



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 9, 2019 – 07:33 PM EST

PDB ID : 6C0F
EMDB ID: : EMD-7324
Title : Yeast nucleolar pre-60S ribosomal subunit (state 2)
Authors : Sanghai, Z.A.; Miller, L.; Barandun, J.; Hunziker, M.; Chaker-Margot, M.;
Klinge, S.
Deposited on : 2017-12-29
Resolution : 3.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

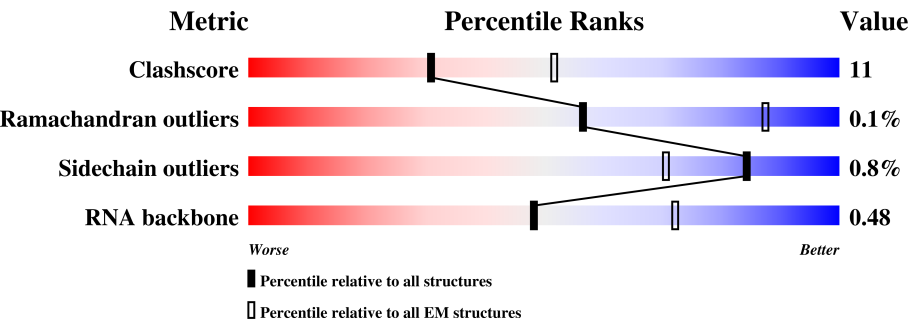
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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.

















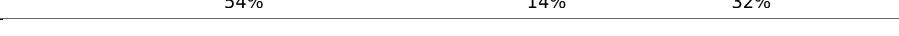
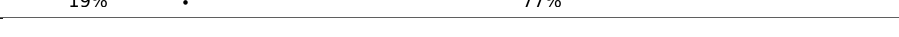
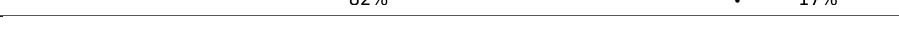

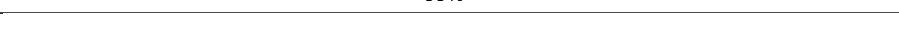



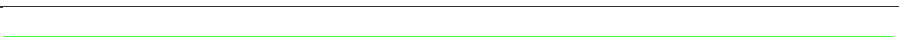


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	1	3395	<div><div>17%17%5%.</div><div>60%</div></div>
2	2	158	<div><div>50%41%8%.</div><div></div></div>
3	6	232	<div><div>12%14%9%.</div><div>62%</div></div>
4	A	463	<div><div>59%26%15%</div><div></div></div>
5	B	387	<div><div>60%24%16%</div><div></div></div>
6	C	362	<div><div>69%17%13%</div><div></div></div>
7	D	306	<div><div>42%19%38%</div><div></div></div>
8	E	176	<div><div>70%26%.</div><div></div></div>



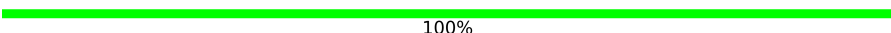







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Mol	Chain	Length	Quality of chain
9	F	244	
10	G	256	
11	I	295	
12	K	376	
13	L	199	
14	M	138	
15	N	204	
16	O	199	
17	P	184	
18	Q	186	
19	S	172	
20	V	137	
21	W	647	
22	Y	127	
23	7	231	
24	8	434	
25	b	291	
26	e	130	
27	f	107	
28	h	120	
29	i	100	
30	j	88	
31	x	28	
32	m	74	
33	n	605	

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Mol	Chain	Length	Quality of chain
34	o	220	 60%40%
35	p	505	 86%13%
36	q	285	 100%
37	s	807	 19%81%
38	t	322	 75%23%
39	u	199	 63%35%
40	v	453	 49%50%
41	w	250	 28%72%
42	y	245	 92%8%
43	z	278	 87%13%

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 91742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* S288c 35S pre-ribosomal RNA miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1357	Total	C	N	O	P	0	0
			29055	12970	5242	9486	1357		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	U	deletion	GB 259147931

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	87	Total	C	N	O	P	0	0
			1838	823	309	619	87		

- Molecule 4 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	394	Total	C	N	O	S	0	0
			3126	1997	525	593	11		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	324	Total	C	N	O	S	0	0
			2577	1635	478	458	6		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	314	Total	C	N	O	S	0	0
			2418	1531	454	430	3		

- Molecule 7 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	190	Total	C	N	O	S	0	0
			1578	996	297	275	10		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	170	Total	C	N	O	S	0	0
			1366	882	244	239	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	242	Total	C	N	O	S	0	0
			1941	1249	352	339	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	187	Total	C	N	O	S	0	0
			1453	934	253	264	2		

- Molecule 11 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	288	Total	C	N	O	S	0	0
			2429	1544	439	442	4		

- Molecule 12 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	260	Total	C	N	O	S	0	0
			2099	1352	346	398	3		

- Molecule 13 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	106	Total	C	N	O	0	0
			845	531	174	140		

- Molecule 14 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	128	Total	C	N	O	S	0
			997	641	190	164	2	0

- Molecule 15 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	N	176	Total	C	N	O	S	0
			1509	946	319	243	1	0

- Molecule 16 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	184	Total	C	N	O	S	0
			1451	936	268	246	1	0

- Molecule 17 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	124	Total	C	N	O	0	0
			975	612	184	179		

- Molecule 18 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	132	Total	C	N	O	S	0
			1015	648	191	175	1	0

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	171	Total	C	N	O	S	0
			1437	925	266	243	3	0

- Molecule 20 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	122	Total	C	N	O	S	0	0
			903	567	169	160	7		

- Molecule 21 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	98	Total	C	N	O	S	0	0
			806	509	132	164	1		

- Molecule 22 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 23 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7	156	Total	C	N	O	S	0	0
			1295	813	250	228	4		

- Molecule 24 is a protein called Ribosomal RNA-processing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	8	98	Total	C	N	O	S	0	0
			836	515	165	154	2		

- Molecule 25 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	242	Total	C	N	O	S	0	0
			1919	1221	344	350	4		

- Molecule 26 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	114	Total	C	N	O	S	0	0
			914	580	181	152	1		

- Molecule 27 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 28 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	84	Total	C	N	O	S	0	0
			665	413	136	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	72	Total	C	N	O	S	0	0
			575	350	125	95	5		

- Molecule 31 is a protein called Brx1-associated peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	x	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 32 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	m	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 33 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	341	Total	C	N	O	S	0	0
			2794	1823	470	492	9		

- Molecule 34 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 35 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	437	Total	C	N	O	S	0	0
			3486	2247	600	627	12		

- Molecule 36 is a protein called Protein MAK11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	285	Total	C	N	O	S	0	0
			1409	839	285	285			

- Molecule 37 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	157	Total	C	N	O	S	0	0
			1069	672	203	191	3		

- Molecule 38 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	248	Total	C	N	O	S	0	0
			1965	1254	350	358	3		

- Molecule 39 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	129	Total	C	N	O	S	0	0
			1088	682	220	178	8		

- Molecule 40 is a protein called Ribosome biogenesis protein SSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	225	Total	C	N	O	S	0	0
			1795	1142	320	324	9		

- Molecule 41 is a protein called Ribosomal RNA-processing protein 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	w	70	Total	C	N	O	0	0
			562	357	96	109		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	226	Total	C	N	O	S	0	0
			1709	1060	296	346	7		

- Molecule 43 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	z	243	Total	C	N	O	S	0	0
			2058	1334	353	366	5		

