



## wwPDB EM Validation Summary Report ⓘ

Oct 23, 2024 – 01:08 AM EDT

PDB ID : 4V6Z  
EMDB ID : EMD-2472  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in classic pre-translocation state (pre1b)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 12.00 Å (reported)  
Based on initial models : 2WRI, 3I1O, 2K4C, 2HGP

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

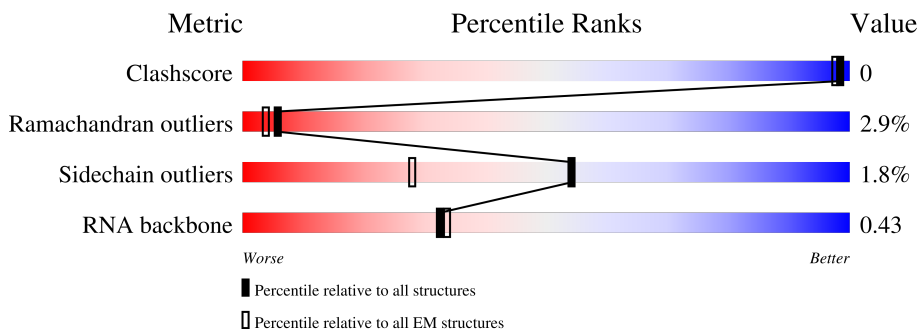
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AB	220	<div> <div>50%</div> <div>94%</div> <div>6%</div> </div>
2	AC	208	<div> <div>46%</div> <div>89%</div> <div>10%</div> </div>
3	AD	206	<div> <div>51%</div> <div>88%</div> <div>11%</div> </div>
4	AE	152	<div> <div>45%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>
5	AF	101	<div> <div>26%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
6	AG	152	<div> <div>36%</div> <div>93%</div> <div>7%</div> </div>
7	AH	130	<div> <div>43%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	AI	128	
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	

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Mol	Chain	Length	Quality of chain
33	BK	123	<div> <div>51%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
34	BL	144	<div> <div>33%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
35	BM	136	<div> <div>54%</div> <div>89%</div> <div>11%</div> <div></div> </div>
36	BN	121	<div> <div>42%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
37	BO	117	<div> <div>11%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
38	BP	115	<div> <div>53%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
39	BQ	118	<div> <div>43%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
40	BR	103	<div> <div>31%</div> <div>89%</div> <div>11%</div> <div></div> </div>
41	BS	110	<div> <div>46%</div> <div>90%</div> <div>10%</div> <div></div> </div>
42	BT	94	<div> <div>36%</div> <div>89%</div> <div>11%</div> <div></div> </div>
43	BU	104	<div> <div>39%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
44	BV	94	<div> <div>34%</div> <div>93%</div> <div>7%</div> <div></div> </div>
45	BW	80	<div> <div>39%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
46	BX	79	<div> <div>49%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
47	BY	63	<div> <div>40%</div> <div>92%</div> <div>8%</div> <div></div> </div>
48	BZ	59	<div> <div>51%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
49	B0	57	<div> <div>23%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
50	B1	52	<div> <div>48%</div> <div>83%</div> <div>17%</div> <div></div> </div>
51	B2	46	<div> <div>57%</div> <div>74%</div> <div>26%</div> <div></div> </div>
52	B3	65	<div> <div>51%</div> <div>91%</div> <div>6%</div> <div>..</div> </div>
53	B4	38	<div> <div>45%</div> <div>87%</div> <div>13%</div> <div></div> </div>
54	BA	2903	<div> <div>35%</div> <div>13%</div> <div>57%</div> <div>26%</div> <div>5%</div> </div>
55	BB	118	<div> <div>23%</div> <div>9%</div> <div>57%</div> <div>31%</div> <div>..</div> </div>
56	B5	234	<div> <div>60%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	amidation	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	acetylation	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	acetylation	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	amidation	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	amidation	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	57	Total	C	N	O		0	1
			459	290	87	82			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	acetylation	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	amidation	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	acetylation	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	amidation	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	amidation	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	amidation	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	amidation	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	amidation	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	acetylation	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	acetylation	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

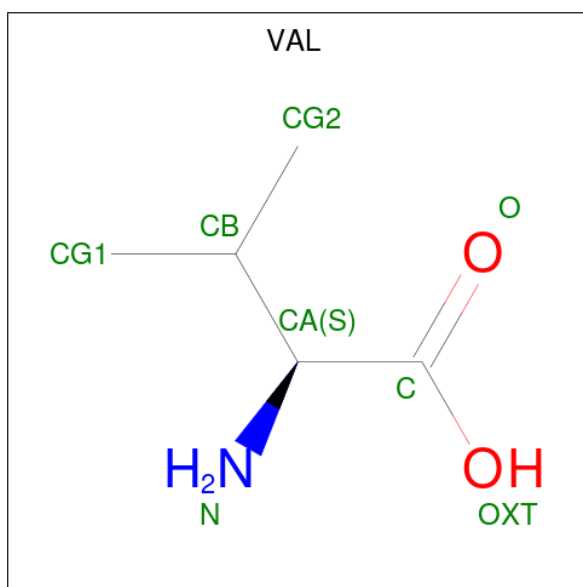
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

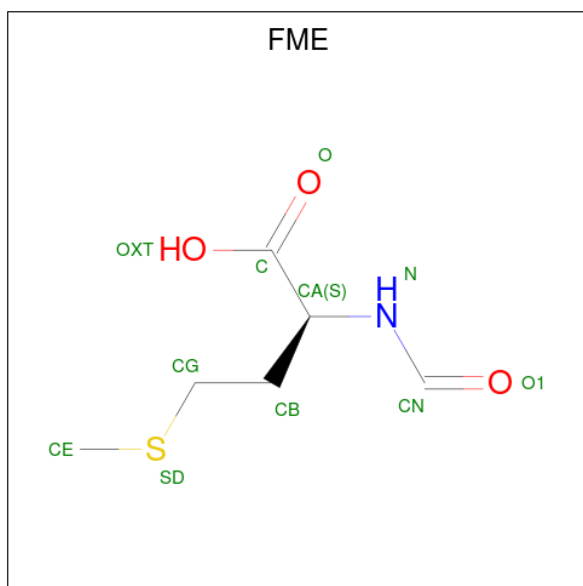
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



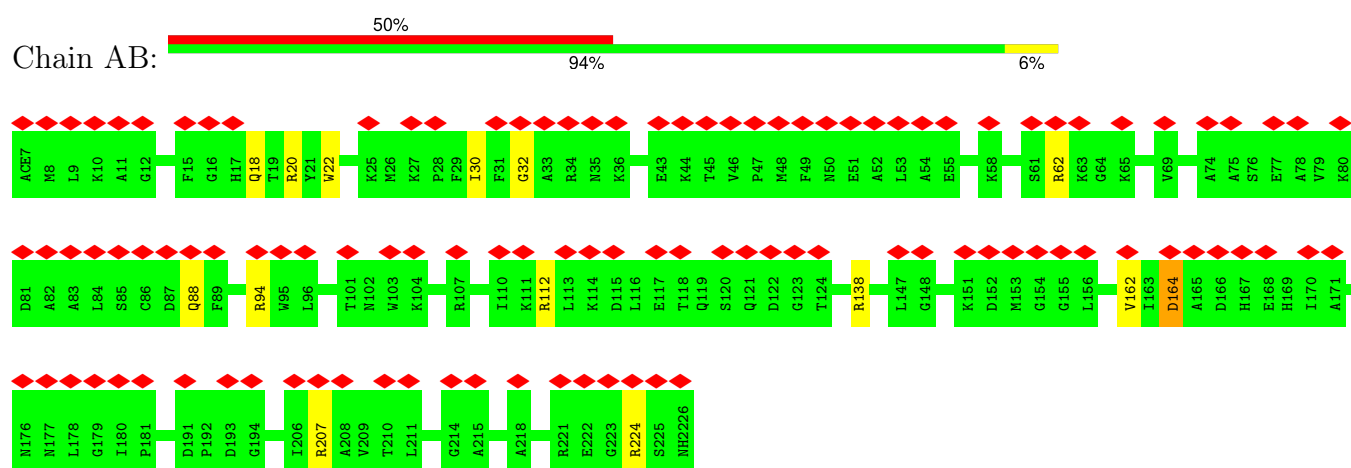
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



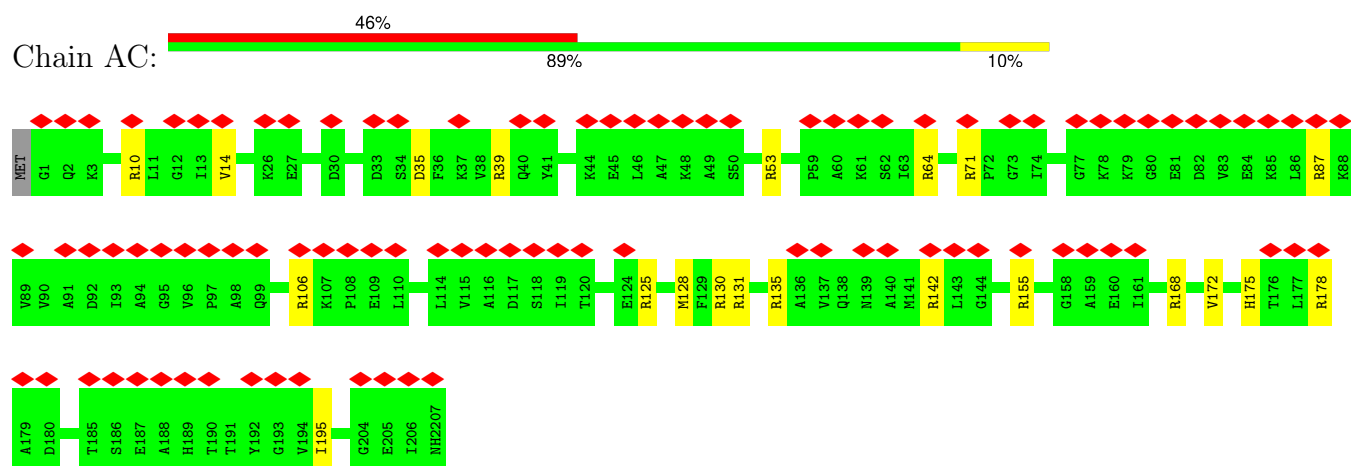
### 3 Residue-property plots

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.

