wwPDB EM Validation Summary Report

Aug 5, 2026 – 09:41 AM EDT

PDB ID	:	8FKR / pdb_00008fkr
EMDB ID	:	EMD-29254
Title	:	Human nucleolar pre-60S ribosomal subunit (State B1)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.89 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 (i) 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 (i)) were used in the production of this report:

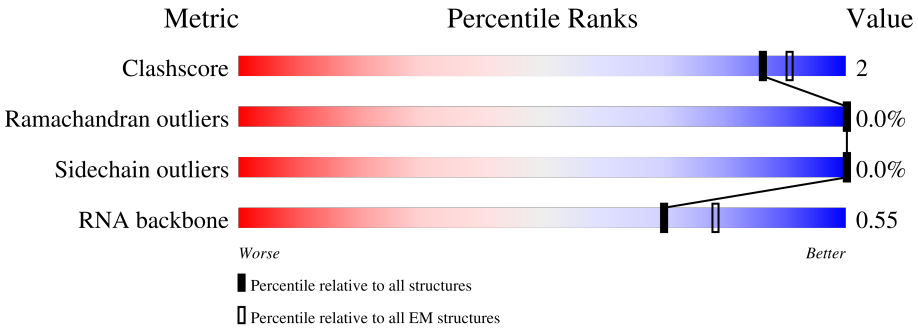
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

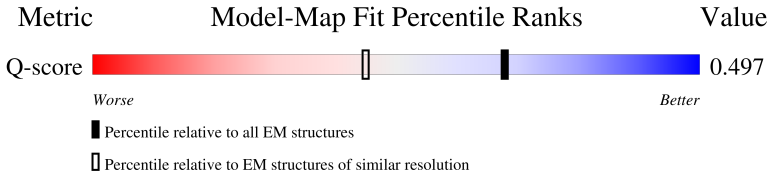
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	33% 85% 10% 5%
2	L1	157	23% 83% 14%
3	L2	1167	5% 94%

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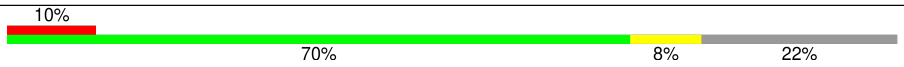
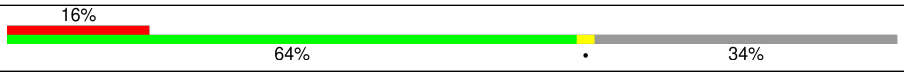
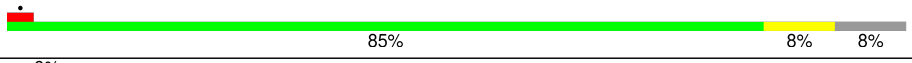
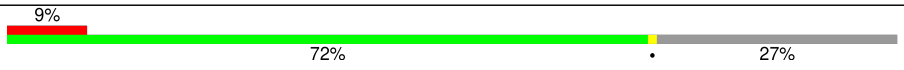
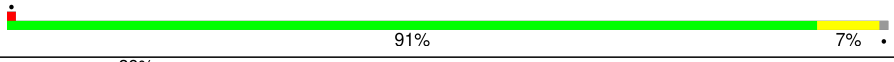
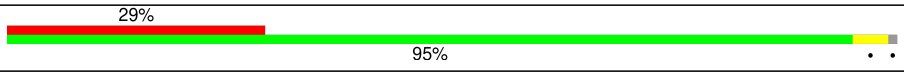
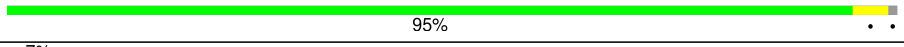
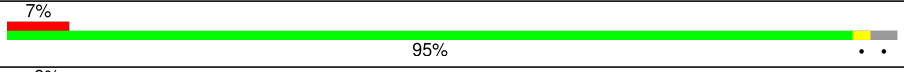
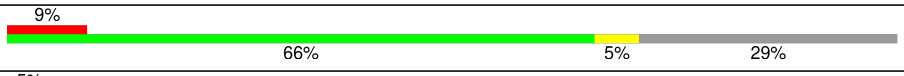
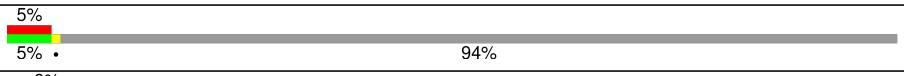
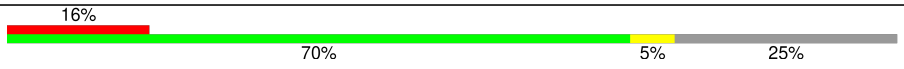
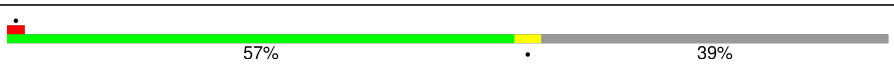
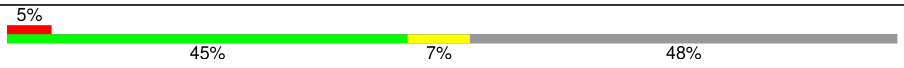
Mol	Chain	Length	Quality of chain
4	L3	5070	
5	L6	211	
6	L7	203	
7	L8	215	
8	L9	204	
9	LA	184	
10	LB	188	
11	LC	176	
12	LE	160	
13	LG	140	
14	LH	156	
15	LI	145	
16	LK	148	
17	LN	403	
18	LQ	135	
19	LS	123	
20	LT	110	
21	LU	105	
22	LW	97	
23	NB	549	
24	NE	361	
25	NF	260	
26	NG	282	
27	NM	300	
28	NN	473	

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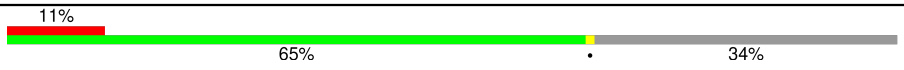
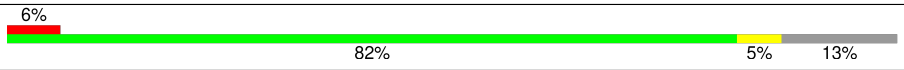
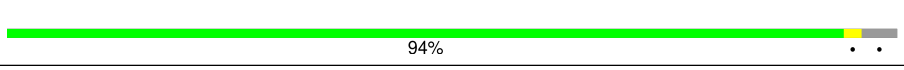
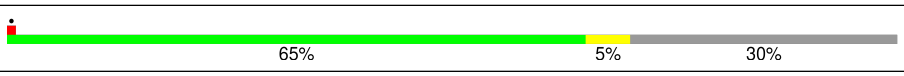
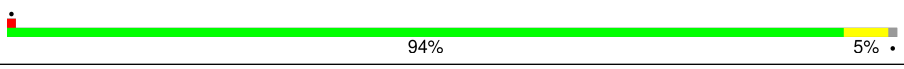
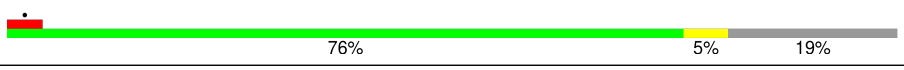
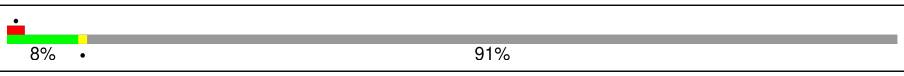
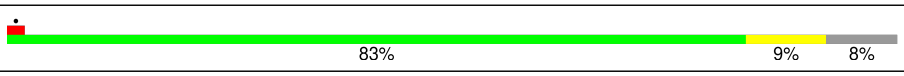
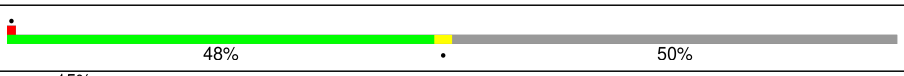
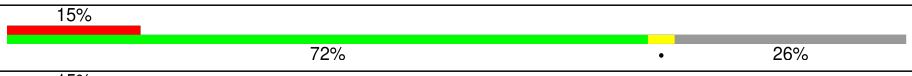
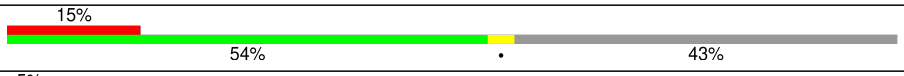
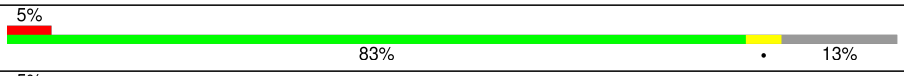
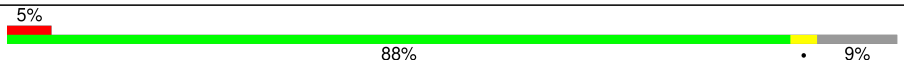
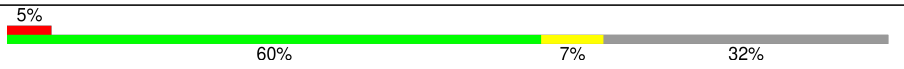
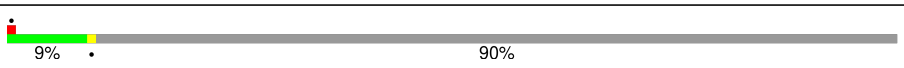
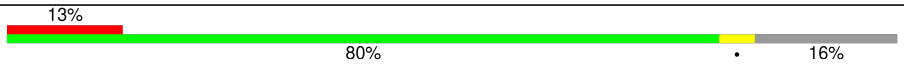
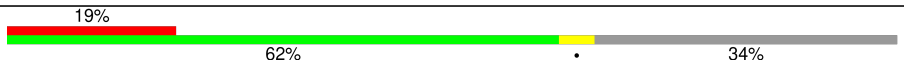
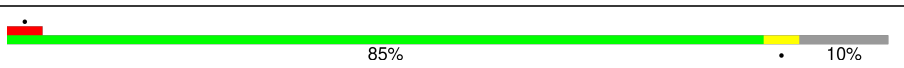
Mol	Chain	Length	Quality of chain
29	NO	461	
30	NQ	385	
31	NS	349	
32	SA	427	
33	SC	288	
34	SD	248	
35	SE	266	
36	SG	192	
37	SH	293	
38	SI	255	
39	SJ	847	
40	SK	245	
41	SL	490	
42	SM	588	
43	SN	306	
44	SO	353	
45	SQ	239	
46	SR	634	
47	SS	746	
48	ST	365	
49	SV	163	
50	SW	670	
51	SZ	178	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 116287 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L12.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	154	3274	1462	579	1080	153	0	0

- Molecule 3 is a RNA chain called ITS2 rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L3	1767	37886	16868	6948	12303	1767	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	143	Total	C	N	O	S	0	0
			1161	732	214	208	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	LE	106	Total	C	N	O	0	0
			686	420	135	131		

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called 60S ribosomal protein L3.

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

- Molecule 18 is a protein called 60S ribosomal protein L32.

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

- Molecule 19 is a protein called 60S ribosomal protein L35.

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

- Molecule 20 is a protein called 60S ribosomal protein L35a.

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

- Molecule 21 is a protein called 60S ribosomal protein L36.

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

- Molecule 22 is a protein called 60S ribosomal protein L37.

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

- Molecule 23 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	NB	31	Total	C	N	O	S	0	0
			257	164	49	43	1		

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

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

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

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

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

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

- Molecule 27 is a protein called Protein MAK16 homolog.

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

- Molecule 28 is a protein called Suppressor of SWI4 1 homolog.

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

- Molecule 29 is a protein called Ribosomal RNA processing protein 1 homolog A.

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

- Molecule 30 is a protein called WD repeat-containing protein 74.

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

- Molecule 31 is a protein called Ribosome production factor 1.

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

- Molecule 32 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SA	331	Total	C	N	O	S	0	0
			2656	1681	524	437	14		

- Molecule 33 is a protein called 60S ribosomal protein L6.

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

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

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

- Molecule 35 is a protein called 60S ribosomal protein L7a.

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

- Molecule 36 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SG	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 37 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 38 is a protein called 60S ribosomal protein L7-like 1.

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

- Molecule 39 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

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

- Molecule 40 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 41 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 42 is a protein called Pescadillo homolog.

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

- Molecule 43 is a protein called Probable rRNA-processing protein EBP2.

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

- Molecule 44 is a protein called Ribosome biogenesis protein BRX1 homolog.

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

- Molecule 45 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 46 is a protein called GTP-binding protein 4.

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

- Molecule 47 is a protein called Ribosome biogenesis protein BOP1.

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

- Molecule 48 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	ST	36	Total	C	N	O	S	0	0
			263	160	51	51	1		

- Molecule 49 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 50 is a protein called ATP-dependent RNA helicase DDX18.

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

- Molecule 51 is a protein called Nucleolar protein 16.

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

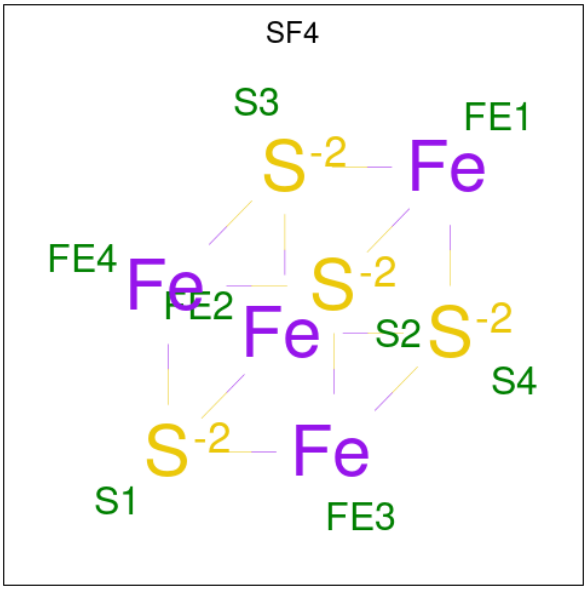
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	L1	3	Total 3	Mg 3	0
52	L2	1	Total 1	Mg 1	0
52	L3	45	Total 45	Mg 45	0
52	L9	1	Total 1	Mg 1	0
52	LN	1	Total 1	Mg 1	0
52	LQ	1	Total 1	Mg 1	0
52	LT	1	Total 1	Mg 1	0
52	SA	1	Total 1	Mg 1	0

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

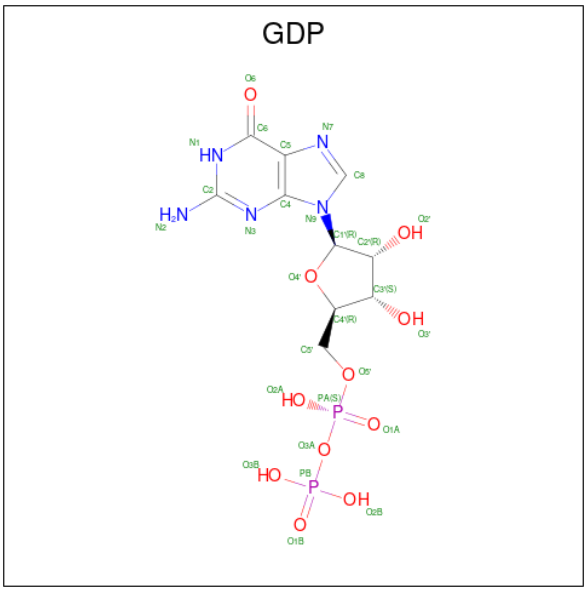
Mol	Chain	Residues	Atoms		AltConf
53	LW	1	Total 1	Zn 1	0
53	SV	1	Total 1	Zn 1	0

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 55 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

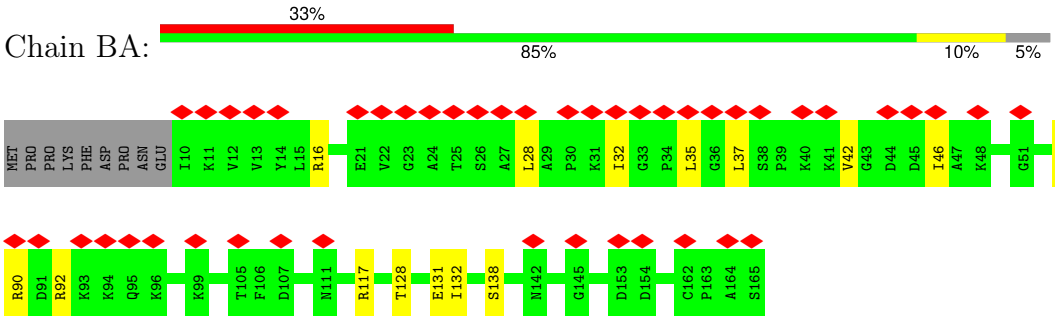
Mol	Chain	Residues	Atoms		AltConf
56	SR	1	Total	K	0
			1	1	

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.

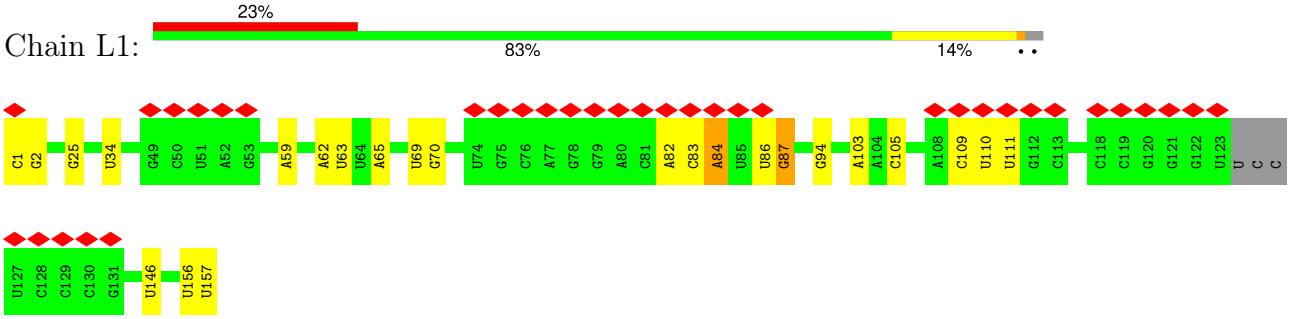
• Molecule 1: 60S ribosomal protein L12

Chain BA:



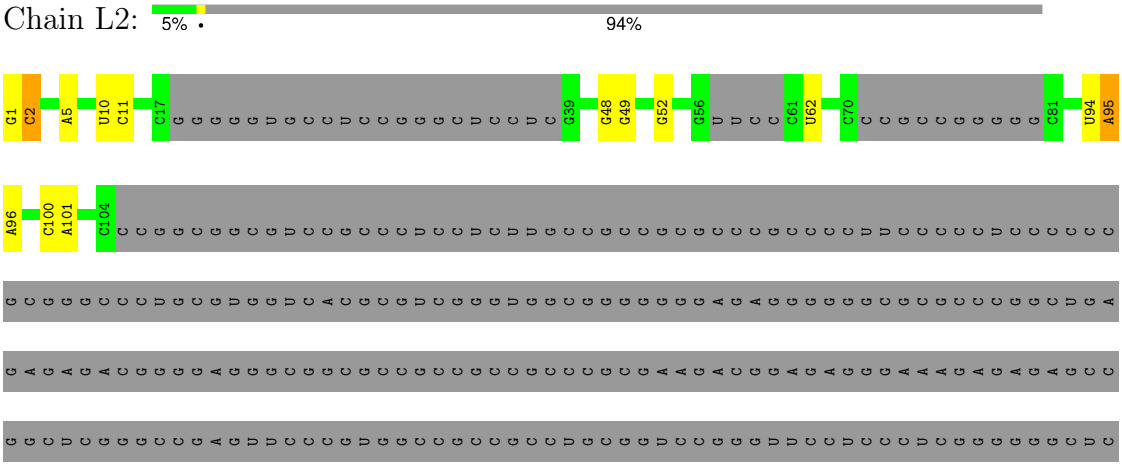
• Molecule 2: 5.8S rRNA

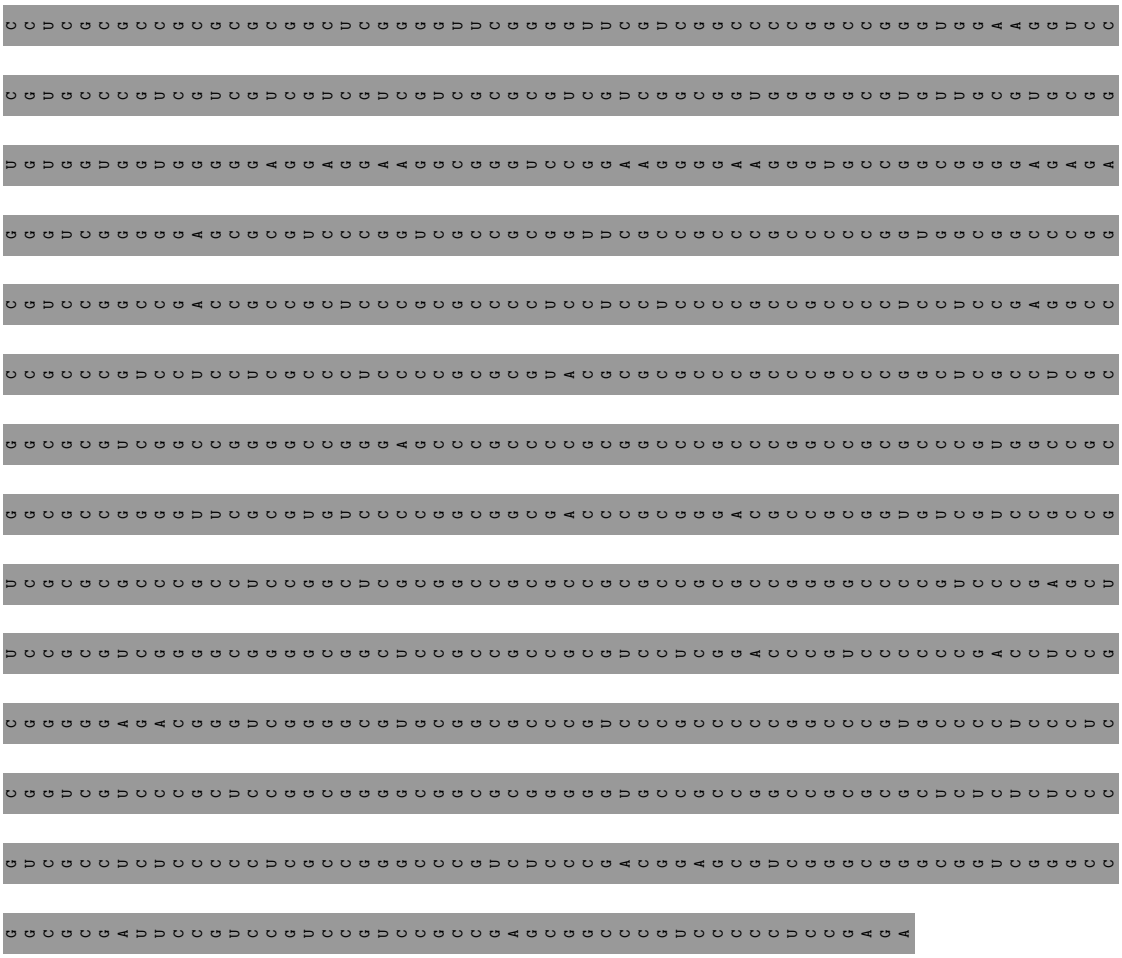
Chain L1:



• Molecule 3: ITS2 rRNA

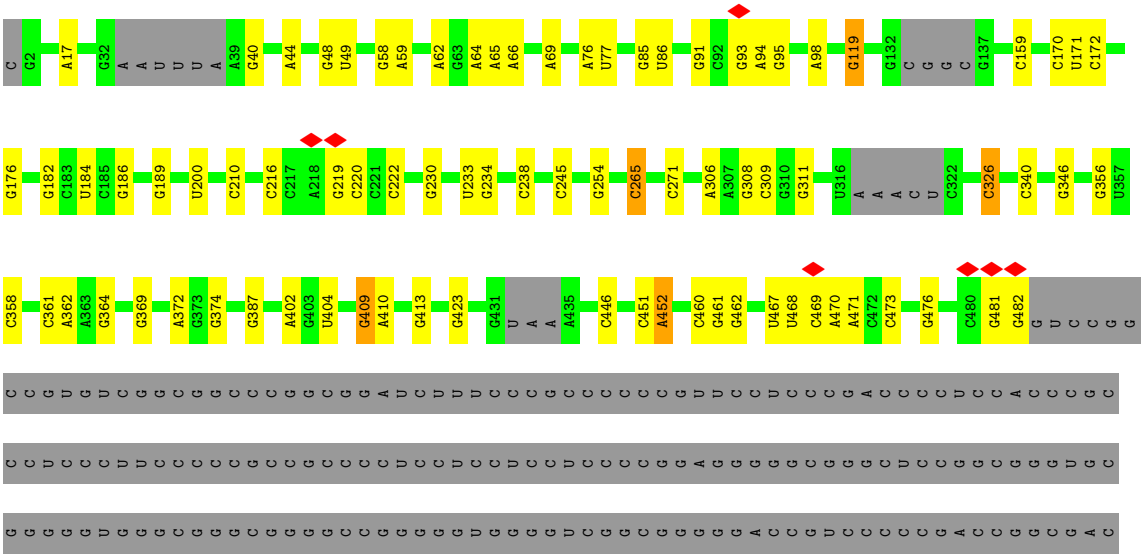
Chain L2:

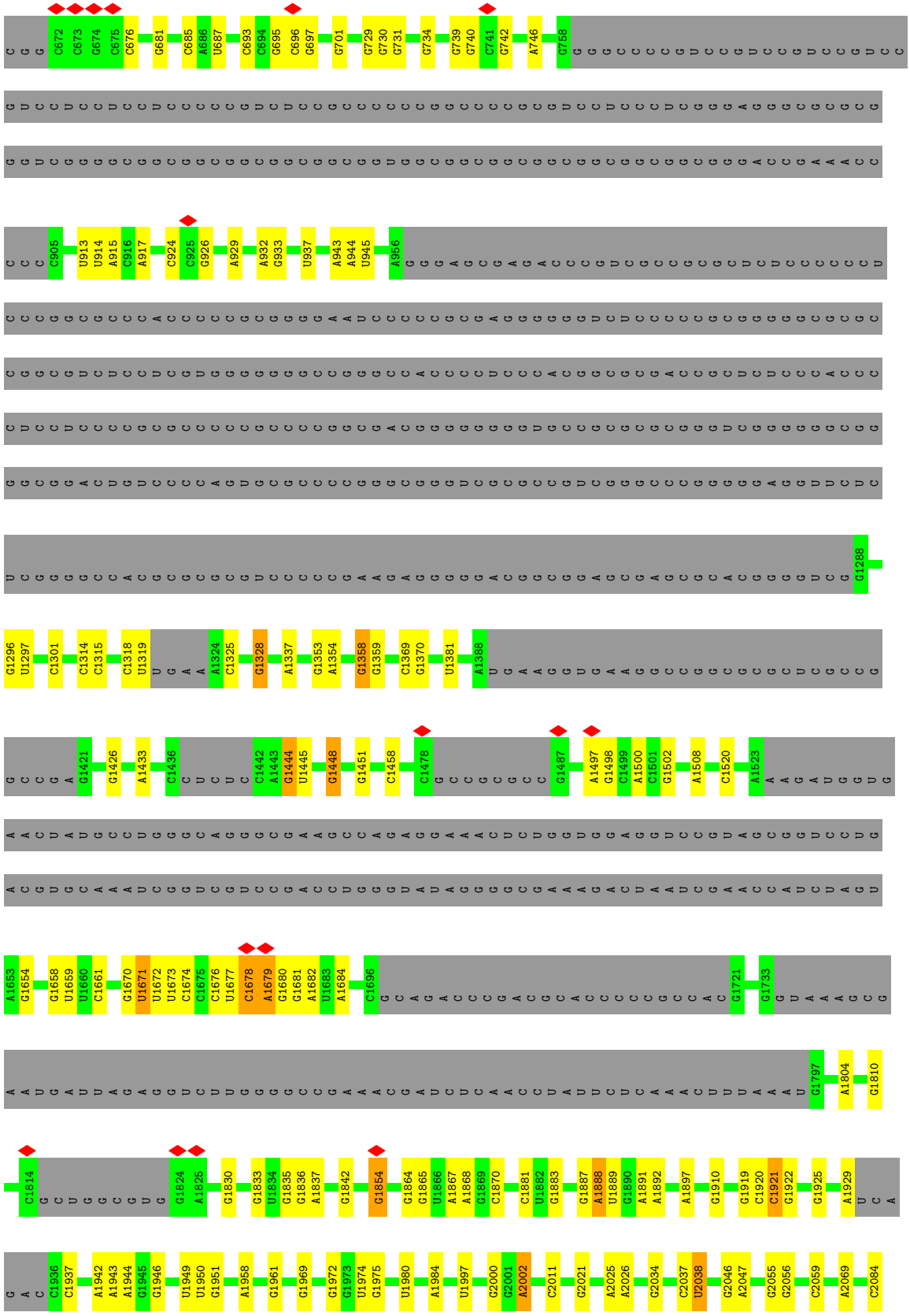


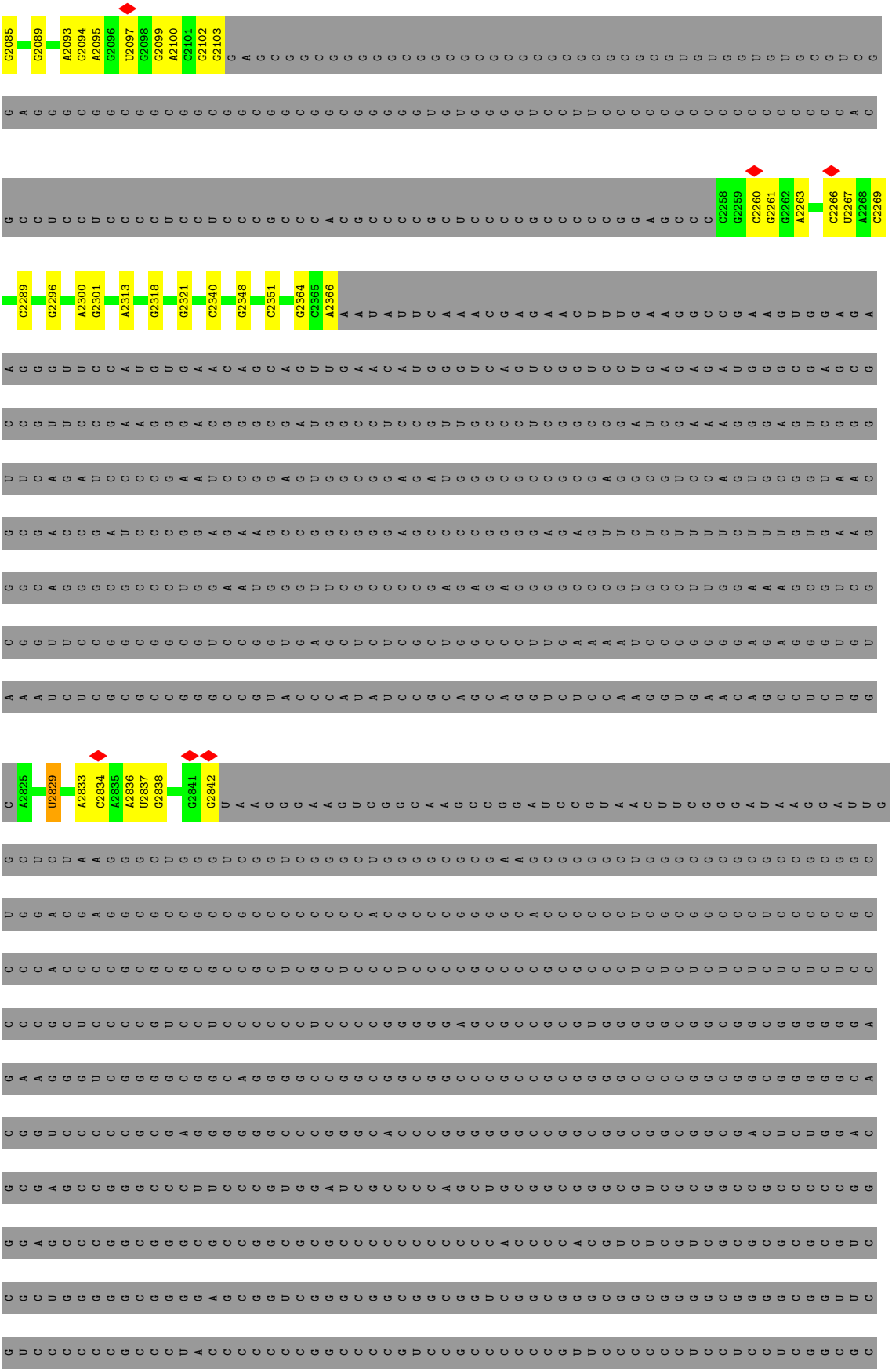


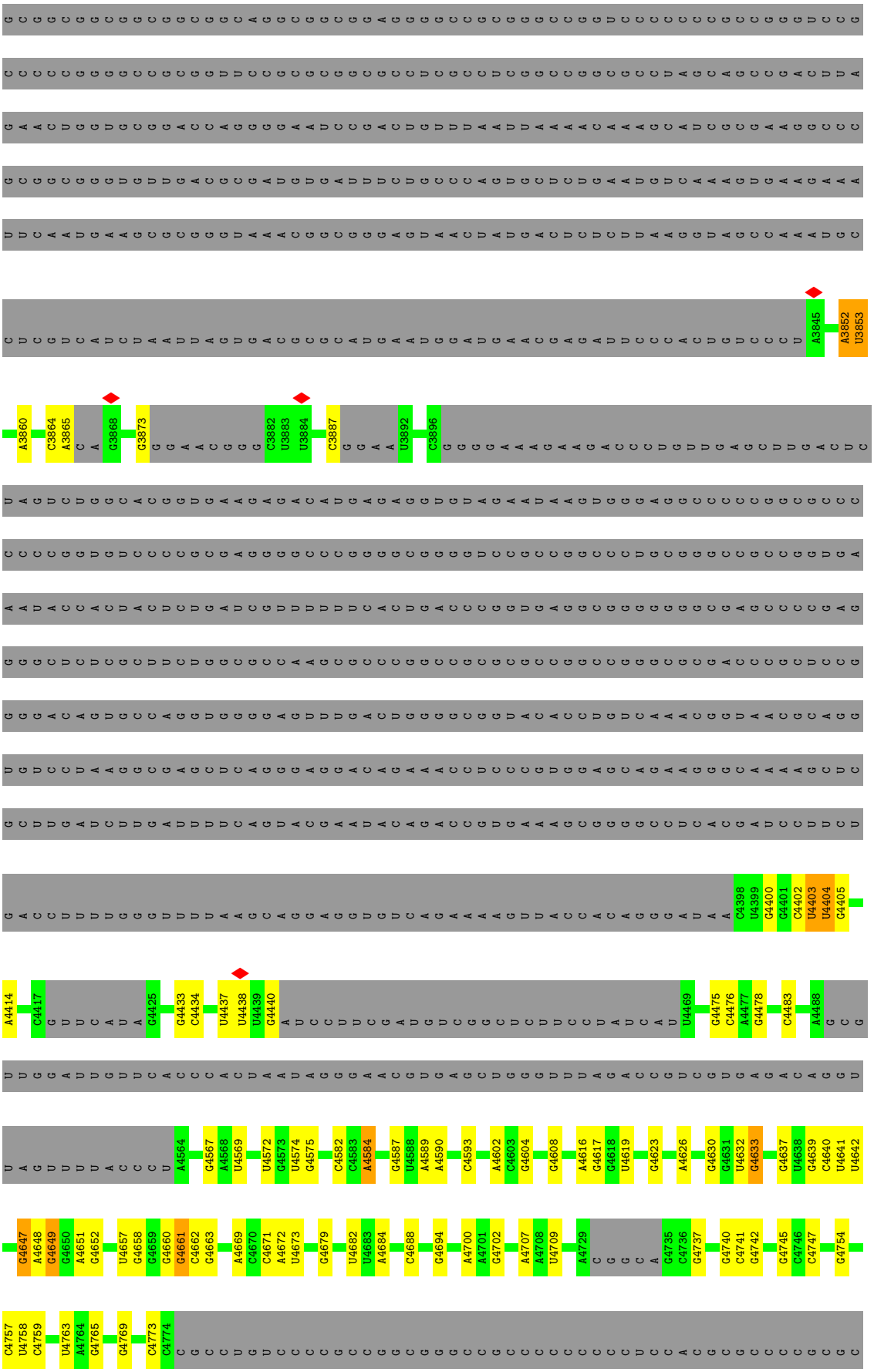
• Molecule 4: 28S rRNA

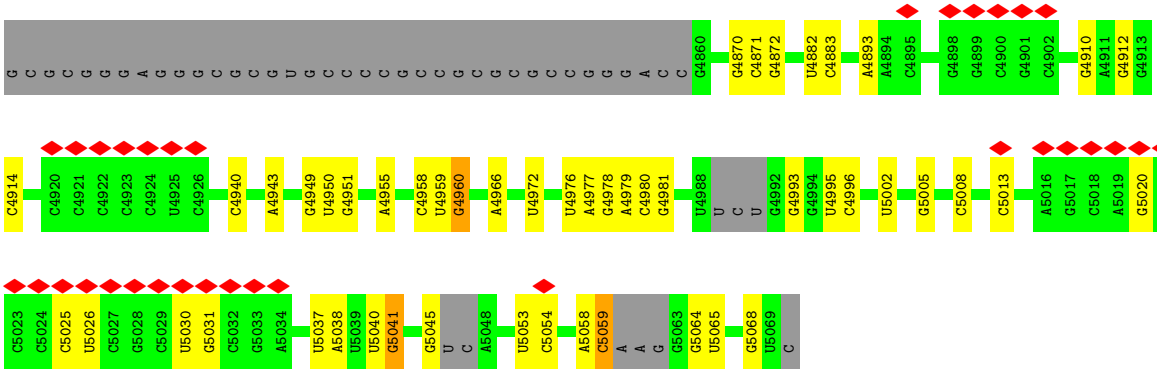
Chain L3:





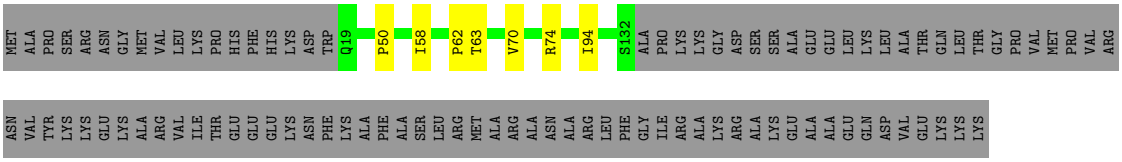

G2085 C2089 A2093 G2094 A2095 G2096 U2097 G2098 G2099 A2100 C2101 G2102 G2103
C2258 G2259 C2260 G2261 G2262 A2263 C2266 U2267 A2268 C2269
C2289 G2296 A2300 G2301 A2313 G2318 G2321 C2340 G2348 C2351 G2364 C2365 A2366
A2825 U2829 A2833 C2834 A2835 A2836 U2837 G2838 G2841 G2842





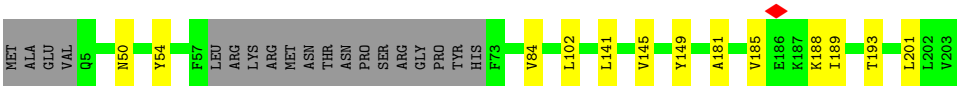
• Molecule 5: 60S ribosomal protein L13

Chain L6:



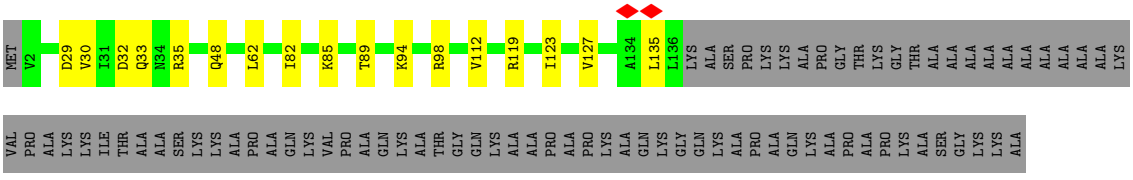
• Molecule 6: 60S ribosomal protein L13a

Chain L7:



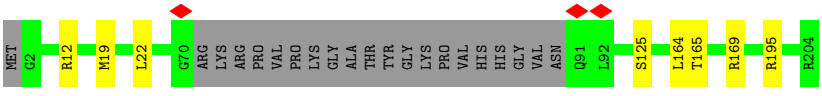
• Molecule 7: 60S ribosomal protein L14

Chain L8:



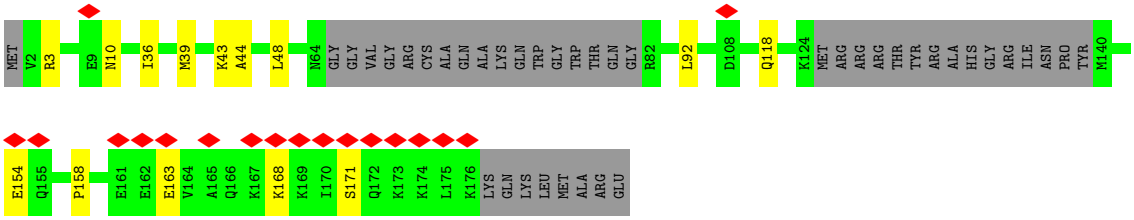
• Molecule 8: 60S ribosomal protein L15

Chain L9:



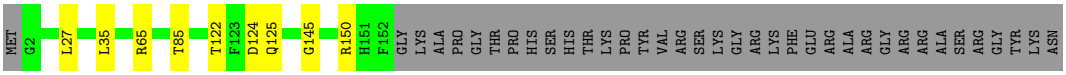
• Molecule 9: 60S ribosomal protein L17

Chain LA:



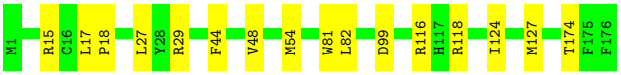
• Molecule 10: 60S ribosomal protein L18

Chain LB:



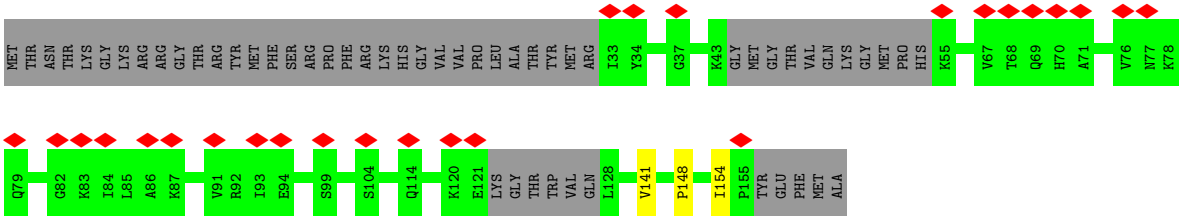
• Molecule 11: 60S ribosomal protein L18a

Chain LC:



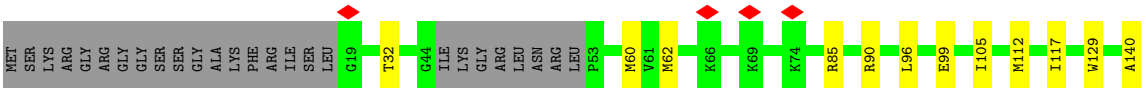
• Molecule 12: 60S ribosomal protein L21

Chain LE:



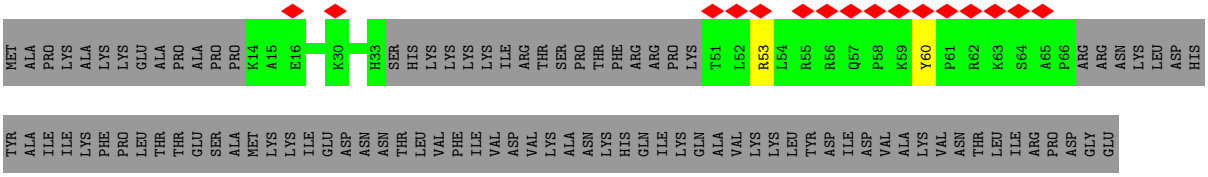
• Molecule 13: 60S ribosomal protein L23

Chain LG:



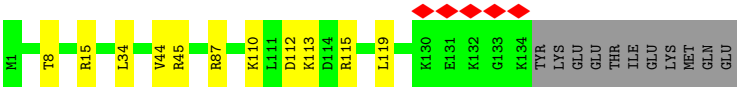
• Molecule 14: 60S ribosomal protein L23a

Chain LH:



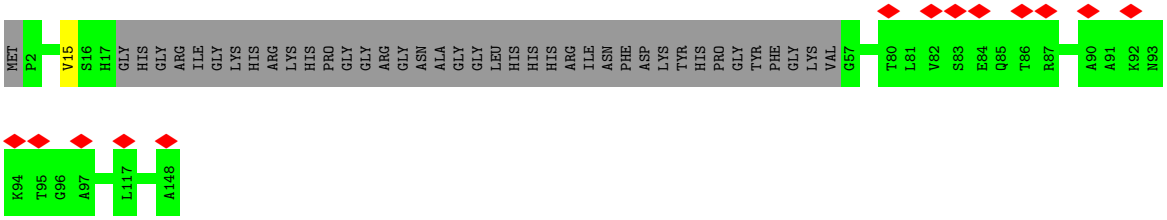
• Molecule 15: 60S ribosomal protein L26

Chain LI:



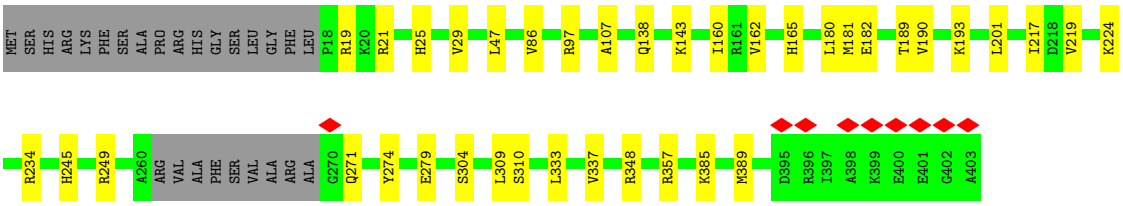
• Molecule 16: 60S ribosomal protein L27a

Chain LK:



• Molecule 17: 60S ribosomal protein L3

Chain LN:

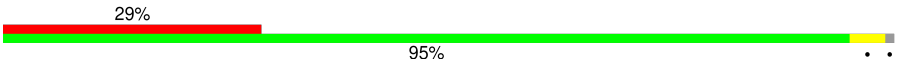


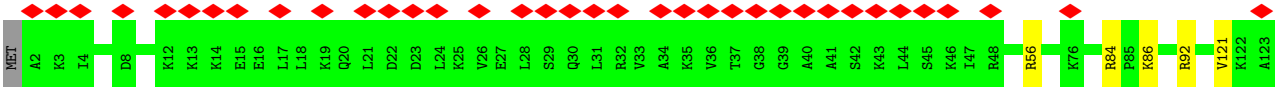
• Molecule 18: 60S ribosomal protein L32

Chain LQ:

• Molecule 19: 60S ribosomal protein L35

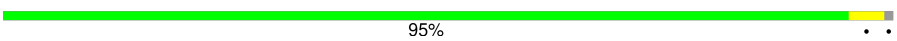
Chain LS:

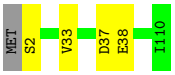




• Molecule 20: 60S ribosomal protein L35a

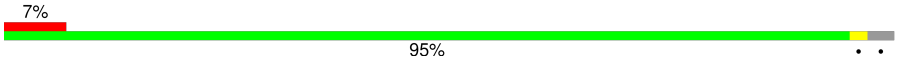
Chain LT:

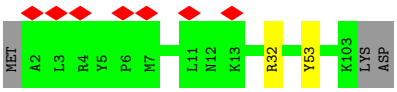




• Molecule 21: 60S ribosomal protein L36

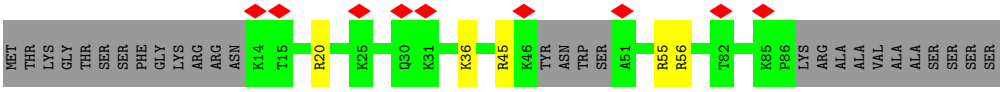
Chain LU:





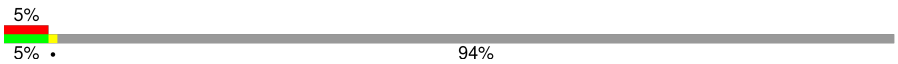
• Molecule 22: 60S ribosomal protein L37

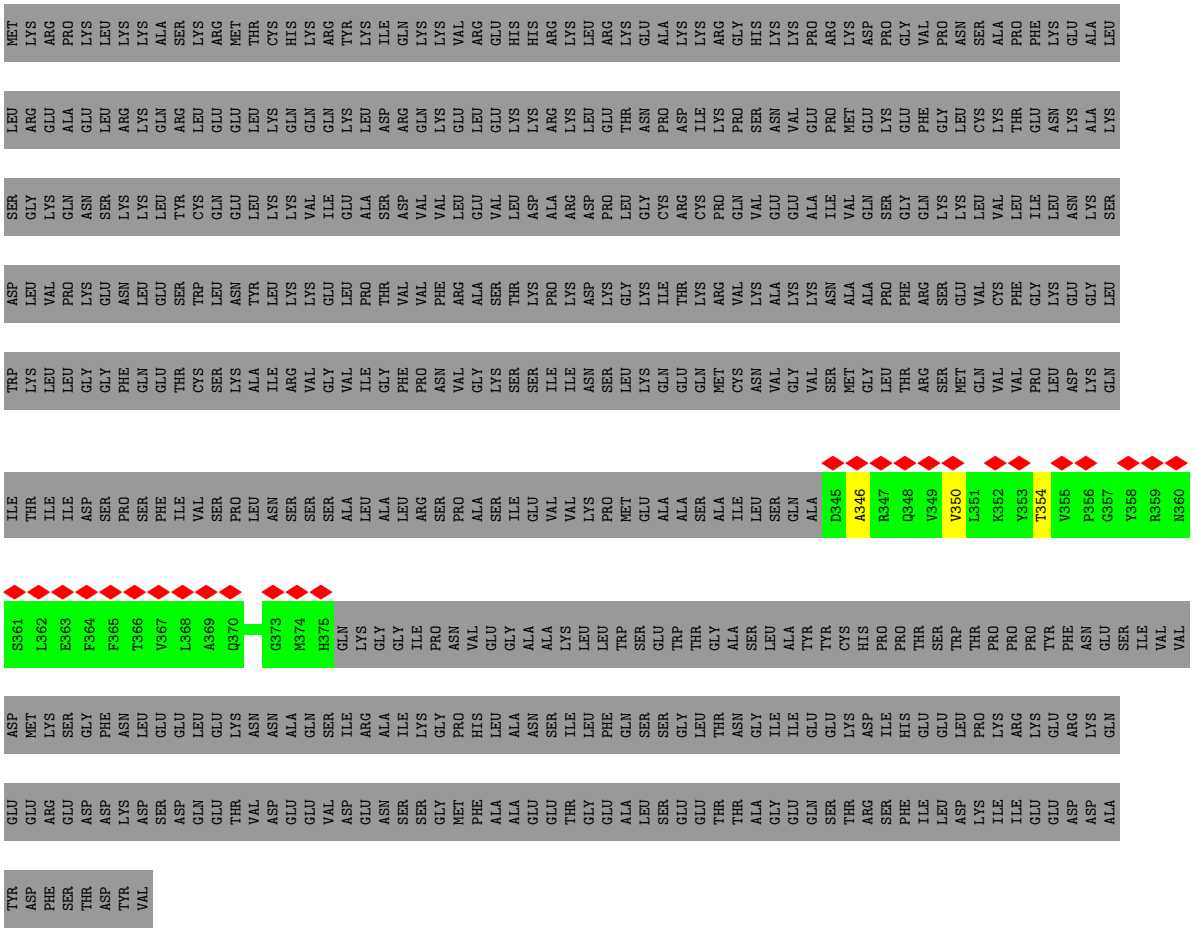
Chain LW:



• Molecule 23: Guanine nucleotide-binding protein-like 3

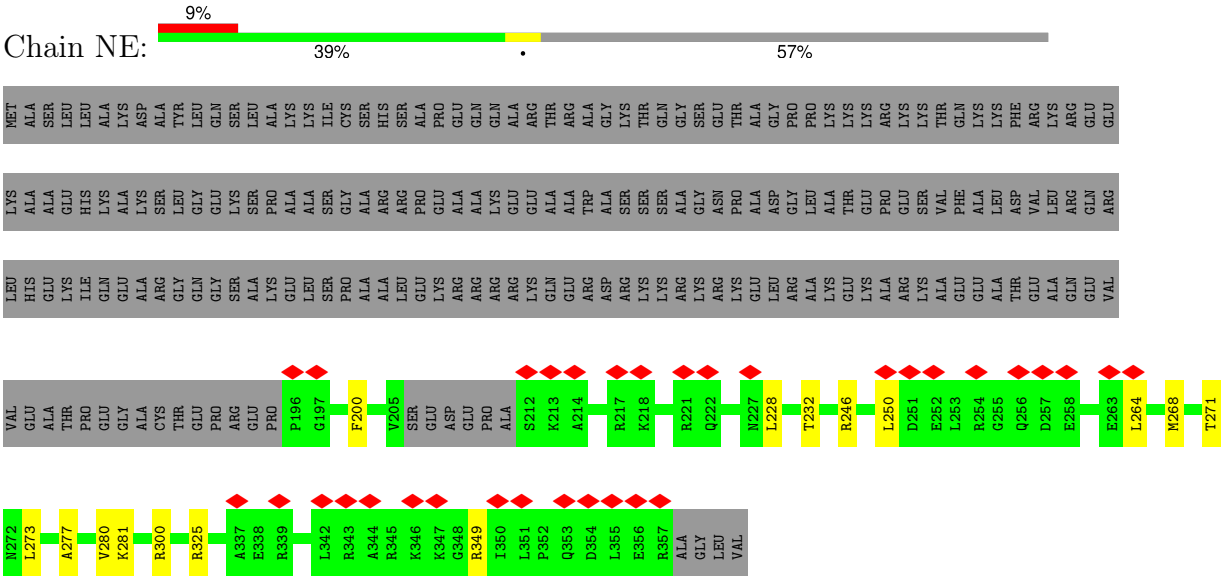
Chain NB:





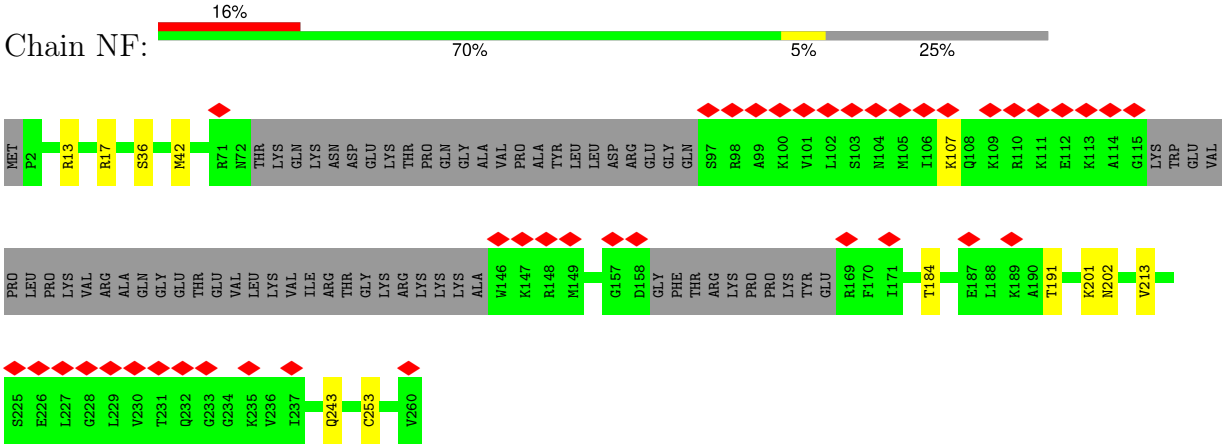
• Molecule 24: Surfeit locus protein 6

Chain NE:



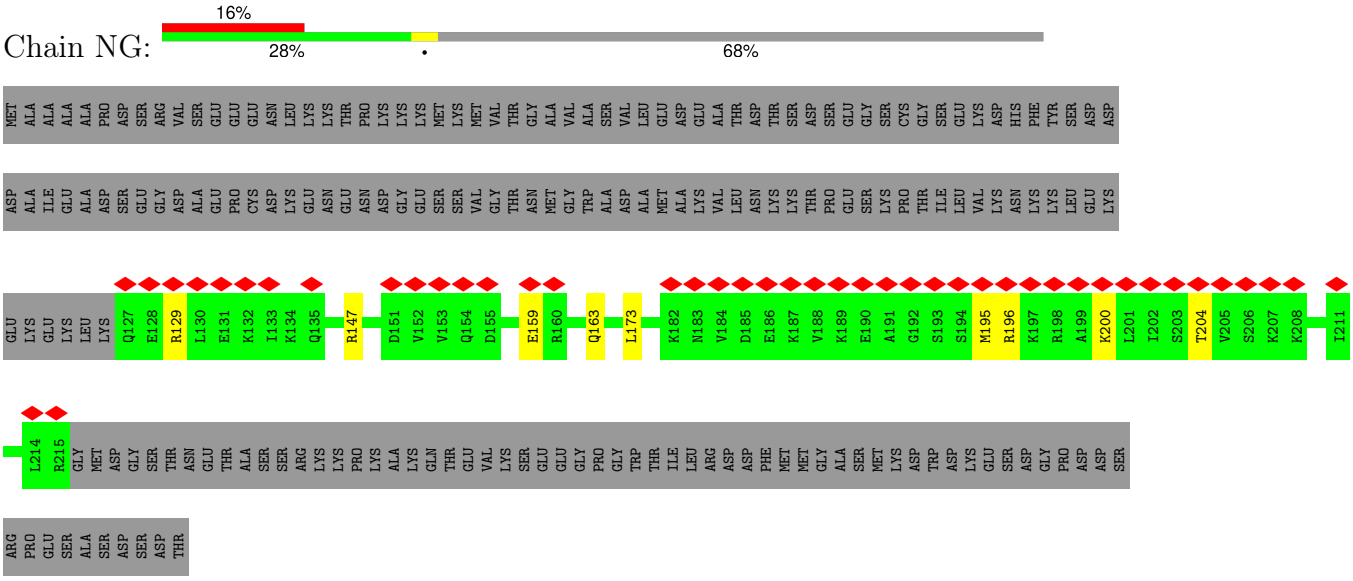
• Molecule 25: Ribosome biogenesis protein NSA2 homolog

Chain NF:



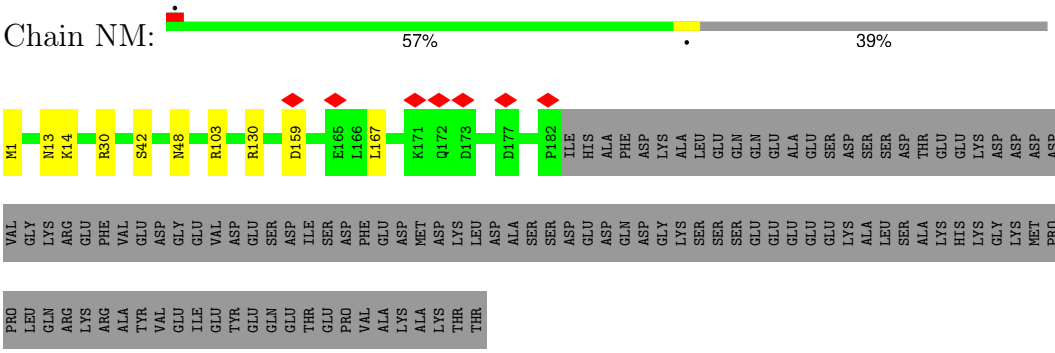
• Molecule 26: RRP15-like protein

Chain NG:



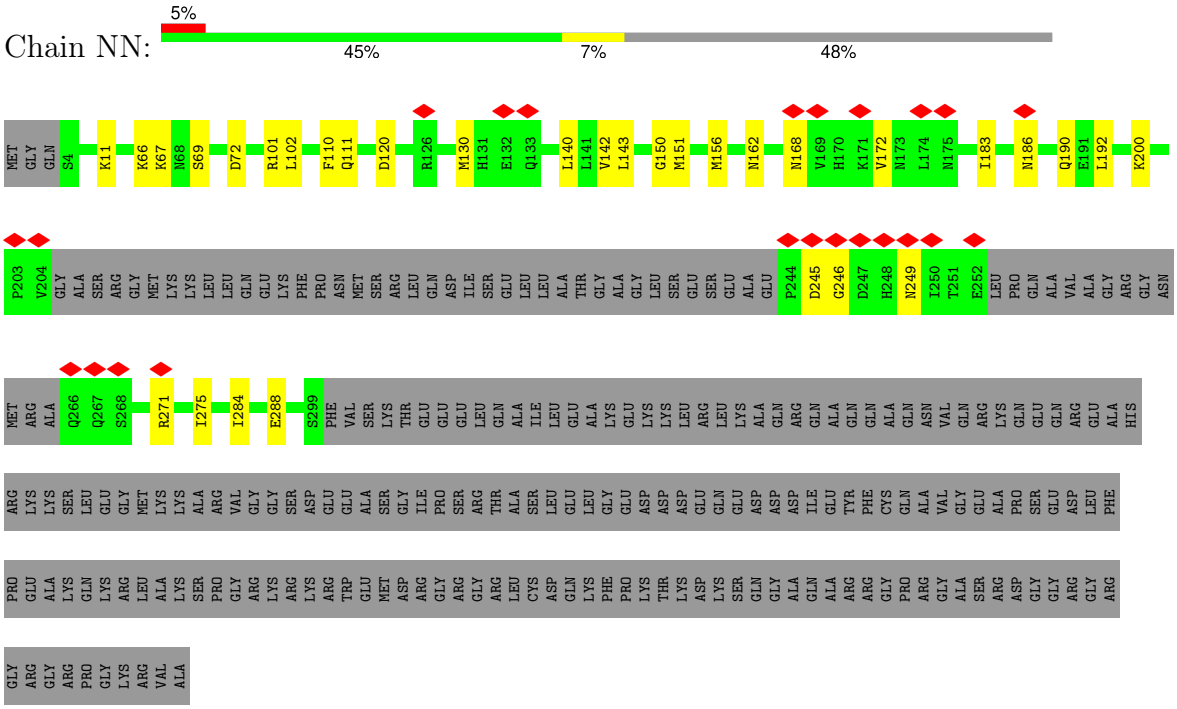
• Molecule 27: Protein MAK16 homolog

Chain NM:



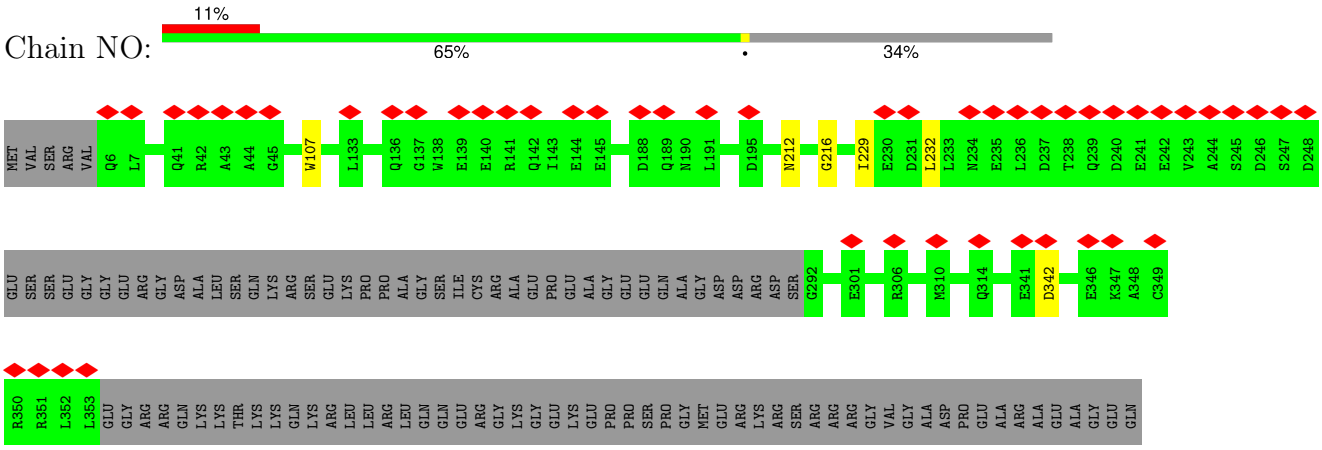
• Molecule 28: Suppressor of SWI4 1 homolog

Chain NN:



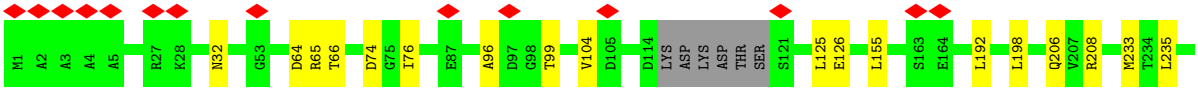
• Molecule 29: Ribosomal RNA processing protein 1 homolog A

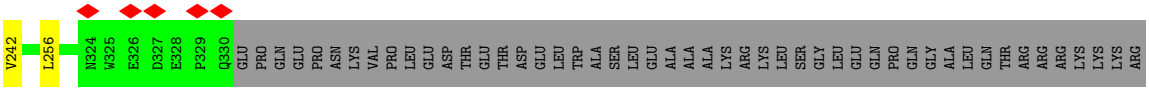
Chain NO:



• Molecule 30: WD repeat-containing protein 74

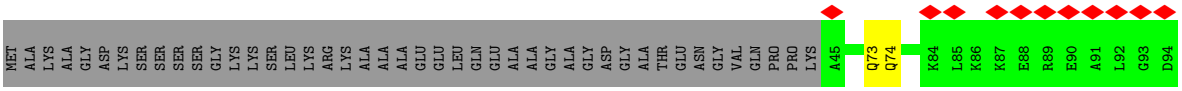
Chain NQ:

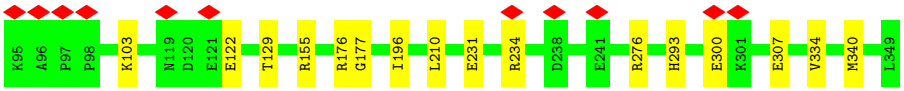




• Molecule 31: Ribosome production factor 1

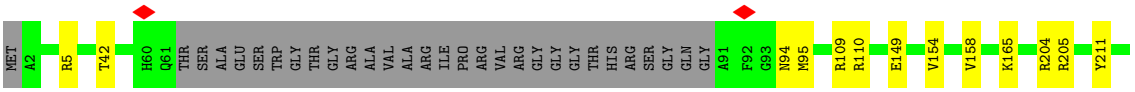
Chain NS:

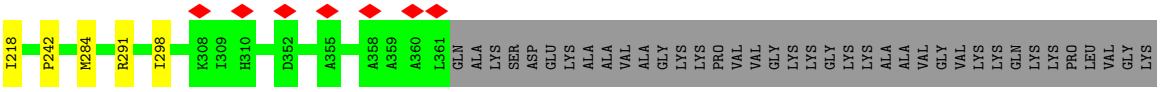




• Molecule 32: 60S ribosomal protein L4

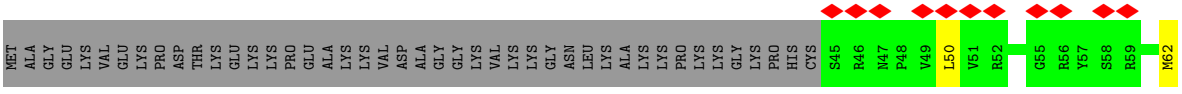
Chain SA:

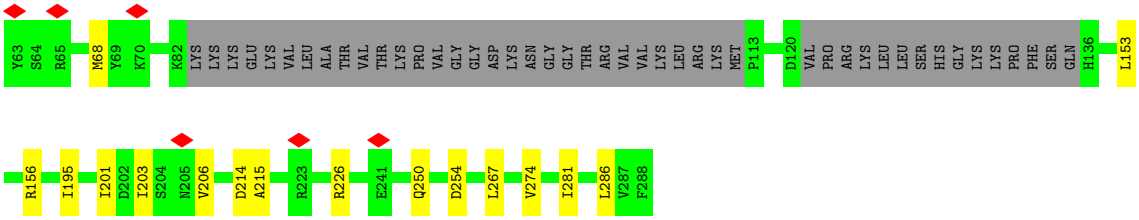




• Molecule 33: 60S ribosomal protein L6

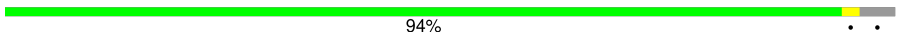
Chain SC:

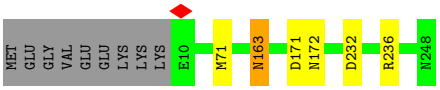




• Molecule 34: 60S ribosomal protein L7

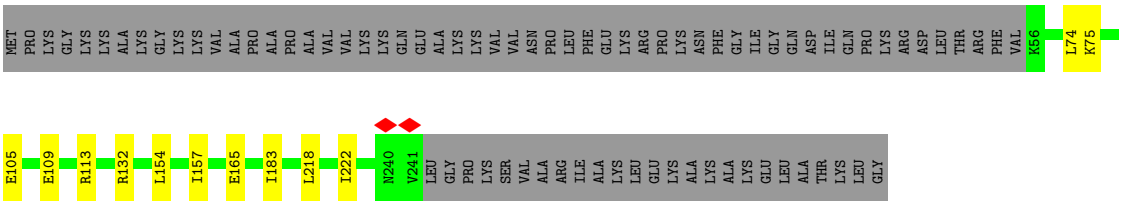
Chain SD:





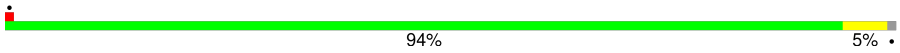
• Molecule 35: 60S ribosomal protein L7a

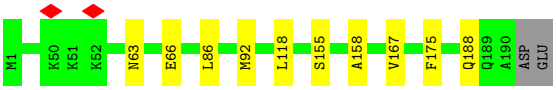
Chain SE:



• Molecule 36: 60S ribosomal protein L9

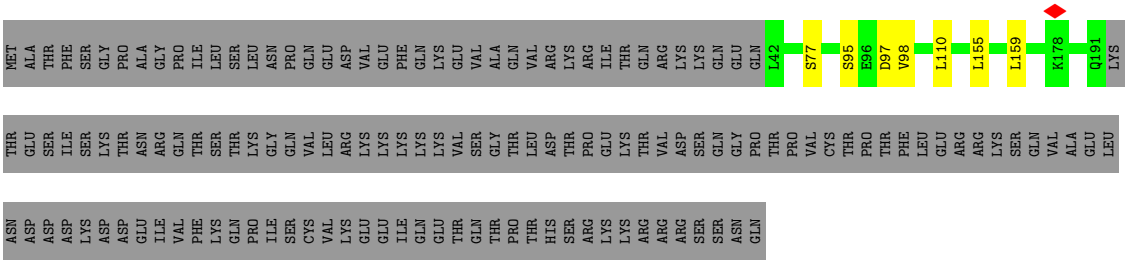
Chain SG:





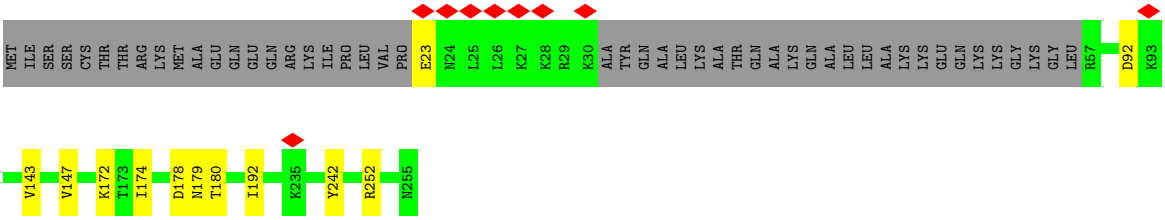
• Molecule 37: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain SH:



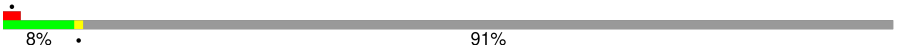
• Molecule 38: 60S ribosomal protein L7-like 1

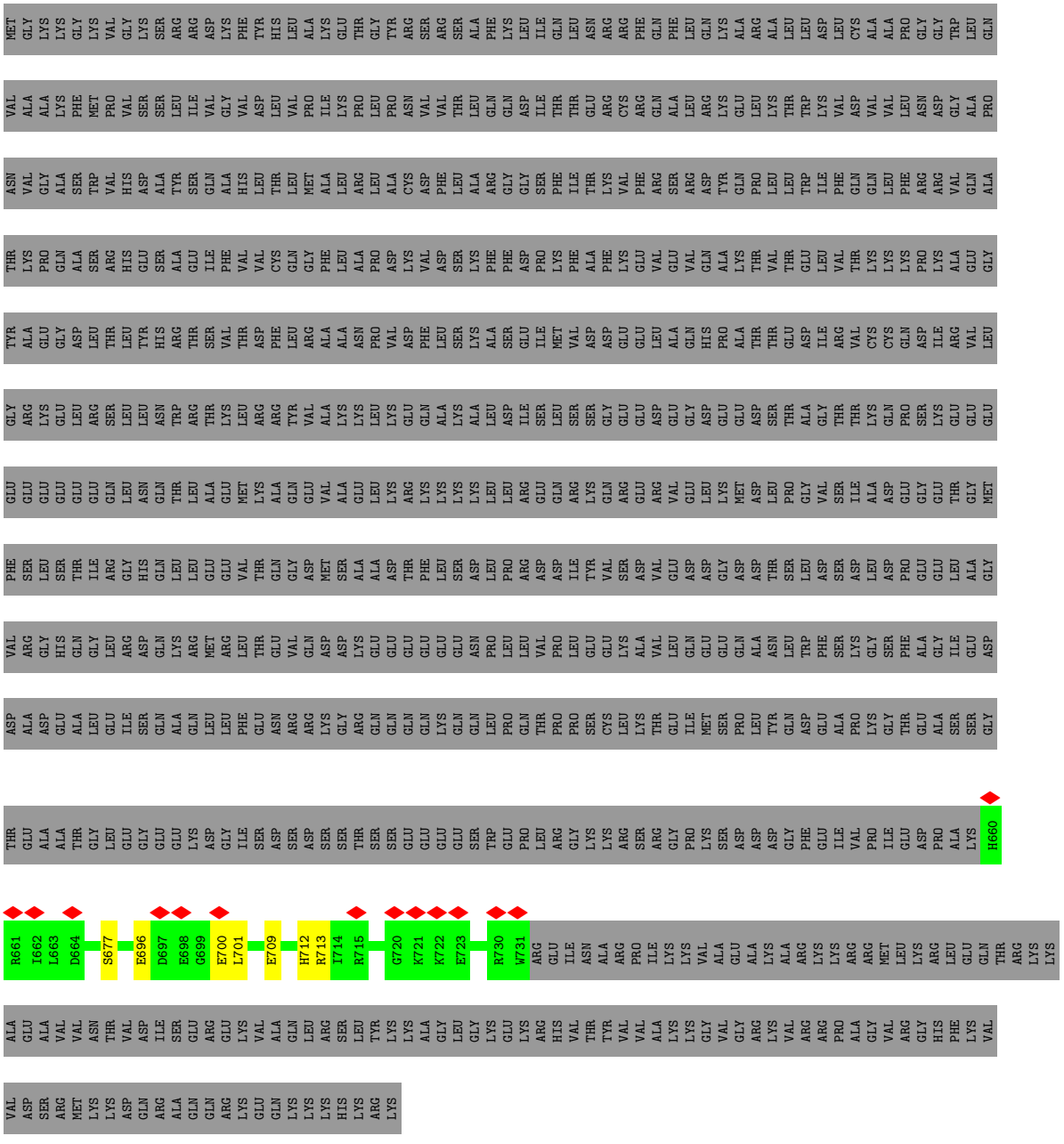
Chain SI:



• Molecule 39: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

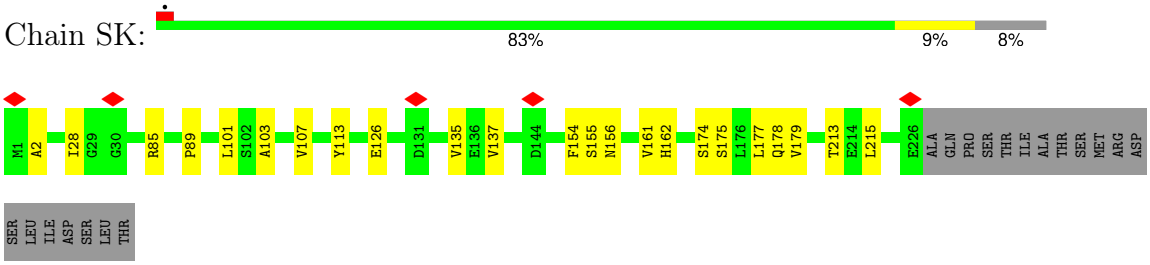
Chain SJ:





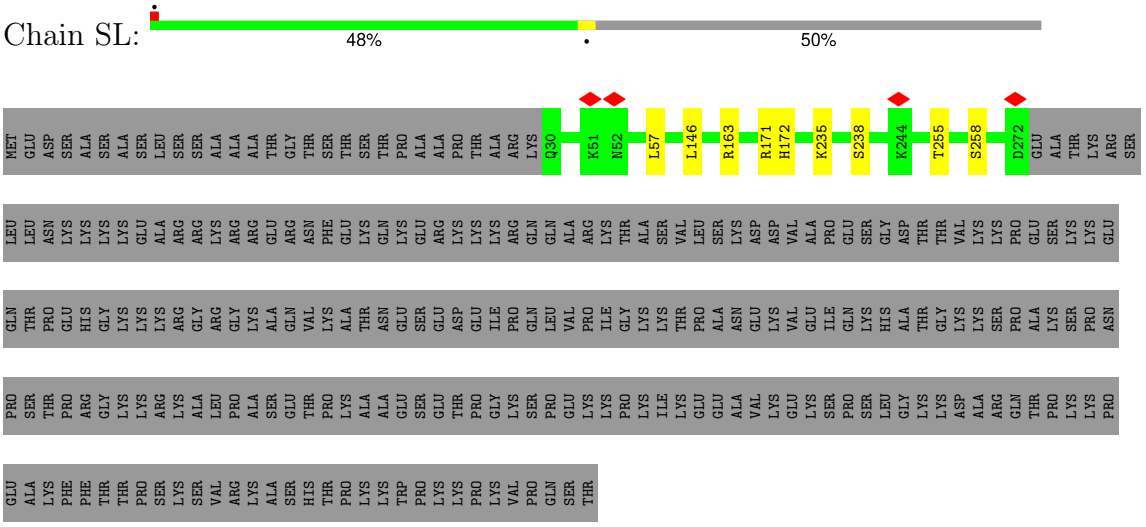
• Molecule 40: Eukaryotic translation initiation factor 6

Chain SK:



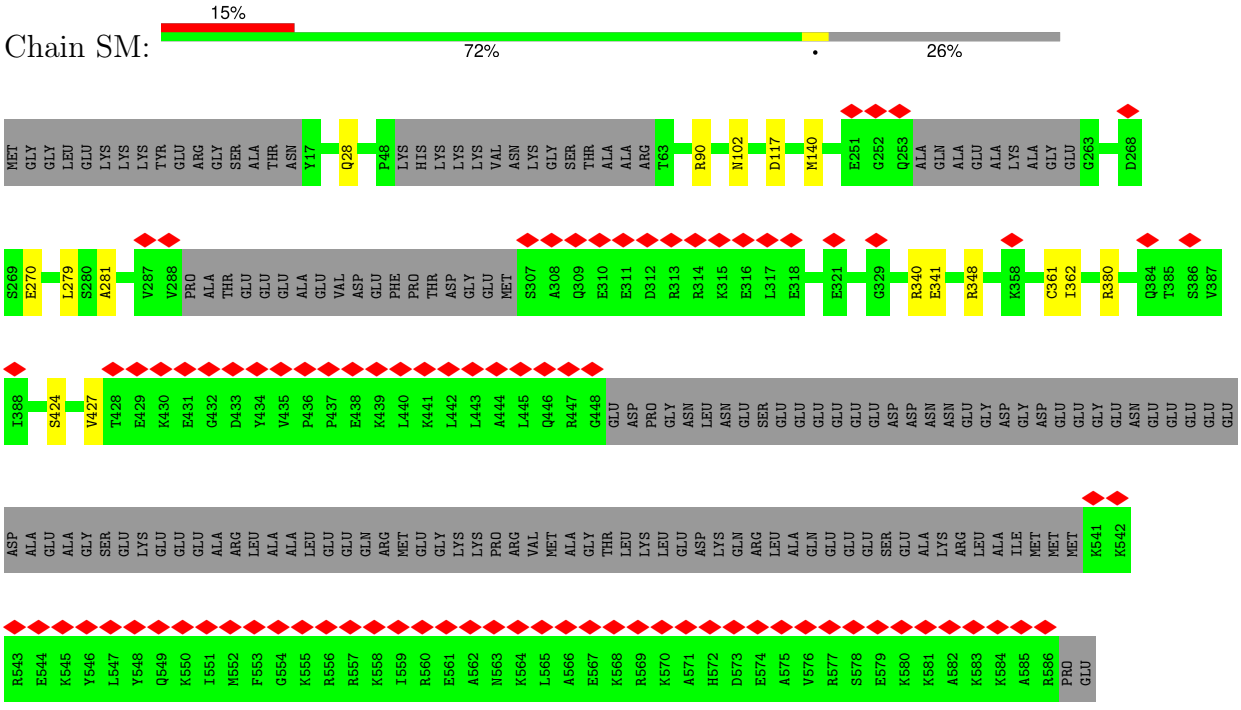
• Molecule 41: Ribosomal L1 domain-containing protein 1

Chain SL:



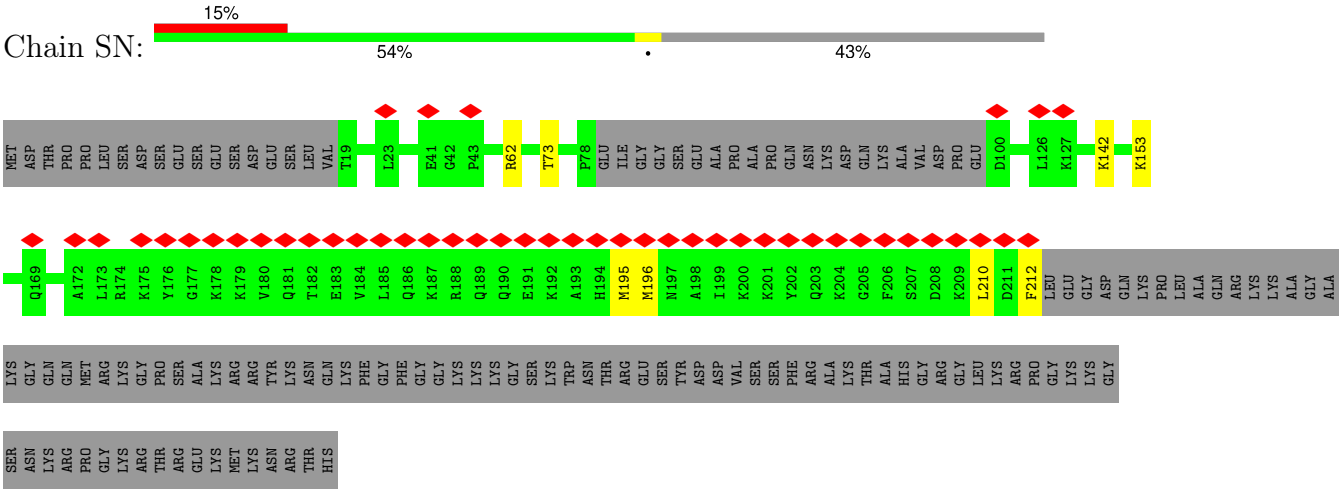
• Molecule 42: Pescadillo homolog

Chain SM:



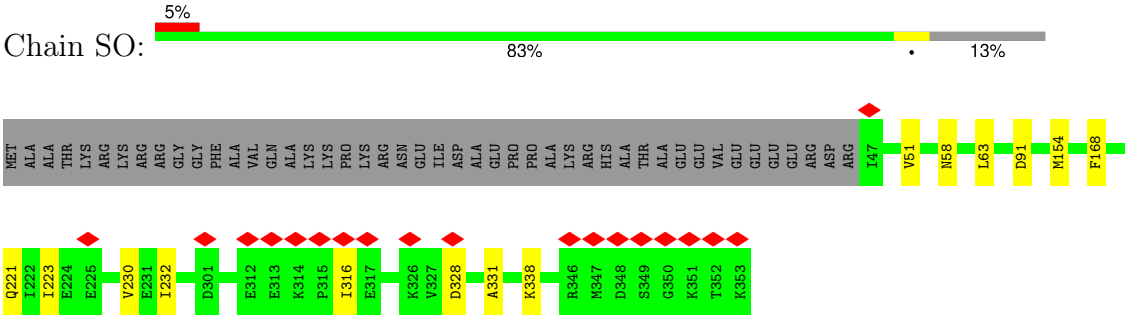
• Molecule 43: Probable rRNA-processing protein EBP2

Chain SN:



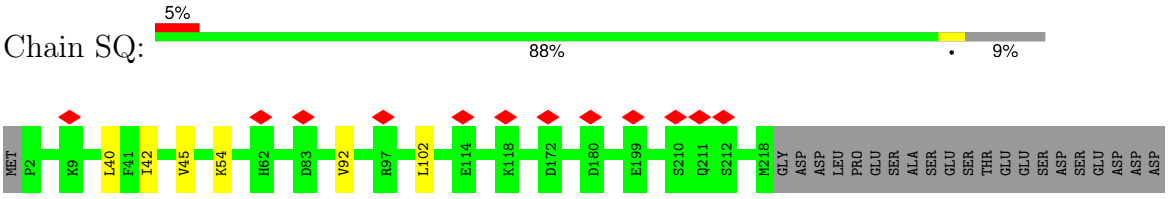
• Molecule 44: Ribosome biogenesis protein BRX1 homolog

Chain SO:



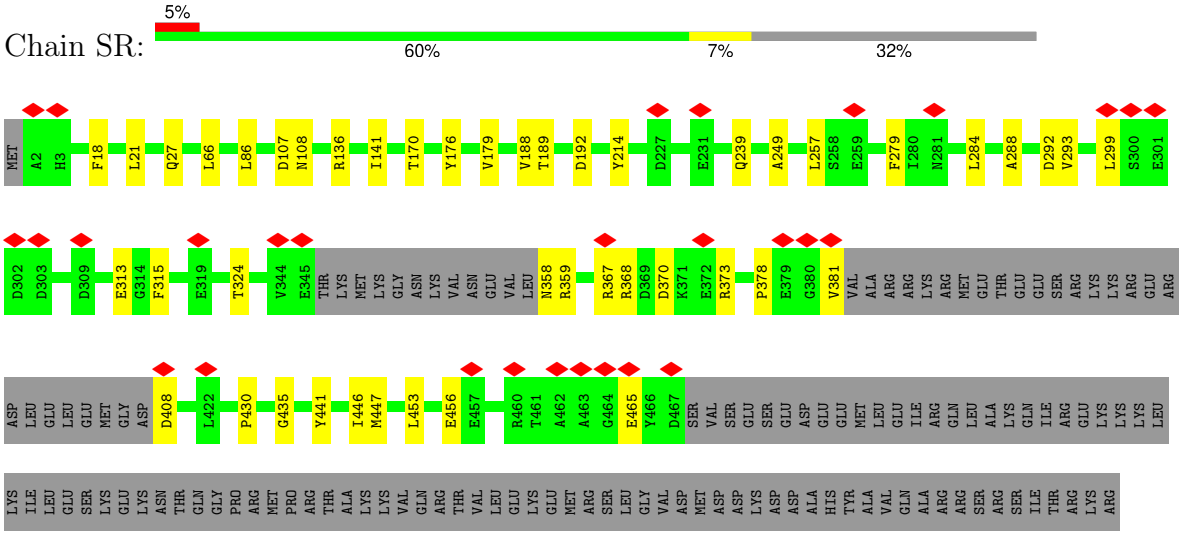
• Molecule 45: mRNA turnover protein 4 homolog

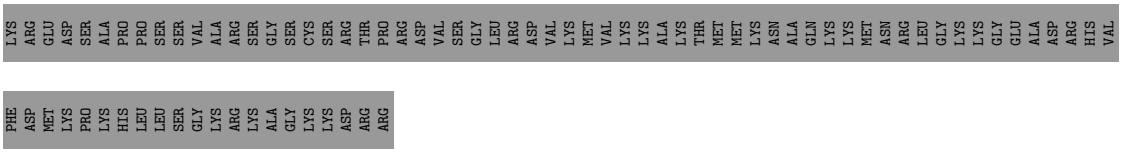
Chain SQ:



• Molecule 46: GTP-binding protein 4

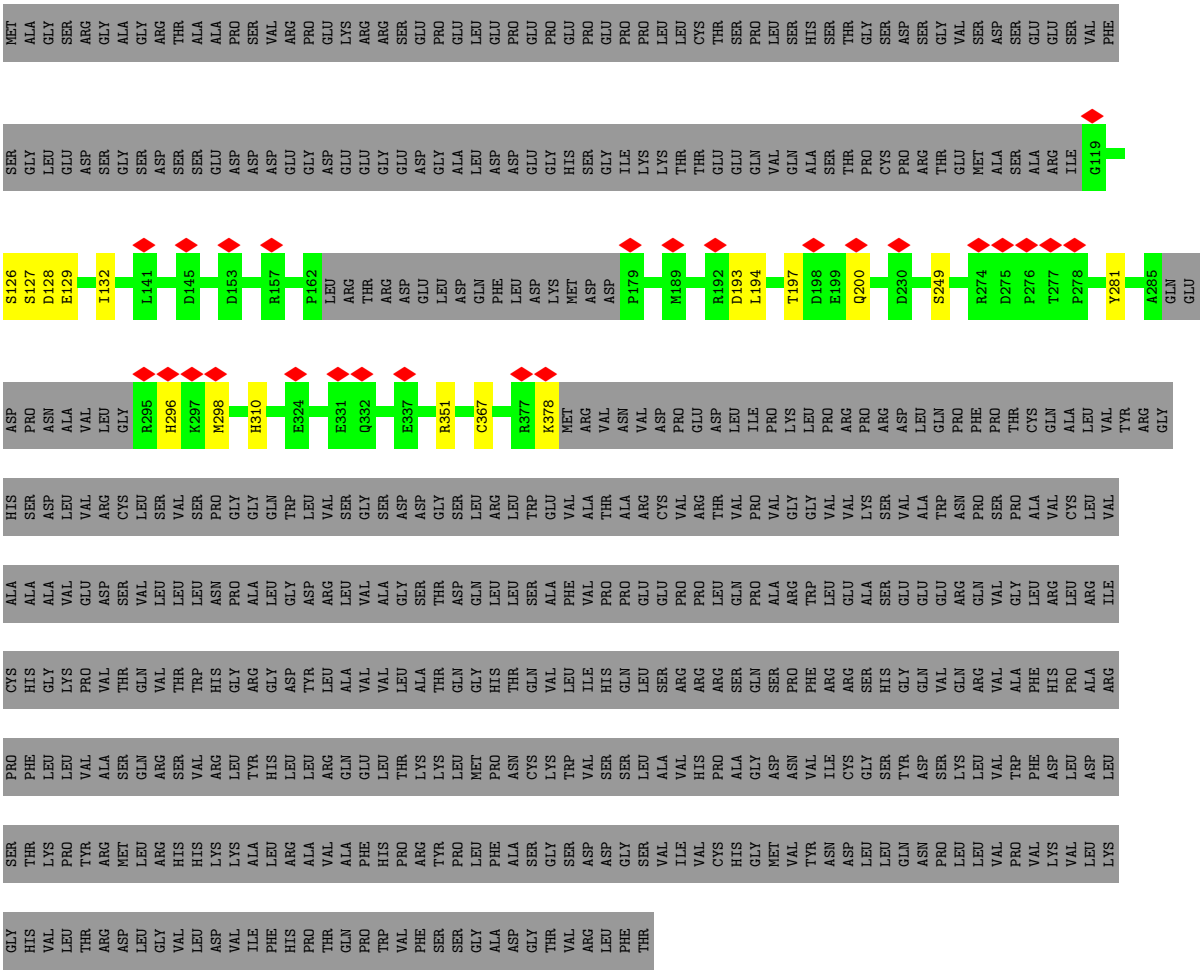
Chain SR:





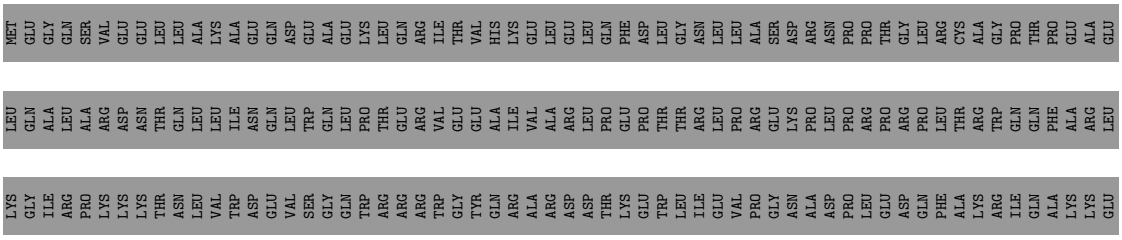
• Molecule 47: Ribosome biogenesis protein BOP1

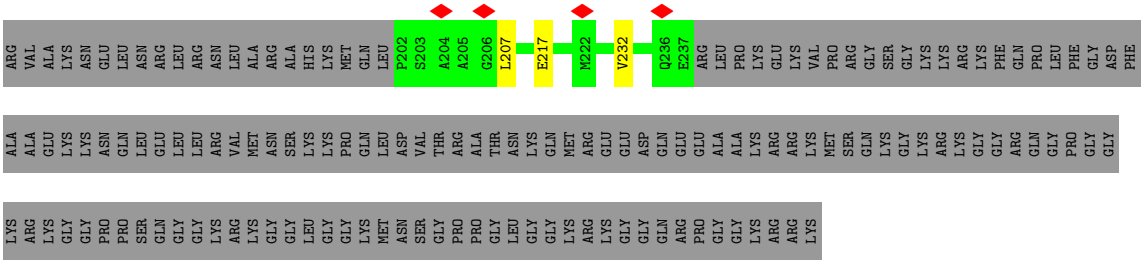
Chain SS:



• Molecule 48: Ribosome biogenesis regulatory protein homolog

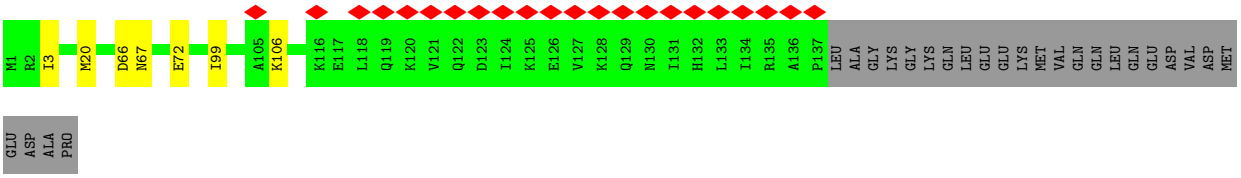
Chain ST:





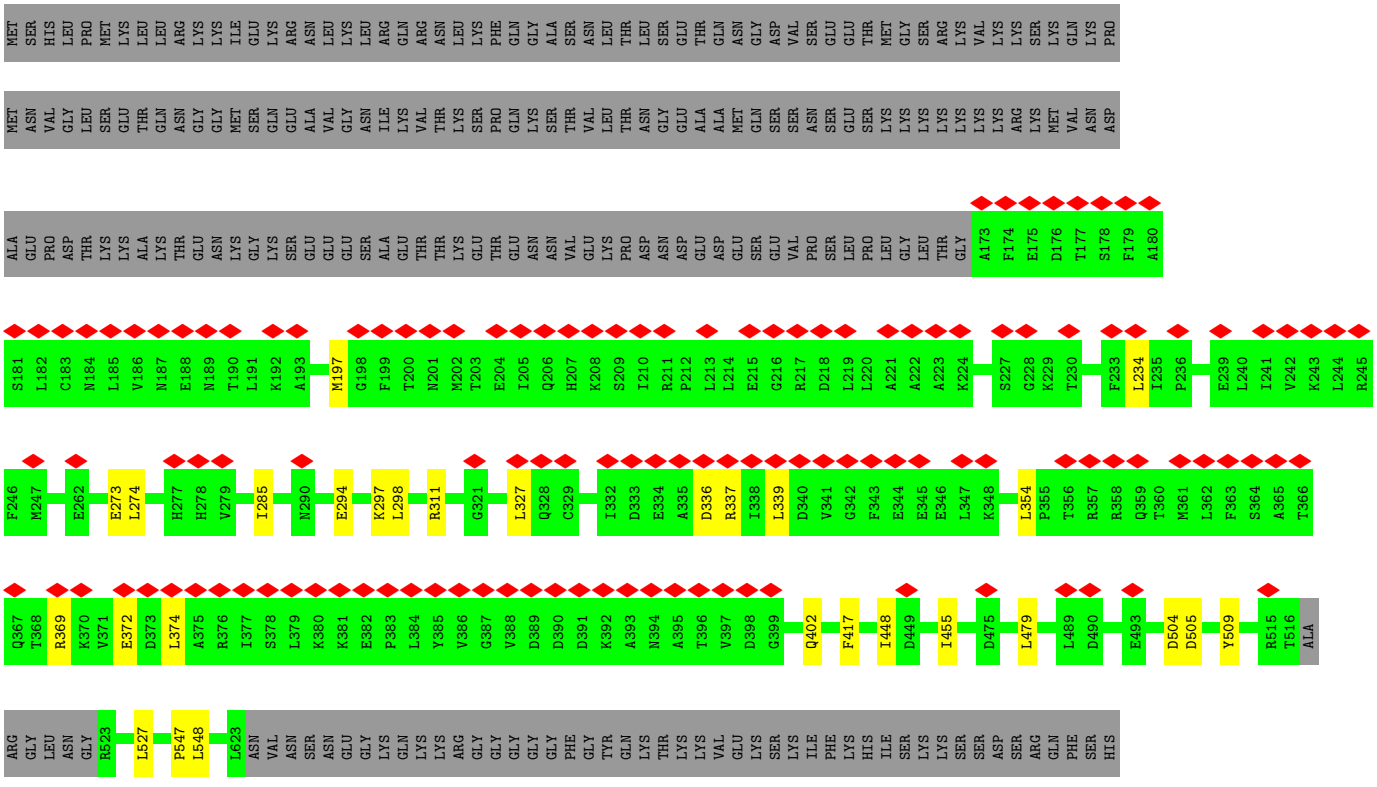
• Molecule 49: Probable ribosome biogenesis protein RLP24

Chain SV:



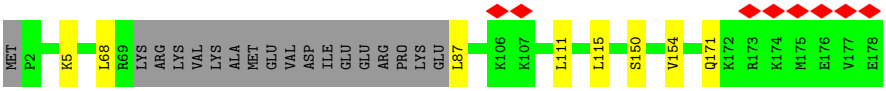
• Molecule 50: ATP-dependent RNA helicase DDX18

Chain SW:



• Molecule 51: Nucleolar protein 16

Chain SZ:


MET
P2
K5
L68
R69
LYS
ARG
LYS
VAL
LYS
ALA
MET
GLU
VAL
ASP
ILE
GLU
GLU
ARG
PRO
LYS
GLU
L87
K106
K107
L111
L115
S150
V154
Q171
K172
R173
K174
M175
E176
V177
E178

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21669	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.579	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.042	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AME, ZN, GDP, SEP, K, HIC, SF4

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	0.17	0/1191	0.34	0/1605
2	L1	0.14	0/3656	0.24	0/5694
3	L2	0.15	0/1634	0.26	0/2538
4	L3	0.15	0/42353	0.27	0/66007
5	L6	0.16	0/953	0.32	0/1276
6	L7	0.16	0/1534	0.34	0/2049
7	L8	0.17	0/1133	0.39	0/1516
8	L9	0.16	0/1584	0.35	0/2117
9	LA	0.15	0/1179	0.32	0/1575
10	LB	0.16	0/1239	0.32	0/1658
11	LC	0.18	0/1501	0.34	0/2013
12	LE	0.18	0/692	0.39	0/936
13	LG	0.14	0/856	0.32	0/1149
14	LH	0.14	0/287	0.32	0/378
15	LI	0.17	0/1132	0.35	0/1504
16	LK	0.13	0/648	0.34	0/880
17	LN	0.17	0/3092	0.33	0/4133
18	LQ	0.15	0/1114	0.31	0/1486
19	LS	0.12	0/1023	0.26	0/1351
20	LT	0.16	0/895	0.30	0/1198
21	LU	0.15	0/854	0.31	0/1129
22	LW	0.12	0/573	0.35	0/755
23	NB	0.08	0/262	0.21	0/352
24	NE	0.12	0/1339	0.27	0/1767
25	NF	0.12	0/1614	0.26	0/2146
26	NG	0.12	0/743	0.27	0/986
27	NM	0.14	0/1566	0.29	0/2097
28	NN	0.17	0/1988	0.37	1/2678 (0.0%)
29	NO	0.12	0/2530	0.26	0/3412
30	NQ	0.14	0/2556	0.29	0/3466
31	NS	0.13	0/2592	0.29	0/3487
32	SA	0.16	0/2705	0.31	0/3632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SC	0.12	0/1657	0.29	0/2219
34	SD	0.14	0/2022	0.31	0/2696
35	SE	0.14	0/1524	0.30	0/2056
36	SG	0.14	0/1537	0.26	0/2066
37	SH	0.15	0/1298	0.27	0/1742
38	SI	0.13	0/1772	0.29	0/2378
39	SJ	0.14	0/623	0.30	0/836
40	SK	0.16	0/1745	0.33	0/2374
41	SL	0.14	0/1994	0.31	0/2684
42	SM	0.12	0/3530	0.25	0/4779
43	SN	0.12	0/1368	0.28	0/1830
44	SO	0.14	0/2608	0.29	0/3506
45	SQ	0.13	0/1817	0.30	0/2435
46	SR	0.14	0/3597	0.30	0/4861
47	SS	0.15	0/1994	0.29	0/2703
48	ST	0.14	0/267	0.31	0/357
49	SV	0.15	0/1194	0.32	0/1582
50	SW	0.13	0/3631	0.27	0/4900
51	SZ	0.13	0/1364	0.26	0/1826
All	All	0.15	0/122560	0.29	1/174800 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	NN	275	ILE	N-CA-C	-5.13	107.83	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1176	0	1234	16	0
2	L1	3274	0	1662	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L2	1468	0	755	5	0
4	L3	37886	0	19186	119	0
5	L6	936	0	1017	6	0
6	L7	1507	0	1649	12	0
7	L8	1111	0	1174	13	0
8	L9	1546	0	1585	7	0
9	LA	1161	0	1221	10	0
10	LB	1223	0	1330	7	0
11	LC	1461	0	1502	14	0
12	LE	686	0	544	4	0
13	LG	844	0	883	7	0
14	LH	284	0	330	2	0
15	LI	1115	0	1205	8	0
16	LK	642	0	455	1	0
17	LN	3044	0	3178	30	0
18	LQ	1096	0	1183	7	0
19	LS	1015	0	1148	4	0
20	LT	876	0	912	3	0
21	LU	840	0	930	2	0
22	LW	563	0	596	4	0
23	NB	257	0	259	2	0
24	NE	1331	0	1430	11	0
25	NF	1588	0	1695	11	0
26	NG	738	0	786	6	0
27	NM	1550	0	1599	8	0
28	NN	1950	0	2005	22	0
29	NO	2487	0	2506	7	0
30	NQ	2502	0	2481	11	0
31	NS	2529	0	2563	14	0
32	SA	2656	0	2833	14	0
33	SC	1627	0	1751	16	0
34	SD	1985	0	2128	4	0
35	SE	1498	0	1601	10	0
36	SG	1518	0	1601	6	0
37	SH	1267	0	1291	5	0
38	SI	1732	0	1837	10	0
39	SJ	609	0	600	7	0
40	SK	1721	0	1695	16	0
41	SL	1960	0	2052	6	0
42	SM	3452	0	3376	13	0
43	SN	1350	0	1345	10	0
44	SO	2544	0	2631	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	SQ	1778	0	1817	5	0
46	SR	3524	0	3558	35	0
47	SS	1955	0	1872	12	0
48	ST	263	0	260	2	0
49	SV	1171	0	1232	7	0
50	SW	3560	0	3641	15	0
51	SZ	1338	0	1352	8	0
52	L1	3	0	0	0	0
52	L2	1	0	0	0	0
52	L3	45	0	0	0	0
52	L9	1	0	0	0	0
52	LN	1	0	0	0	0
52	LQ	1	0	0	0	0
52	LT	1	0	0	0	0
52	SA	1	0	0	0	0
53	LW	1	0	0	0	0
53	SV	1	0	0	0	0
54	NM	8	0	0	0	0
55	SR	28	0	12	0	0
56	SR	1	0	0	0	0
All	All	116287	0	97488	431	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 431 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)
7:L8:32:ASP:OD2	7:L8:33:GLN:N	2.11	0.83
47:SS:197:THR:OG1	47:SS:200:GLN:OE1	1.94	0.83
4:L3:2059:C:O2'	11:LC:118:ARG:NH1	2.12	0.83
1:BA:37:LEU:HD11	1:BA:64:ILE:HD11	1.60	0.82
4:L3:254:G:OP2	44:SO:338:LYS:NZ	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	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
5	L6	112/211 (53%)	110 (98%)	2 (2%)	0	100	100
6	L7	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
7	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
8	L9	179/204 (88%)	178 (99%)	1 (1%)	0	100	100
9	LA	137/184 (74%)	136 (99%)	1 (1%)	0	100	100
10	LB	149/188 (79%)	149 (100%)	0	0	100	100
11	LC	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
12	LE	100/160 (62%)	100 (100%)	0	0	100	100
13	LG	110/140 (79%)	109 (99%)	1 (1%)	0	100	100
14	LH	32/156 (20%)	32 (100%)	0	0	100	100
15	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
16	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
17	LN	372/403 (92%)	366 (98%)	6 (2%)	0	100	100
18	LQ	131/135 (97%)	130 (99%)	1 (1%)	0	100	100
19	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
20	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
21	LU	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
22	LW	65/97 (67%)	64 (98%)	1 (2%)	0	100	100
23	NB	29/549 (5%)	29 (100%)	0	0	100	100
24	NE	152/361 (42%)	149 (98%)	3 (2%)	0	100	100
25	NF	187/260 (72%)	185 (99%)	2 (1%)	0	100	100
26	NG	87/282 (31%)	86 (99%)	1 (1%)	0	100	100
27	NM	180/300 (60%)	175 (97%)	5 (3%)	0	100	100
28	NN	238/473 (50%)	234 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	NO	301/461 (65%)	299 (99%)	2 (1%)	0	100	100
30	NQ	320/385 (83%)	315 (98%)	5 (2%)	0	100	100
31	NS	303/349 (87%)	301 (99%)	2 (1%)	0	100	100
32	SA	327/427 (77%)	322 (98%)	5 (2%)	0	100	100
33	SC	193/288 (67%)	191 (99%)	2 (1%)	0	100	100
34	SD	237/248 (96%)	234 (99%)	3 (1%)	0	100	100
35	SE	184/266 (69%)	182 (99%)	2 (1%)	0	100	100
36	SG	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
37	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
38	SI	204/255 (80%)	202 (99%)	2 (1%)	0	100	100
39	SJ	70/847 (8%)	69 (99%)	1 (1%)	0	100	100
40	SK	224/245 (91%)	220 (98%)	4 (2%)	0	100	100
41	SL	241/490 (49%)	237 (98%)	4 (2%)	0	100	100
42	SM	427/588 (73%)	426 (100%)	1 (0%)	0	100	100
43	SN	169/306 (55%)	169 (100%)	0	0	100	100
44	SO	305/353 (86%)	299 (98%)	6 (2%)	0	100	100
45	SQ	216/239 (90%)	212 (98%)	4 (2%)	0	100	100
46	SR	422/634 (67%)	418 (99%)	4 (1%)	0	100	100
47	SS	227/746 (30%)	225 (99%)	1 (0%)	1 (0%)	30	59
48	ST	34/365 (9%)	33 (97%)	1 (3%)	0	100	100
49	SV	135/163 (83%)	135 (100%)	0	0	100	100
50	SW	441/670 (66%)	431 (98%)	10 (2%)	0	100	100
51	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	8937/14481 (62%)	8828 (99%)	108 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
47	SS	128	ASP

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	128/137 (93%)	128 (100%)	0	100	100
5	L6	98/177 (55%)	98 (100%)	0	100	100
6	L7	157/174 (90%)	157 (100%)	0	100	100
7	L8	115/161 (71%)	115 (100%)	0	100	100
8	L9	155/172 (90%)	155 (100%)	0	100	100
9	LA	132/163 (81%)	132 (100%)	0	100	100
10	LB	136/165 (82%)	136 (100%)	0	100	100
11	LC	157/157 (100%)	157 (100%)	0	100	100
12	LE	45/140 (32%)	45 (100%)	0	100	100
13	LG	87/107 (81%)	87 (100%)	0	100	100
14	LH	28/133 (21%)	28 (100%)	0	100	100
15	LI	124/135 (92%)	124 (100%)	0	100	100
16	LK	29/121 (24%)	29 (100%)	0	100	100
17	LN	328/348 (94%)	328 (100%)	0	100	100
18	LQ	119/121 (98%)	119 (100%)	0	100	100
19	LS	109/110 (99%)	109 (100%)	0	100	100
20	LT	88/89 (99%)	88 (100%)	0	100	100
21	LU	87/89 (98%)	87 (100%)	0	100	100
22	LW	58/80 (72%)	58 (100%)	0	100	100
23	NB	27/485 (6%)	27 (100%)	0	100	100
24	NE	136/294 (46%)	136 (100%)	0	100	100
25	NF	172/228 (75%)	172 (100%)	0	100	100
26	NG	83/246 (34%)	83 (100%)	0	100	100
27	NM	168/272 (62%)	168 (100%)	0	100	100
28	NN	218/398 (55%)	218 (100%)	0	100	100
29	NO	269/392 (69%)	269 (100%)	0	100	100
30	NQ	265/318 (83%)	265 (100%)	0	100	100
31	NS	276/305 (90%)	276 (100%)	0	100	100
32	SA	280/348 (80%)	280 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	SC	178/252 (71%)	178 (100%)	0	100	100
34	SD	207/215 (96%)	206 (100%)	1 (0%)	81	93
35	SE	159/223 (71%)	159 (100%)	0	100	100
36	SG	169/171 (99%)	169 (100%)	0	100	100
37	SH	140/274 (51%)	140 (100%)	0	100	100
38	SI	190/228 (83%)	190 (100%)	0	100	100
39	SJ	64/733 (9%)	64 (100%)	0	100	100
40	SK	196/213 (92%)	196 (100%)	0	100	100
41	SL	226/437 (52%)	226 (100%)	0	100	100
42	SM	350/509 (69%)	350 (100%)	0	100	100
43	SN	133/260 (51%)	133 (100%)	0	100	100
44	SO	283/319 (89%)	283 (100%)	0	100	100
45	SQ	195/214 (91%)	195 (100%)	0	100	100
46	SR	390/574 (68%)	390 (100%)	0	100	100
47	SS	208/648 (32%)	208 (100%)	0	100	100
48	ST	27/300 (9%)	27 (100%)	0	100	100
49	SV	127/149 (85%)	127 (100%)	0	100	100
50	SW	394/591 (67%)	394 (100%)	0	100	100
51	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	7851/12533 (63%)	7850 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	SD	163	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
45	SQ	113	ASN
50	SW	572	ASN
46	SR	37	HIS
47	SS	299	HIS
28	NN	149	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	16 (10%)	0
3	L2	65/1167 (5%)	9 (13%)	0
4	L3	1735/5070 (34%)	280 (16%)	2 (0%)
All	All	1952/6394 (30%)	305 (15%)	2 (0%)

5 of 305 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	34	U
2	L1	59	A
2	L1	62	A
2	L1	63	U
2	L1	82	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	2266	C
4	L3	3852	A

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

4 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	$\#\|Z\| > 2$
17	HIC	LN	245	17	10,11,12	1.51	1 (10%)	9,14,16	1.21	2 (22%)
47	SEP	SS	127	47	8,9,10	1.58	1 (12%)	7,12,14	1.23	1 (14%)
47	SEP	SS	126	47	8,9,10	1.58	1 (12%)	7,12,14	1.20	1 (14%)
27	AME	NM	1	27	9,10,11	1.52	2 (22%)	9,11,13	1.35	1 (11%)

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
17	HIC	LN	245	17	-	0/5/6/8	0/1/1/1
47	SEP	SS	127	47	-	2/6/8/10	-
47	SEP	SS	126	47	-	0/6/8/10	-
27	AME	NM	1	27	-	3/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	SS	127	SEP	P-O1P	3.48	1.61	1.50
47	SS	126	SEP	P-O1P	3.45	1.61	1.50
27	NM	1	AME	CT1-N	3.43	1.45	1.34
17	LN	245	HIC	CD2-CG	3.01	1.41	1.36
27	NM	1	AME	OT-CT1	-2.01	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	LN	245	HIC	NE2-CE1-ND1	-2.57	111.68	112.66
47	SS	126	SEP	OG-CB-CA	2.53	110.61	108.14
47	SS	127	SEP	OG-CB-CA	2.48	110.56	108.14
27	NM	1	AME	CT2-CT1-N	2.45	120.18	116.12
17	LN	245	HIC	CB-CG-CD2	-2.12	124.85	129.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	SS	127	SEP	N-CA-CB-OG
27	NM	1	AME	N-CA-CB-CG
27	NM	1	AME	C-CA-N-CT1
27	NM	1	AME	CB-CG-SD-CE
47	SS	127	SEP	C-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 59 ligands modelled in this entry, 57 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	$\#\|Z\| > 2$
54	SF4	NM	401	27	0,12,12	-	-	-		
55	GDP	SR	1001	56	29,30,30	3.04	12 (41%)	45,47,47	2.69	17 (37%)

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
54	SF4	NM	401	27	-	-	0/6/5/5
55	GDP	SR	1001	56	-	2/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	SR	1001	GDP	O6-C6	8.80	1.40	1.23
55	SR	1001	GDP	C5-N7	6.53	1.52	1.39
55	SR	1001	GDP	PA-O3A	5.01	1.64	1.59
55	SR	1001	GDP	C2-N2	4.82	1.45	1.34
55	SR	1001	GDP	C8-N9	-4.06	1.28	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	SR	1001	GDP	C8-N9-C4	7.94	120.91	106.03
55	SR	1001	GDP	N9-C4-N3	6.69	139.33	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	SR	1001	GDP	C5-C4-N3	-6.64	117.82	128.39
55	SR	1001	GDP	C2-N3-C4	5.30	121.42	112.30
55	SR	1001	GDP	C6-C5-N7	4.80	139.03	130.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

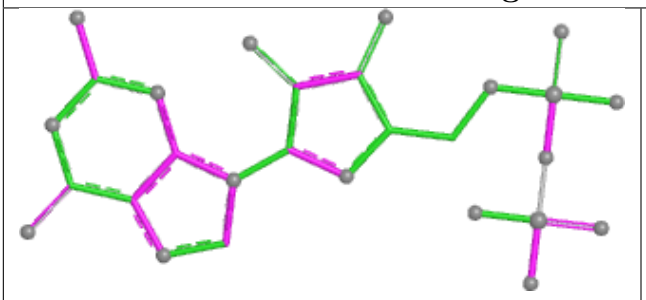
Mol	Chain	Res	Type	Atoms
55	SR	1001	GDP	PA-O3A-PB-O3B
55	SR	1001	GDP	PA-O3A-PB-O2B

There are no ring outliers.

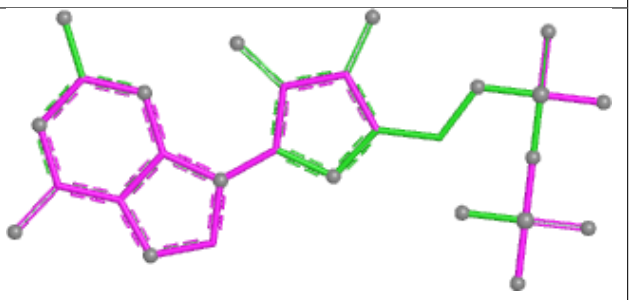
No monomer is involved in short contacts.

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.

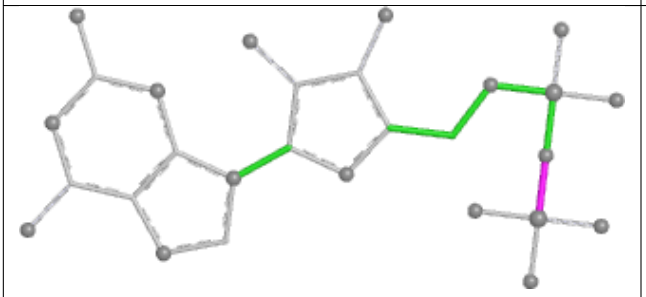
Ligand GDP SR 1001



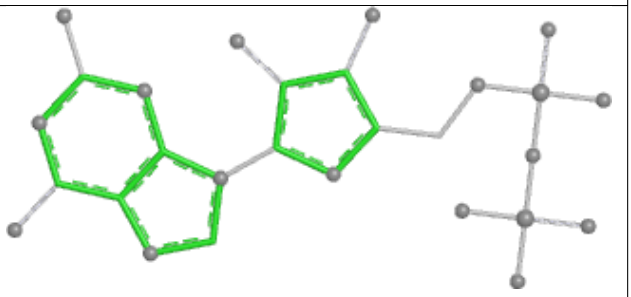
Bond lengths



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.

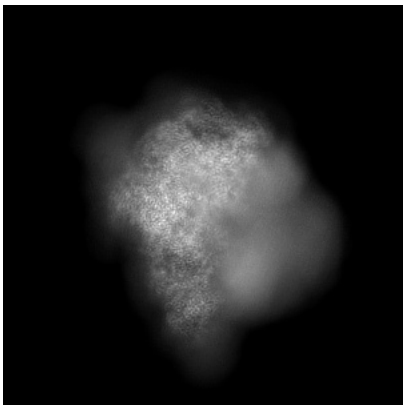
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29254. These allow visual inspection of the internal detail of the map and identification of artifacts.