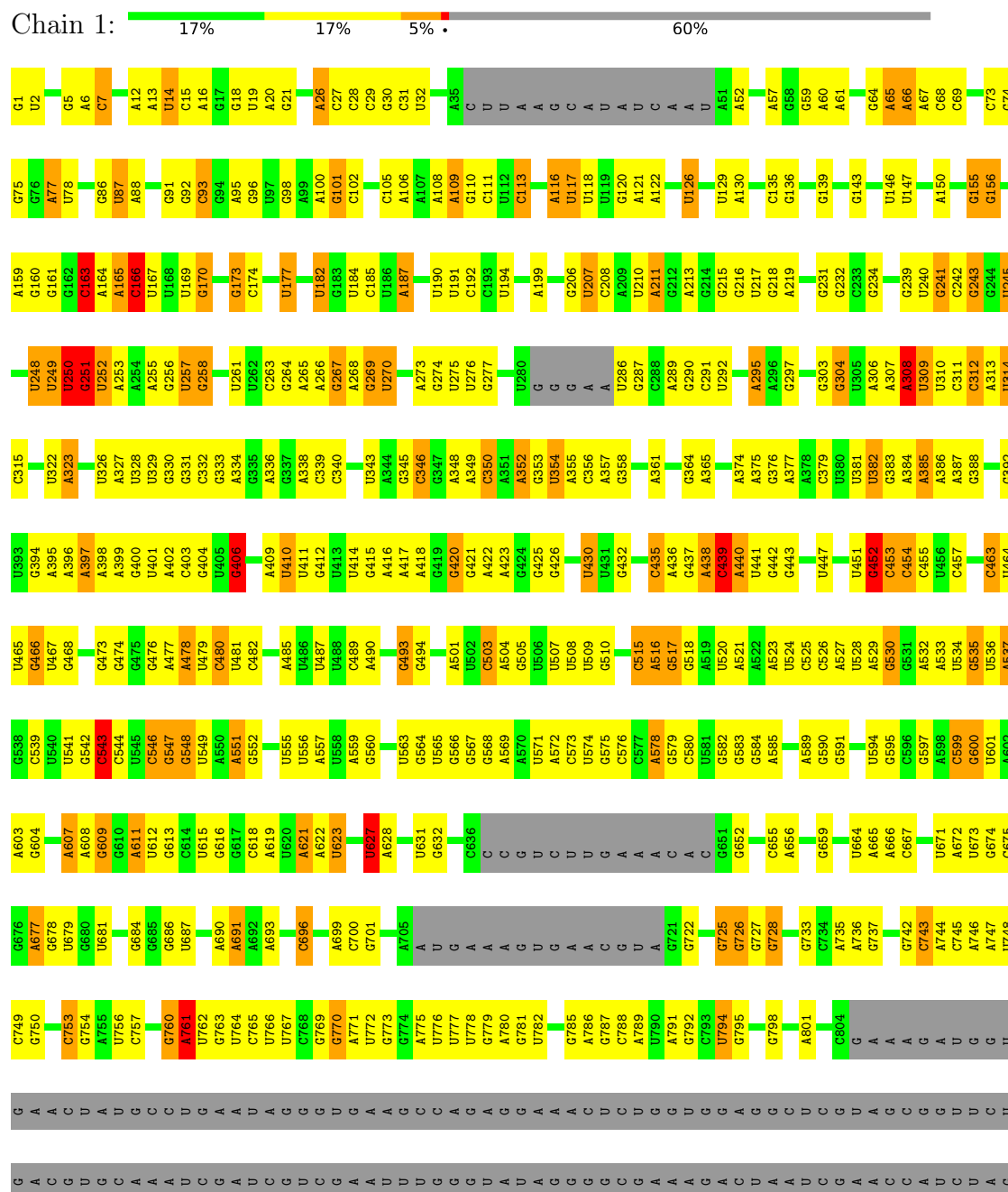
- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

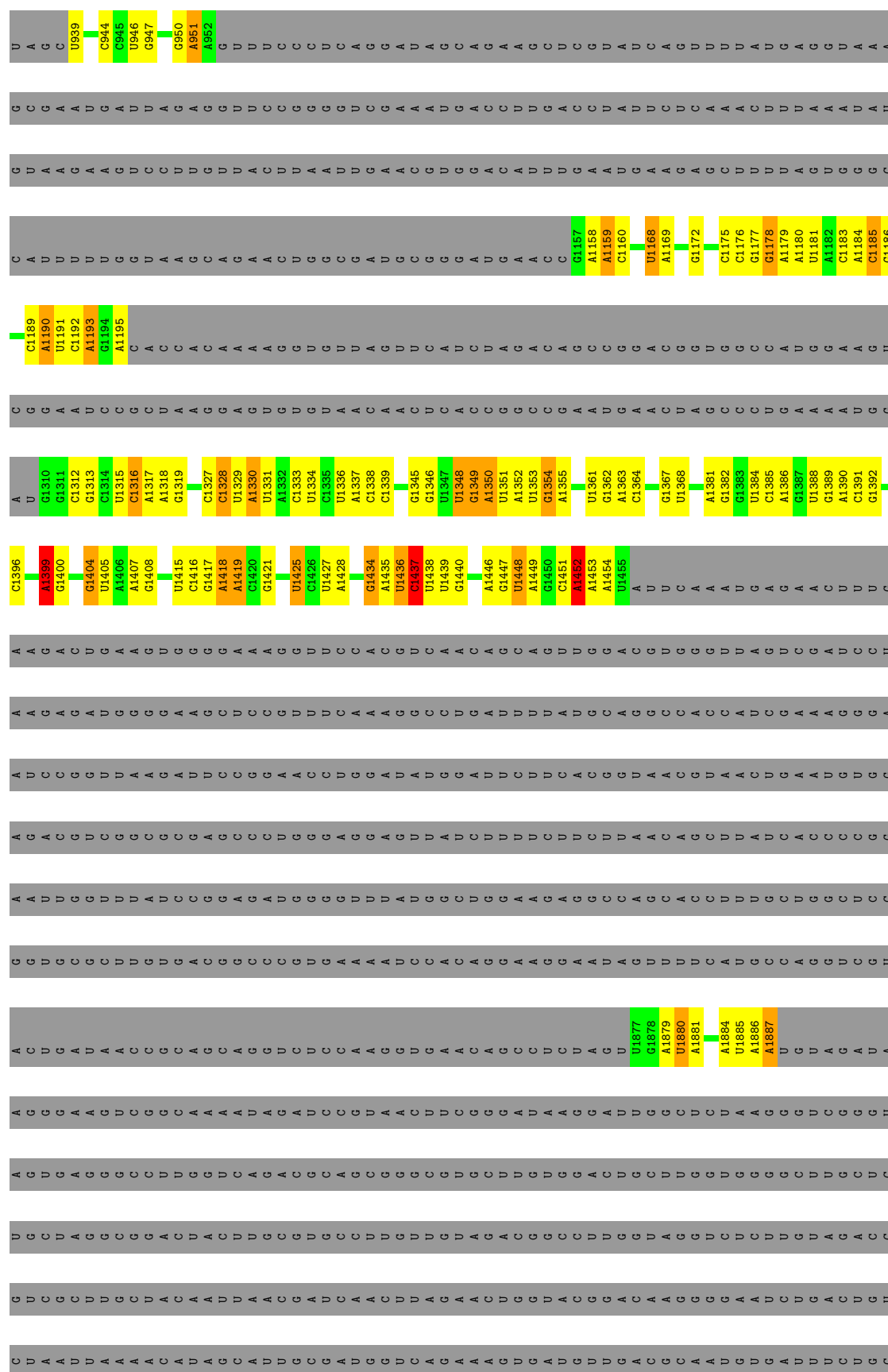
Mol	Chain	Residues	Atoms		AltConf
44	j	1	Total	Zn	0
			1	1	
44	D	1	Total	Zn	0
			1	1	
44	u	1	Total	Zn	0
			1	1	

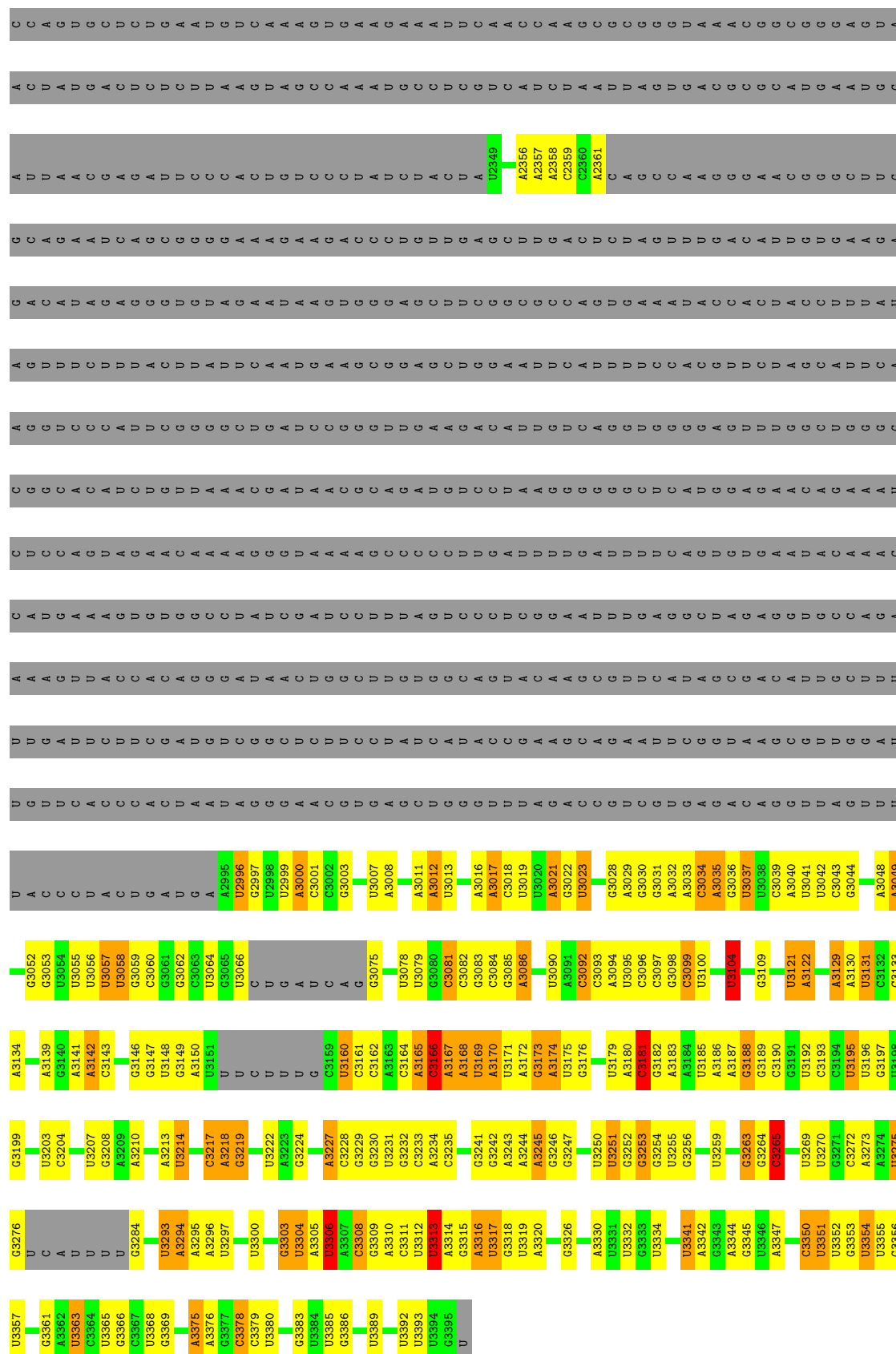
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