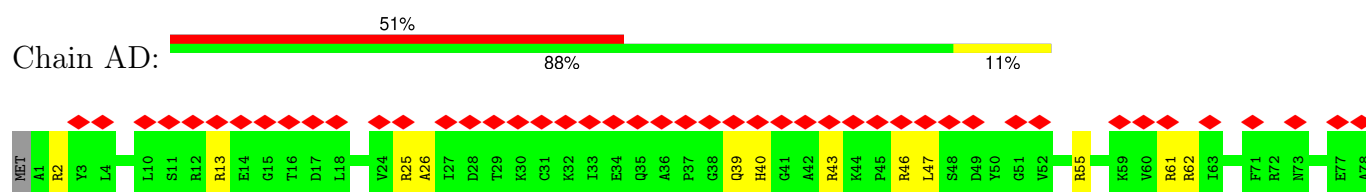
#### • Molecule 1: 30S ribosomal protein S2

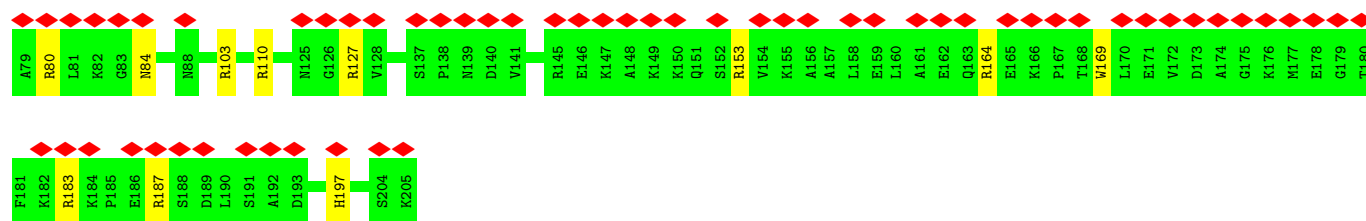


#### • Molecule 2: 30S ribosomal protein S3

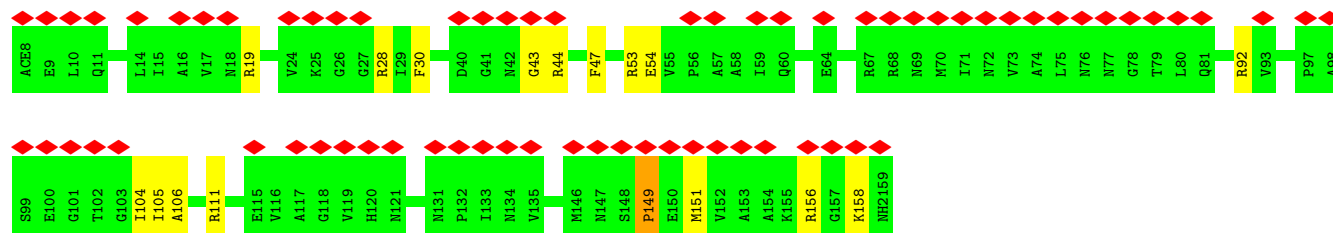
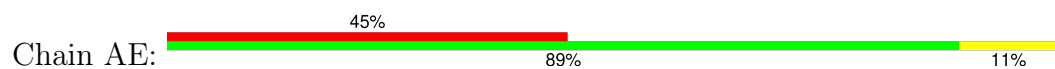


#### • Molecule 3: 30S ribosomal protein S4

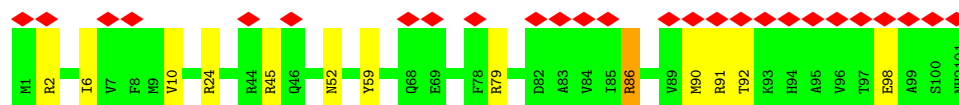
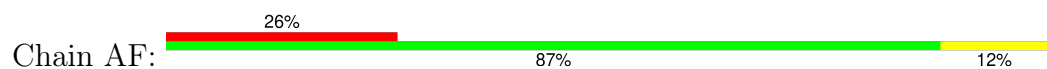




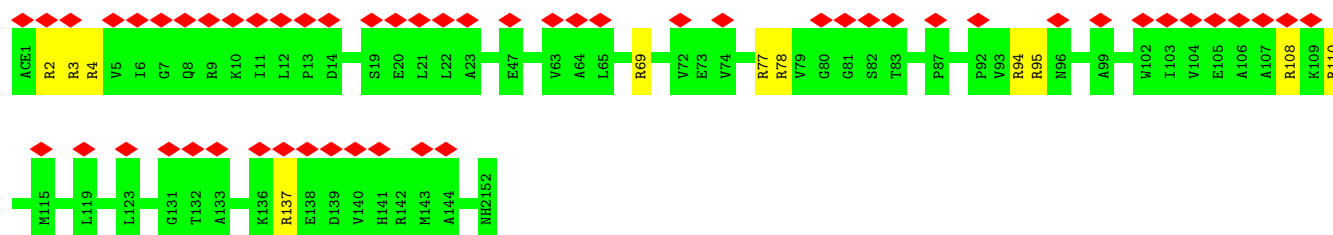
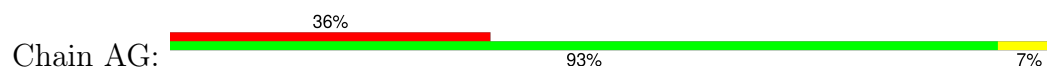
• Molecule 4: 30S ribosomal protein S5



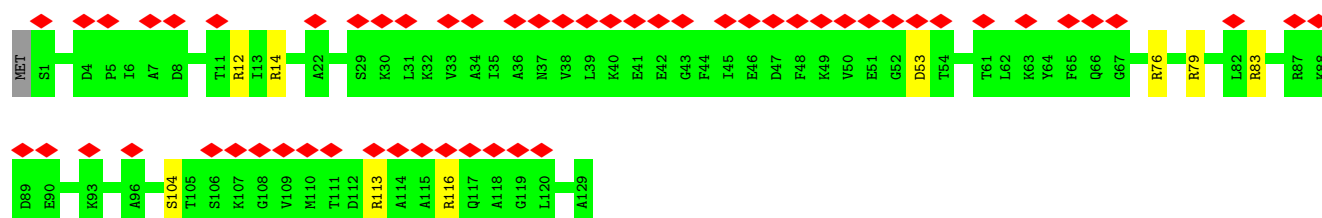
• Molecule 5: 30S ribosomal protein S6



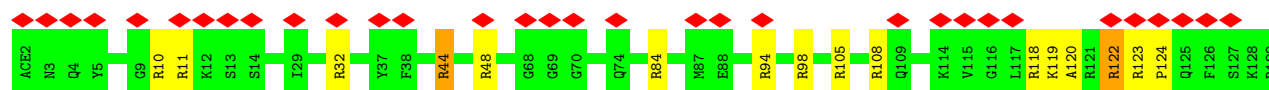
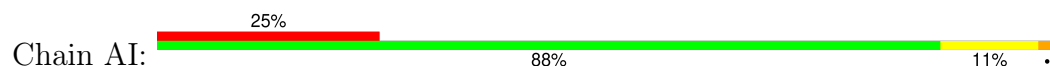
• Molecule 6: 30S ribosomal protein S7



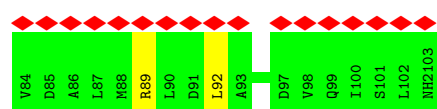
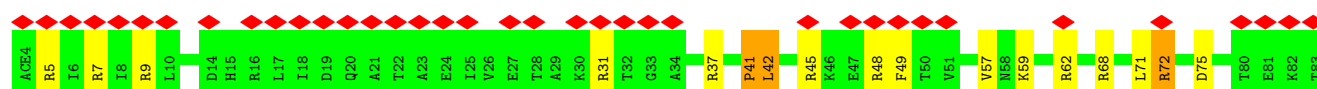
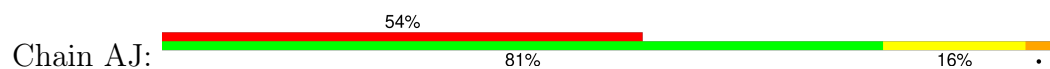
• Molecule 7: 30S ribosomal protein S8



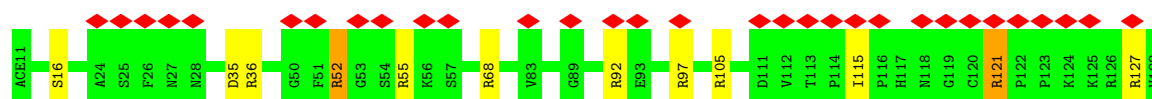
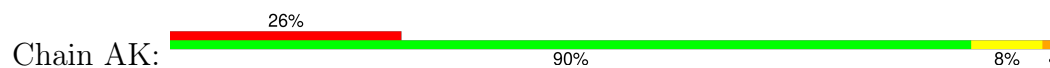
- Molecule 8: 30S ribosomal protein S9



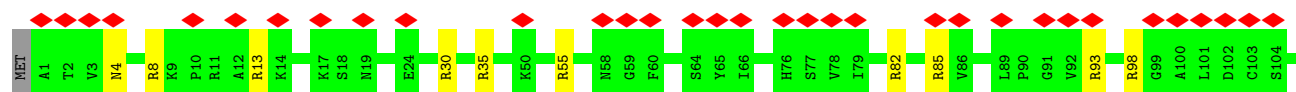
- Molecule 9: 30S ribosomal protein S10



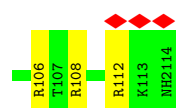
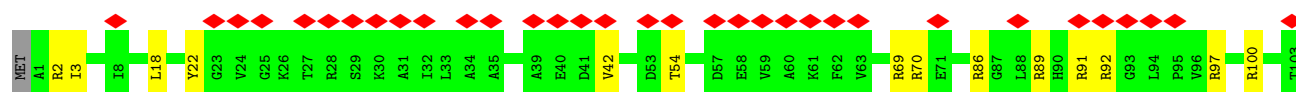
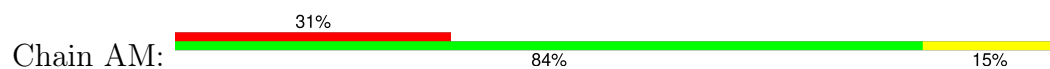
- Molecule 10: 30S ribosomal protein S11



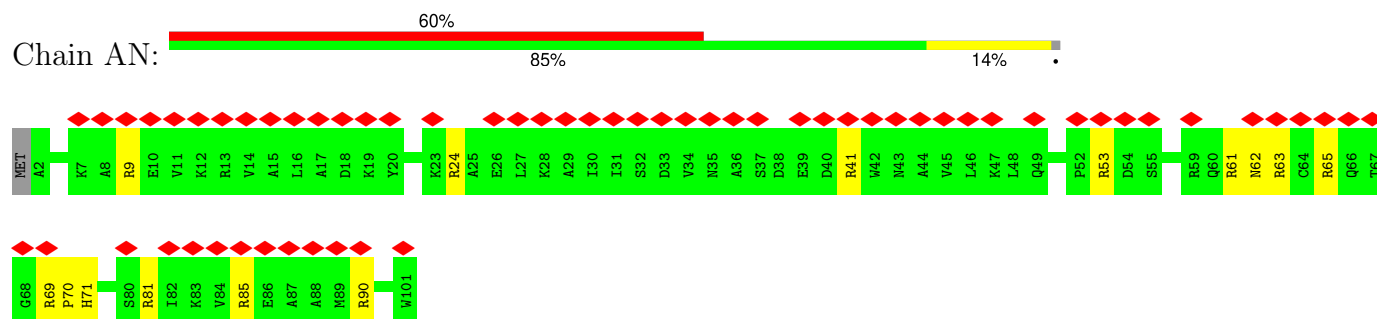
- Molecule 11: 30S ribosomal protein S12



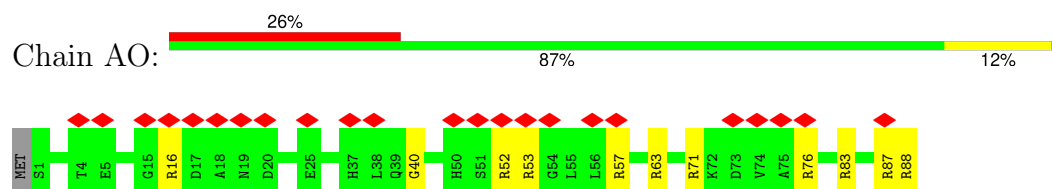
- Molecule 12: 30S ribosomal protein S13



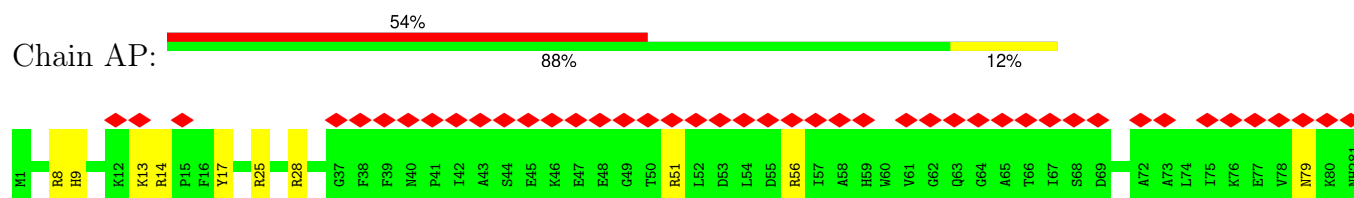
- Molecule 13: 30S ribosomal protein S14



