



# wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:42 AM UTC

PDB ID : 1ML5 / pdb\_00001ml5  
EMDB ID : EMD-1005  
Title : Structure of the E. coli ribosomal termination complex with release factor 2  
Authors : Klaholz, B.P.; Pape, T.; Zavialov, A.V.; Myasnikov, A.G.; Orlova, E.V.; Vestergaard, B.; Ehrenberg, M.; van Heel, M.  
Deposited on : 2002-08-30  
Resolution : 14.00 Å (reported)  
Based on initial models : 1GIX, 1GIY, 1GQE

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

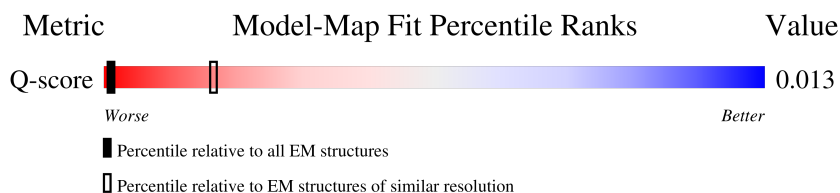
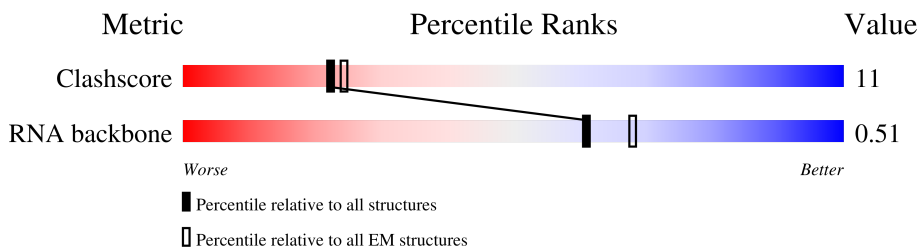
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 14.00 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	61 ( 13.50 - 14.50 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	1522	
2	B	76	
3	C	6	
4	a	2916	
5	b	123	

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Mol	Chain	Length	Quality of chain
6	Z	365	87% 98%
7	E	256	73% 91% 9%
8	F	239	71% 85% 14%
9	G	209	79% 99%
10	H	162	81% 92% 7%
11	I	101	72% 100%
12	J	156	64% 99%
13	K	138	85% 100%
14	L	128	84% 97%
15	M	105	66% 90% 7%
16	N	129	60% 92% 8%
17	O	135	59% 91% 8%
18	P	126	77% 98%
19	Q	61	93% 93% 5%
20	R	89	73% 99%
21	S	91	89% 91% 9%
22	T	105	90% 99%
23	U	88	74% 83% 17%
24	V	93	80% 86% 14%
25	W	106	79% 93% 7%
26	X	26	92% 92% 8%
27	c	228	96% 96%
28	d	178	90% 92% 5%
29	e	338	48% 54% 43%
30	f	246	54% 72% 23%

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Mol	Chain	Length	Quality of chain
31	g	176	
32	h	177	
33	l	141	
34	m	145	
35	n	122	
36	o	164	
37	p	138	
38	q	186	
39	r	66	
40	s	113	
41	t	84	
42	u	119	
43	v	94	
44	w	70	
45	x	60	

## 2 Entry composition [i](#)

There are 45 unique types of molecules in this entry. The entry contains 11392 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 30S 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	1519	Total	P	0	1519
			1519	1519		

- Molecule 2 is a RNA chain called T-RNA(PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 3 is a RNA chain called A- AND P-SITE MESSENGER RNA CODONS.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

- Molecule 4 is a RNA chain called 50S 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	a	2889	Total	P	0	2889
			2889	2889		

- Molecule 5 is a RNA chain called 50S 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	b	123	Total	P	0	123
			123	123		

- Molecule 6 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	Z	362	Total	C	0	362
			362	362		

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	E	234	Total C 234 234	0	234

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	F	206	Total C 206 206	0	206

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	G	208	Total C 208 208	0	208

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	H	150	Total C 150 150	0	150

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	I	101	Total C 101 101	0	101

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	J	155	Total C 155 155	0	155

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	K	138	Total C 138 138	0	138

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		AltConf	Trace
14	L	127	Total 127	C 127	0	127

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	M	98	Total 98	C 98	0	98

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms		AltConf	Trace
16	N	119	Total 119	C 119	0	119

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms		AltConf	Trace
17	O	124	Total 124	C 124	0	124

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	P	125	Total 125	C 125	0	125

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	Q	60	Total 60	C 60	0	60

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	R	88	Total 88	C 88	0	88

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	S	83	Total C 83 83	0	83

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	T	104	Total C 104 104	0	104

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	U	73	Total C 73 73	0	73

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	V	80	Total C 80 80	0	80

- Molecule 25 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	W	99	Total C 99 99	0	99

- Molecule 26 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	X	24	Total C 24 24	0	24

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	c	224	Total C 224 224	0	224

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	d	173	Total	C	0	173
			173	173		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	e	191	Total	C	0	191
			191	191		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	f	189	Total	C	0	189
			189	189		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	g	122	Total	C	0	122
			122	122		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	h	164	Total	C	0	164
			164	164		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	l	133	Total	C	0	133
			133	133		

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms		AltConf	Trace
34	m	117	Total	C	0	117
			117	117		

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	n	122	Total	C	0	122
			122	122		

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	o	84	Total	C	0	84
			84	84		

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	p	138	Total	C	0	138
			138	138		

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	q	113	Total	C	0	113
			113	113		

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms		AltConf	Trace
39	r	52	Total	C	0	52
			52	52		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		AltConf	Trace
40	s	110	Total	C	0	110
			110	110		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms		AltConf	Trace
41	t	76	Total	C	0	76
			76	76		

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	AltConf	Trace
42	u	110	Total C 110 110	0	110

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms	AltConf	Trace
43	v	89	Total C 89 89	0	89

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	AltConf	Trace
44	w	64	Total C 64 64	0	64

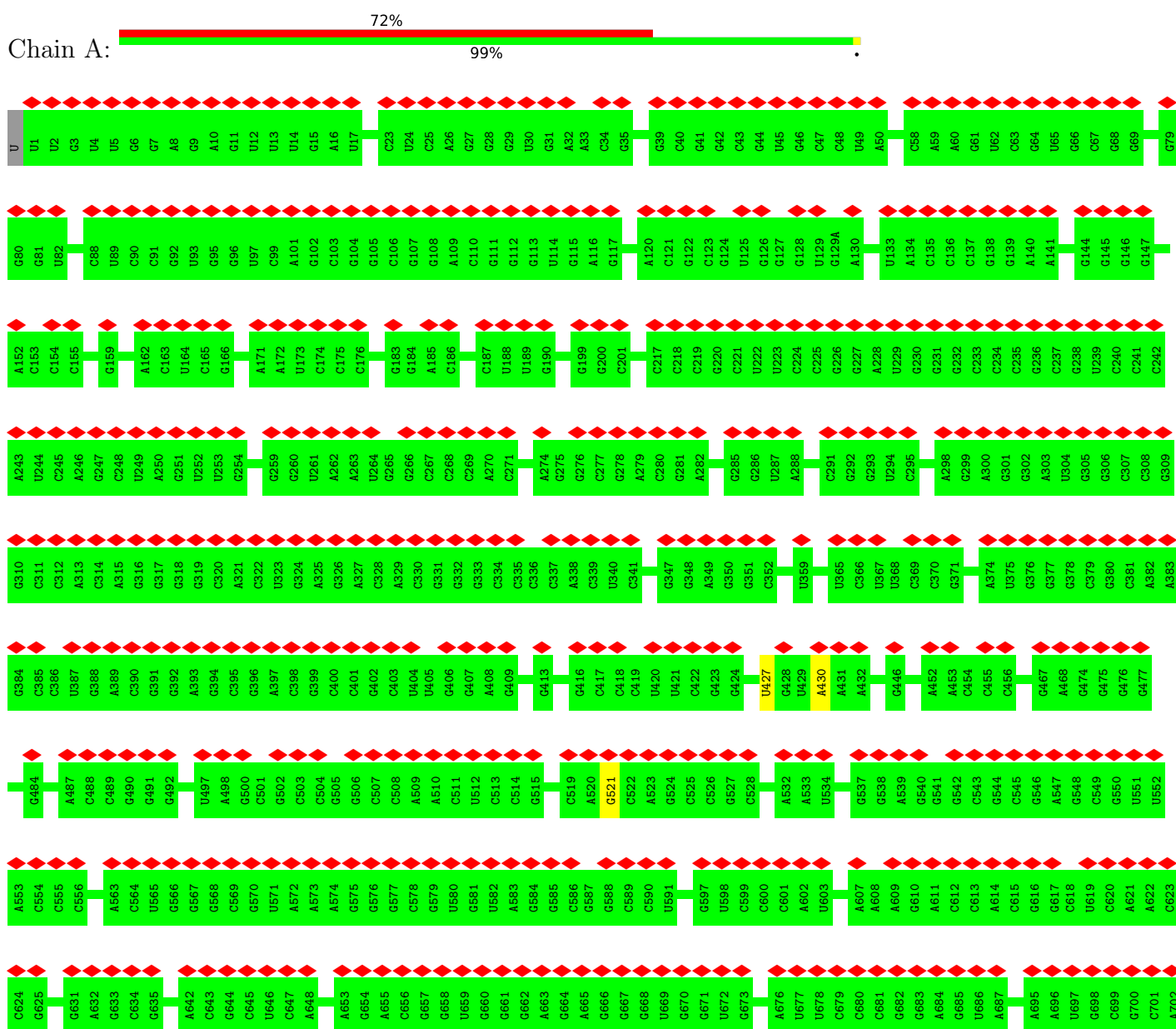
- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

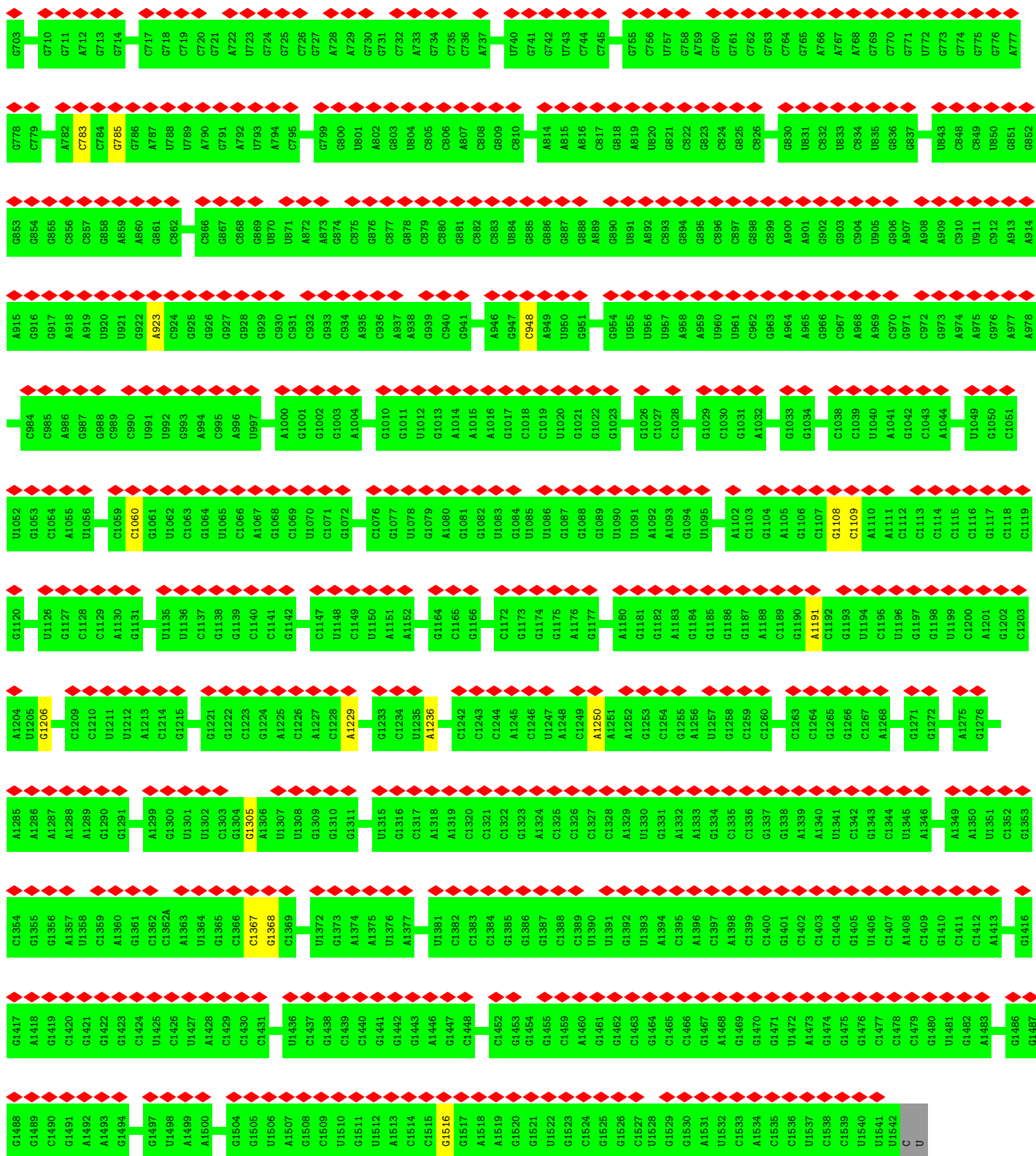
Mol	Chain	Residues	Atoms	AltConf	Trace
45	x	60	Total C 60 60	0	60

### 3 Residue-property plots

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.