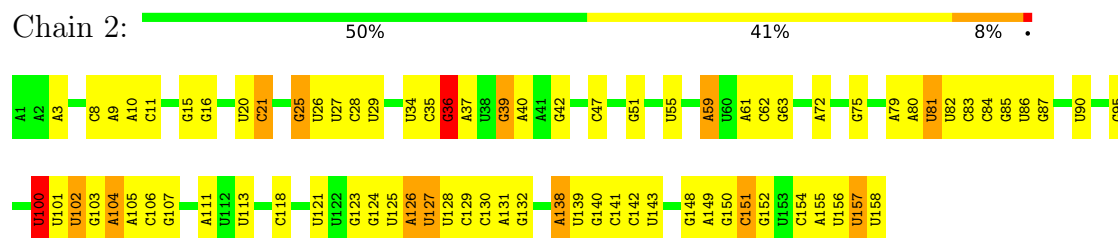
- Molecule 1: *Saccharomyces cerevisiae* S288c 35S pre-ribosomal RNA miscRNA



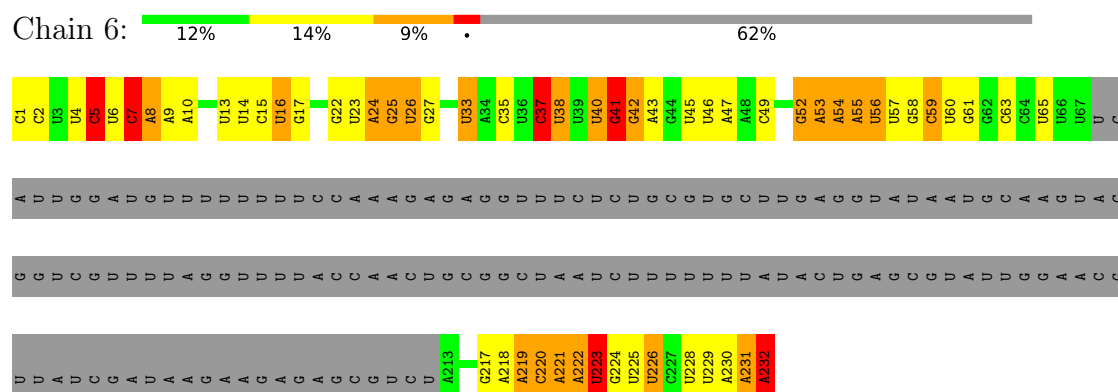




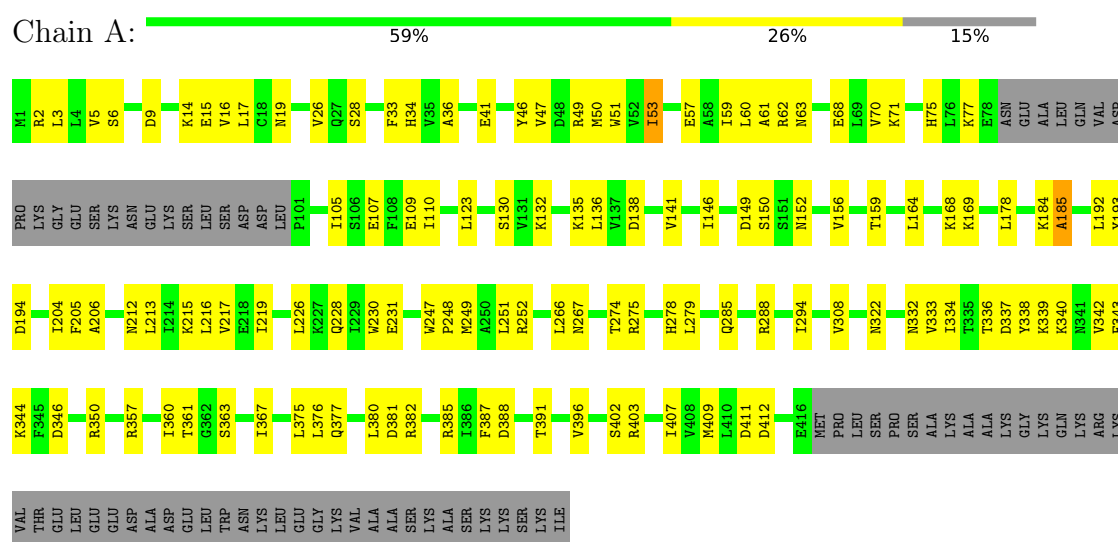
- Molecule 2: 5.8S rRNA



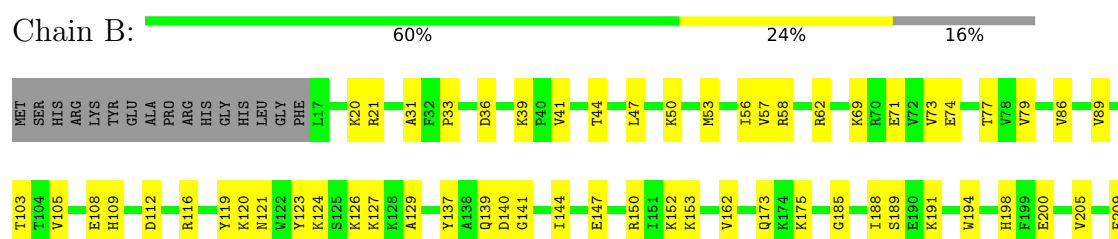
• Molecule 3: ITS2

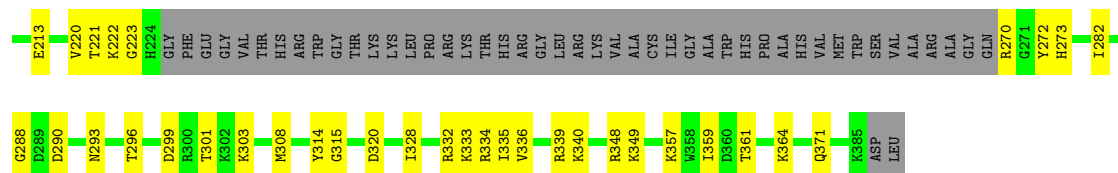


• Molecule 4: Ribosome biogenesis protein NSA1

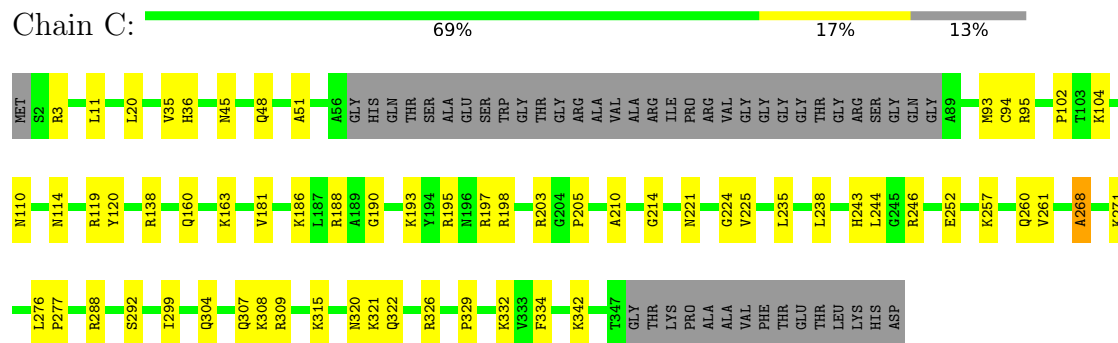


• Molecule 5: 60S ribosomal protein L3

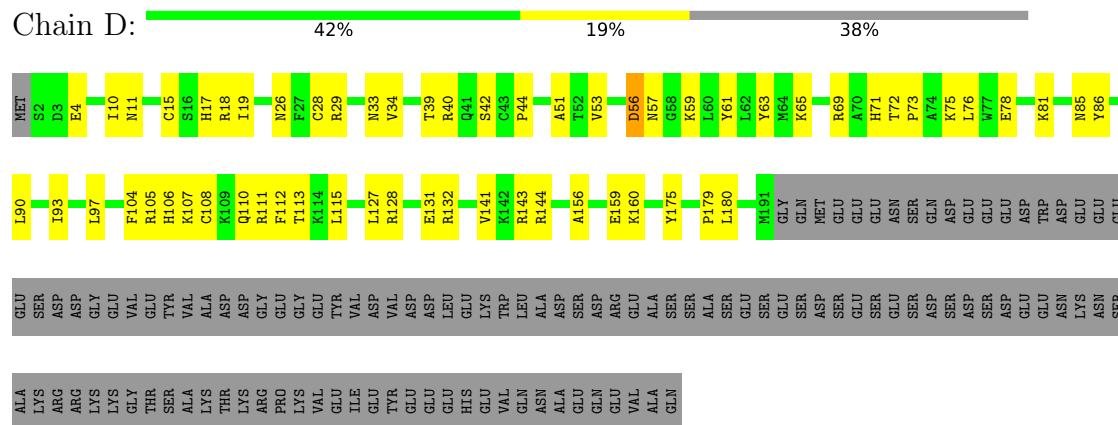




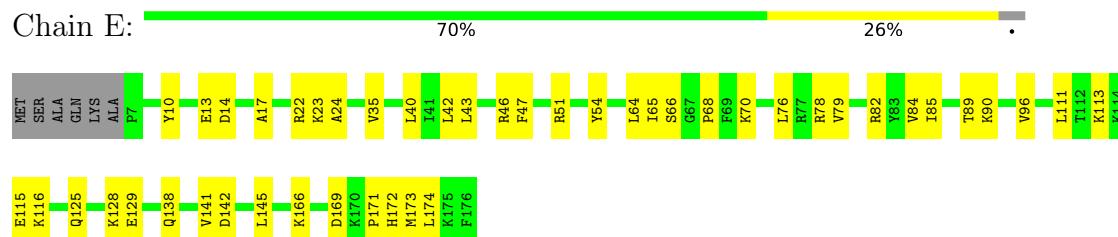
• Molecule 6: 60S ribosomal protein L4-A



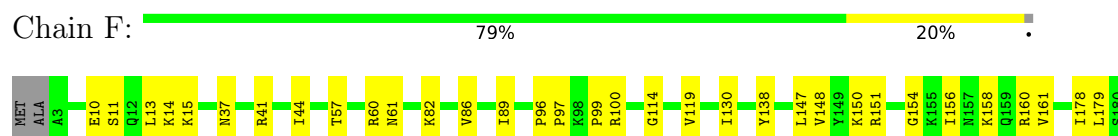
• Molecule 7: Protein MAK16