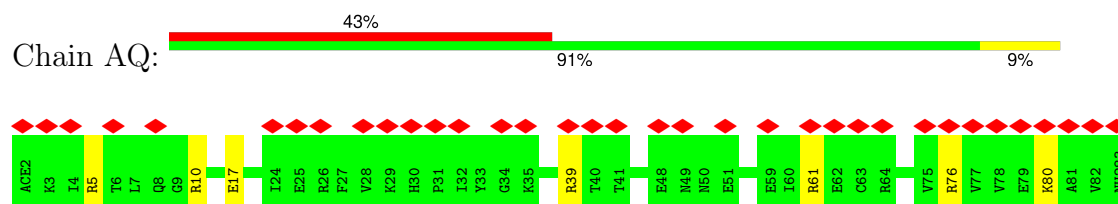
- Molecule 14: 30S ribosomal protein S15



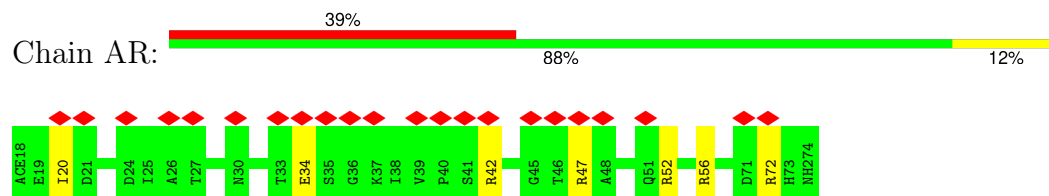
- Molecule 15: 30S ribosomal protein S16



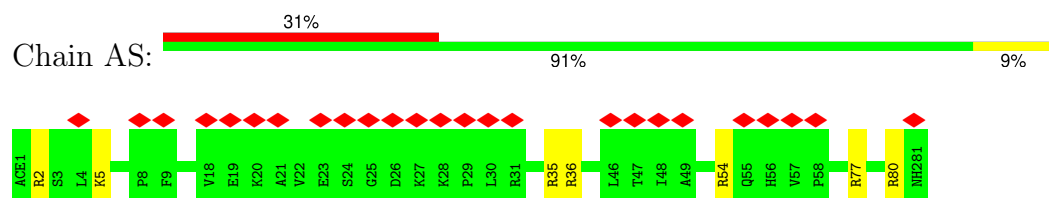
- Molecule 16: 30S ribosomal protein S17



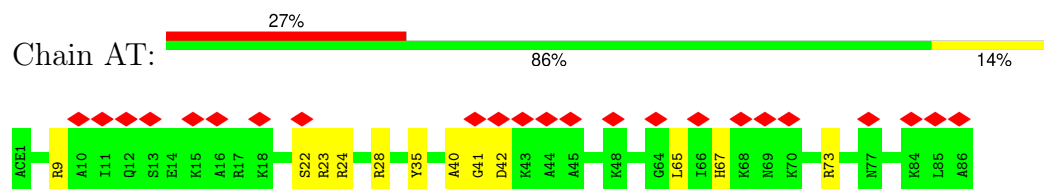
- Molecule 17: 30S ribosomal protein S18



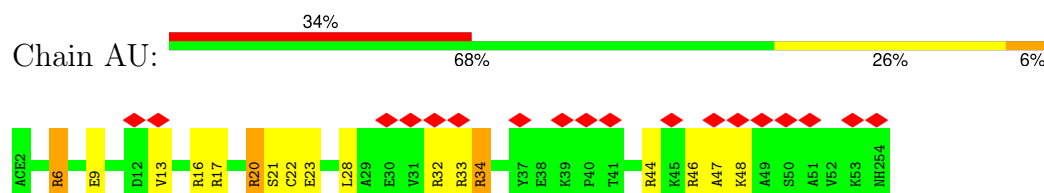
- Molecule 18: 30S ribosomal protein S19



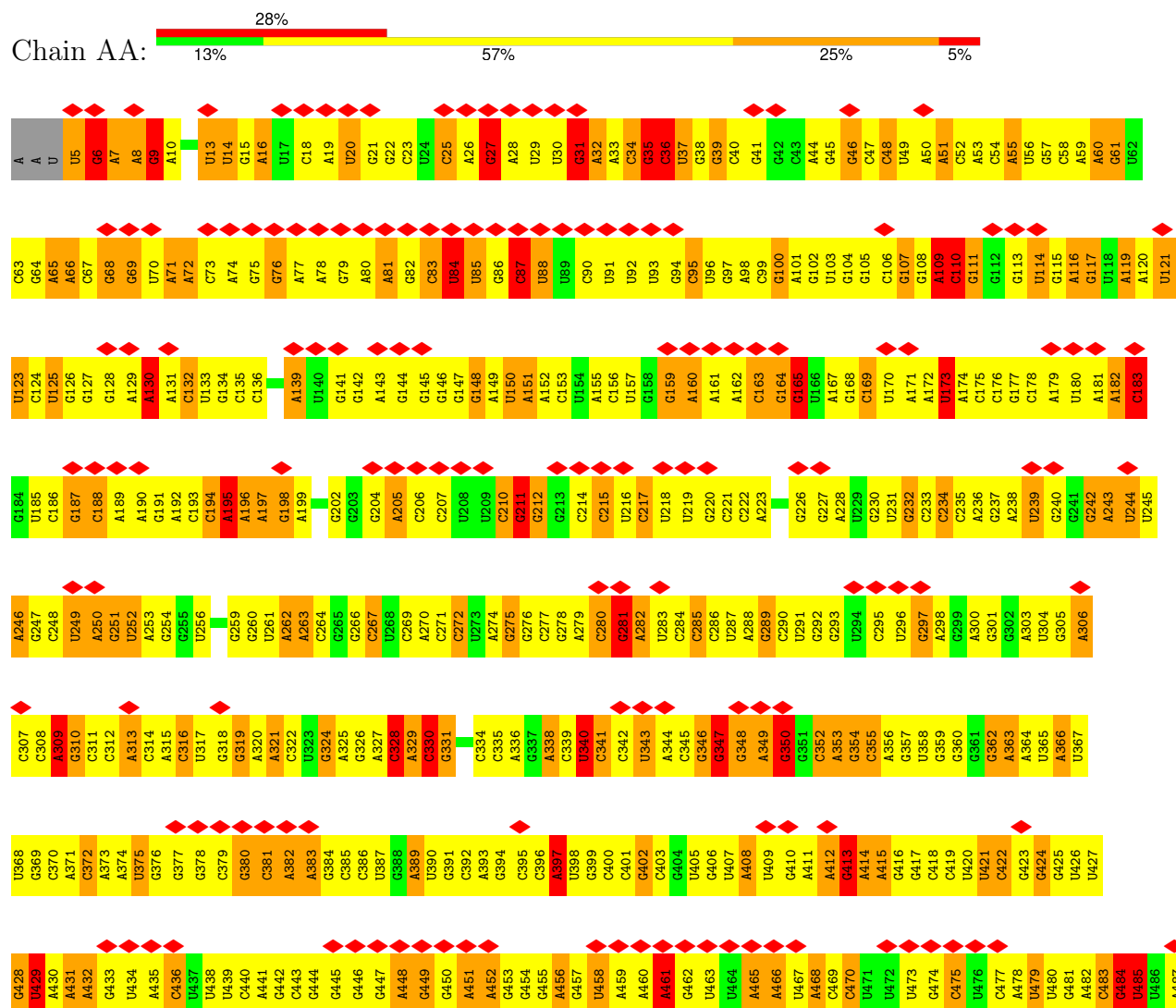
- Molecule 19: 30S ribosomal protein S20