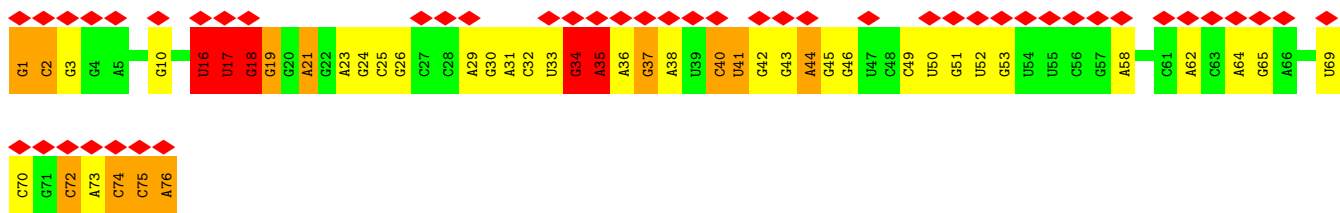
#### • Molecule 1: 30S 16S RIBOSOMAL RNA





• Molecule 2: T-RNA(PHE)

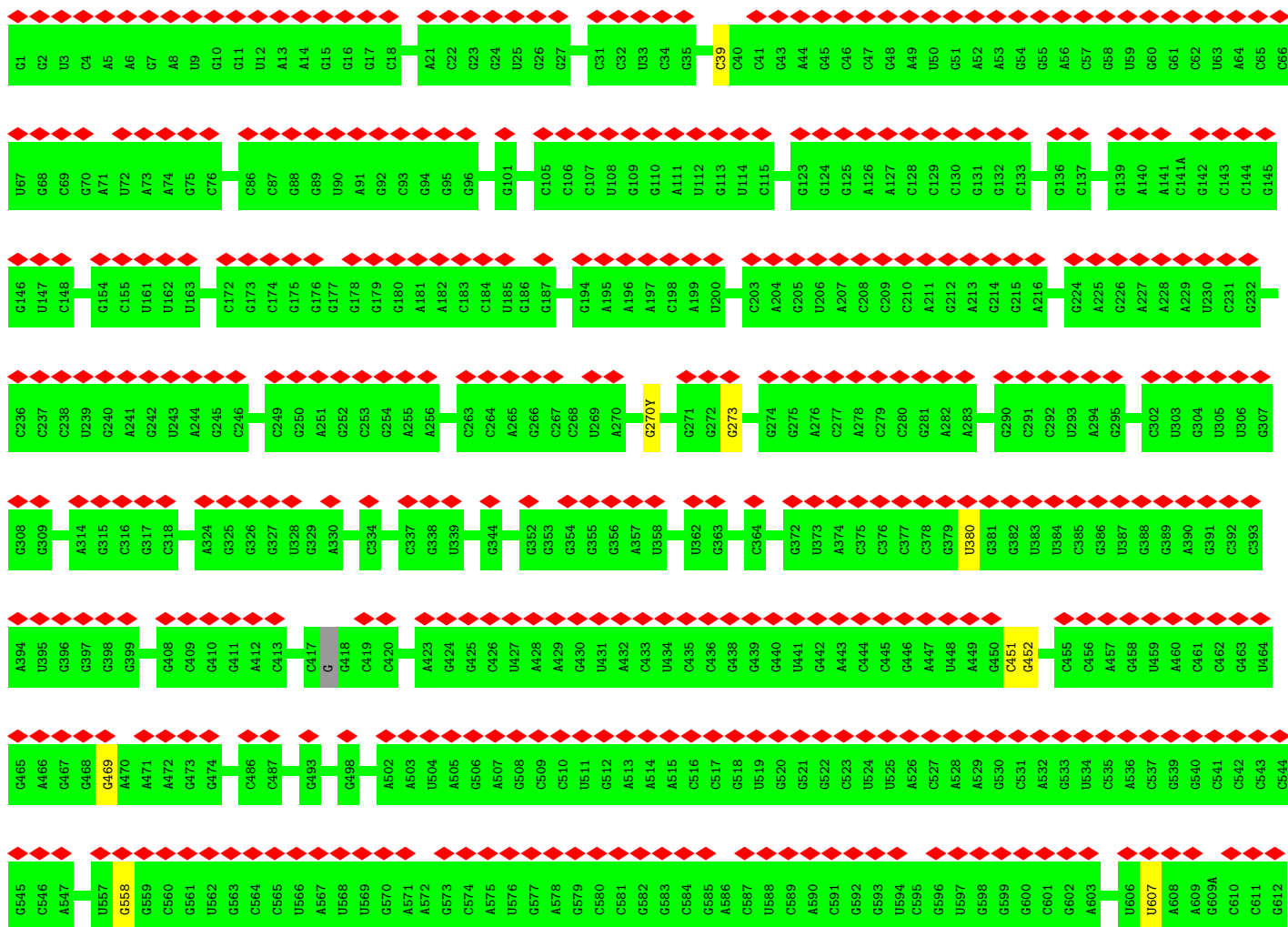




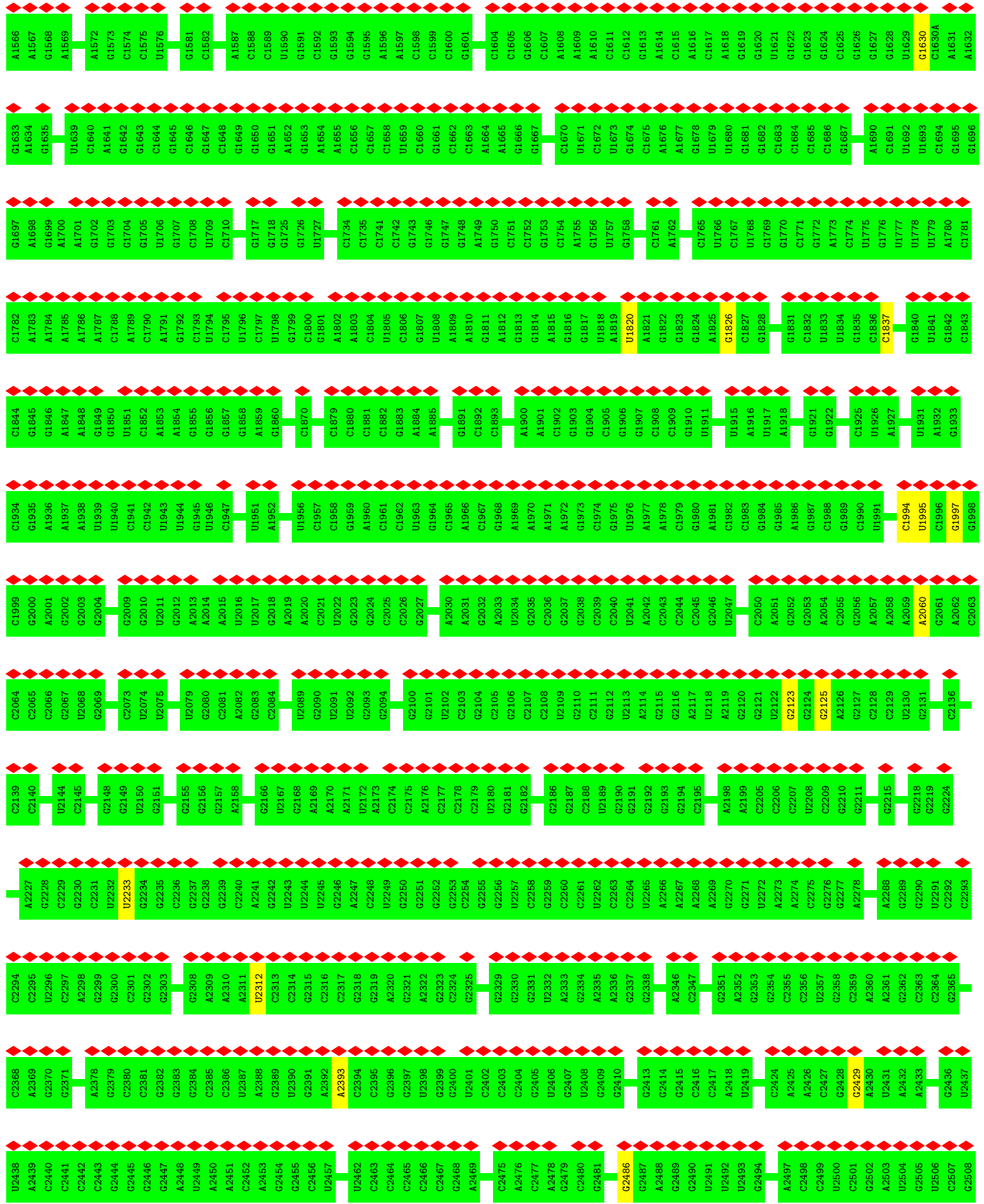
• Molecule 3: A- AND P-SITE MESSENGER RNA CODONS

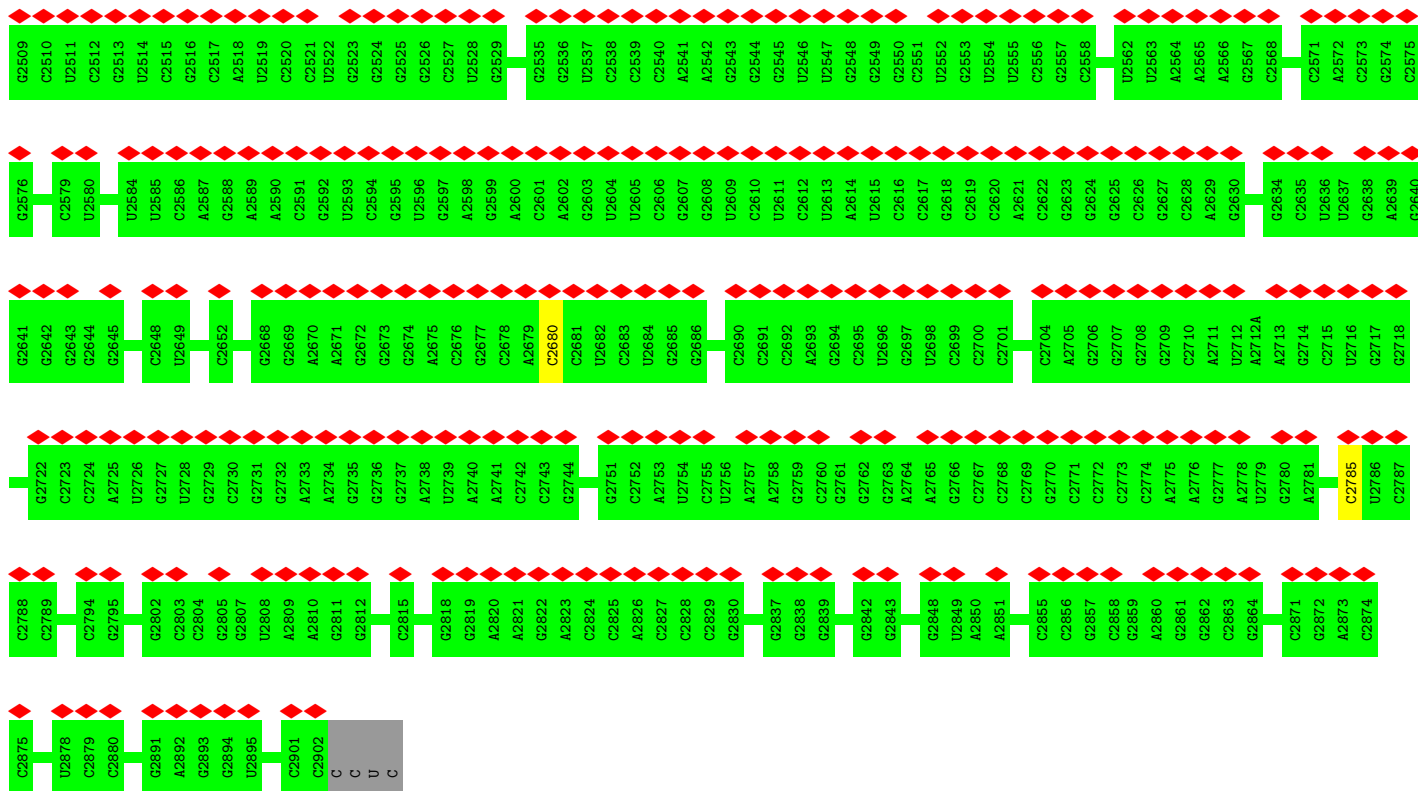


• Molecule 4: 50S 23S RIBOSOMAL RNA

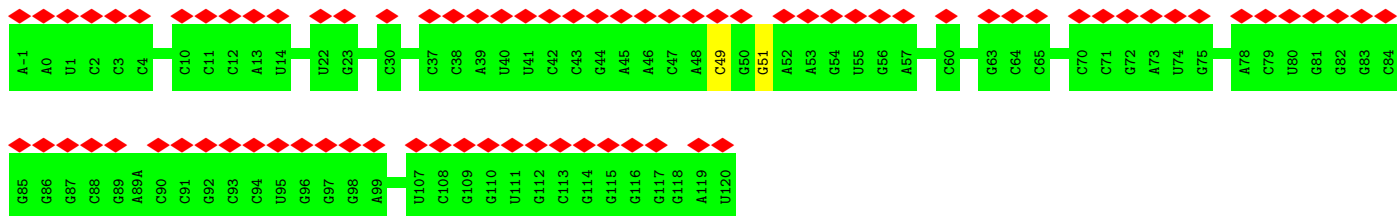




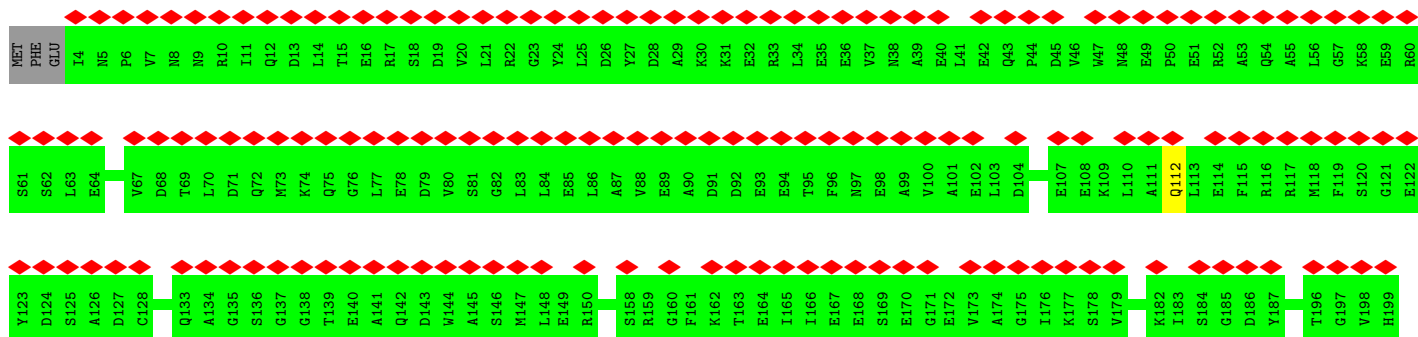
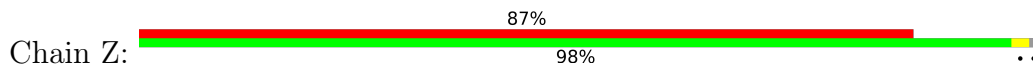