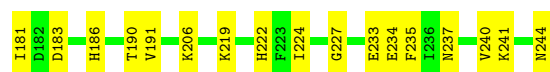


• Molecule 8: 60S ribosomal protein L6-A



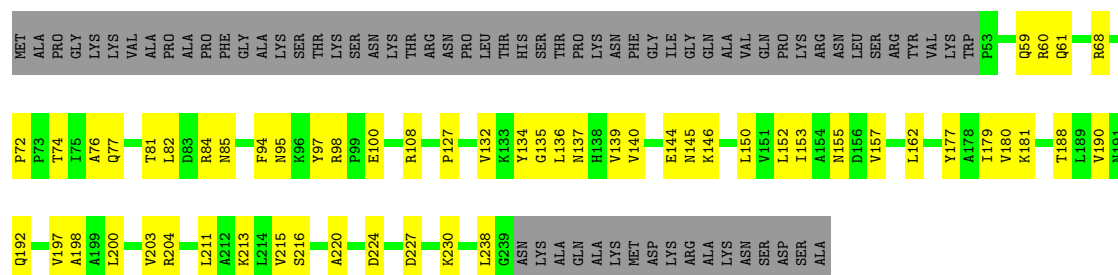
• Molecule 9: 60S ribosomal protein L7-A





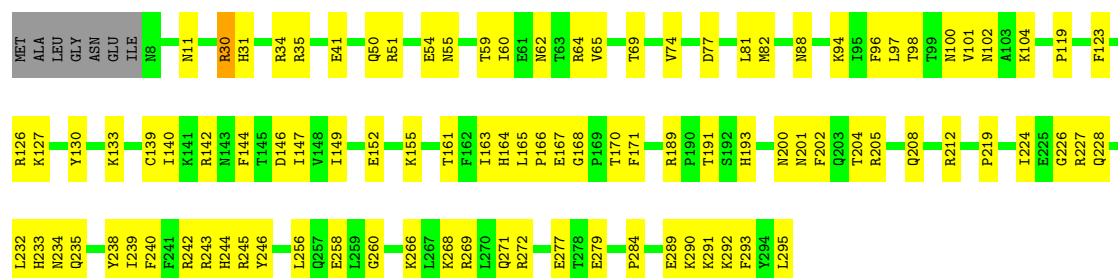
• Molecule 10: 60S ribosomal protein L8-A

Chain G: 51% 22% 27%



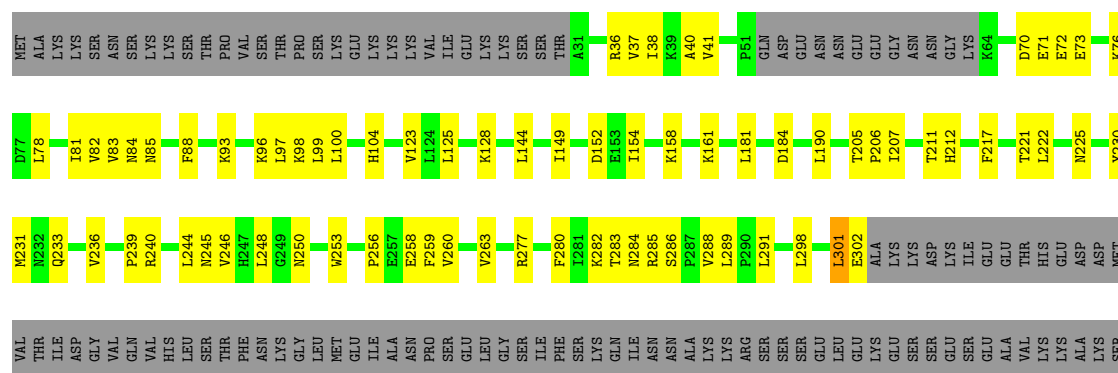
• Molecule 11: Ribosome production factor 1

Chain I: 65% 33%



• Molecule 12: Proteasome-interacting protein CIC1

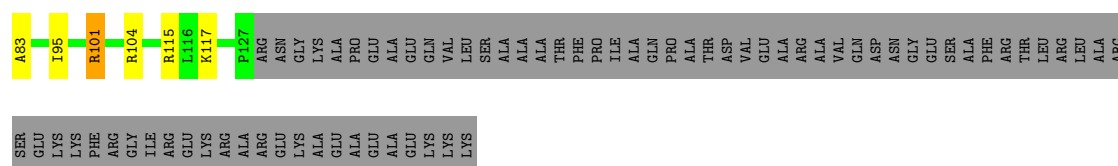
Chain K: 49% 20% 31%



• Molecule 13: 60S ribosomal protein L13-A

Chain L: 38% 14% 47%





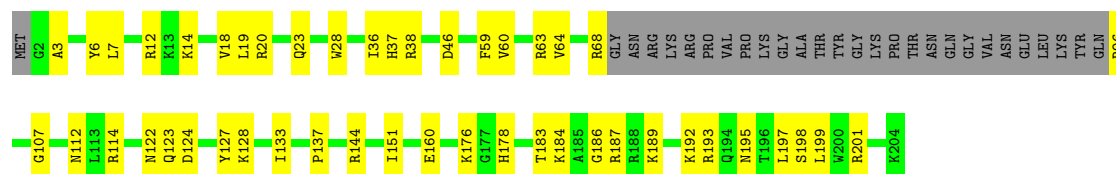
- Molecule 14: 60S ribosomal protein L14-A