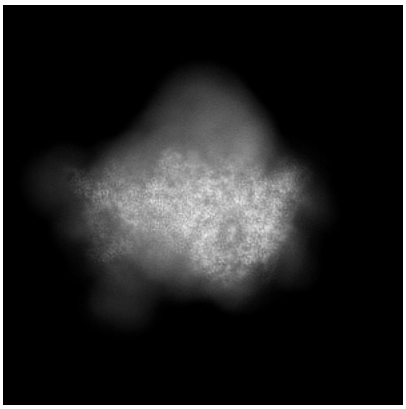
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

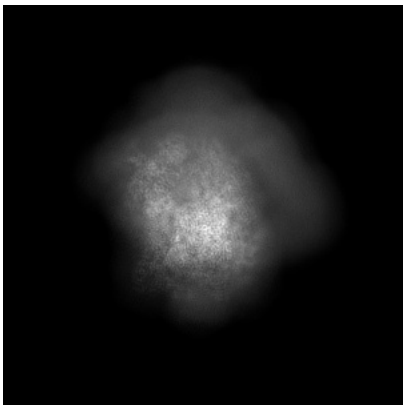
6.1.1 Primary map



X

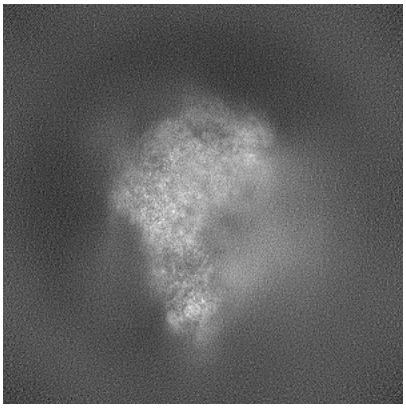


Y

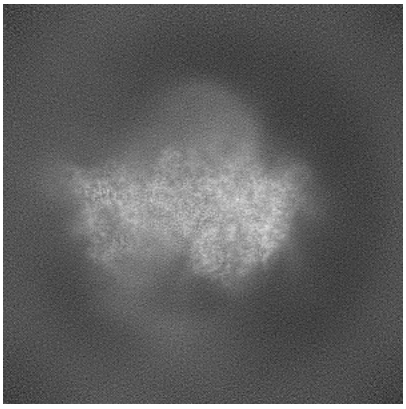


Z

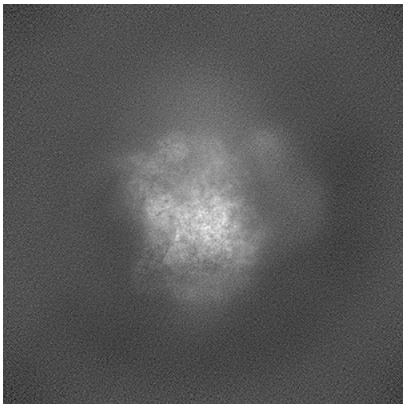
6.1.2 Raw map



X



Y

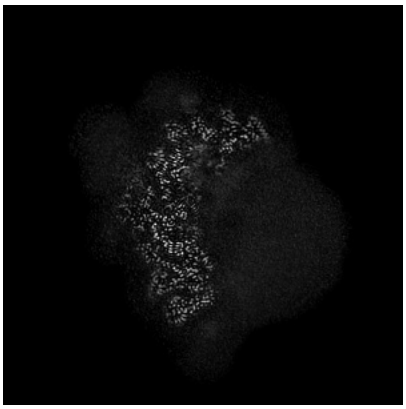


Z

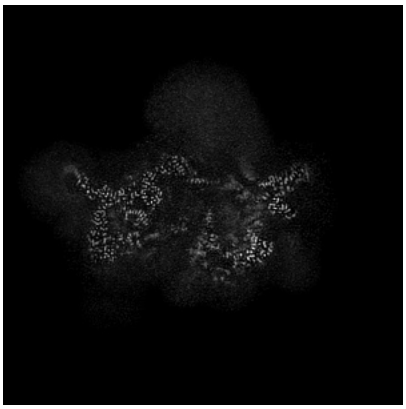
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

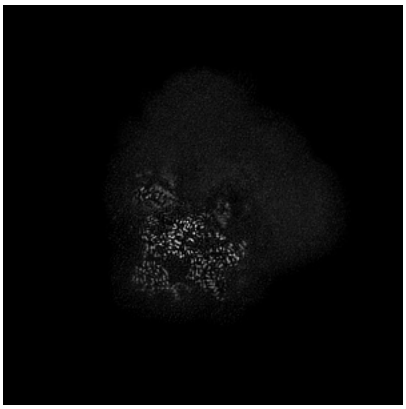
6.2.1 Primary map



X Index: 240

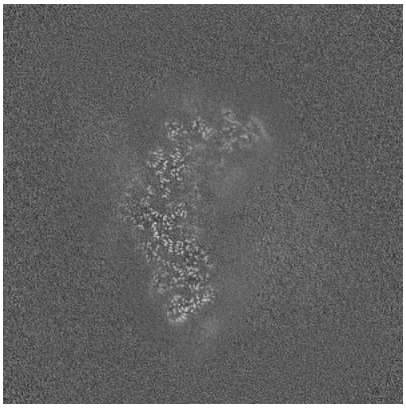


Y Index: 240

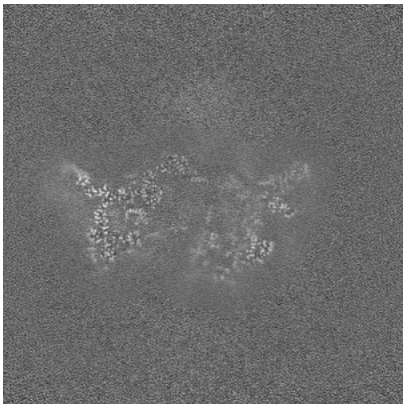


Z Index: 240

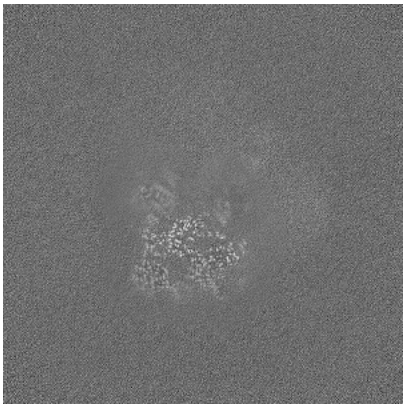
6.2.2 Raw map



X Index: 240



Y Index: 240

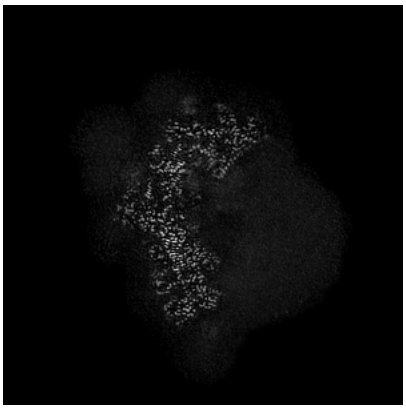


Z Index: 240

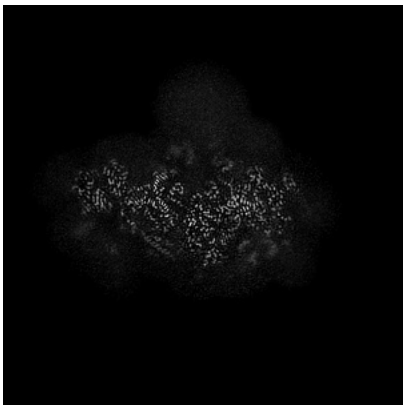
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

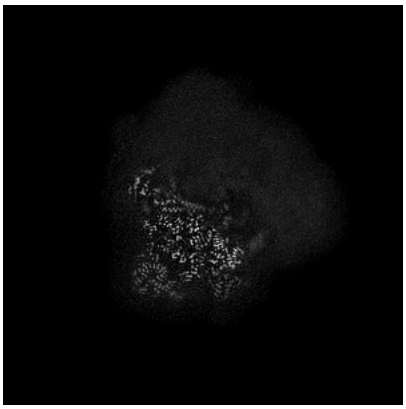
6.3.1 Primary map



X Index: 244

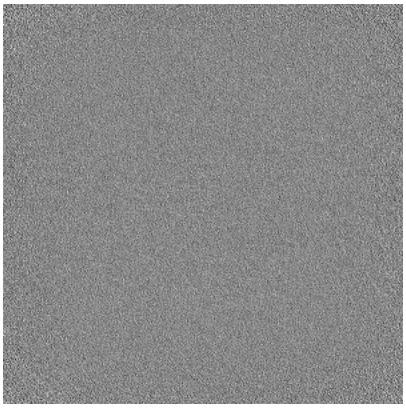


Y Index: 210

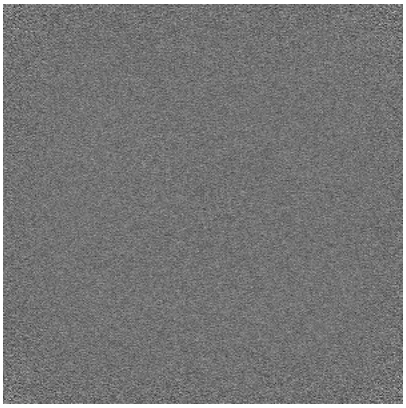


Z Index: 246

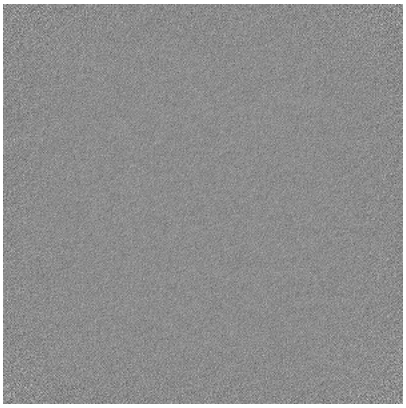
6.3.2 Raw map



X Index: 0



Y Index: 0

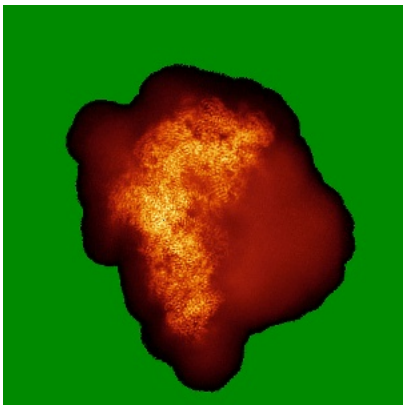


Z Index: 0

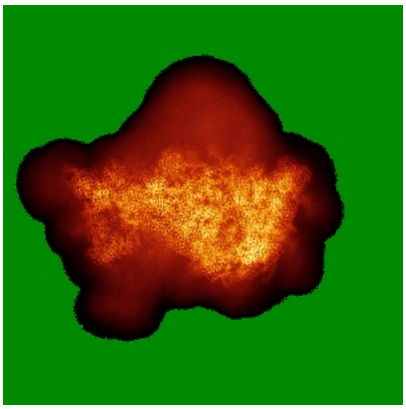
The images above show the largest variance slices of the map in three orthogonal directions.

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

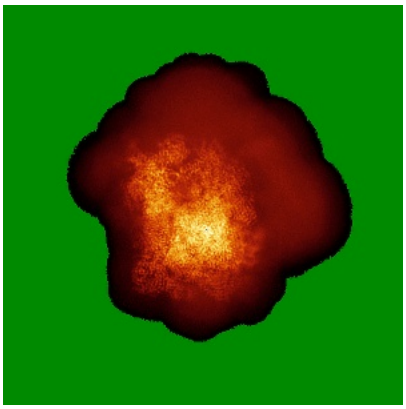
6.4.1 Primary map



X

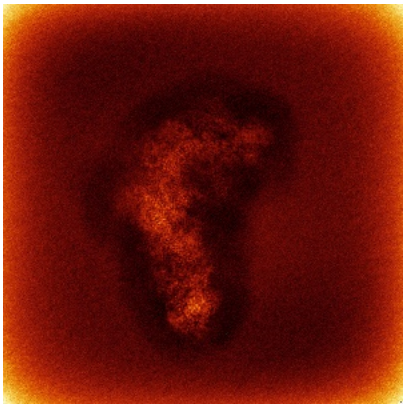


Y

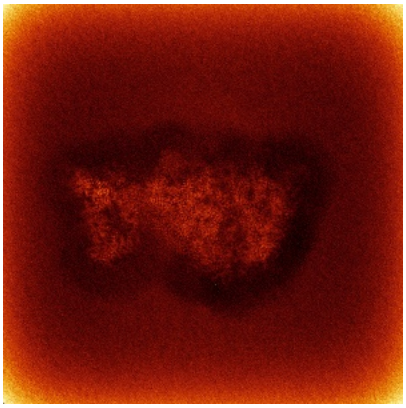


Z

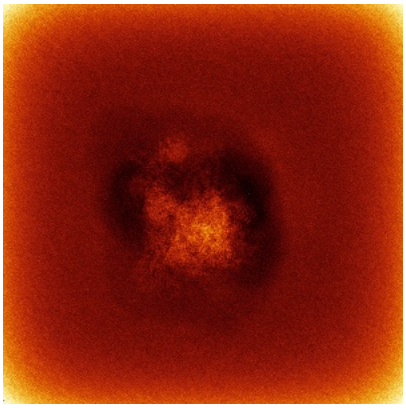
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

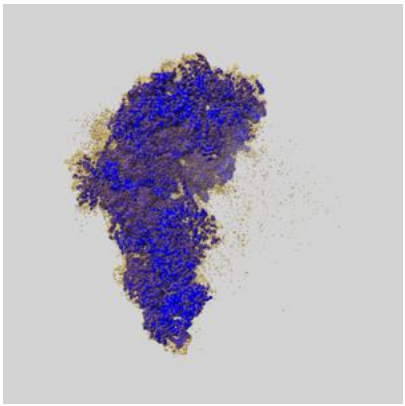
6.6 Mask visualisation

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

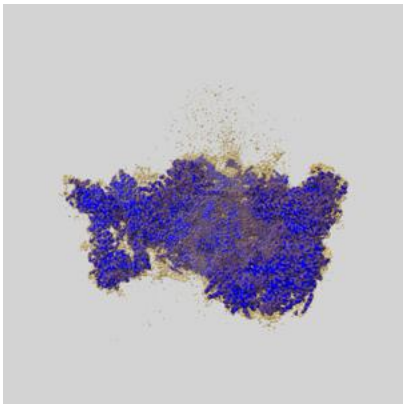
A mask typically either:

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

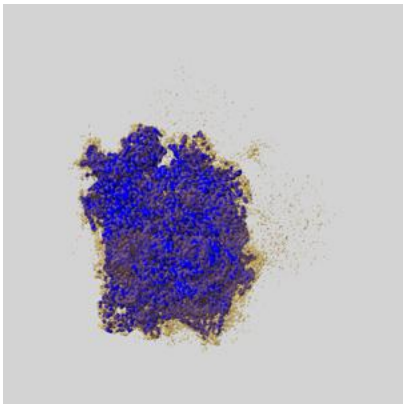
6.6.1 emd_29254_msk_1.map



X



Y

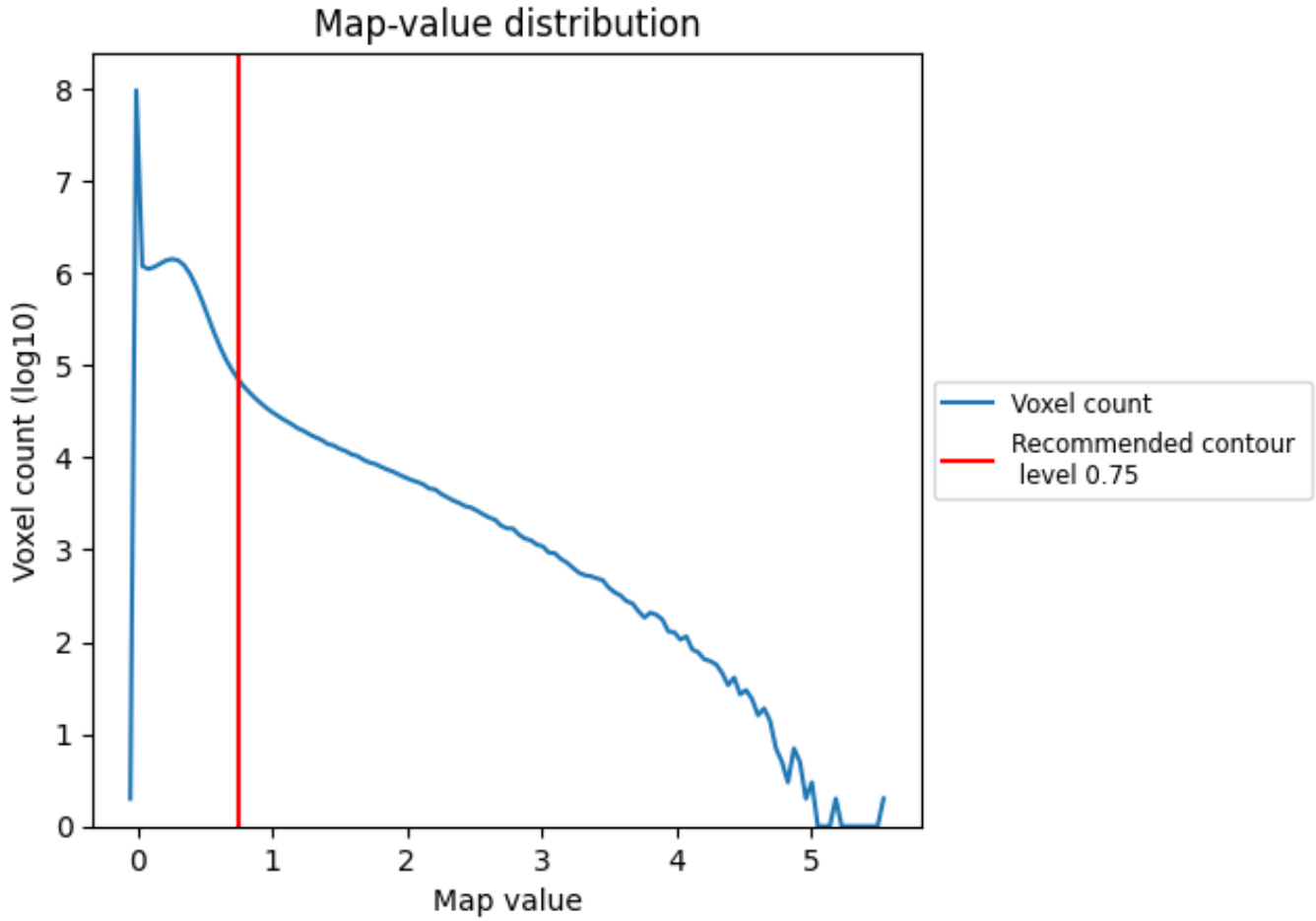


Z

7 Map analysis

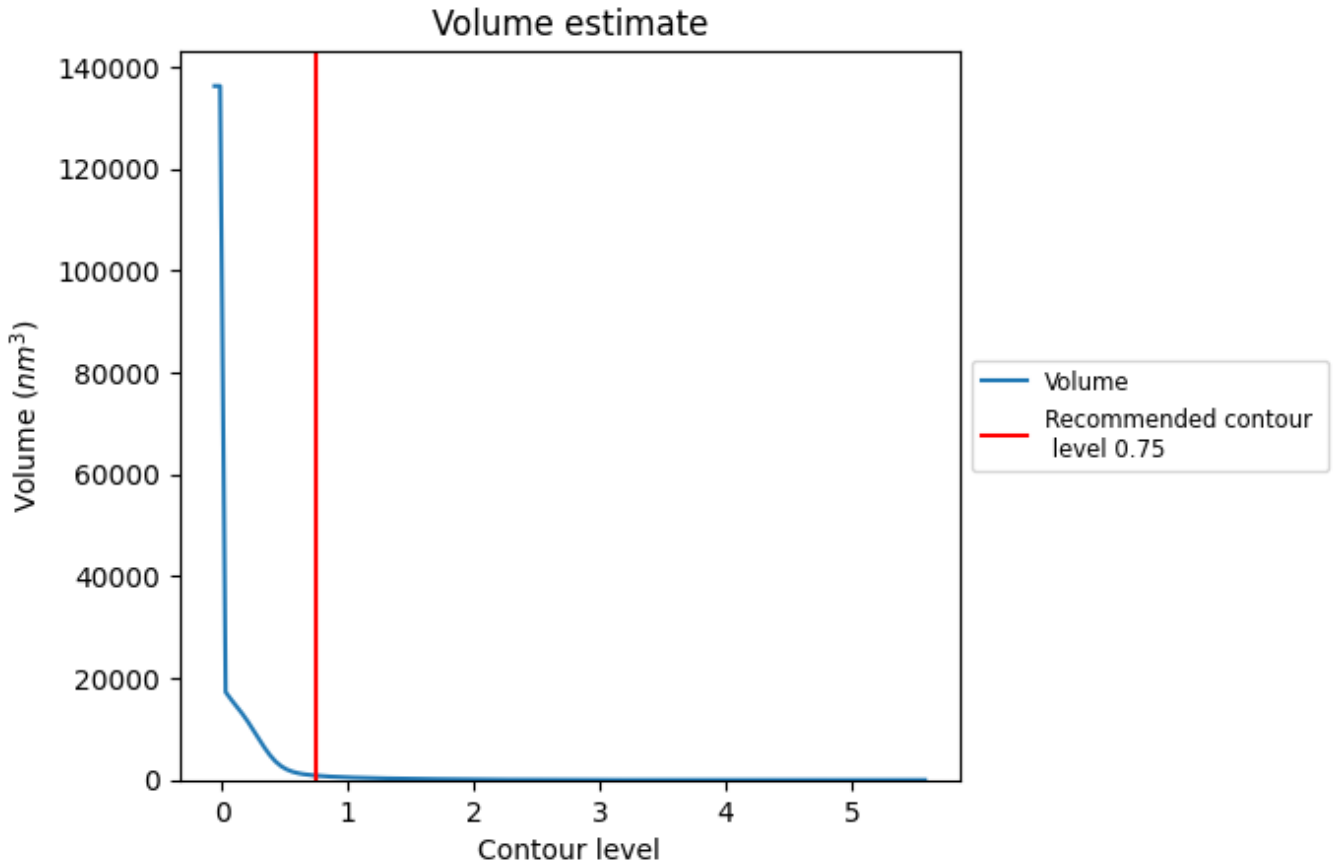
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