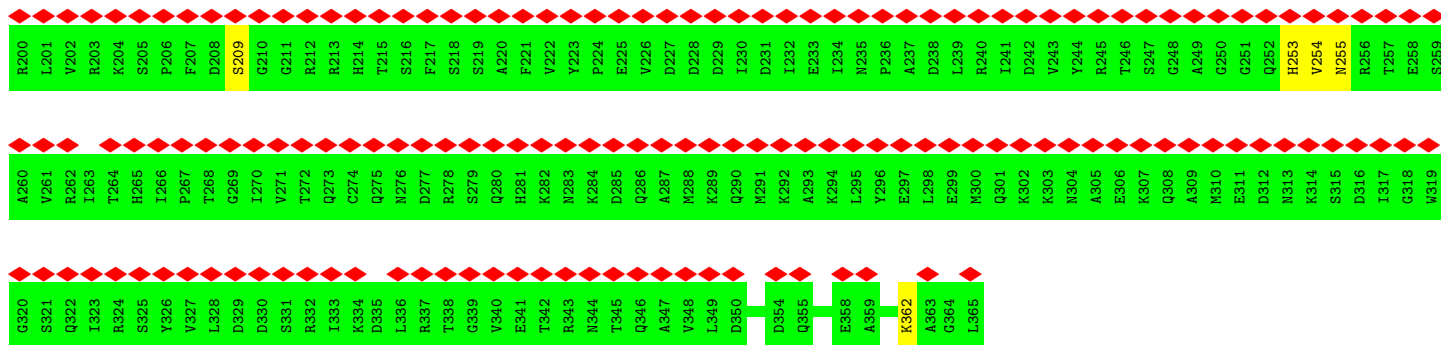


• Molecule 5: 50S 5S RIBOSOMAL RNA

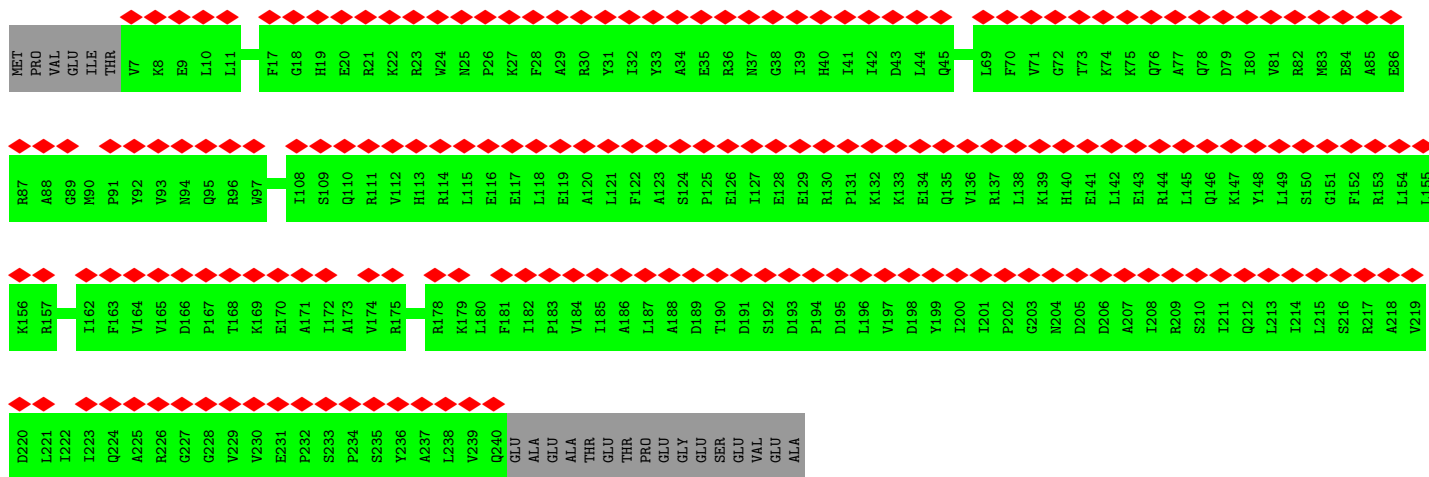
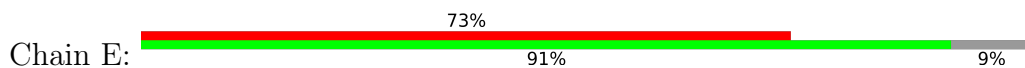


• Molecule 6: Peptide chain release factor 2

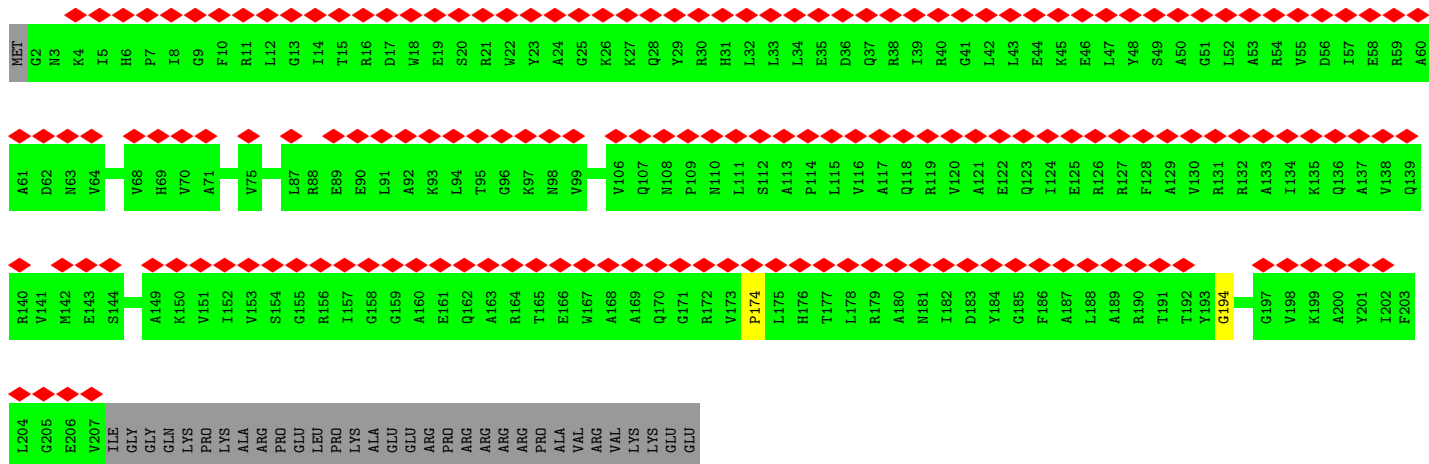
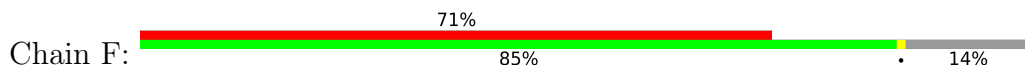




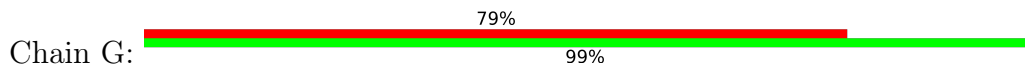
• Molecule 7: 30S RIBOSOMAL PROTEIN S2

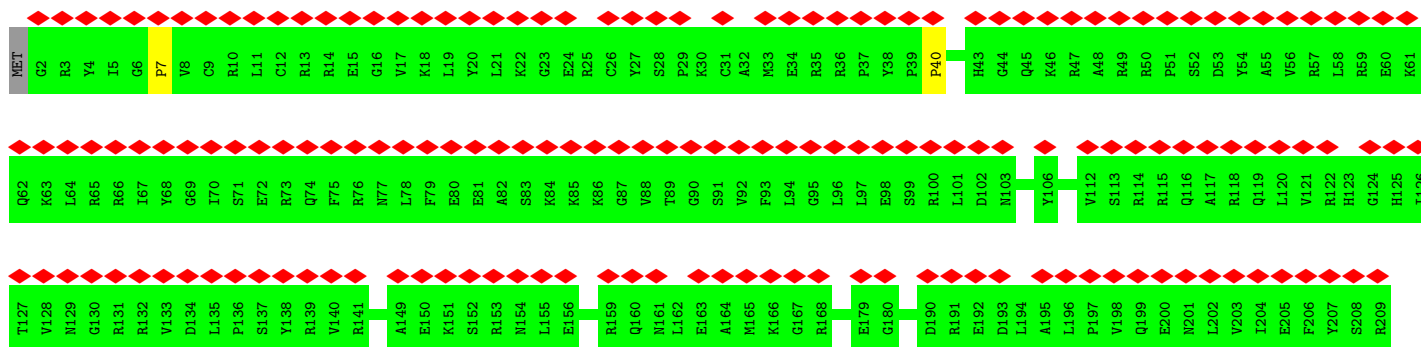


• Molecule 8: 30S RIBOSOMAL PROTEIN S3

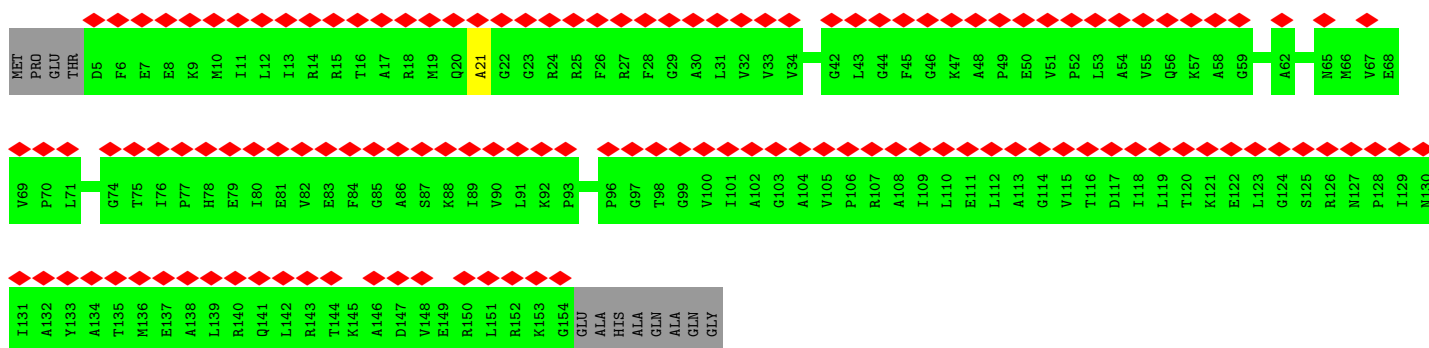
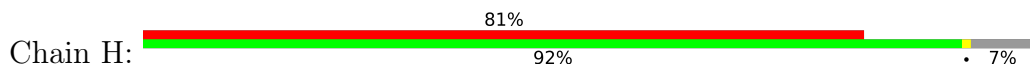