Chain M: 75% 17% 7%



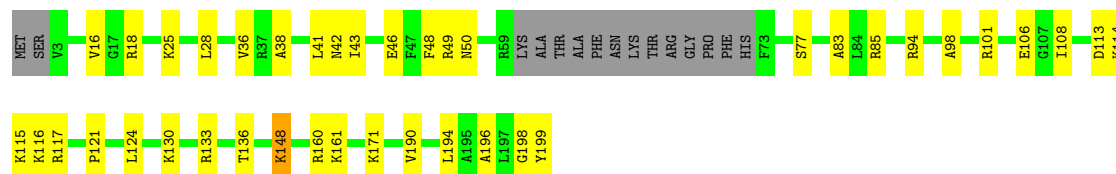
- Molecule 15: 60S ribosomal protein L15-A

Chain N: 63% 23% 14%



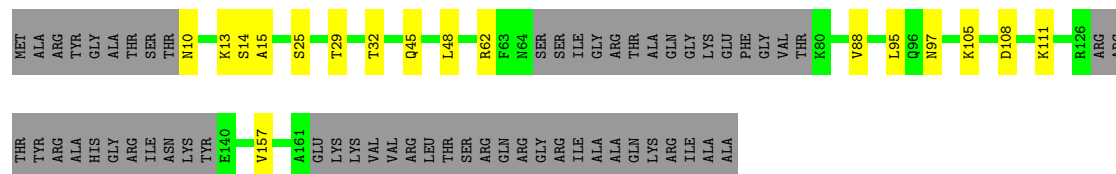
- Molecule 16: 60S ribosomal protein L16-A

Chain O: 72% 20% 8%



- Molecule 17: 60S ribosomal protein L17-A

Chain P: 58% 9% 33%



- Molecule 18: 60S ribosomal protein L18-A

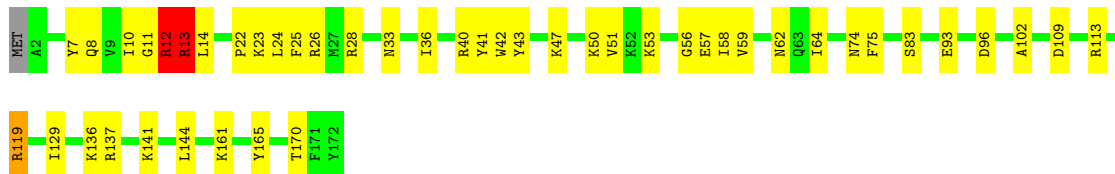
Chain Q: 61% 10% 29%



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

- Molecule 19: 60S ribosomal protein L20-A

Chain S: 73% 25% ...



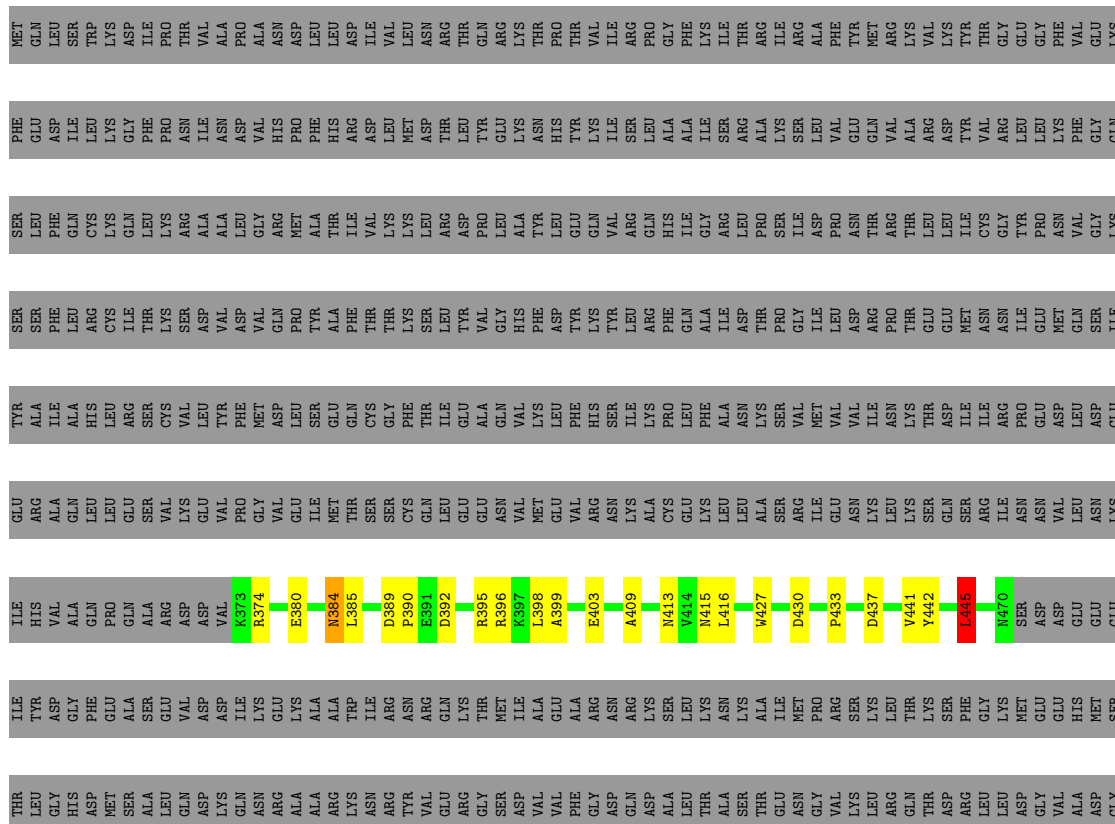
- Molecule 20: 60S ribosomal protein L23-A

Chain V:  67% 22% 11%



- Molecule 21: Nucleolar GTP-binding protein 1

Chain W:  12% . 85%



SER	MET	SER	LYS	ALA	ASP	ARG	MET	ALA	LYS	GLU	ARG	ARG	ASN	ASN	HIS	ALA	LYS	GLN	GLY	GLU	SER	SER	ASP	ARG	HIS	ASN	ALA	VAL	SER	SER	LEU	HIS	LEU	PHE	SER	GLY	LYS	GLY	VAL	LYS	LYS	THR	ASP	PHE	ARG
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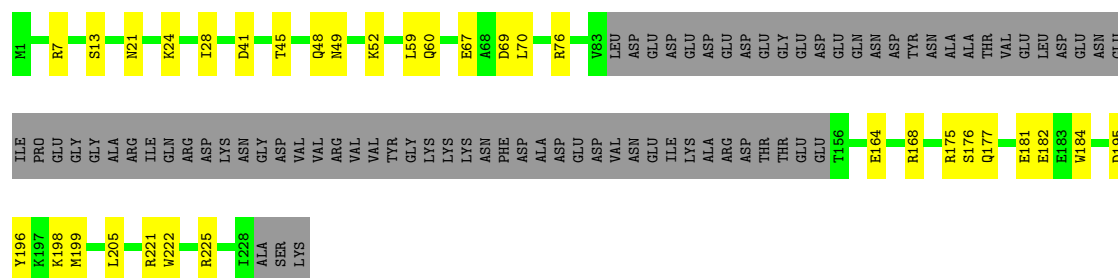
- Molecule 22: 60S ribosomal protein L26-A