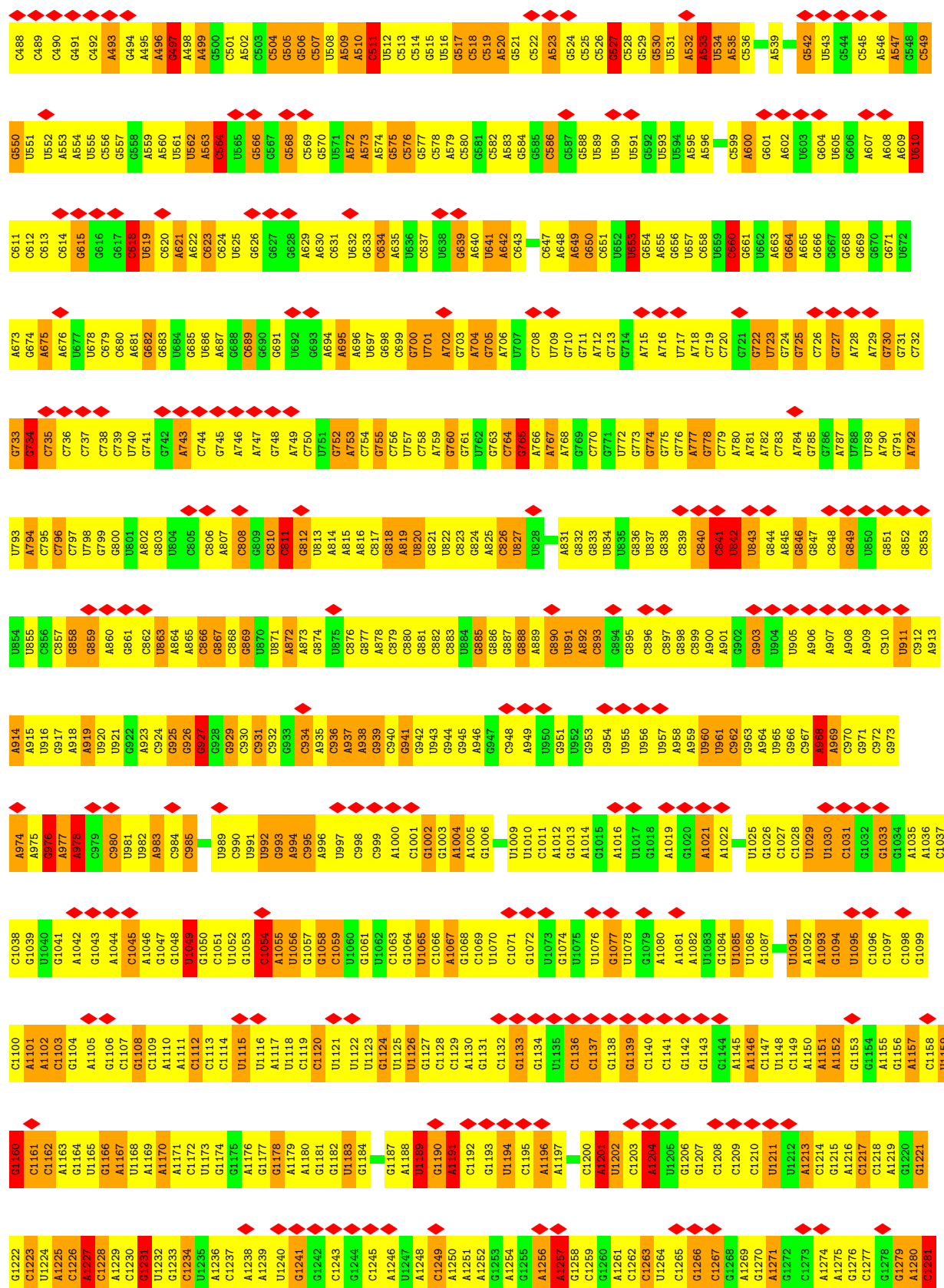


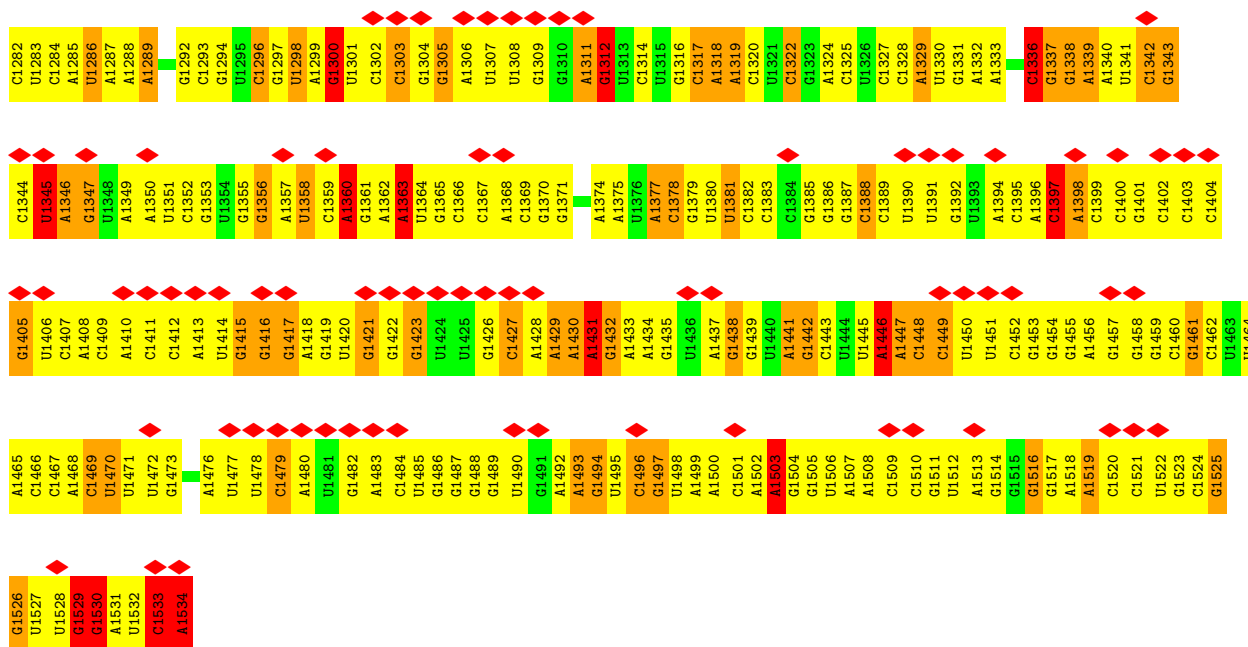
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



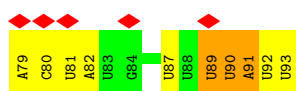




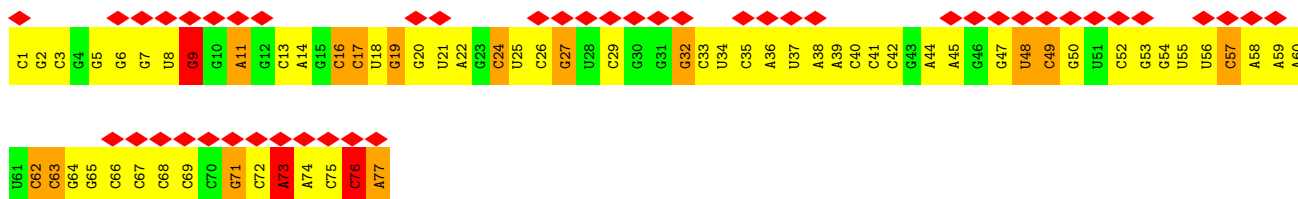
• Molecule 22: fMet-Val-tRNA-Val



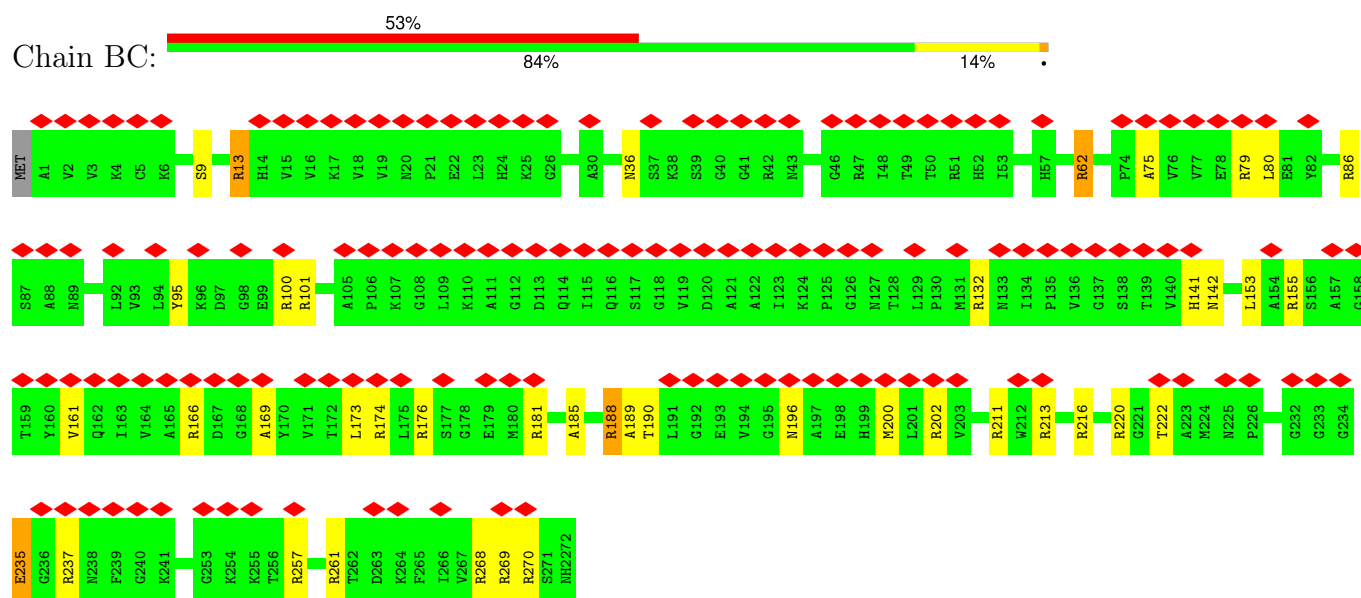
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'



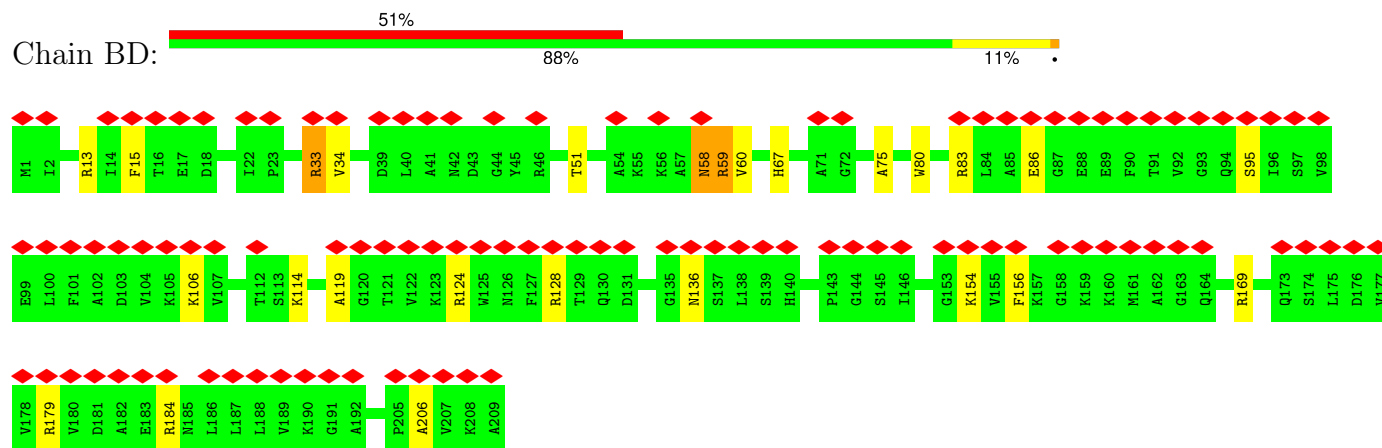
• Molecule 24: tRNA-fMet



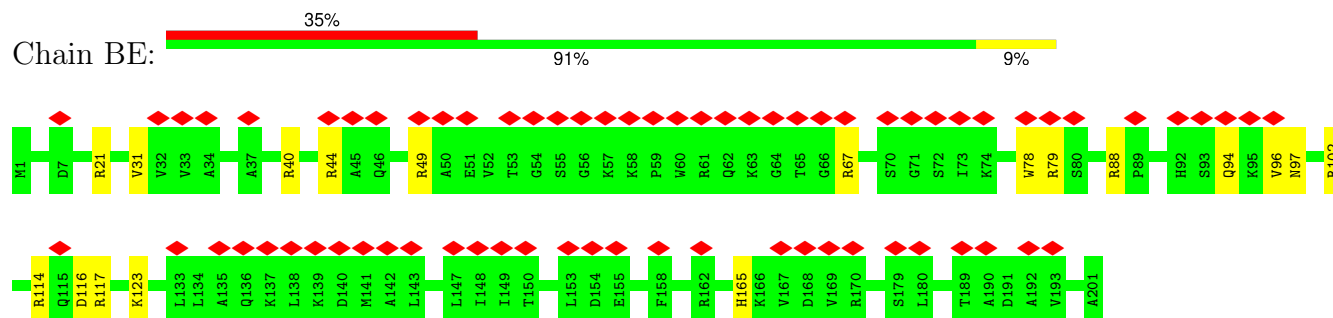
• Molecule 25: 50S ribosomal protein L2



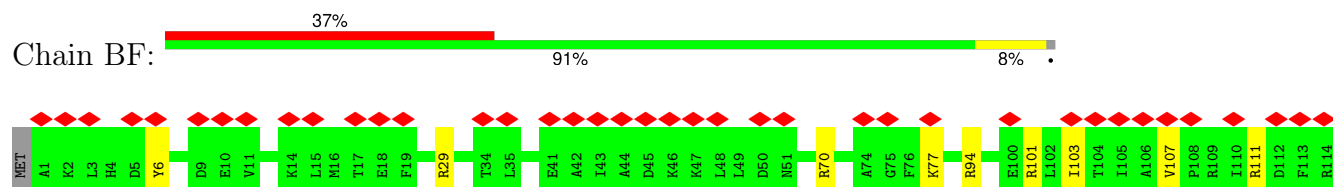
- Molecule 26: 50S ribosomal protein L3



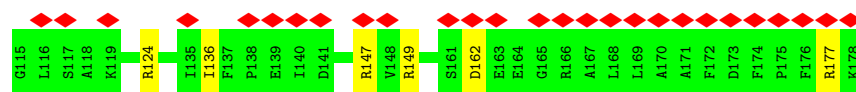
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5