• Molecule 9: 30S RIBOSOMAL PROTEIN S4

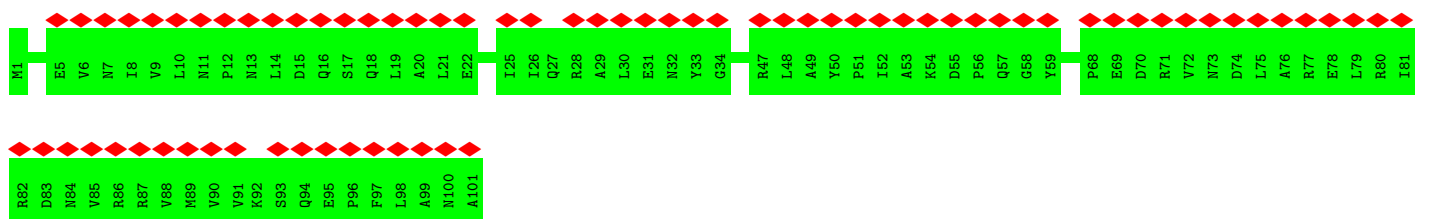




• Molecule 10: 30S RIBOSOMAL PROTEIN S5



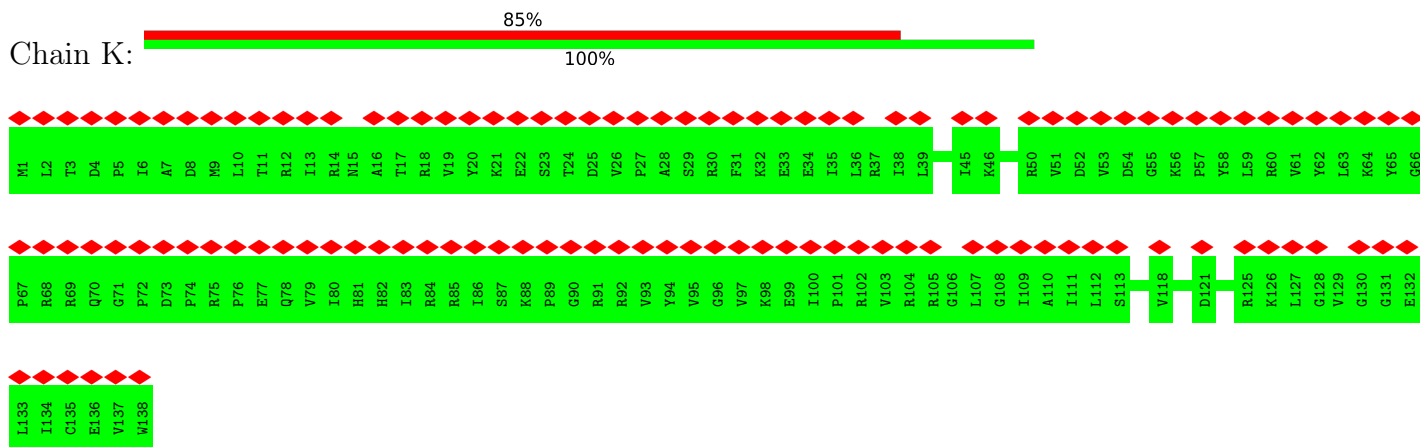
• Molecule 11: 30S RIBOSOMAL PROTEIN S6



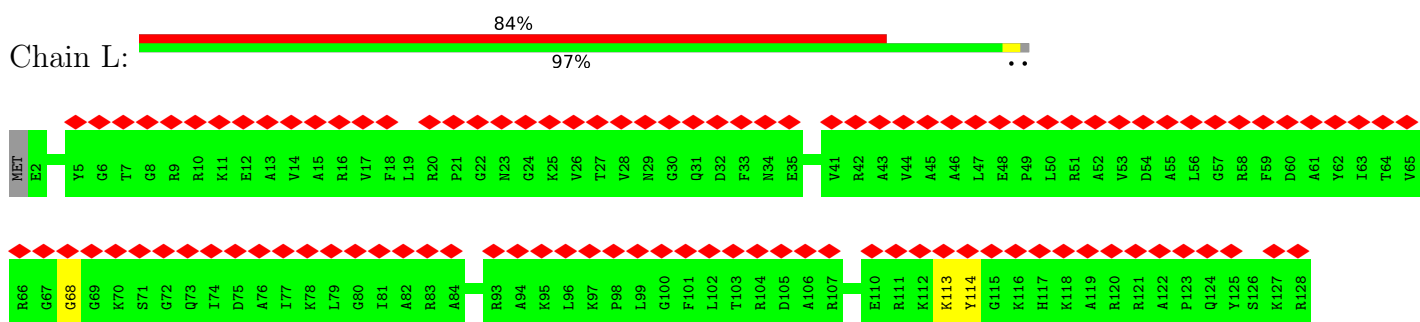
• Molecule 12: 30S RIBOSOMAL PROTEIN S7



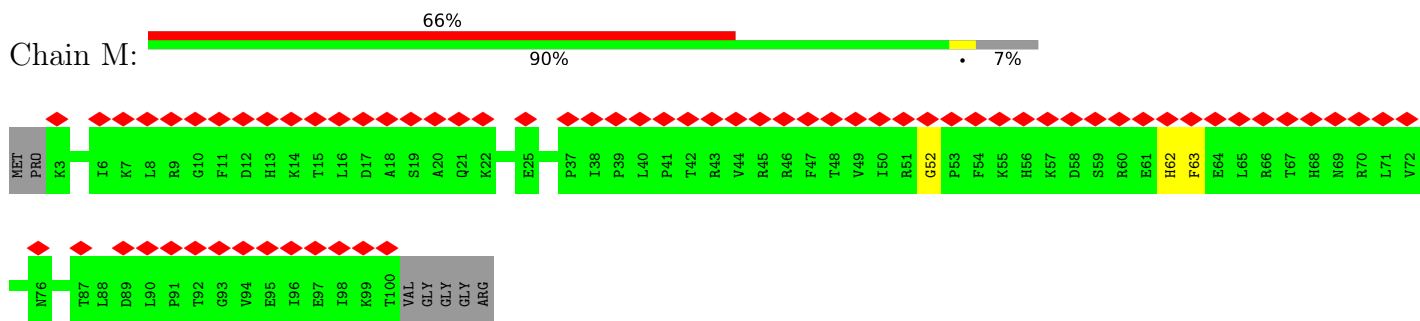
• Molecule 13: 30S RIBOSOMAL PROTEIN S8



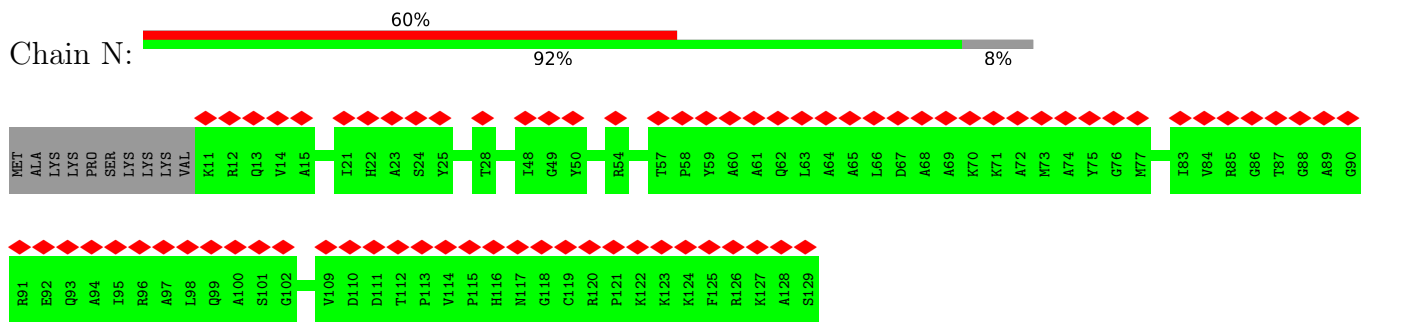
• Molecule 14: 30S RIBOSOMAL PROTEIN S9



• Molecule 15: 30S RIBOSOMAL PROTEIN S10

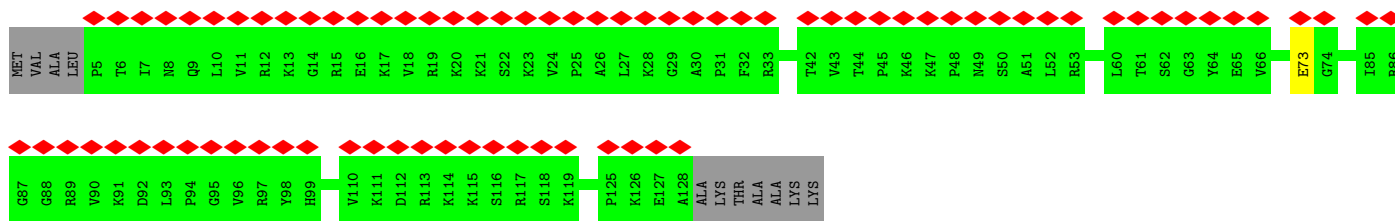


• Molecule 16: 30S RIBOSOMAL PROTEIN S11

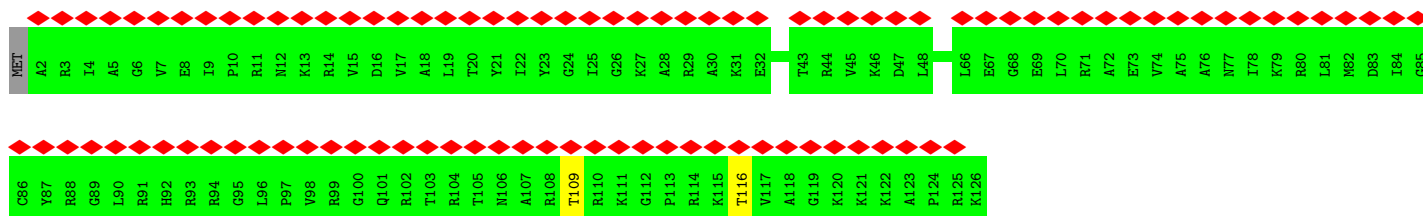
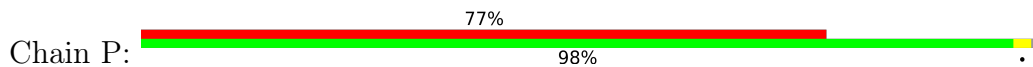


• Molecule 17: 30S RIBOSOMAL PROTEIN S12

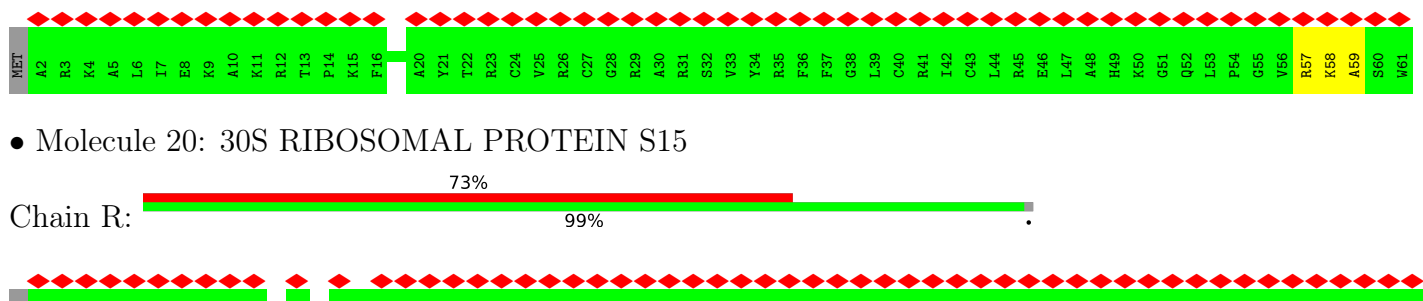
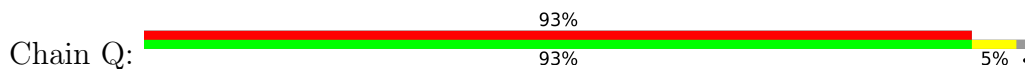




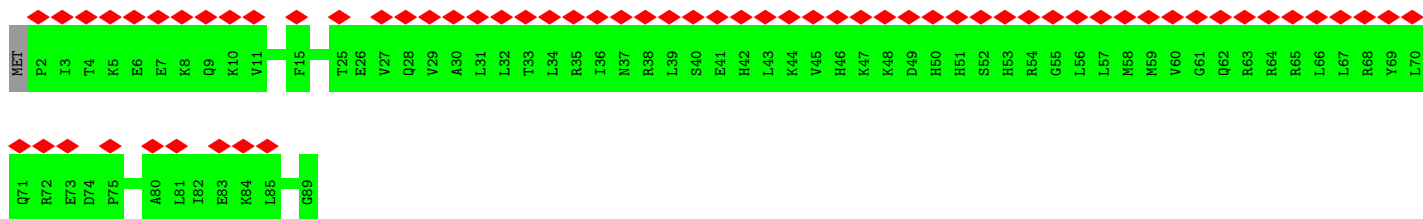
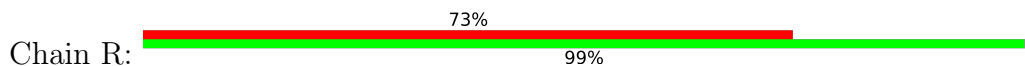
- Molecule 18: 30S RIBOSOMAL PROTEIN S13



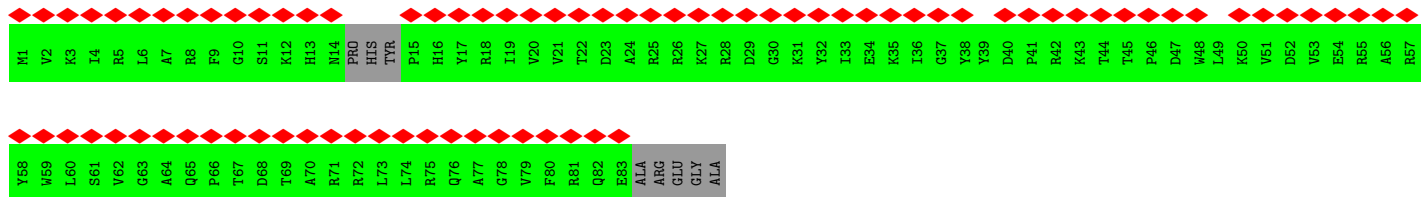
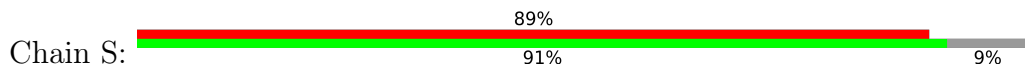
- Molecule 19: 30S RIBOSOMAL PROTEIN S14