Chain Y: 81% 18%



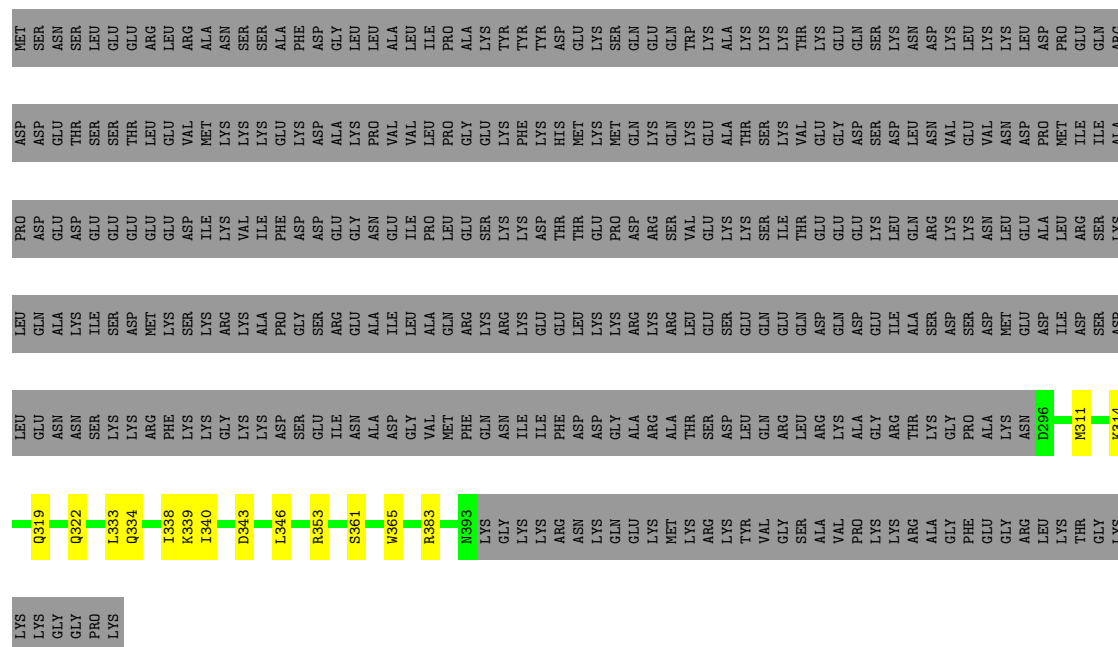
- Molecule 23: Nucleolar protein 16

Chain 7:  54% 14% 32%

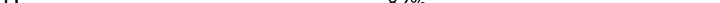


- Molecule 24: Ribosomal RNA-processing protein 14

Chain 8:  19% . 77%



- Molecule 25: Ribosome biogenesis protein BRX1

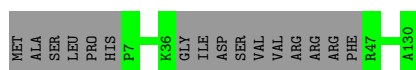
Chain b:  82% . 17%



LYS

- Molecule 26: 60S ribosomal protein L32

Chain e: 88% 12%



- Molecule 27: 60S ribosomal protein L33-A

Chain f: 99% .



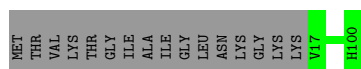
- Molecule 28: 60S ribosomal protein L35-A

Chain h: 97% ..



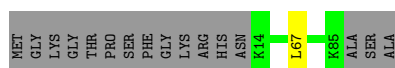
- Molecule 29: 60S ribosomal protein L36-A

Chain i: 84% 16%



- Molecule 30: 60S ribosomal protein L37-A

Chain j: 81% . 18%



- Molecule 31: Brx1-associated peptide

Chain x: 100%

There are no outlier residues recorded for this chain.

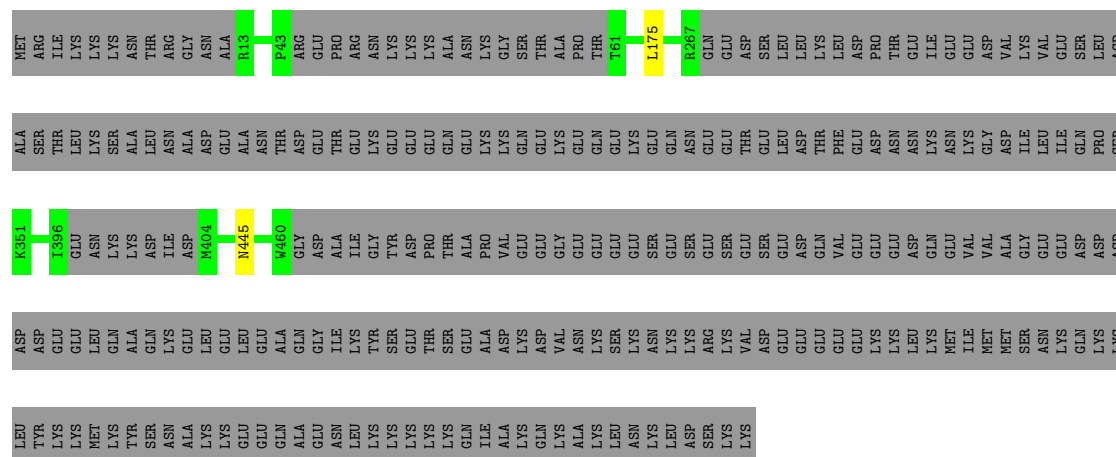
- Molecule 32: rRNA-processing protein EBP2

Chain m: 100%

There are no outlier residues recorded for this chain.

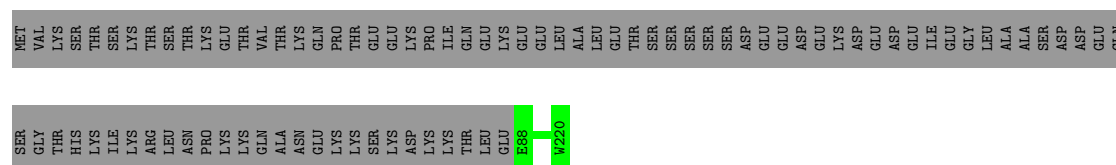
- Molecule 33: Pescadillo homolog

Chain n:  56% 44%



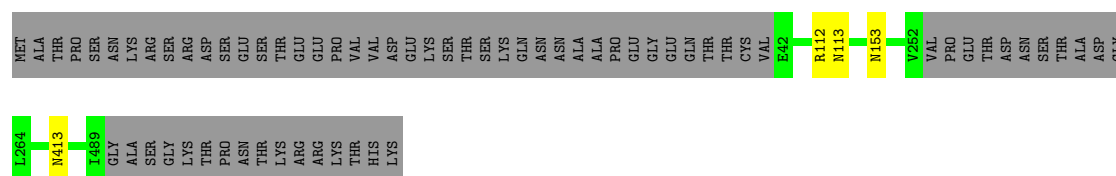
- Molecule 34: Ribosome biogenesis protein 15