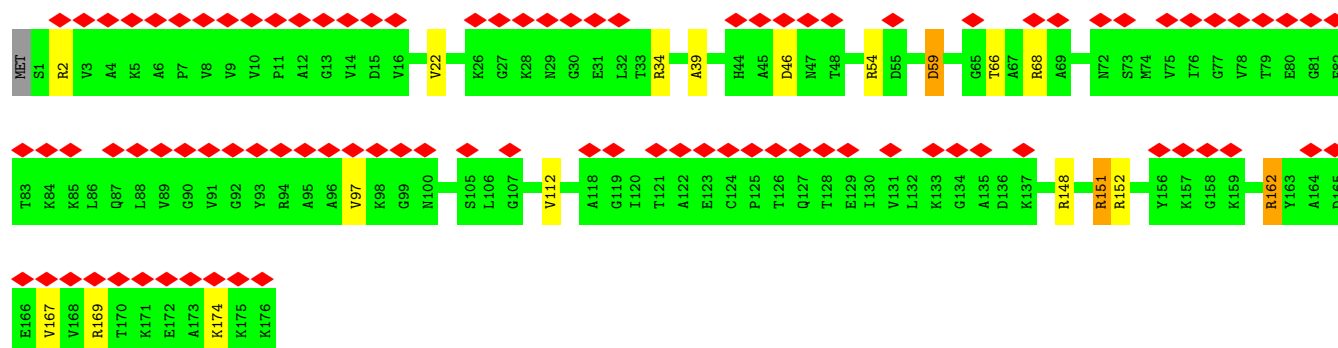






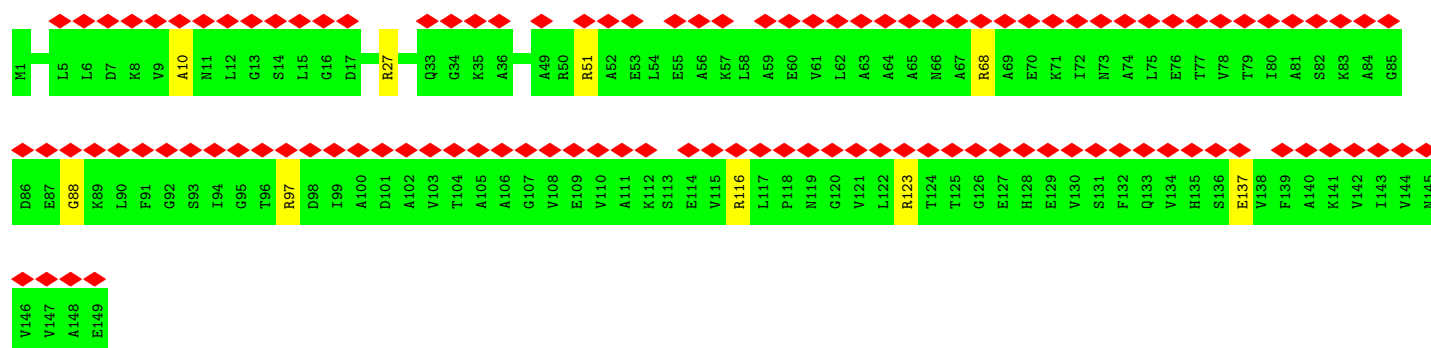
- Molecule 29: 50S ribosomal protein L6

Chain BG: 53% 89% 8% ..



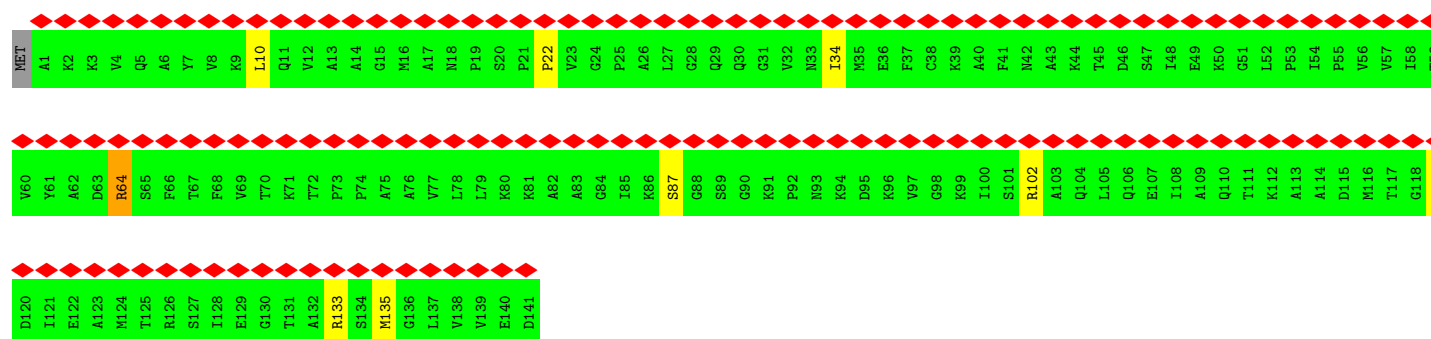
- Molecule 30: 50S ribosomal protein L9

Chain BH: 76% 94% 6%

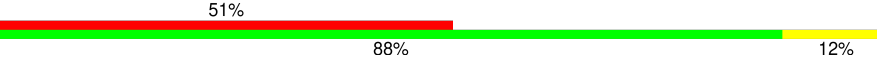


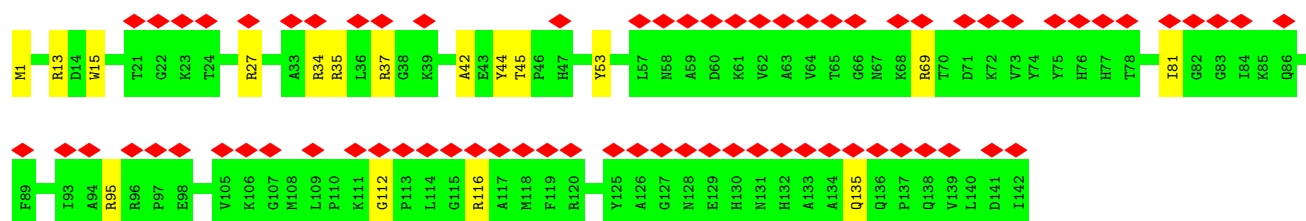
- Molecule 31: 50S ribosomal protein L11

Chain BI: 99% 93% 6% ..




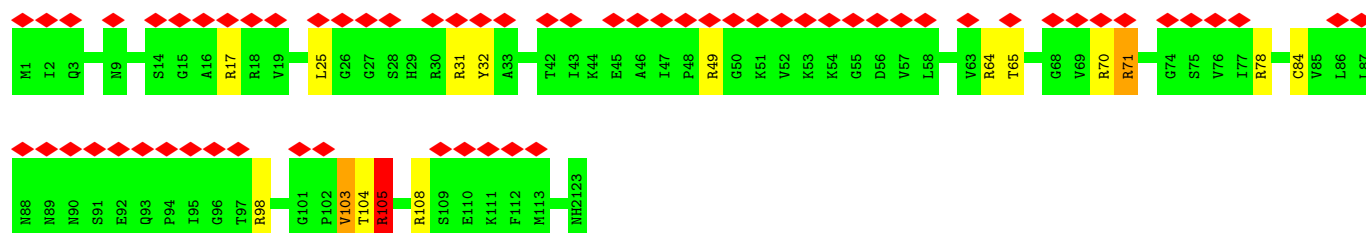
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 




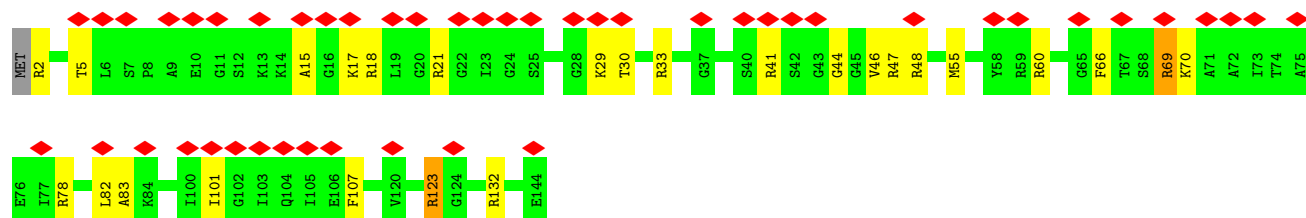
- Molecule 33: 50S ribosomal protein L14

Chain BK: 

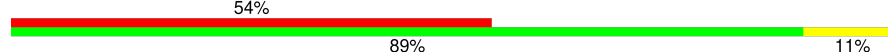


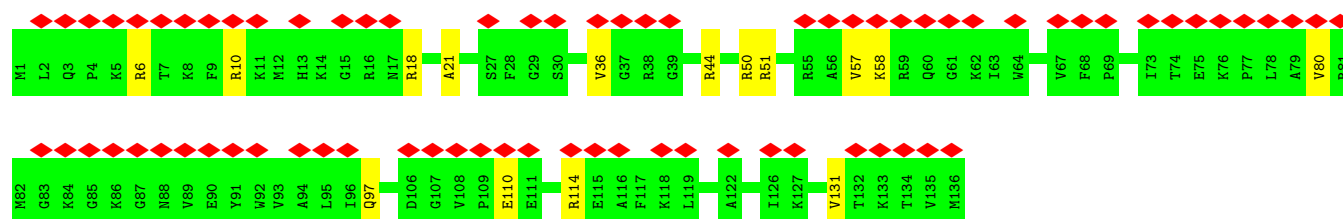
- Molecule 34: 50S ribosomal protein L15

Chain BL: 




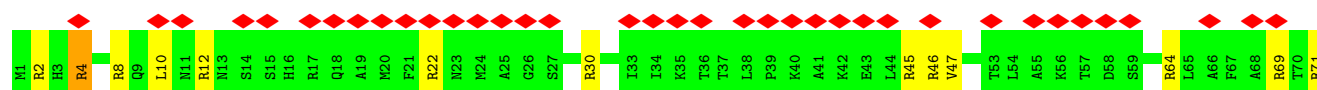
- Molecule 35: 50S ribosomal protein L16

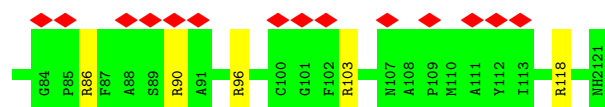
Chain BM: 



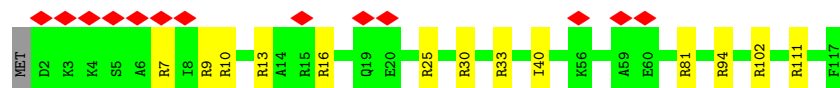
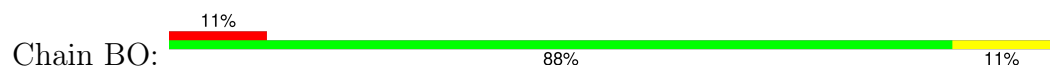
- Molecule 36: 50S ribosomal protein L17

Chain BN: 

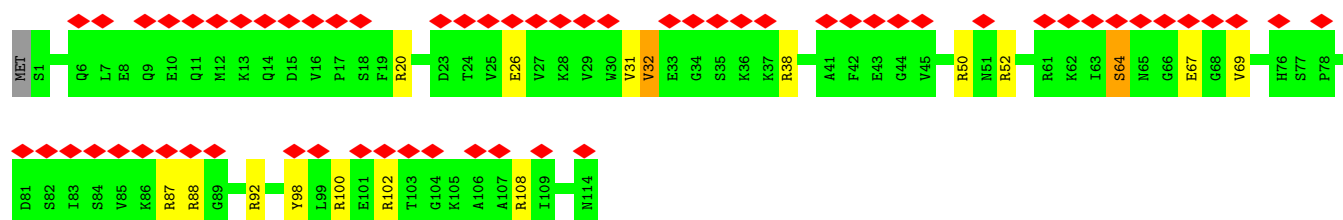
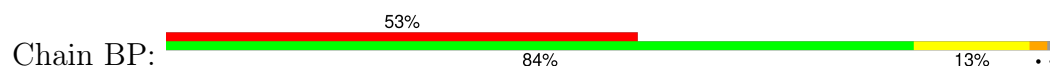