- Molecule 20: 30S RIBOSOMAL PROTEIN S15

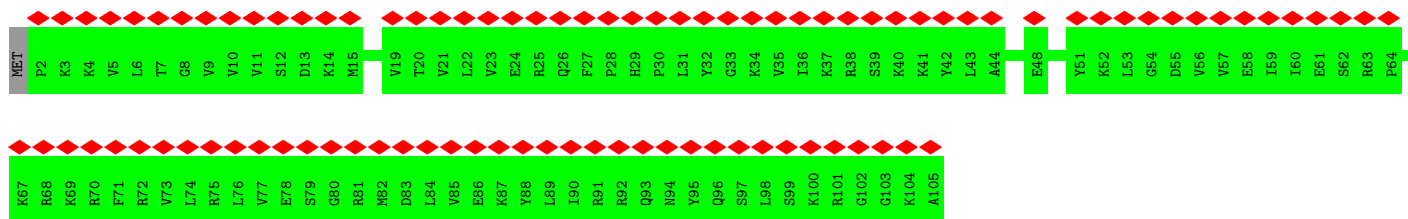


- Molecule 21: 30S RIBOSOMAL PROTEIN S16

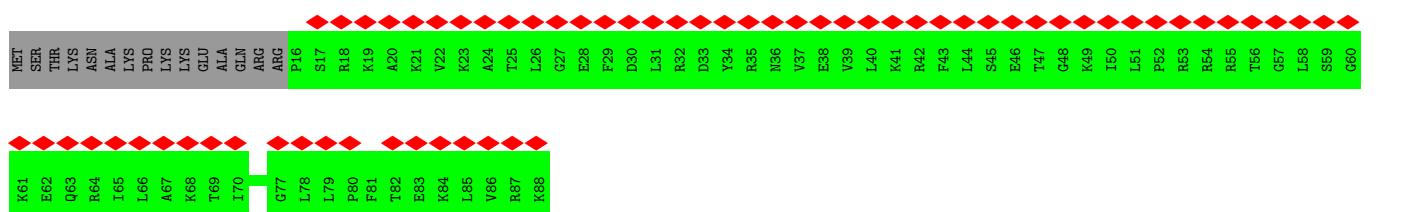
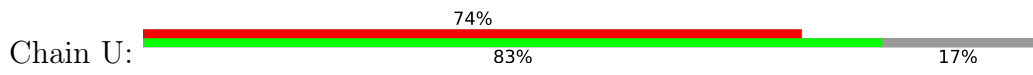


- Molecule 22: 30S RIBOSOMAL PROTEIN S17

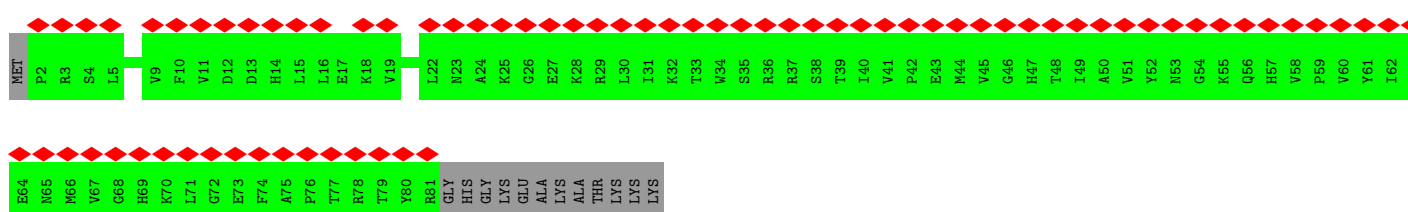
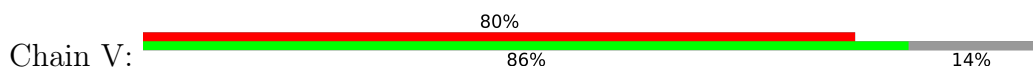




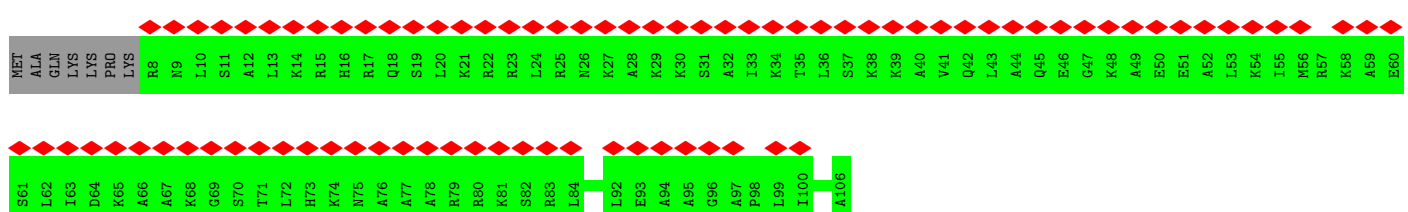
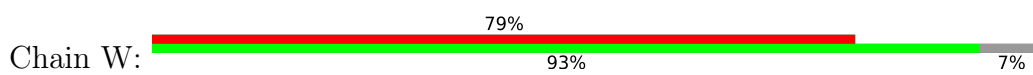
• Molecule 23: 30S RIBOSOMAL PROTEIN S18



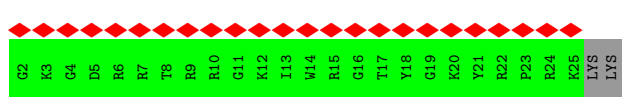
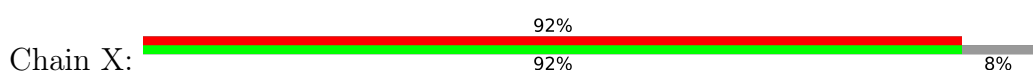
• Molecule 24: 30S RIBOSOMAL PROTEIN S19



• Molecule 25: 30S RIBOSOMAL PROTEIN S20



• Molecule 26: 30S RIBOSOMAL PROTEIN THX

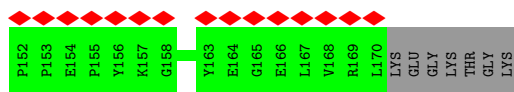


• Molecule 27: 50S RIBOSOMAL PROTEIN L1

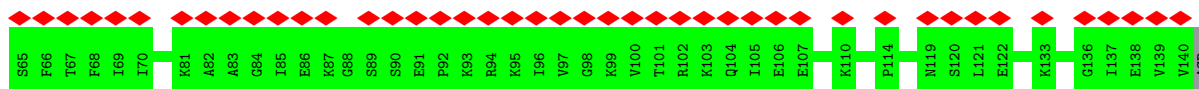
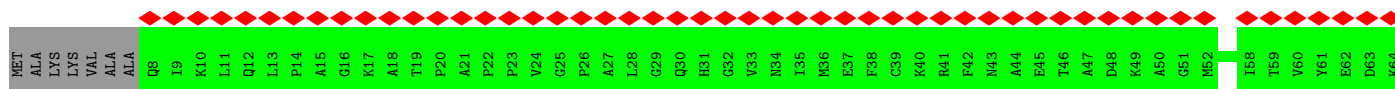
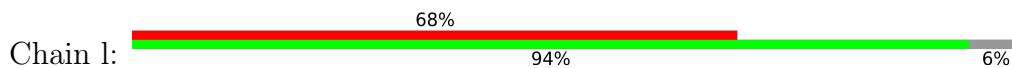




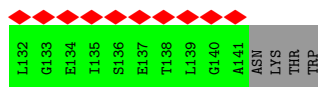
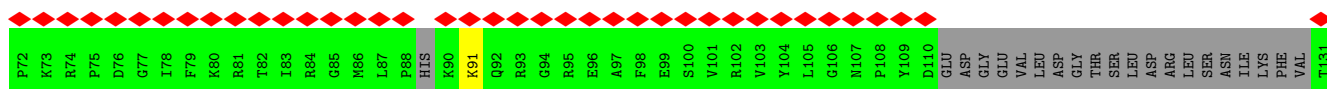
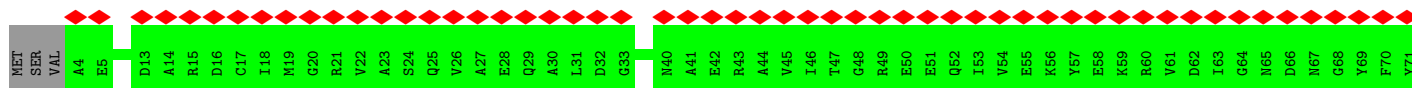
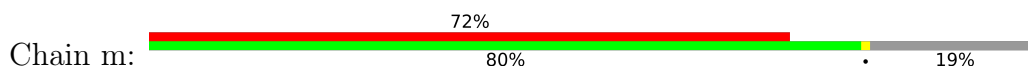




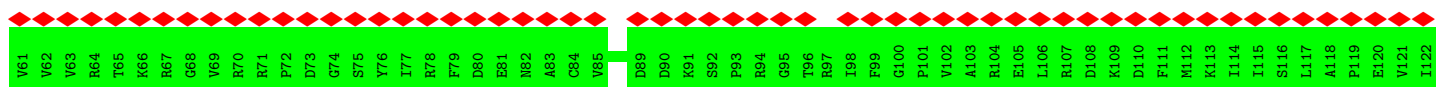
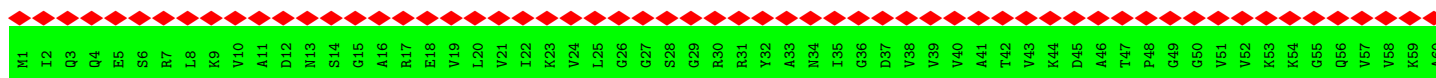
- Molecule 33: 50S RIBOSOMAL PROTEIN L11



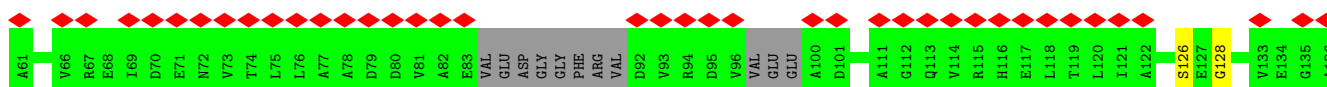
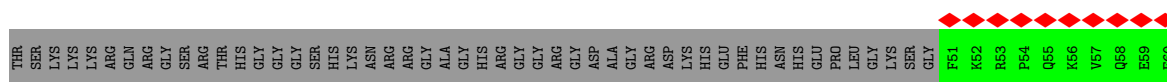
- Molecule 34: 50S RIBOSOMAL PROTEIN L13

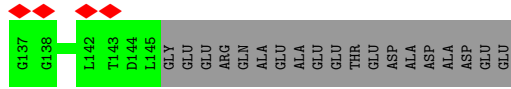


- Molecule 35: 50S RIBOSOMAL PROTEIN L14

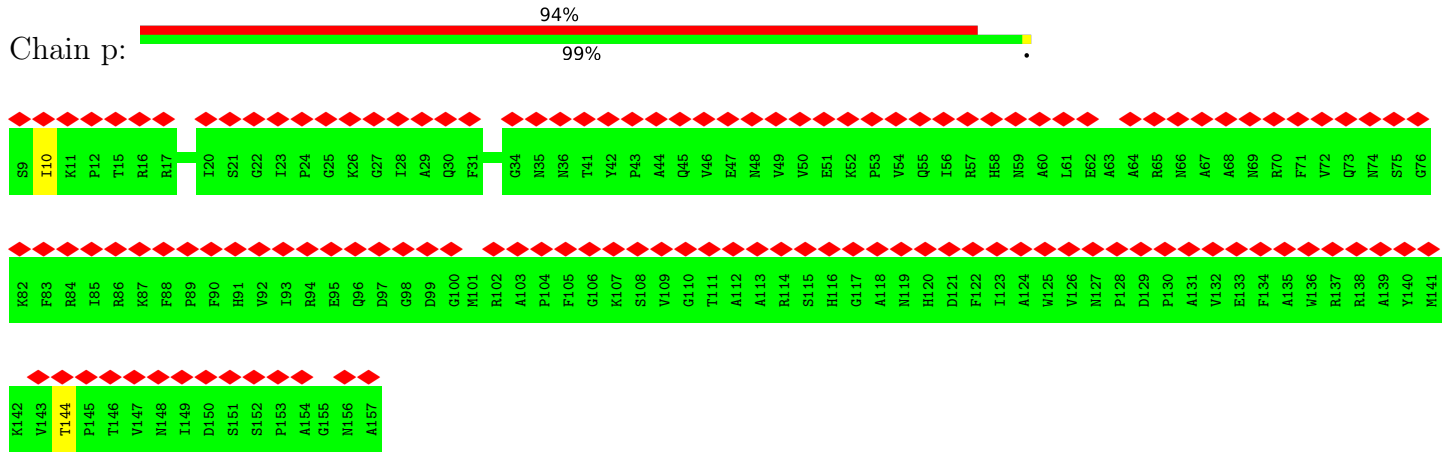


- Molecule 36: 50S RIBOSOMAL PROTEIN L15

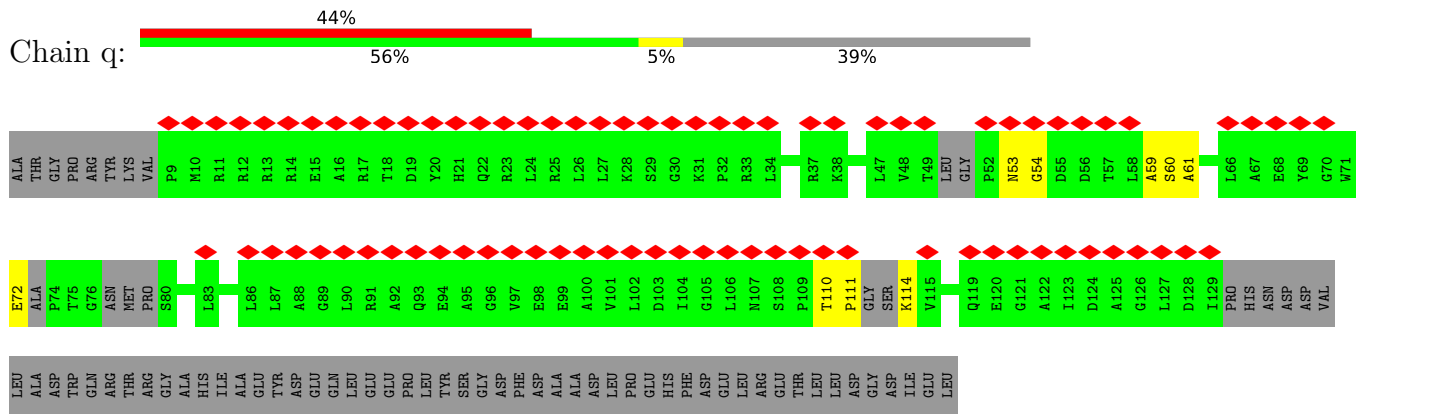




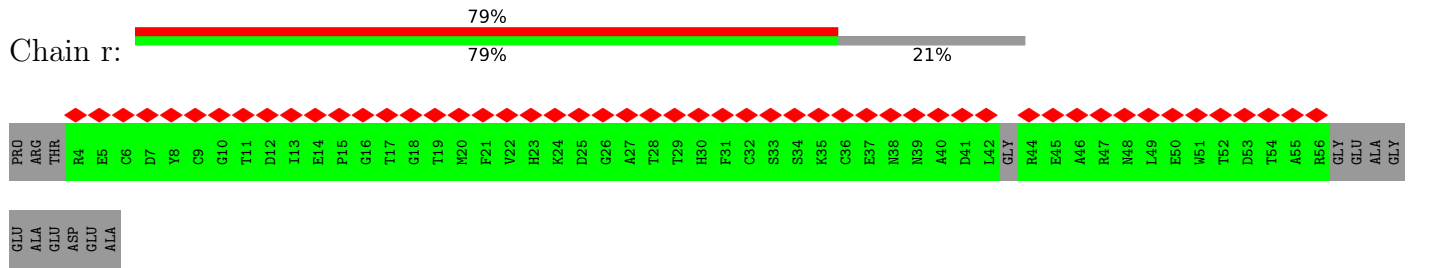
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



