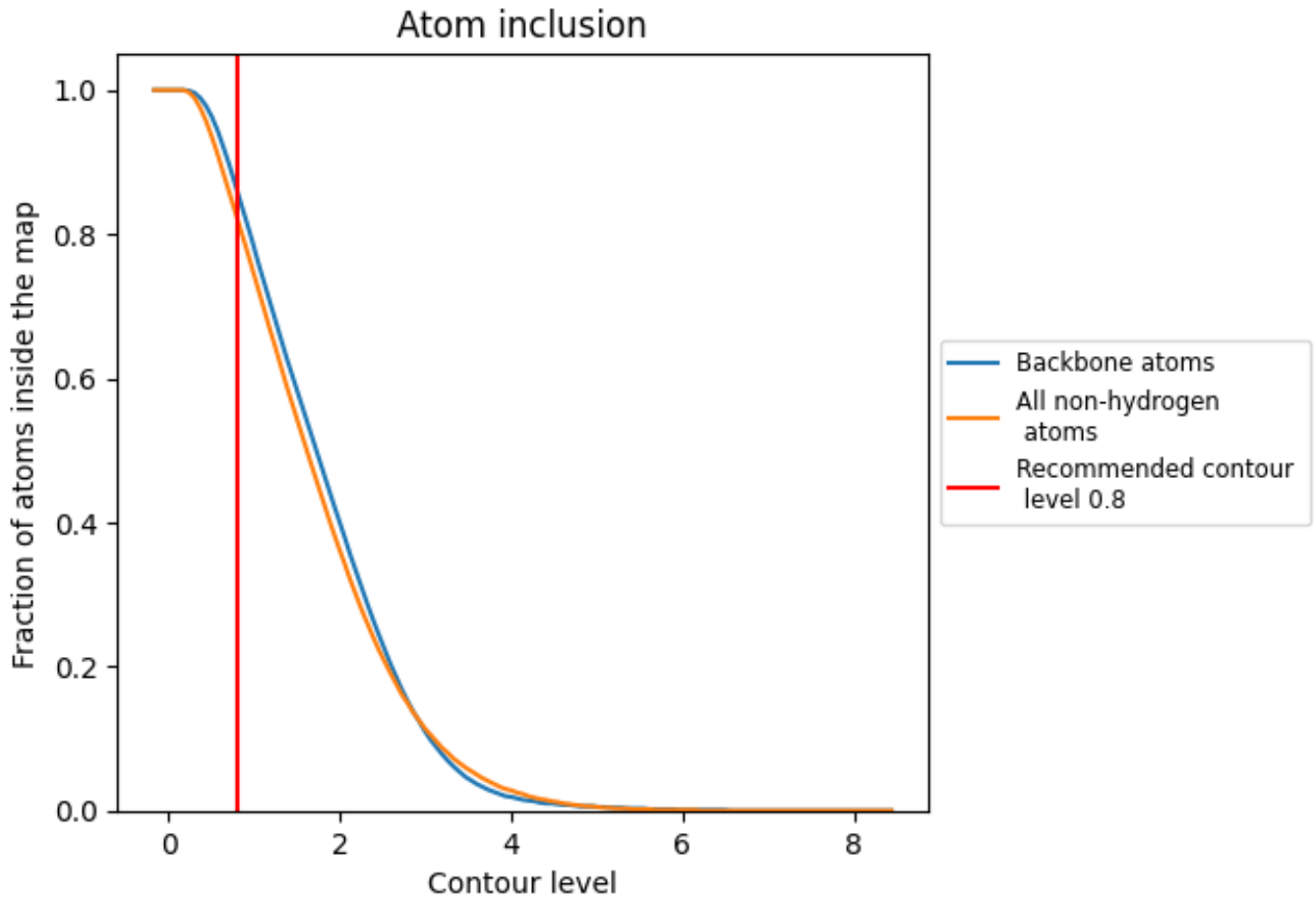
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.5490
BA	0.3420	0.3900
BB	0.3170	0.2800
L1	0.8950	0.5710
L2	0.9440	0.5930
L3	0.8780	0.5560
L6	0.9280	0.6120
L7	0.9460	0.6230
L8	0.9490	0.6350
L9	0.9630	0.6400
LA	0.8560	0.6020
LB	0.9460	0.6230
LC	0.9480	0.6390
LE	0.6130	0.4520
LG	0.8640	0.5840
LH	0.3830	0.3360
LI	0.9040	0.6110
LK	0.7760	0.4410
LN	0.8820	0.6050
LP	0.4960	0.4240
LQ	0.9630	0.6420
LS	0.7710	0.5290
LT	0.9740	0.6540
LU	0.8520	0.5980
LW	0.9250	0.6130
NA	0.7360	0.3980
NB	0.3350	0.3380
NF	0.8700	0.5850
NH	0.9160	0.5640
NI	0.7950	0.5260
NK	0.7950	0.5500
NM	0.8670	0.5850
NO	0.7370	0.5350
NQ	0.8660	0.5830
NS	0.8650	0.5990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SA	0.9160	0.6170
SC	0.8660	0.5940
SD	0.9230	0.6220
SE	0.9240	0.6260
SG	0.8900	0.6190
SH	0.8730	0.5960
SI	0.8510	0.5810
SJ	0.6940	0.4780
SK	0.8750	0.5800
SL	0.8340	0.5850
SM	0.7800	0.5440
SN	0.7540	0.5210
SO	0.8450	0.5780
SQ	0.6980	0.5570
SR	0.8140	0.5650
SS	0.8090	0.5630
ST	0.5440	0.4530
SU	0.7720	0.4660
SV	0.6540	0.5050
SW	0.5820	0.4880
SY	0.8590	0.5510
SZ	0.8510	0.5630