Chain o:  60% 40%



- Molecule 35: ATP-dependent RNA helicase HAS1

Chain p:  86% 13%



- Molecule 36: Protein MAK11

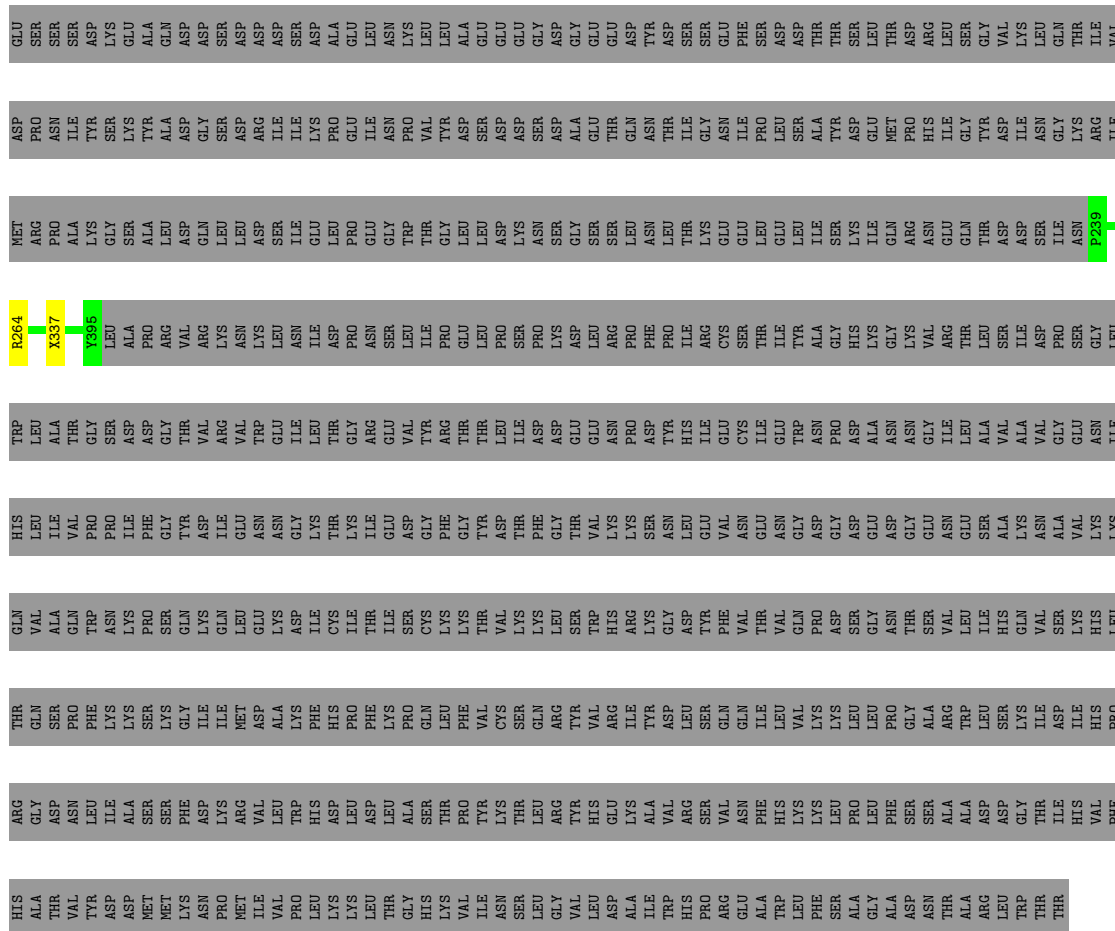
Chain q:  100%



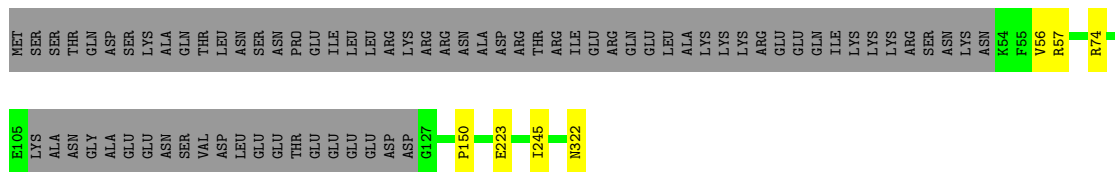
- Molecule 37: Ribosome biogenesis protein ERB1

Chain s:  19% 81%

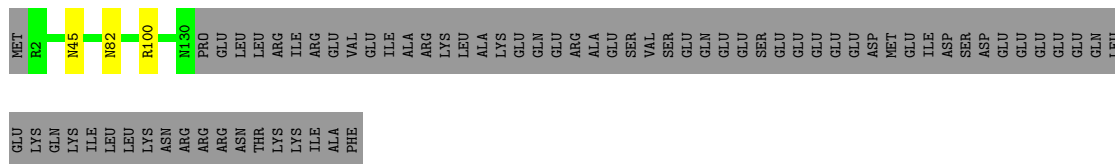




- Molecule 38: Ribosome biogenesis protein RLP7

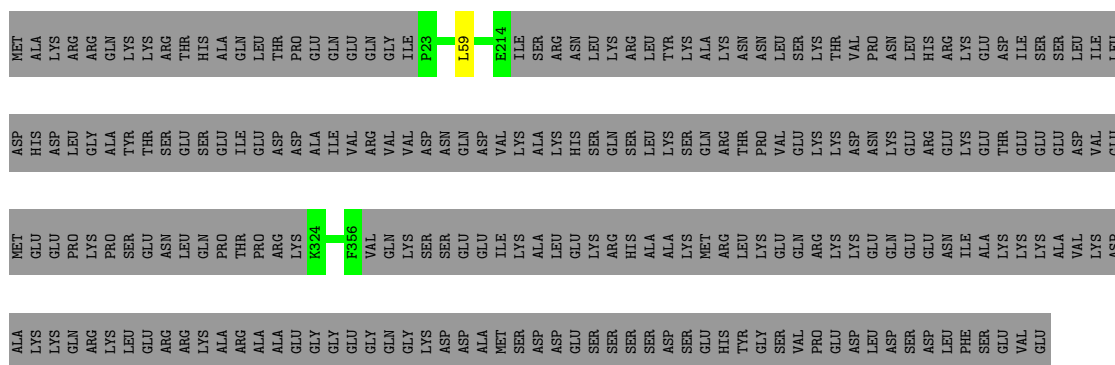


- Molecule 39: Ribosome biogenesis protein RLP24

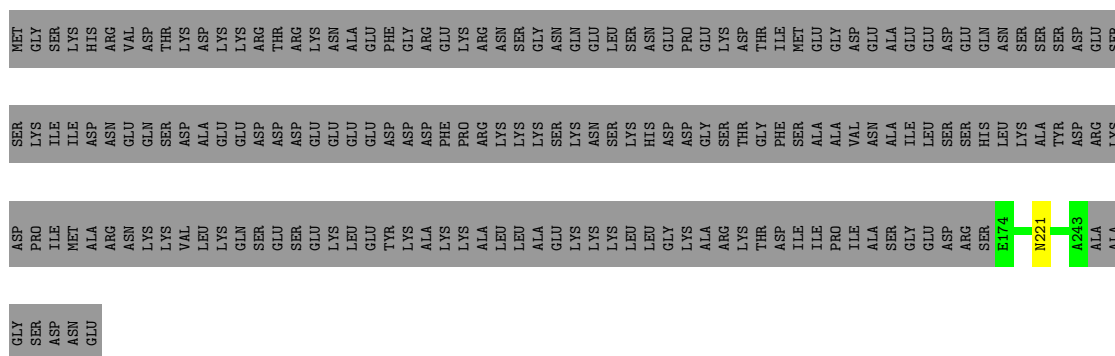


- Molecule 40: Ribosome biogenesis protein SSF1

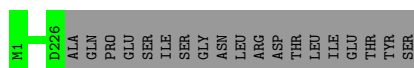




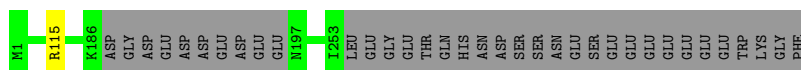
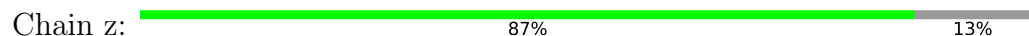
- Molecule 41: Ribosomal RNA-processing protein 15



- Molecule 42: Eukaryotic translation initiation factor 6



- Molecule 43: Ribosomal RNA-processing protein 1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201114	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.72	0/32512	1.16	224/50669 (0.4%)
10	G	0.39	0/1477	0.67	0/1994
11	I	0.41	0/2476	0.58	0/3323
12	K	0.35	0/2133	0.59	1/2879 (0.0%)
13	L	0.42	0/858	0.64	2/1154 (0.2%)
14	M	0.36	0/1012	0.53	0/1362
15	N	0.42	0/1540	0.55	0/2060
16	O	0.37	0/1476	0.52	0/1980
17	P	0.35	0/991	0.50	0/1334
18	Q	0.39	0/1030	0.59	0/1393
19	S	0.37	0/1473	0.57	1/1980 (0.1%)
2	2	0.71	0/3746	1.09	13/5832 (0.2%)
20	V	0.29	0/917	0.50	0/1235
21	W	0.32	0/821	0.51	1/1106 (0.1%)
22	Y	0.40	0/1004	0.60	0/1341
23	7	0.40	0/1312	0.62	1/1744 (0.1%)
24	8	0.28	0/840	0.42	0/1105
25	b	0.36	0/1868	0.58	0/2522
26	e	0.36	0/931	0.53	0/1243
27	f	0.42	0/868	0.57	0/1168
28	h	0.36	0/978	0.62	1/1301 (0.1%)
29	i	0.34	0/672	0.57	0/894
3	6	0.63	0/2050	1.33	34/3186 (1.1%)
30	j	0.34	0/587	0.54	0/778
33	n	0.36	0/2862	0.56	0/3870
34	o	0.37	0/1129	0.54	0/1502
35	p	0.37	0/3552	0.61	0/4789
37	s	0.40	0/720	0.55	0/964
38	t	0.36	0/1991	0.61	0/2679
39	u	0.34	0/1109	0.50	0/1474
4	A	0.39	0/3182	0.59	0/4288
40	v	0.31	0/1825	0.62	1/2453 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
41	w	0.29	0/563	0.51	0/748
42	y	0.31	0/1730	0.58	0/2354
43	z	0.40	0/2104	0.55	0/2832
5	B	0.34	0/2628	0.58	0/3529
6	C	0.41	0/2462	0.60	0/3333
7	D	0.44	0/1609	0.55	0/2157
8	E	0.39	0/1390	0.56	0/1866
9	F	0.37	0/1979	0.58	0/2661
All	All	0.54	0/94407	0.88	279/135082 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	G	0	1
19	S	0	4
28	h	0	1
33	n	0	1
36	q	0	1
37	s	0	1
38	t	0	3
4	A	0	2
7	D	0	1
9	F	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3217	C	N1-C2-O2	13.30	126.88	118.90
1	1	3217	C	N3-C2-O2	-10.79	114.35	121.90
1	1	3217	C	C2-N1-C1'	10.48	130.33	118.80
1	1	406	G	O4'-C1'-N9	9.94	116.15	108.20
1	1	3058	U	N1-C2-O2	9.91	129.74	122.80

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	185	ALA	Peptide
4	A	53	ILE	Peptide
7	D	56	ASP	Peptide
9	F	158	LYS	Peptide
10	G	76	ALA	Peptide