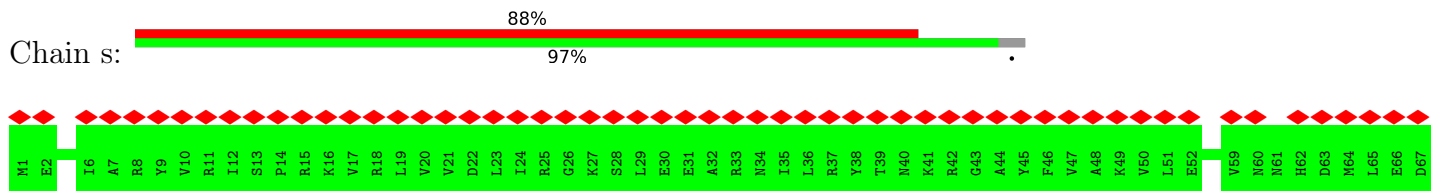
• Molecule 38: 50S RIBOSOMAL PROTEIN L18



• Molecule 39: 50S RIBOSOMAL PROTEIN L19

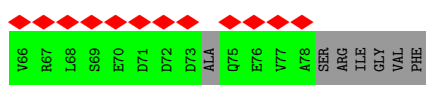
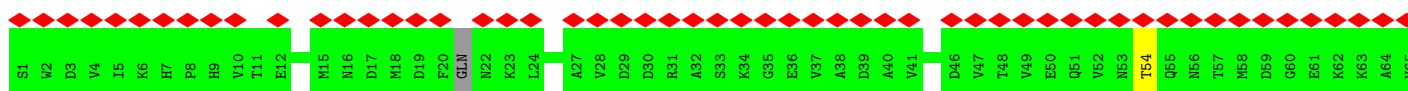
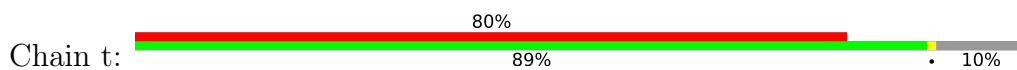


• Molecule 40: 50S RIBOSOMAL PROTEIN L22

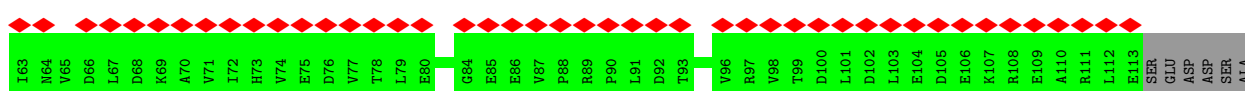
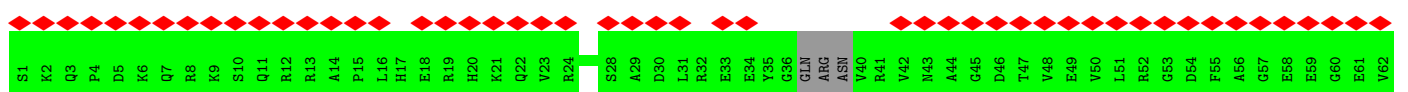
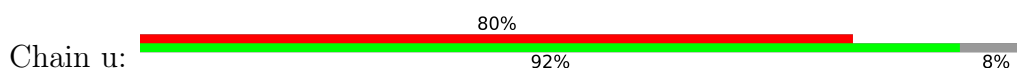




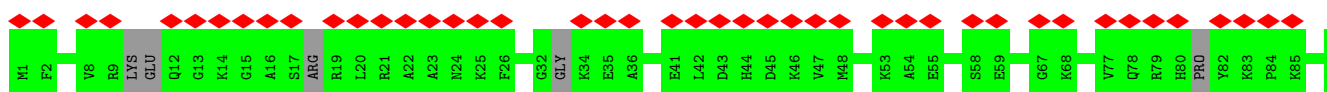
• Molecule 41: 50S RIBOSOMAL PROTEIN L23



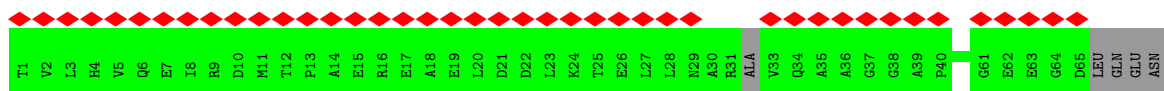
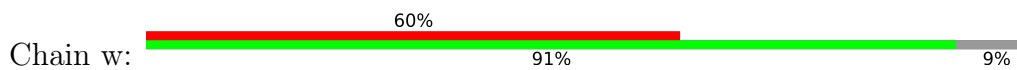
• Molecule 42: 50S RIBOSOMAL PROTEIN L24



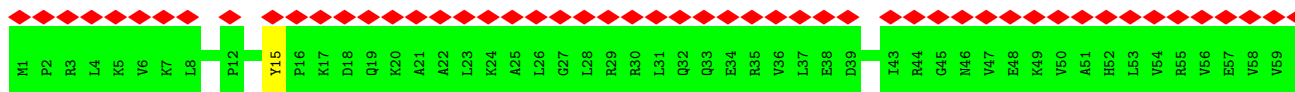
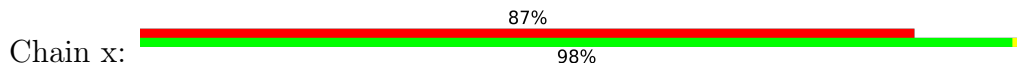
• Molecule 43: 50S RIBOSOMAL PROTEIN L25



• Molecule 44: 50S RIBOSOMAL PROTEIN L29



• Molecule 45: 50S RIBOSOMAL PROTEIN L30



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15800	Depositor
Resolution determination method	Not provided	
CTF correction method	phase flipping CTF correction of each particle as function of position in the micrograph	Depositor
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	48000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.160	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0401	Depositor
Map size ( $\text{\AA}$ )	290.28, 290.28, 290.28	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.419, 2.419, 2.419	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: 5MC, M2G, OMC, 5MU, YG, 2MG, OMG, PSU, 1MA, H2U, 7MG

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
2	B	1.10	6/1487 (0.4%)	1.44	23/2315 (1.0%)
3	C	1.89	5/131 (3.8%)	2.09	3/200 (1.5%)
All	All	1.18	11/1618 (0.7%)	1.50	26/2515 (1.0%)

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
2	B	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	C	O3'-P	-21.57	1.28	1.61
2	B	75	C	O3'-P	-20.59	1.30	1.61
2	B	44	A	O3'-P	-13.56	1.40	1.61
2	B	72	C	O3'-P	-12.66	1.42	1.61
3	C	14	U	O3'-P	-9.78	1.46	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	C	O3'-P-O5'	30.97	150.46	104.00
3	C	13	U	P-O3'-C3'	21.83	152.94	120.20
2	B	35	A	P-O3'-C3'	21.29	152.14	120.20
2	B	72	C	O3'-P-O5'	17.66	130.50	104.00
3	C	13	U	O3'-P-O5'	17.05	129.58	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	18	G	Sidechain
2	B	19	G	Sidechain
2	B	62	A	Sidechain

## 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	A	1519	0	0	16	0
2	B	1652	0	862	65	0
3	C	120	0	61	11	0
4	a	2889	0	0	29	0
5	b	123	0	0	2	0
6	Z	362	0	0	23	0
7	E	234	0	0	0	0
8	F	206	0	0	2	0
9	G	208	0	0	2	0
10	H	150	0	0	1	0
11	I	101	0	0	0	0
12	J	155	0	0	0	0
13	K	138	0	0	0	0
14	L	127	0	0	3	0
15	M	98	0	0	5	0
16	N	119	0	0	0	0
17	O	124	0	0	1	0
18	P	125	0	0	2	0
19	Q	60	0	0	4	0
20	R	88	0	0	0	0
21	S	83	0	0	0	0
22	T	104	0	0	0	0
23	U	73	0	0	0	0
24	V	80	0	0	0	0
25	W	99	0	0	0	0
26	X	24	0	0	0	0
27	c	224	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	173	0	0	6	0
29	e	191	0	0	7	0
30	f	189	0	0	9	0
31	g	122	0	0	1	0
32	h	164	0	0	0	0
33	l	133	0	0	0	0
34	m	117	0	0	1	0
35	n	122	0	0	0	0
36	o	84	0	0	2	0
37	p	138	0	0	2	0
38	q	113	0	0	6	0
39	r	52	0	0	0	0
40	s	110	0	0	0	0
41	t	76	0	0	1	0
42	u	110	0	0	0	0
43	v	89	0	0	0	0
44	w	64	0	0	0	0
45	x	60	0	0	1	0
All	All	11392	0	923	140	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 140 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)
30:f:100:LEU:CA	30:f:101:ASP:CA	1.80	1.58
2:B:73:A:H3'	6:Z:255:ASN:CA	1.33	1.51
1:A:430:A:P	9:G:7:PRO:CA	2.16	1.34
2:B:73:A:C3'	6:Z:255:ASN:CA	2.05	1.33
28:d:196:ASN:CA	28:d:197:GLY:CA	2.06	1.33

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1522	-	-
2	B	73/76 (96%)	12 (16%)	3 (4%)
3	C	5/6 (83%)	1 (20%)	0
4	a	0/2916	-	-
5	b	0/123	-	-
All	All	78/4643 (1%)	13 (16%)	3 (3%)

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	17	H2U
2	B	18	G
2	B	19	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	H2U
2	B	18	G
2	B	35	A

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

14 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
2	YG	B	37	2	38,42,43	0.90	2 (5%)	45,62,65	2.32	10 (22%)
2	7MG	B	46	2	23,26,27	0.98	2 (8%)	27,39,42	1.26	2 (7%)
2	1MA	B	58	2	21,25,26	2.09	2 (9%)	30,37,40	1.86	7 (23%)
2	OMC	B	32	2	19,22,23	0.45	0	25,31,34	0.59	0
2	PSU	B	55	2	18,21,22	0.74	0	21,30,33	0.89	0
2	OMG	B	34	2,3	23,26,27	0.54	0	32,38,41	0.51	0
2	M2G	B	26	2	24,27,28	0.47	0	33,40,43	0.42	0
2	H2U	B	17	2	18,21,22	0.70	1 (5%)	19,30,33	0.93	1 (5%)
2	PSU	B	39	2	18,21,22	0.70	0	21,30,33	0.73	0
2	5MU	B	54	2	19,22,23	0.46	0	27,32,35	0.67	0
2	2MG	B	10	2	23,26,27	0.49	0	33,38,41	0.43	0
2	5MC	B	49	2	19,22,23	0.73	0	26,32,35	0.76	1 (3%)
2	H2U	B	16	2	18,21,22	0.76	1 (5%)	19,30,33	1.02	1 (5%)
2	5MC	B	40	2	19,22,23	0.71	1 (5%)	26,32,35	0.71	1 (3%)

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
2	YG	B	37	2	-	7/24/42/43	0/4/4/4
2	7MG	B	46	2	-	2/7/37/38	0/3/3/3
2	1MA	B	58	2	-	0/7/25/26	0/3/3/3
2	OMC	B	32	2	-	0/9/27/28	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	OMG	B	34	2,3	-	1/9/27/28	0/3/3/3
2	M2G	B	26	2	-	0/11/29/30	0/3/3/3
2	H2U	B	17	2	-	0/7/38/39	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
2	5MC	B	49	2	-	0/7/25/26	0/2/2/2
2	H2U	B	16	2	-	4/7/38/39	0/2/2/2
2	5MC	B	40	2	-	1/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	1MA	C6-N6	8.47	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	1MA	C2-N3	3.74	1.37	1.30
2	B	37	YG	C2-N2	3.11	1.38	1.33
2	B	46	7MG	C4-N9	2.75	1.41	1.37
2	B	16	H2U	C2-N1	2.62	1.39	1.35

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	YG	C11-C12-N1	8.59	111.36	105.31
2	B	37	YG	C24-O23-C21	6.39	123.03	115.63
2	B	58	1MA	CM1-N1-C6	-4.99	112.41	120.15
2	B	46	7MG	C4-C5-N7	4.85	111.11	105.38
2	B	37	YG	C5-C4-N3	4.76	127.86	123.99

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C6
2	B	16	H2U	C2'-C1'-N1-C6
2	B	37	YG	C15-C16-O18-C19
2	B	46	7MG	C2'-C1'-N9-C8

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	37	YG	6	0
2	B	32	OMC	1	0
2	B	34	OMG	4	0
2	B	26	M2G	6	0
2	B	17	H2U	3	0
2	B	10	2MG	3	0
2	B	16	H2U	3	0
2	B	40	5MC	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
2	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	25:C	O3'	26:M2G	P	2.12
1	B	75:C	O3'	76:A	P	1.30
1	B	74:C	O3'	75:C	P	1.28
1	B	36:A	O3'	37:YG	P	1.18

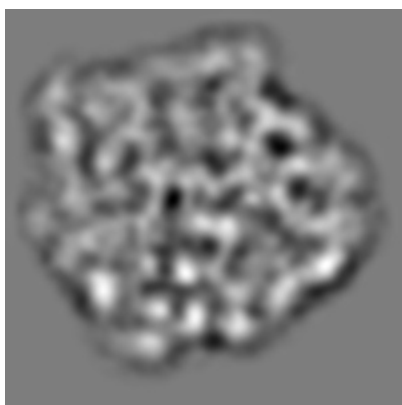
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1005. These allow visual inspection of the internal detail of the map and identification of artifacts.