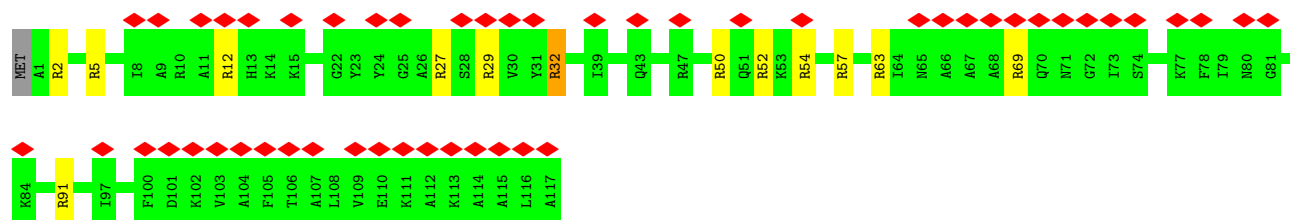
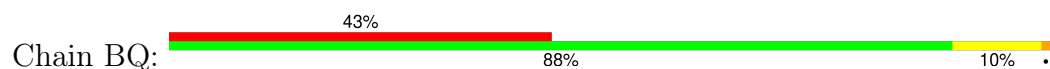
- Molecule 37: 50S ribosomal protein L18



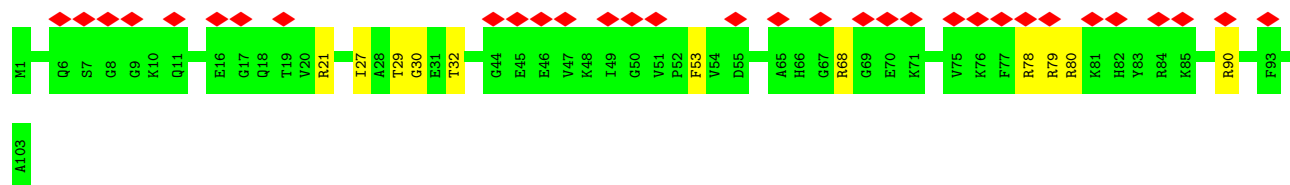
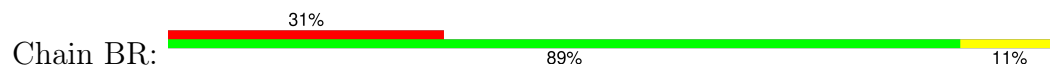
- Molecule 38: 50S ribosomal protein L19



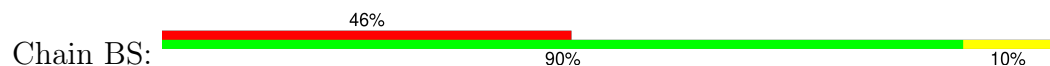
- Molecule 39: 50S ribosomal protein L20

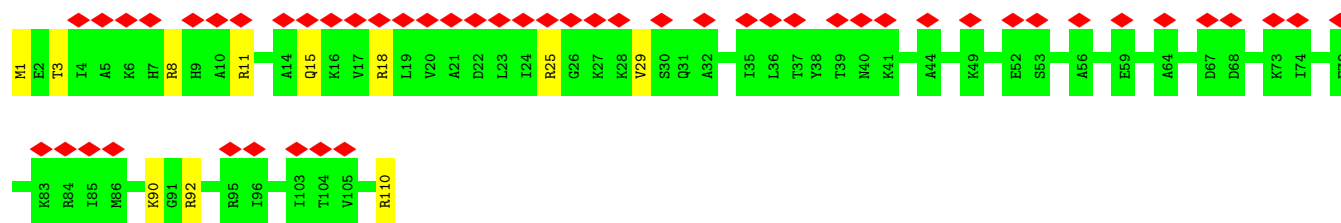


- Molecule 40: 50S ribosomal protein L21

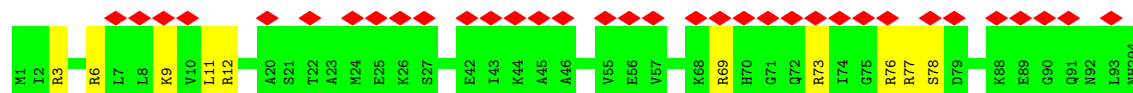
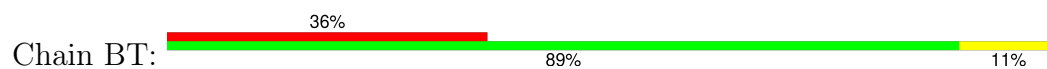


- Molecule 41: 50S ribosomal protein L22

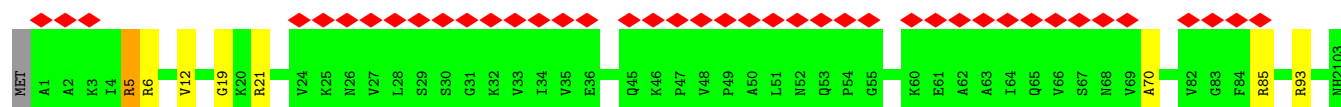
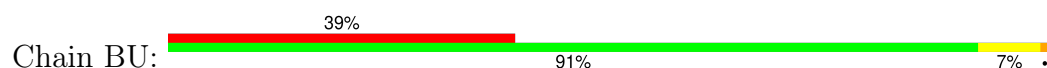




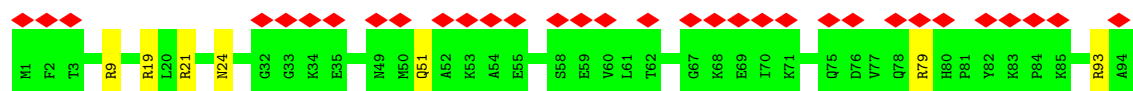
- Molecule 42: 50S ribosomal protein L23



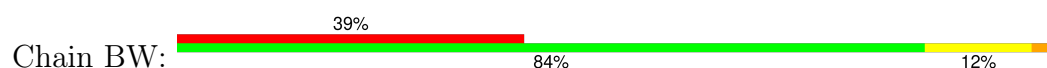
- Molecule 43: 50S ribosomal protein L24



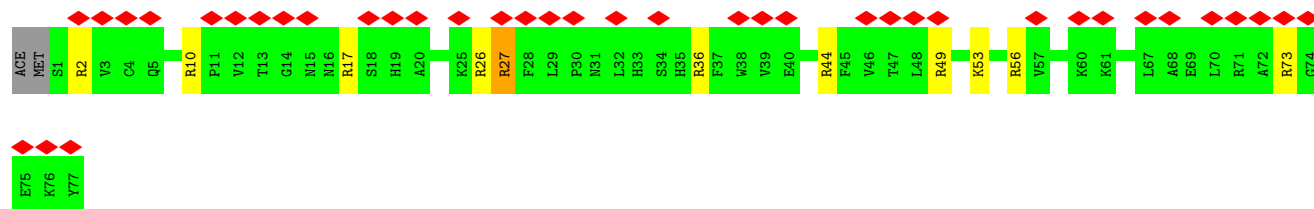
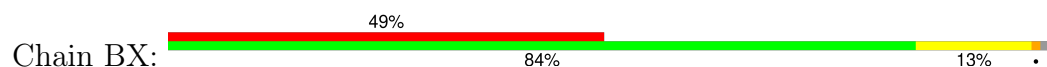
- Molecule 44: 50S ribosomal protein L25



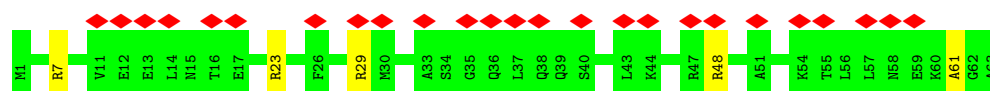
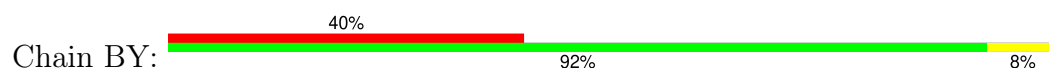
- Molecule 45: 50S ribosomal protein L27



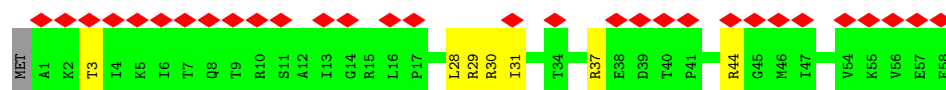
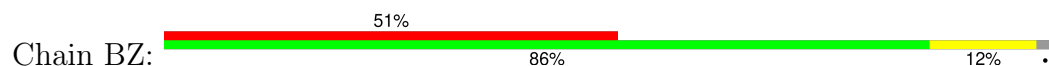
- Molecule 46: 50S ribosomal protein L28



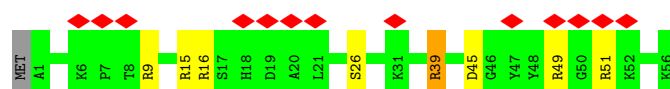
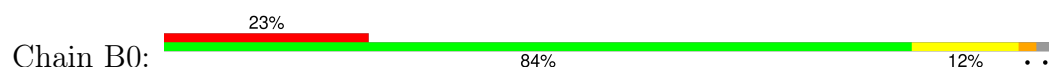
- Molecule 47: 50S ribosomal protein L29



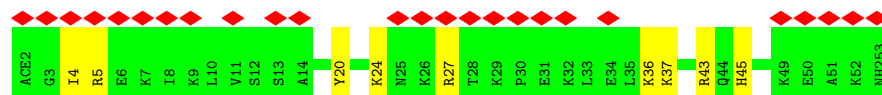
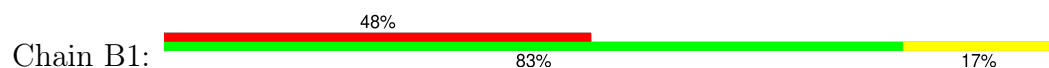
- Molecule 48: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L32



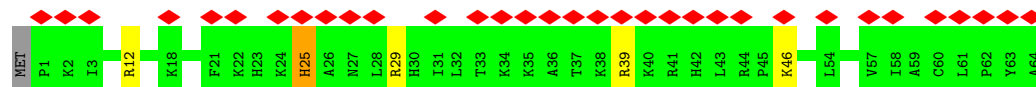
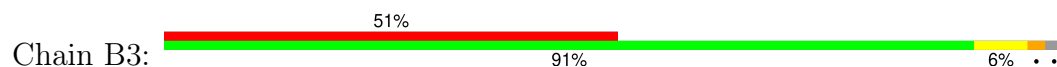
- Molecule 50: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L34