5.2 Too-close contacts

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	1	29055	0	14598	480	0
2	2	3353	0	1695	48	0
3	6	1838	0	927	33	0
4	A	3126	0	3178	93	0
5	B	2577	0	2655	71	0
6	C	2418	0	2541	56	0
7	D	1578	0	1619	49	0
8	E	1366	0	1466	36	0
9	F	1941	0	2037	40	0
10	G	1453	0	1536	41	0
11	I	2429	0	2472	88	0
12	K	2099	0	2180	54	0
13	L	845	0	898	28	0
14	M	997	0	1090	24	0
15	N	1509	0	1561	40	0
16	O	1451	0	1554	35	0
17	P	975	0	988	12	0
18	Q	1015	0	1096	13	0
19	S	1437	0	1475	32	0
20	V	903	0	946	23	0
21	W	806	0	777	13	0
22	Y	993	0	1081	20	0
23	7	1295	0	1383	24	0
24	8	836	0	897	10	0
25	b	1919	0	1858	0	0
26	e	914	0	977	0	0
27	f	850	0	880	0	0
28	h	969	0	1078	0	0
29	i	665	0	721	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	575	0	579	0	0
31	x	140	0	34	0	0
32	m	370	0	76	0	0
33	n	2794	0	2845	0	0
34	o	1107	0	1159	0	0
35	p	3486	0	3618	0	0
36	q	1409	0	308	0	0
37	s	1069	0	820	0	0
38	t	1965	0	2077	0	0
39	u	1088	0	1118	0	0
40	v	1795	0	1877	0	0
41	w	562	0	614	0	0
42	y	1709	0	1701	0	0
43	z	2058	0	2096	0	0
44	D	1	0	0	0	0
44	j	1	0	0	0	0
44	u	1	0	0	0	0
All	All	91742	0	75086	1109	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 11.

The worst 5 of 1109 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)
1:1:182:U:H3	1:1:234:G:H1	1.07	0.97
1:1:160:G:H1	1:1:261:U:H3	1.09	0.97
4:A:57:GLU:OE2	4:A:169:LYS:NZ	1.99	0.96
1:1:509:U:H3	1:1:582:G:H1	1.10	0.95
1:1:528:U:H3	1:1:564:G:H1	1.09	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	390/463 (84%)	368 (94%)	22 (6%)	0	100	100
5	B	320/387 (83%)	302 (94%)	18 (6%)	0	100	100
6	C	310/362 (86%)	285 (92%)	23 (7%)	2 (1%)	27	68
7	D	188/306 (61%)	177 (94%)	11 (6%)	0	100	100
8	E	168/176 (96%)	158 (94%)	10 (6%)	0	100	100
9	F	240/244 (98%)	225 (94%)	15 (6%)	0	100	100
10	G	185/256 (72%)	170 (92%)	14 (8%)	1 (0%)	31	71
11	I	286/295 (97%)	272 (95%)	14 (5%)	0	100	100
12	K	256/376 (68%)	243 (95%)	13 (5%)	0	100	100
13	L	104/199 (52%)	96 (92%)	7 (7%)	1 (1%)	17	59
14	M	126/138 (91%)	123 (98%)	3 (2%)	0	100	100
15	N	172/204 (84%)	162 (94%)	10 (6%)	0	100	100
16	O	180/199 (90%)	173 (96%)	7 (4%)	0	100	100
17	P	118/184 (64%)	113 (96%)	5 (4%)	0	100	100
18	Q	130/186 (70%)	128 (98%)	2 (2%)	0	100	100
19	S	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
20	V	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
21	W	96/647 (15%)	94 (98%)	2 (2%)	0	100	100
22	Y	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
23	7	152/231 (66%)	137 (90%)	15 (10%)	0	100	100
24	8	96/434 (22%)	96 (100%)	0	0	100	100
25	b	220/291 (76%)	207 (94%)	13 (6%)	0	100	100
26	e	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
27	f	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
28	h	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
29	i	82/100 (82%)	78 (95%)	4 (5%)	0	100	100
30	j	70/88 (80%)	66 (94%)	4 (6%)	0	100	100
33	n	333/605 (55%)	322 (97%)	11 (3%)	0	100	100
34	o	131/220 (60%)	123 (94%)	8 (6%)	0	100	100
35	p	433/505 (86%)	422 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	s	82/807 (10%)	77 (94%)	5 (6%)	0	100	100
38	t	244/322 (76%)	220 (90%)	23 (9%)	1 (0%)	36	75
39	u	127/199 (64%)	127 (100%)	0	0	100	100
40	v	221/453 (49%)	207 (94%)	14 (6%)	0	100	100
41	w	68/250 (27%)	64 (94%)	4 (6%)	0	100	100
42	y	224/245 (91%)	214 (96%)	10 (4%)	0	100	100
43	z	239/278 (86%)	228 (95%)	11 (5%)	0	100	100
All	All	6735/10443 (64%)	6380 (95%)	350 (5%)	5 (0%)	56	87

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	268	ALA
6	C	292	SER
13	L	63	VAL
10	G	127	PRO
38	t	56	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	352/410 (86%)	352 (100%)	0	100	100
5	B	272/323 (84%)	271 (100%)	1 (0%)	92	97
6	C	257/289 (89%)	253 (98%)	4 (2%)	65	86
7	D	171/274 (62%)	170 (99%)	1 (1%)	87	94
8	E	149/153 (97%)	148 (99%)	1 (1%)	85	93
9	F	204/205 (100%)	203 (100%)	1 (0%)	90	96
10	G	152/208 (73%)	150 (99%)	2 (1%)	71	88
11	I	271/276 (98%)	268 (99%)	3 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	241/346 (70%)	240 (100%)	1 (0%)	92	97
13	L	85/159 (54%)	84 (99%)	1 (1%)	74	89
14	M	100/109 (92%)	100 (100%)	0	100	100
15	N	153/176 (87%)	151 (99%)	2 (1%)	71	88
16	O	150/162 (93%)	148 (99%)	2 (1%)	71	88
17	P	100/146 (68%)	99 (99%)	1 (1%)	78	90
18	Q	108/151 (72%)	106 (98%)	2 (2%)	60	83
19	S	155/156 (99%)	153 (99%)	2 (1%)	71	88
20	V	94/105 (90%)	94 (100%)	0	100	100
21	W	87/573 (15%)	82 (94%)	5 (6%)	23	60
22	Y	109/110 (99%)	108 (99%)	1 (1%)	81	91
23	7	141/205 (69%)	141 (100%)	0	100	100
24	8	90/388 (23%)	90 (100%)	0	100	100
25	b	203/247 (82%)	200 (98%)	3 (2%)	67	86
26	e	97/111 (87%)	97 (100%)	0	100	100
27	f	90/91 (99%)	90 (100%)	0	100	100
28	h	104/105 (99%)	103 (99%)	1 (1%)	78	90
29	i	70/82 (85%)	70 (100%)	0	100	100
30	j	60/71 (84%)	59 (98%)	1 (2%)	63	85
33	n	309/548 (56%)	308 (100%)	1 (0%)	93	97
34	o	118/199 (59%)	118 (100%)	0	100	100
35	p	381/440 (87%)	377 (99%)	4 (1%)	78	90
37	s	77/653 (12%)	76 (99%)	1 (1%)	71	88
38	t	219/287 (76%)	216 (99%)	3 (1%)	69	87
39	u	114/180 (63%)	111 (97%)	3 (3%)	49	77
40	v	208/413 (50%)	208 (100%)	0	100	100
41	w	63/219 (29%)	62 (98%)	1 (2%)	65	86
42	y	194/211 (92%)	194 (100%)	0	100	100
43	z	225/257 (88%)	224 (100%)	1 (0%)	92	97
All	All	5973/9038 (66%)	5924 (99%)	49 (1%)	84	92

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	12	ARG
21	W	415	ASN
39	u	82	ASN
21	W	374	ARG
21	W	445	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	8	GLN
24	8	322	GLN
42	y	79	GLN
19	S	74	ASN
21	W	415	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1343/3395 (39%)	352 (26%)	28 (2%)
2	2	157/158 (99%)	35 (22%)	3 (1%)
3	6	85/232 (36%)	44 (51%)	5 (5%)
All	All	1585/3785 (41%)	431 (27%)	36 (2%)

5 of 431 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	7	C
1	1	12	A
1	1	13	A
1	1	14	U

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	3121	U
1	1	3218	A
3	6	60	U
1	1	3168	A
1	1	3228	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
36	q	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	398:UNK	C	400:UNK	N	14.84
1	q	136:UNK	C	137:UNK	N	9.43
1	q	114:UNK	C	115:UNK	N	7.34
1	q	257:UNK	C	259:UNK	N	6.77
1	q	242:UNK	C	247:UNK	N	4.06