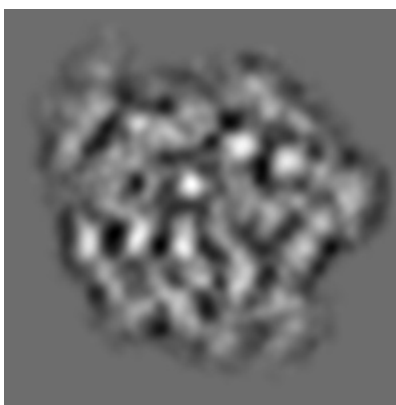
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

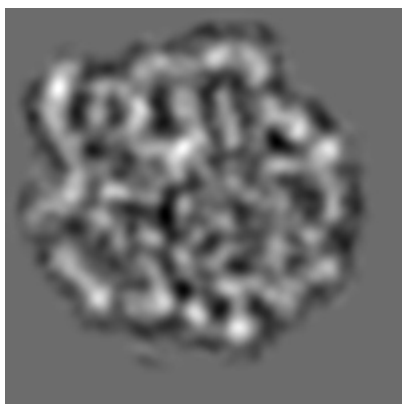


Z

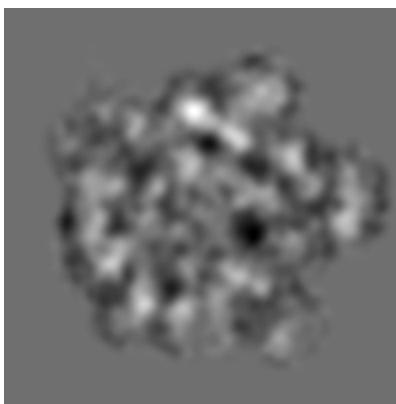
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

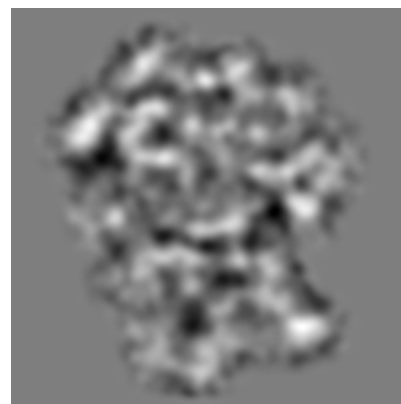
#### 6.2.1 Primary map



X Index: 60



Y Index: 60

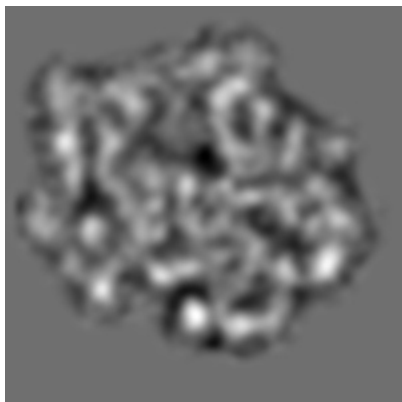


Z Index: 60

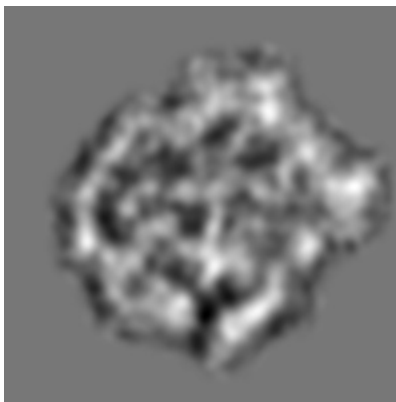
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

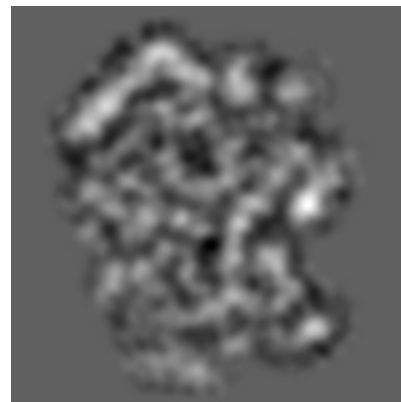
### 6.3.1 Primary map



X Index: 53



Y Index: 74

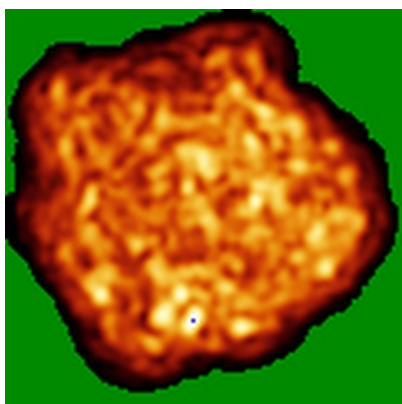


Z Index: 56

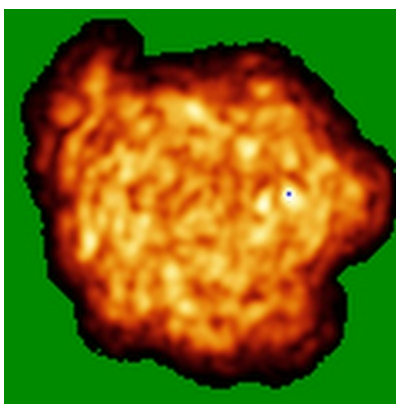
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

### 6.4.1 Primary map



X



Y



Z

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

This section was not generated.

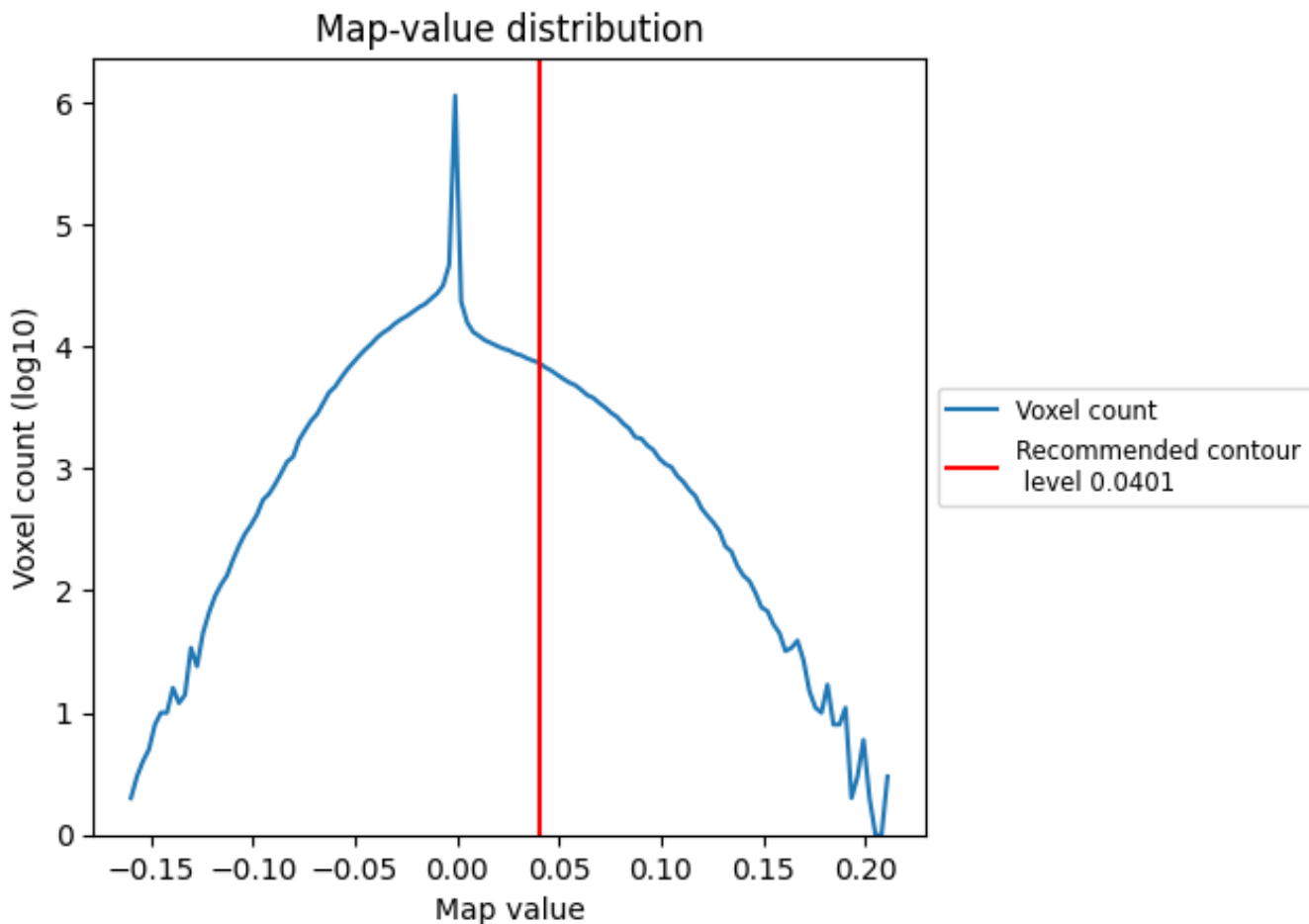
## 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

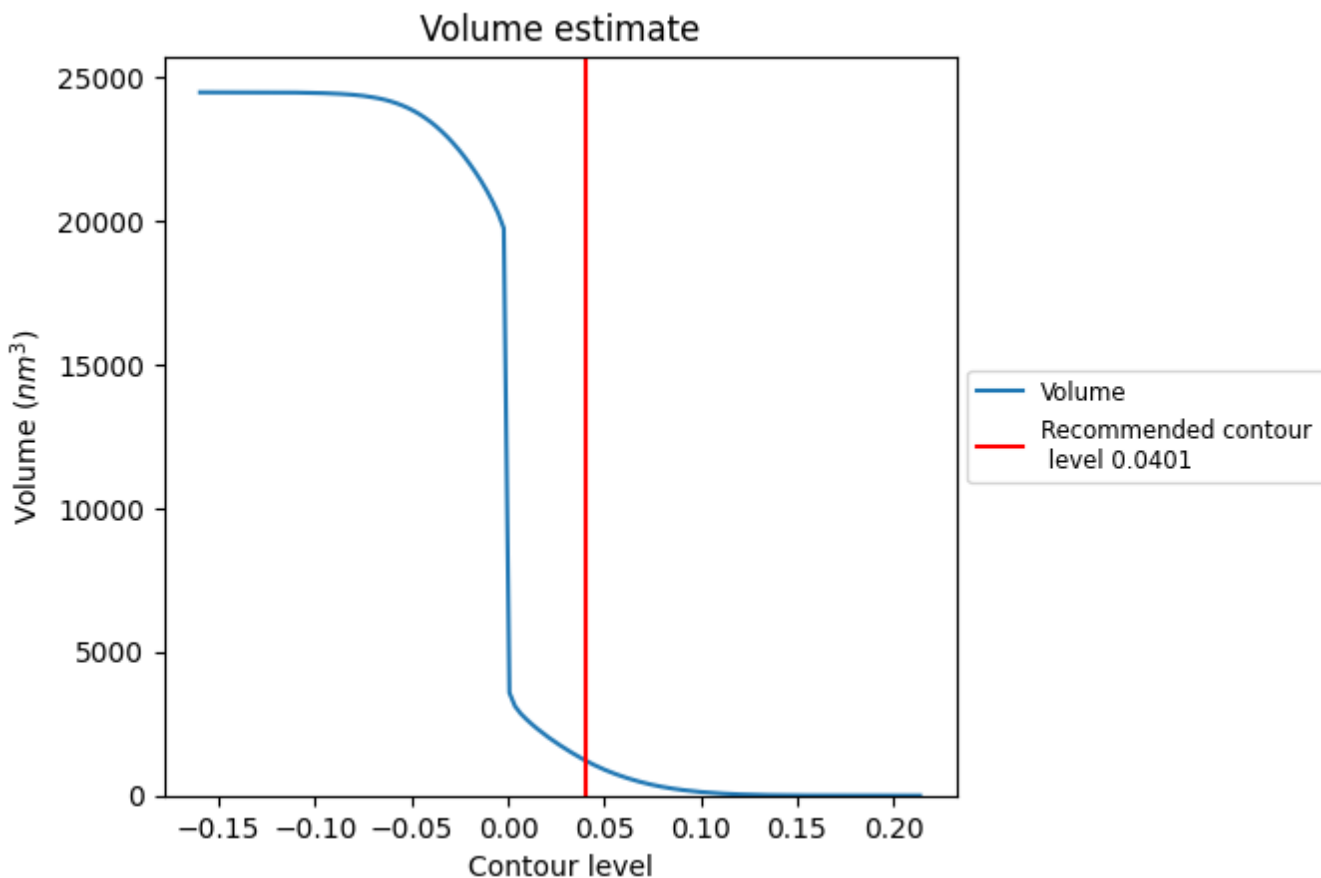
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