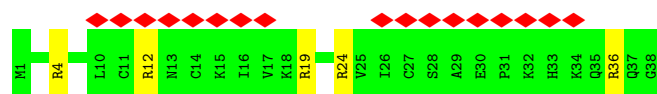


- Molecule 52: 50S ribosomal protein L35

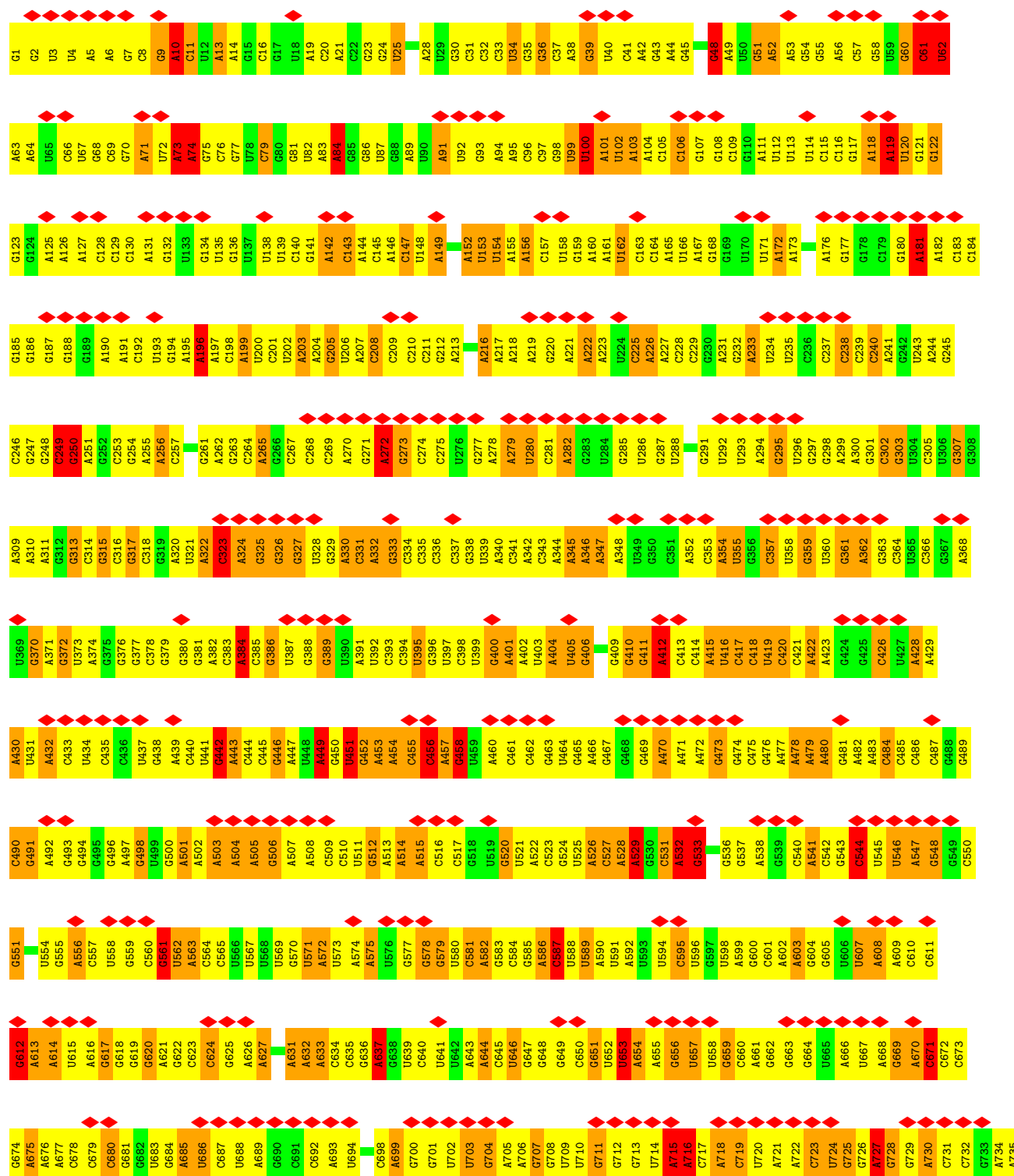
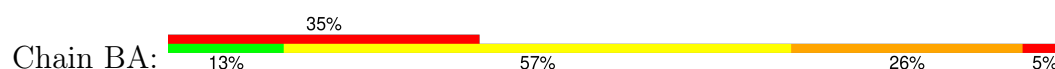


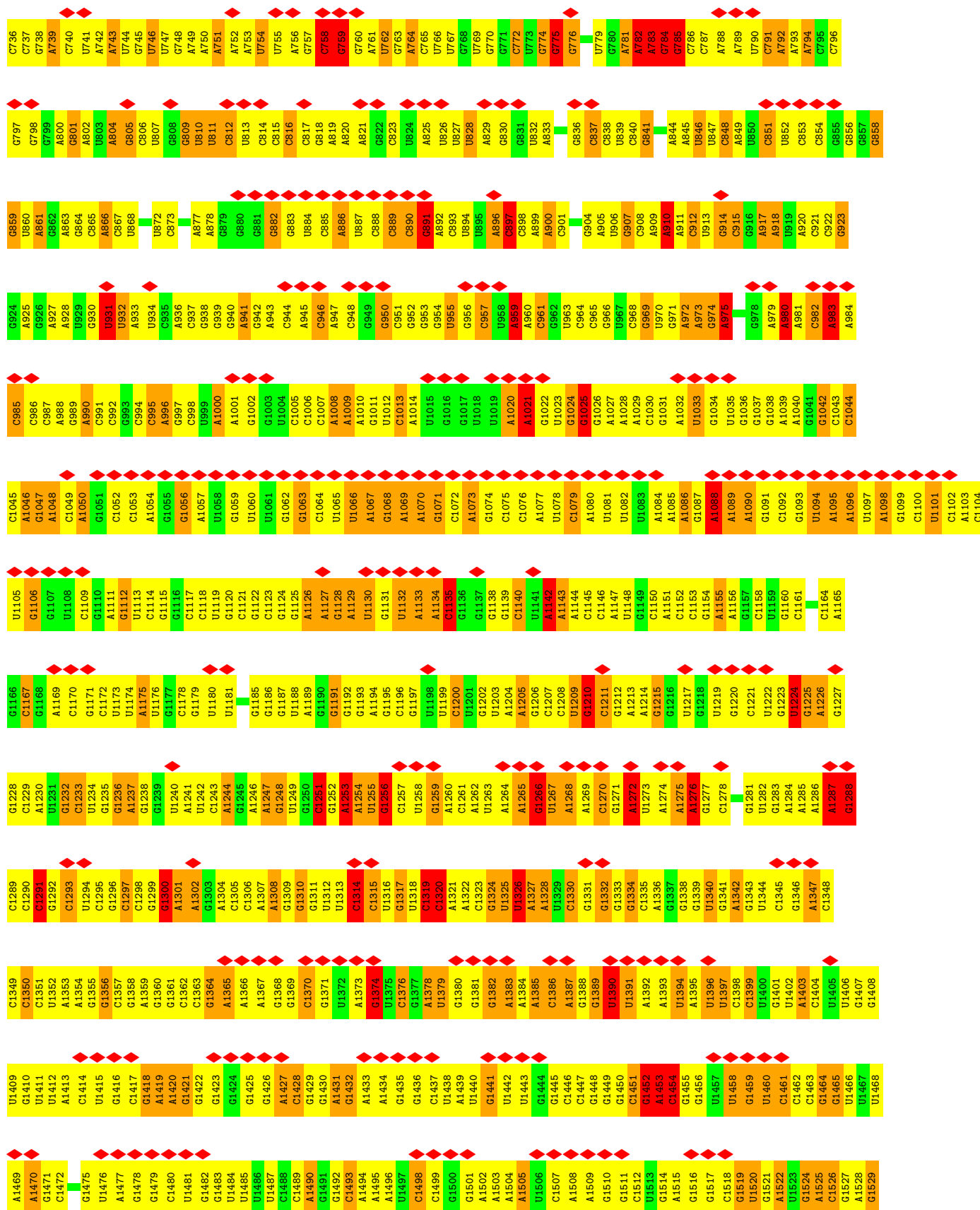
- Molecule 53: 50S ribosomal protein L36





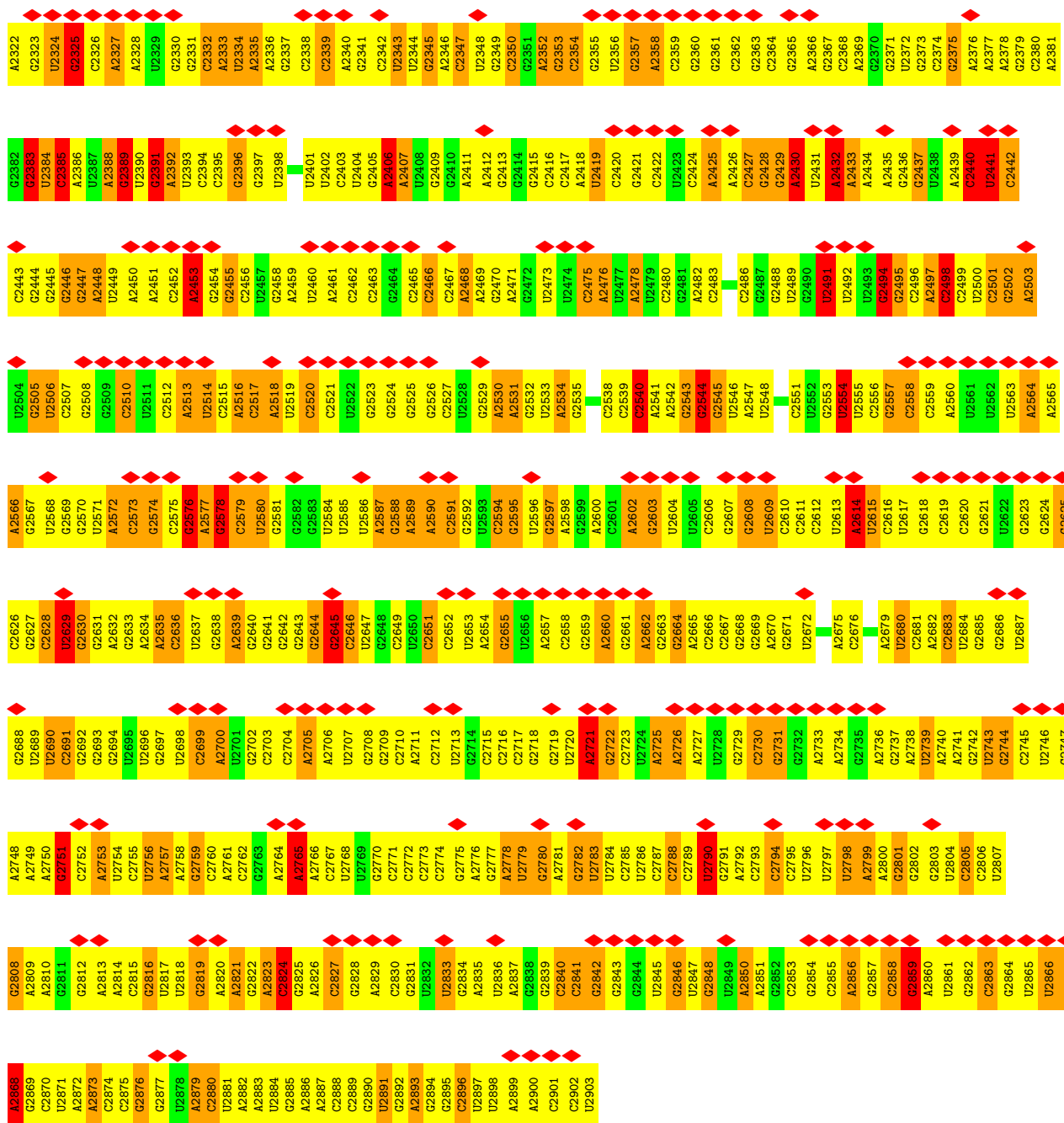
• Molecule 54: 23S ribosomal RNA



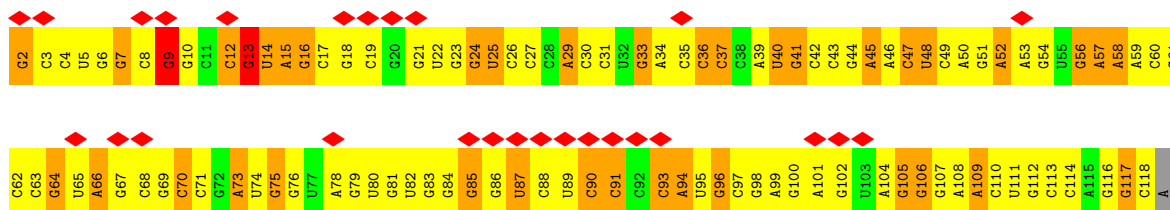
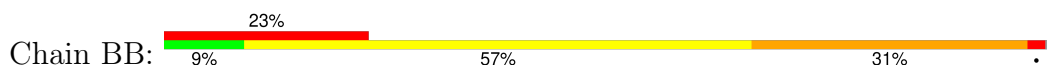