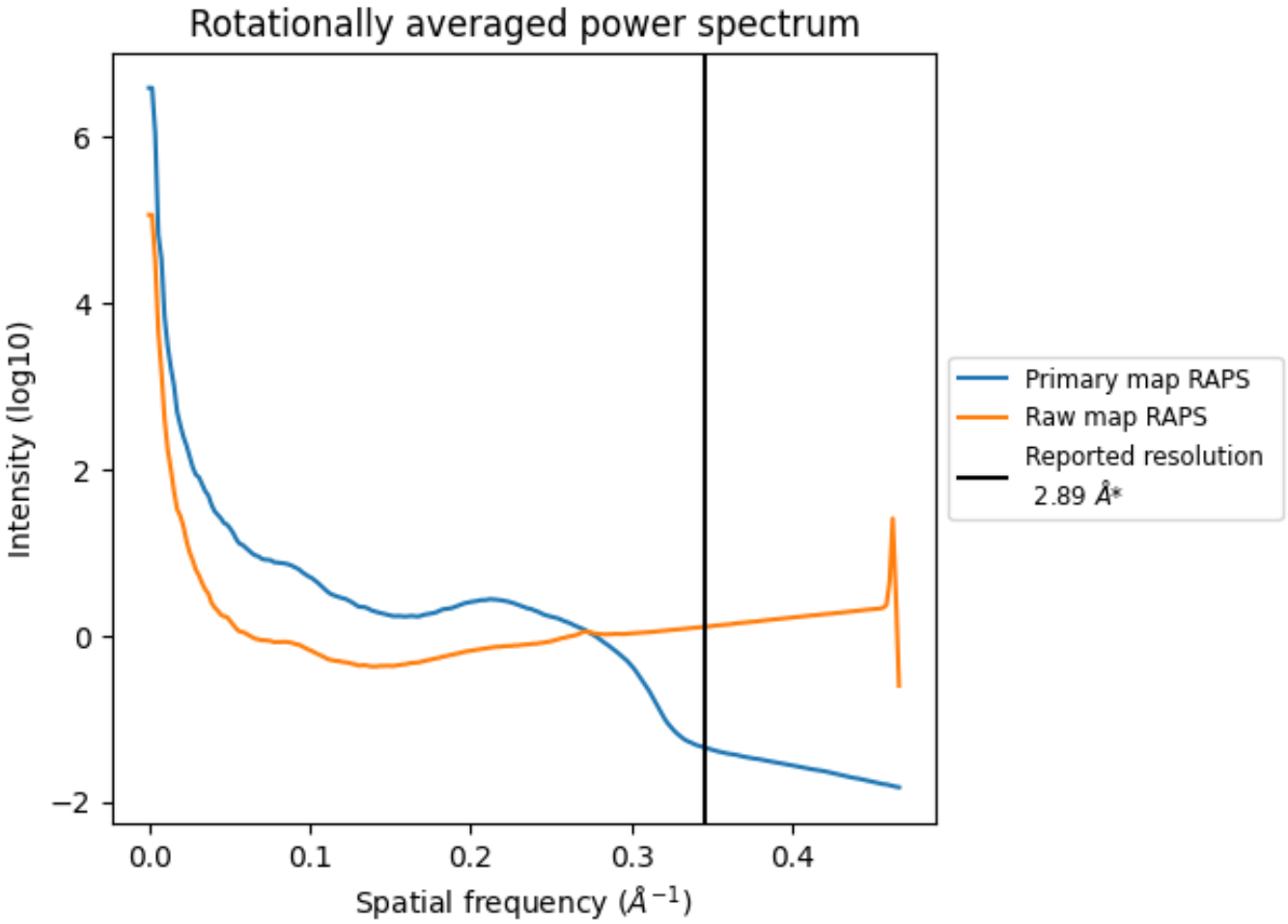
7.2 Volume estimate (i)



The volume at the recommended contour level is 854 nm^3; this corresponds to an approximate mass of 771 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)

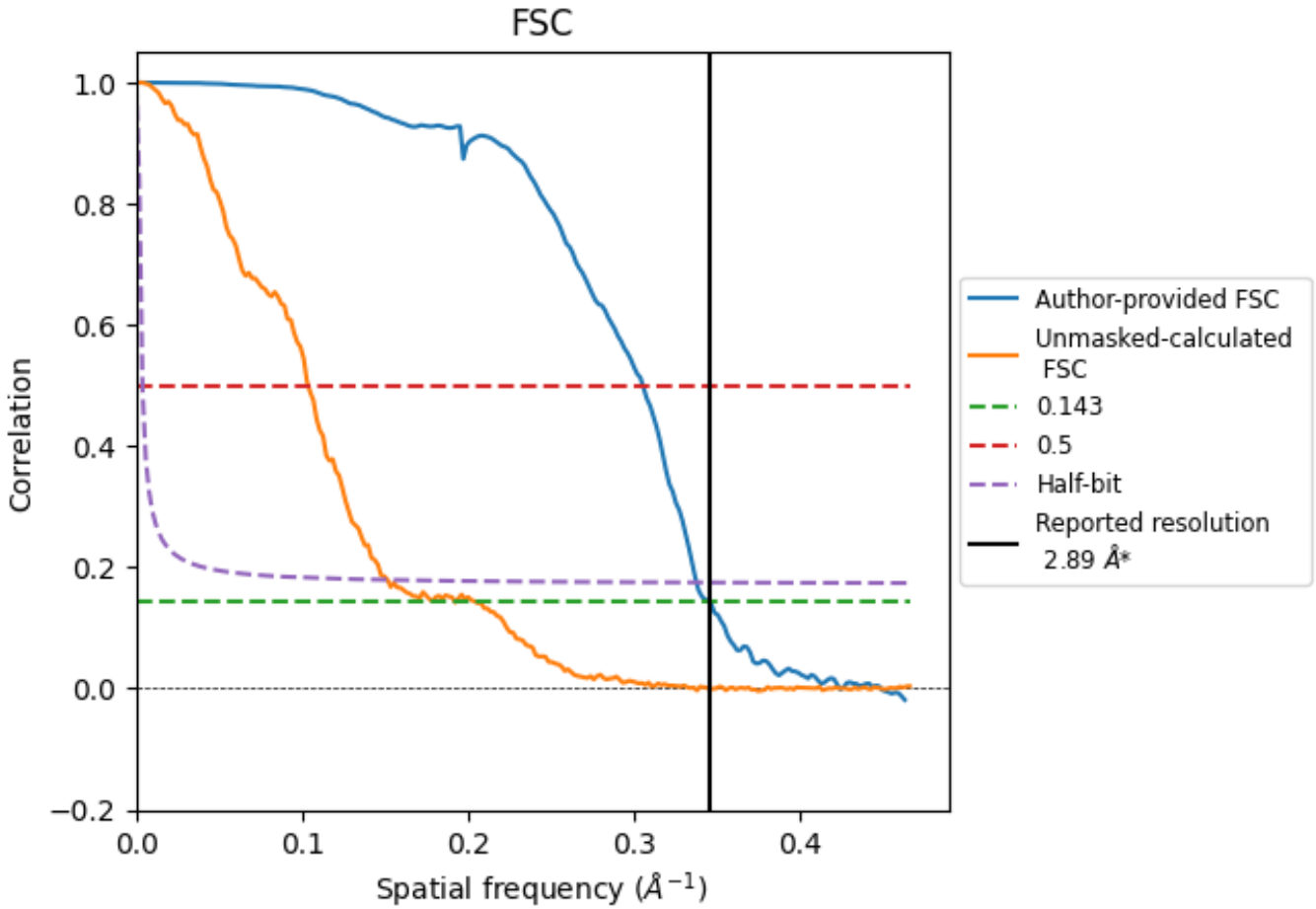


*Reported resolution corresponds to spatial frequency of 0.346 $Å^{-1}$

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 0.346 Å^{-1}

8.2 Resolution estimates (i)

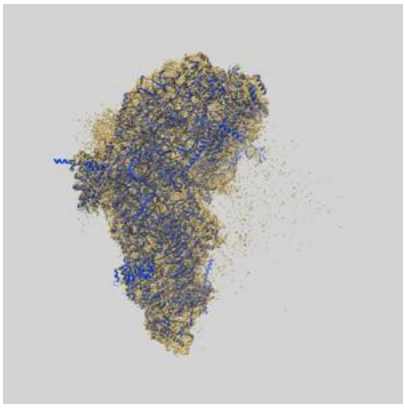
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.27	2.96
Unmasked-calculated*	5.20	9.63	6.60

*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 5.20 differs from the reported value 2.89 by more than 10 %

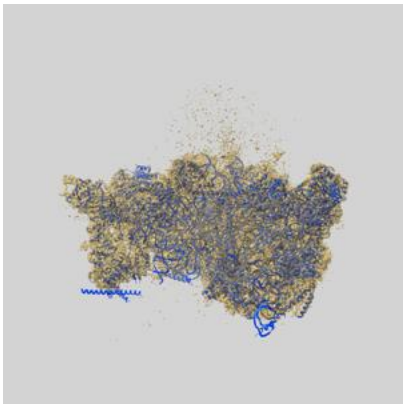
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29254 and PDB model 8FKR. Per-residue inclusion information can be found in section 3 on page 15.

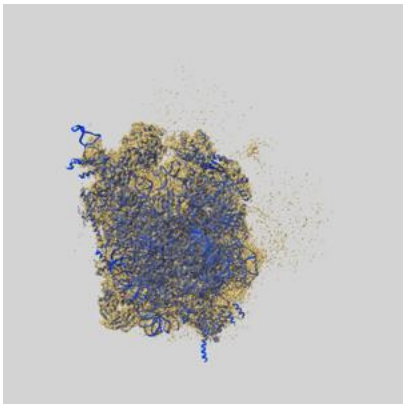
9.1 Map-model overlay



X



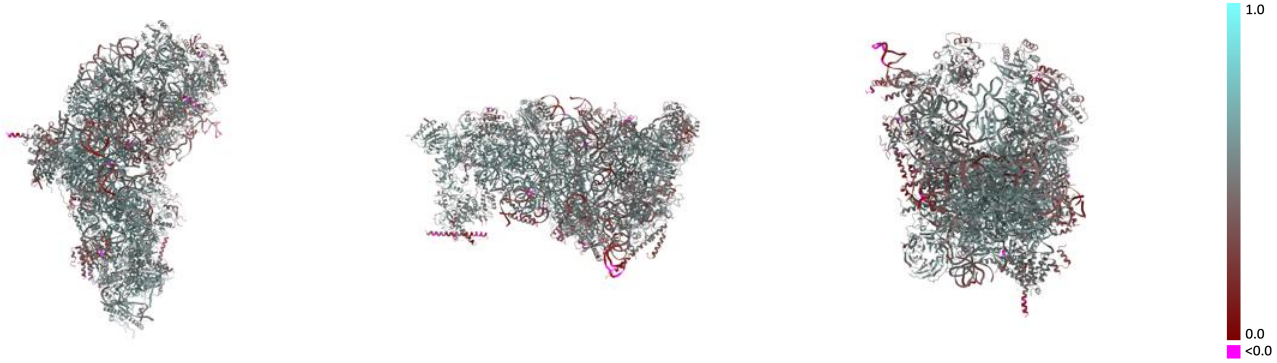
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

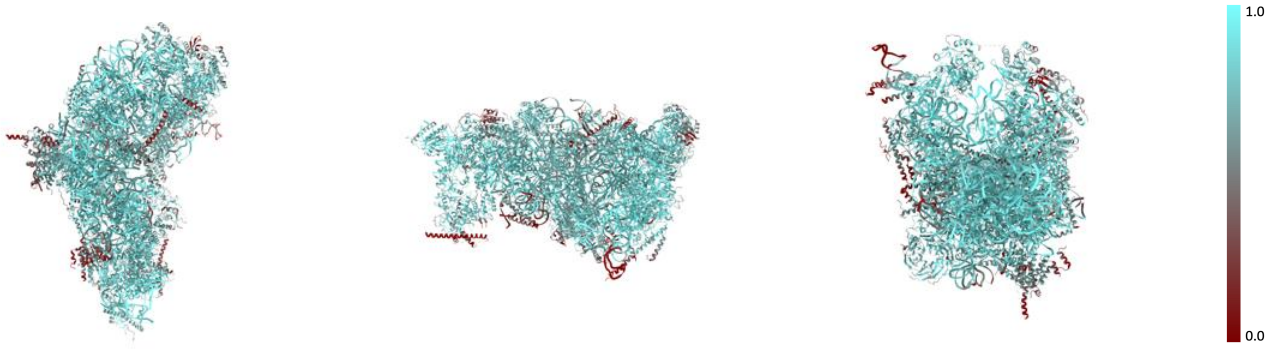
9.2 Q-score mapped to coordinate model



X Y Z

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

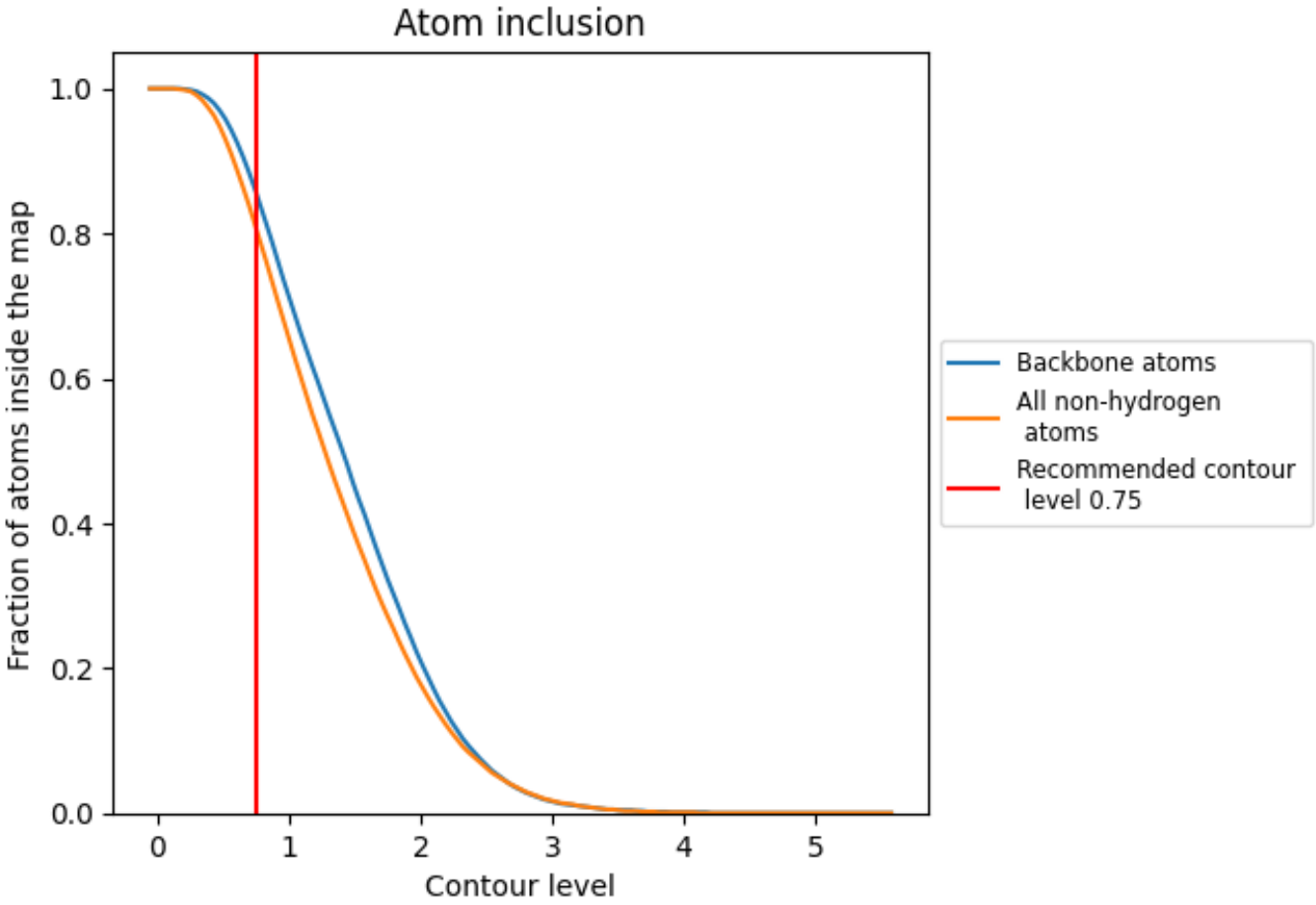
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4970
BA	0.5140	0.3850
L1	0.7150	0.4510
L2	0.9230	0.5290
L3	0.8940	0.4950
L6	0.9410	0.5820
L7	0.9080	0.4910
L8	0.8880	0.5240
L9	0.9290	0.5930
LA	0.7240	0.5020
LB	0.9340	0.5890
LC	0.9100	0.5410
LE	0.5920	0.3610
LG	0.8010	0.4420
LH	0.4140	0.4380
LI	0.8620	0.5680
LK	0.8000	0.4320
LN	0.8920	0.5160
LQ	0.9220	0.5870
LS	0.5900	0.4610
LT	0.9500	0.5850
LU	0.8020	0.5380
LW	0.6910	0.5110
NB	0.1820	0.3150
NE	0.6060	0.3710
NF	0.6180	0.4500
NG	0.3720	0.2560
NM	0.8250	0.5550
NN	0.7760	0.4480
NO	0.6240	0.4760
NQ	0.7660	0.5120
NS	0.7850	0.5340
SA	0.9020	0.5740
SC	0.7320	0.5160
SD	0.8870	0.5560

Continued on next page...

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Chain	Atom inclusion	Q-score
SE	0.8880	0.5570
SG	0.8340	0.5480
SH	0.8420	0.5450
SI	0.7860	0.5290
SJ	0.6070	0.4740
SK	0.8370	0.4540
SL	0.8050	0.5360
SM	0.6900	0.4680
SN	0.5610	0.4170
SO	0.7900	0.5260
SQ	0.7280	0.4950
SR	0.7440	0.4760
SS	0.7160	0.4750
ST	0.6220	0.4490
SV	0.6870	0.4160
SW	0.5950	0.4430
SZ	0.8110	0.5160