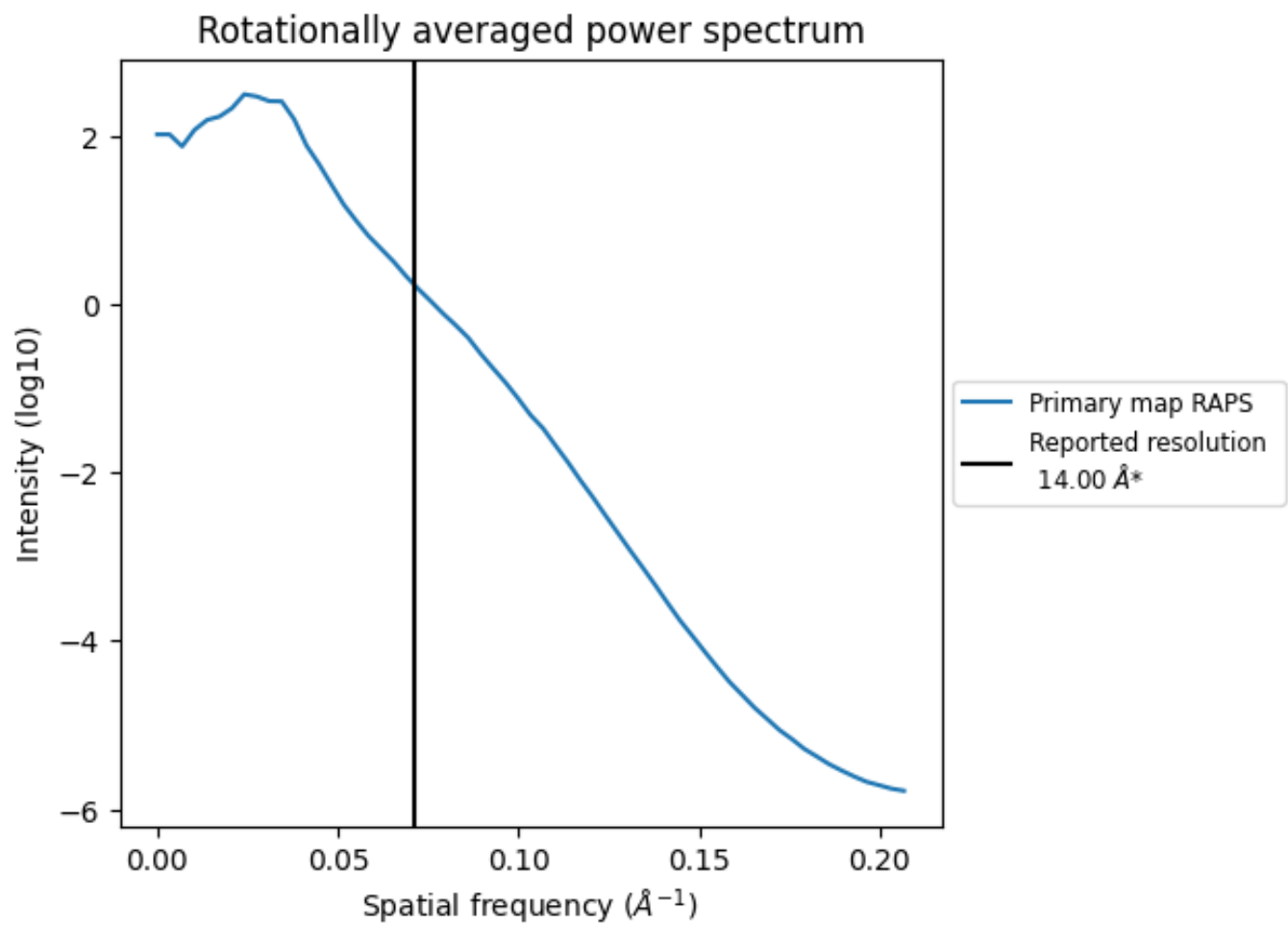
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1226 nm<sup>3</sup>; this corresponds to an approximate mass of 1107 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  $0.071 \text{\AA}^{-1}$

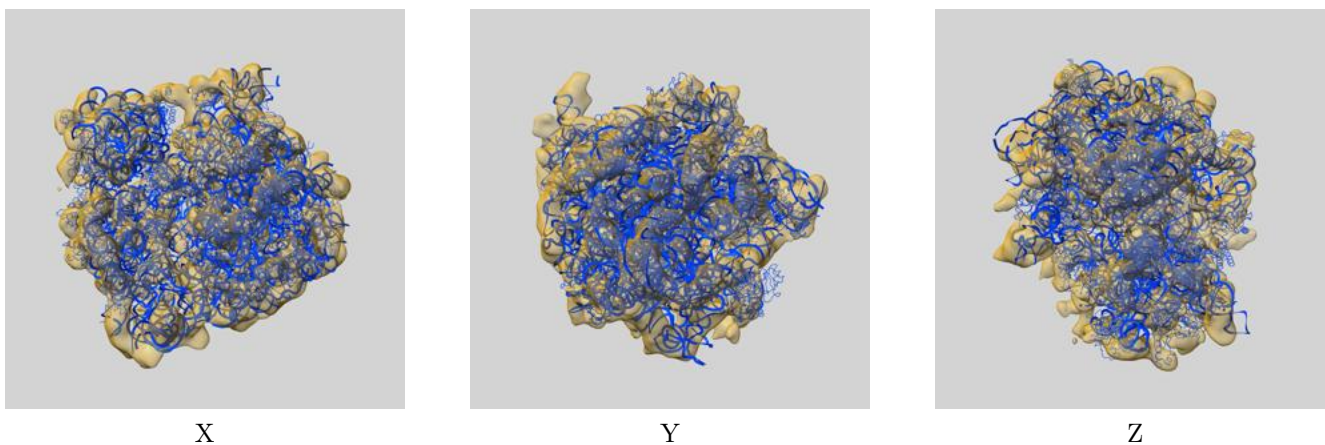
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

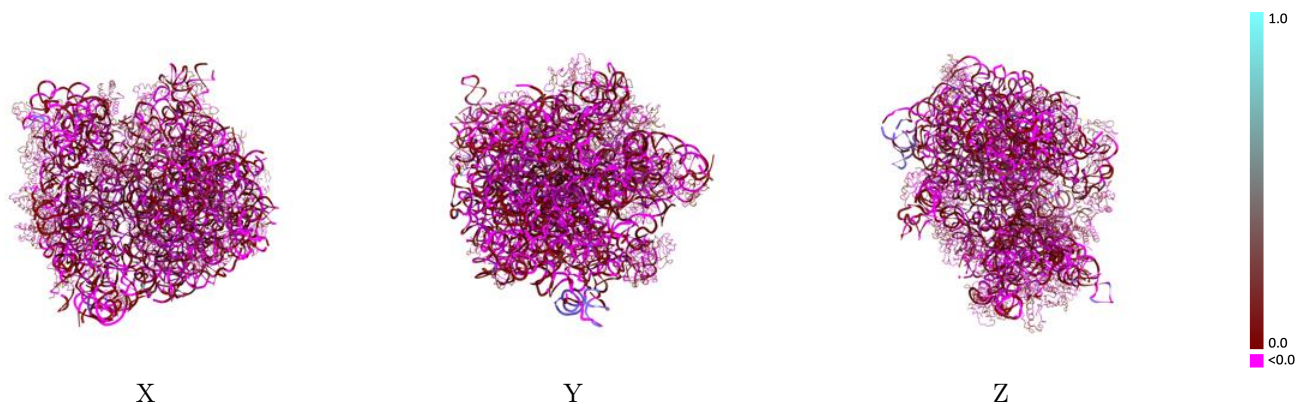
This section contains information regarding the fit between EMDB map EMD-1005 and PDB model 1ML5. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0401 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)

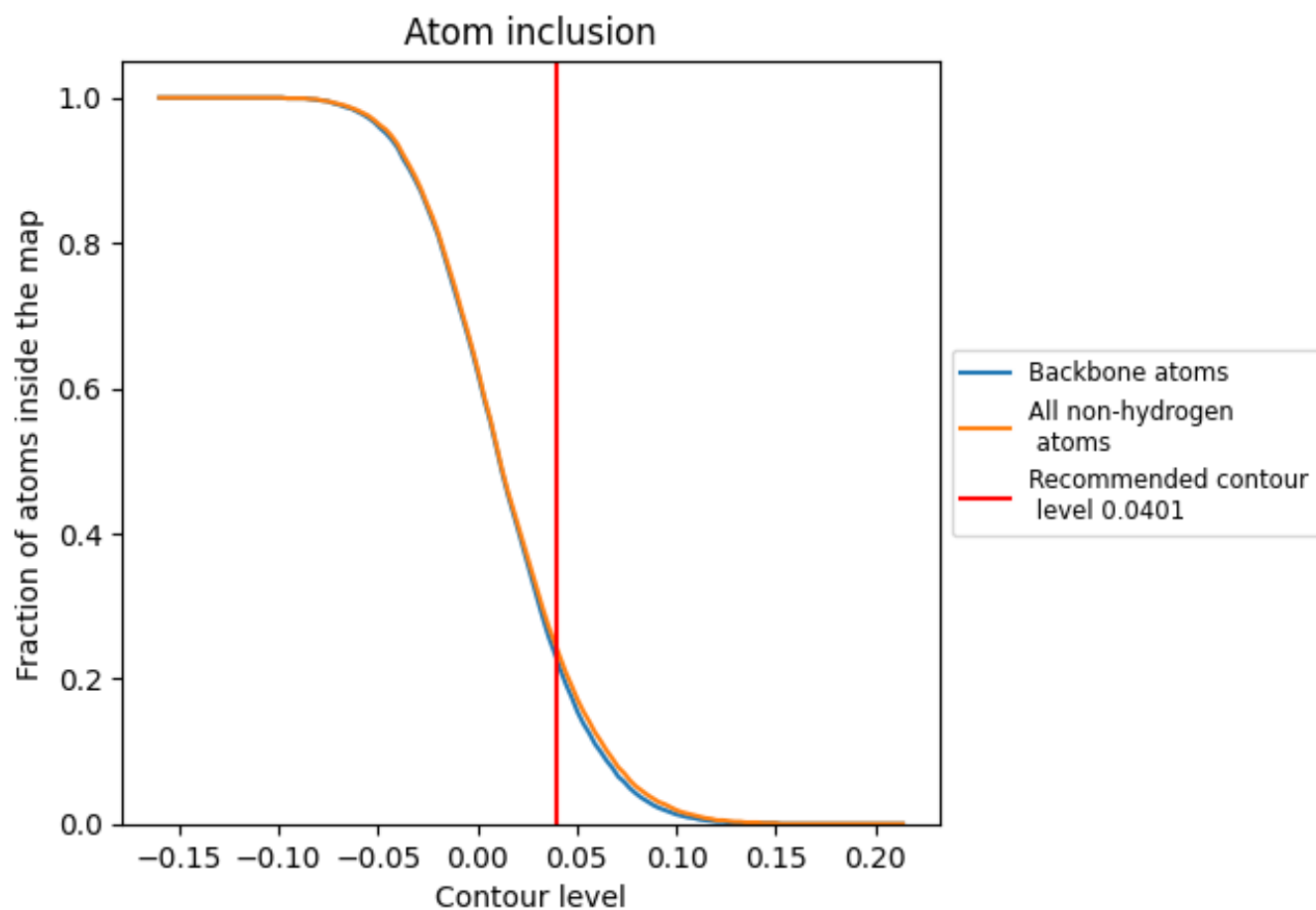


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 23% of all backbone atoms, 24% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)























The table lists the average atom inclusion at the recommended contour level (0.0401) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2410	0.0130
A	0.2630	0.0080
B	0.3490	0.0370
C	0.0000	-0.0190
E	0.2050	0.0140
F	0.1750	0.0200
G	0.2070	0.0190
H	0.1270	0.0090
I	0.2770	0.0010
J	0.3550	0.0190
K	0.1520	-0.0160
L	0.1580	0.0120
M	0.2960	0.0050
N	0.3530	0.0310
O	0.3630	0.0280
P	0.2240	0.0190
Q	0.0500	-0.0220
R	0.2610	0.0430
S	0.0240	0.0070
T	0.0960	0.0070
U	0.1100	-0.0070
V	0.0750	0.0320
W	0.1510	-0.0240
X	0.0000	-0.0200
Z	0.1270	0.0250
a	0.2740	0.0090
b	0.3500	0.0050
c	0.0270	-0.0150
d	0.0690	0.0200
e	0.1570	0.0030
f	0.2960	0.0060
g	0.1470	-0.0100
h	0.3110	0.0200
l	0.2780	0.0250
m	0.1110	-0.0110



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Chain	Atom inclusion	Q-score
n	 0.0330	 0.0130
o	 0.3570	 0.0110
p	 0.0580	 -0.0190
q	 0.2740	 0.0160
r	 0.0000	 -0.0410
s	 0.1000	 -0.0170
t	 0.1180	 0.0430
u	 0.1360	 -0.0120
v	 0.5060	 0.0340
w	 0.3440	 0.0800
x	 0.1330	 0.0170