C2261	U2262	C2263	C2264	U2265	A2266	A2267	A2268	G2269	U2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	A2281	G2282	C2283	A2284	G2285	G2286	A2287	A2288	G2289	U2290	U2291	U2292	U2293	G2294	C2295	U2296	A2297	A2298	U2299	C2300	C2301	U2302	G2303	U2304	U2305	C2306	G2307	G2308	C2309	C2310	A2311	U2312	C2313	A2314	C2315	G2316	A2317	U2320	U2321			
C2200	G2201	U2202	U2203	A2205	C2206	C2207	C2208	C2209	U2210	A2211	A2212	U2213	C2214	C2215	C2216	C2217	U2220	G2221	C2222	G2223	G2224	A2225	C2226	A2227	C2228	U2229	G2230	U2231	U2232	C2233	U2234	G2235	U2236	C2237	G2238	C2301	U2302	U2303	U2304	U2305	C2306	G2307	G2308	C2309	C2310	A2311	U2312	C2313	A2314	C2315	G2316	U2317	U2320	U2321							
U2139	G2140	G2141	U2142	C2143	G2144	C2145	C2146	A2147	C2150	U2151	U2152	C2153	A2154	U2155	C2156	U2157	A2158	U2159	C2160	G2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185	U2186	U2187	U2188	U2189	A2191	U2192	G2193	U2194	U2195	C2196	U2197						
C2078	U2079	U2080	U2081	U2082	G2083	C2084	U2085	U2086	U2087	A2088	C2089	A2090	C2091	U2092	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	C2104	U2106	U2107	A2108	U2109	U2110	U2111	G2112	U2113	A2114	C2115	G2116	U2117	U2118	A2119	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138				
G2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	C2035	C2036	A2037	G2038	U2039	G2040	U2041	A2042	C2043	C2044	C2045	U2046	G2047	U2048	G2049	C2050	A2051	U2052	G2053	A2054	C2055	U2056	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	A2073	U2074	U2075	U2076	A2077			
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U2139	G2140	G2141	U2142	C2143	G2144	C2145	C2146	A2147	C2150	U2151	U2152	C2153	A2154	U2155	C2156	U2157	A2158	U2159	C2160	G2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185	U2186	U2187	U2188	U2189	A2191	U2192	G2193	U2194	U2195	C2196	U2197						
C2200	C2201	U2202	U2203	A2205	C2206	C2207	C2208	C2209	U2210	A2211	A2212	U2213	C2214	C2215	C2216	C2217	U2220	G2221	C2222	G2223	G2224	A2225	C2226	A2227	C2228	U2229	G2230	U2231	U2232	C2233	U2234	G2235	U2236	C2237	G2238	C2301	U2302	U2303	U2304	U2305	C2306	G2307	G2308	C2309	C2310	A2311	U2312	C2313	A2314	C2315	G2316	U2317	U2320	U2321							
U2261	U2262	C2263	C2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	C2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2320	U2321			
G1530	C1531	A1532	C1533	U1534	A1535	C1536	C1537	G1538	U1539	G1540	C1541	U1542	G1543	A1544	G1545	G1546	C1547	A1548	A1549	C1550	A1551	A1552	A1553	U1554	G1555	C1556	C1557	C1558	U1559	G1560	C1561	U1562	U1563	C1564	C1565	A1566	G1567	U1568	A1569	A1570	A1571	A1572	U1573	C1574	C1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	U1584	C1585	A1586	G1587	U1588	U1589		
A1590	A1591	C1592	A1593	U1594	C1595	A1596	A1597	U1598	U1599	C1600	G1601	U1602	G1603	A1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	C1612	G1613	A1614	C1615	A1616	C1617	A1618	G1619	U1620	U1621	G1622	U1623	U1624	C1625	A1626	G1627	G1628	U1629	A1630	G1631	A1632	G1633	A1634	A1635	U1636	A1637	C1638	C1639	A1640	A1641	G1642	G1643	A1644	G1645	C1646	U1647	U1648	G1649		
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A1773	C1774	U1775	G1776	U1777	U1778	A1779	U1780	U1781	U1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	A1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1803	C1804	A1805	C1806	G1807	A1808	A1809	A1810	G1813	G1814	A1815	C1816	U1817	U1818	A1819	U1820	A1821	C1822	G1823	G1824	U1825	U1826	G1827	U1828	A1829	C1830	G1831	C1832	C1833			
U1834	G1835	C1836	U1837	C1838	G1839	C1843	C1844	G1845	G1846	A1847	A1848	G1849	G1850	U1851	U1852	A1853	A1854	G1857	A1858	U1859	G1860	G1861	G1862	U1863	U1864	U1865	A1866	G1867	G1868	G1869	C1870	A1871	G1872	A1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	U1883	G1884	A1885	U1886	C1887	G1888	A1889	A1890	G1891	C1892	C1893	A1894	C1895	G1896				
G1897	U1898	A1899	A1900	A1901	C1902	G1903	U1904	C1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	A1913	A1914	U1915	A1916	U1917	A1918	A1919	C1920	U1923	C1924	C1925	U1926	A1927	U1928	G1929	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	U1938	U1939	U1940	C1941	C1942	U1943	U1944	G1945	U1946	C1947	G1948	G1949	G1950	U1951	A1952	A1953	G1954	U1955	C1957				
C1958	G1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	U1967	G1968	A1969	U1970	U1971	G1972	C1973	C1974	G1975	U1976	A1977	A1978	U1979	G1980	A1981	U1982	G1983	G1984	C1985	C1986	A1987	G1988	G1989	C1990	U1991	G1992	U1993	C1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	G2002	A2003	U2004	A2005	C2006	U2007	C2008	A2009	U2010	G2012	A2013	A2014	A2015	U2016	U2017			
G2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	C2035	C2036	A2037	G2038	U2039	G2040	U2041	A2042	C2043	C2044	C2045	U2046	G2047	U2048	G2049	C2050	A2051	U2052	G2053	A2054	C2055	U2056	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	A2073	U2074	U2075	U2076	A2077			
C2078	U2079	U2080	U2081	U2082	G2083	C2084	U2085	U2086	U2087	A2088	C2089	A2090	C2091	U2092	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	C2104	U2106	U2107	A2108	U2109	U2110	U2111	G2112	U2113	A2114	C2115	G2116	U2117	U2118	A2119	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138				
U2139	G2140	G2141	U2142	C2143	G2144	C2145	C2146	A2147	C2150	U2151	U2152	C2153	A2154	U2155	C2156	U2157	A2158	U2159	C2160	G2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2182																						

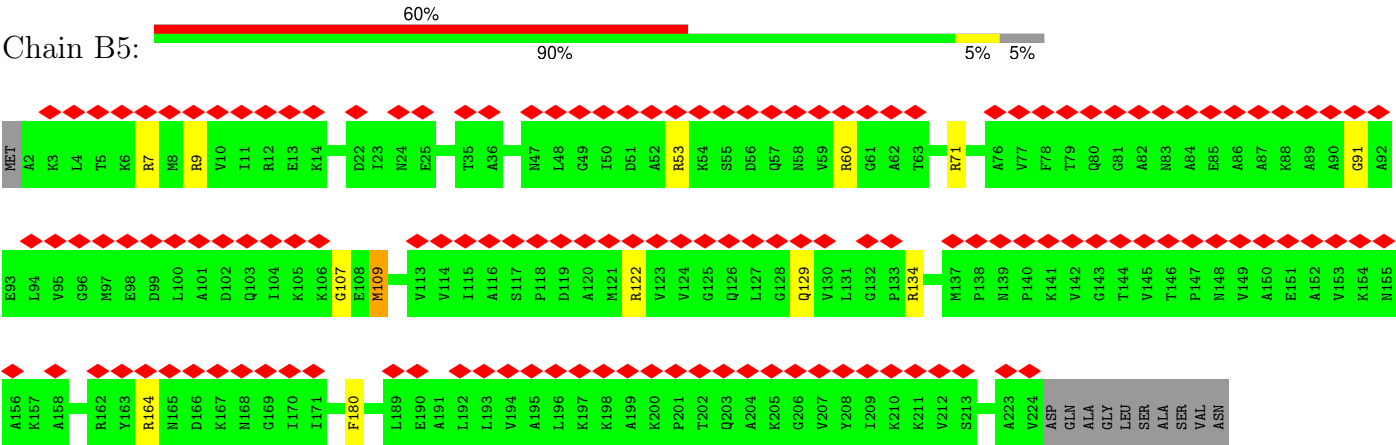




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13091	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	191.487	Depositor
Minimum map value	-133.057	Depositor
Average map value	-0.914	Depositor
Map value standard deviation	20.362	Depositor
Recommended contour level	25	Depositor
Map size ( $\text{\AA}$ )	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.8, 2.8, 2.8	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, OMC, H2U, CM0, PSU, NH2, 6MZ, 5MU, 4SU, ACE, 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$
1	AB	0.76	0/1736	1.10	10/2340 (0.4%)
2	AC	0.81	0/1651	1.19	17/2225 (0.8%)
3	AD	0.83	0/1665	1.27	20/2227 (0.9%)
4	AE	0.79	0/1119	1.16	9/1506 (0.6%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
6	AG	0.81	0/1188	1.19	11/1593 (0.7%)
7	AH	0.80	0/989	1.09	8/1326 (0.6%)
8	AI	0.88	0/1035	1.34	14/1377 (1.0%)
9	AJ	0.81	0/797	1.22	11/1079 (1.0%)
10	AK	0.85	0/894	1.20	10/1207 (0.8%)
11	AL	0.85	0/969	1.25	13/1300 (1.0%)
12	AM	0.84	0/884	1.30	14/1181 (1.2%)
13	AN	0.88	1/817 (0.1%)	1.43	16/1088 (1.5%)
14	AO	0.86	0/722	1.26	12/964 (1.2%)
15	AP	0.88	0/648	1.25	6/870 (0.7%)
16	AQ	0.78	0/658	1.13	5/883 (0.6%)
17	AR	0.85	0/463	1.25	8/623 (1.3%)
18	AS	0.84	0/653	1.26	8/879 (0.9%)
19	AT	0.79	0/672	1.24	8/890 (0.9%)
20	AU	0.96	0/431	1.57	12/572 (2.1%)
21	AA	2.03	752/36759 (2.0%)	2.33	2571/57346 (4.5%)
22	A1	2.04	28/1668 (1.7%)	2.30	106/2595 (4.1%)
23	A2	1.81	3/343 (0.9%)	2.39	25/531 (4.7%)
24	A3	2.06	38/1722 (2.2%)	2.29	111/2685 (4.1%)
25	BC	0.85	0/2121	1.31	31/2852 (1.1%)
26	BD	0.77	0/1586	1.22	10/2134 (0.5%)
27	BE	0.75	0/1571	1.20	13/2113 (0.6%)
28	BF	0.79	0/1444	1.21	11/1937 (0.6%)
29	BG	0.76	0/1343	1.18	10/1816 (0.6%)
30	BH	0.72	0/1122	1.10	7/1515 (0.5%)
31	BI	0.71	0/1046	1.07	3/1410 (0.2%)
32	BJ	0.77	0/1152	1.24	12/1551 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BK	0.79	0/947	1.30	11/1268 (0.9%)
34	BL	0.82	0/1054	1.36	14/1403 (1.0%)
35	BM	0.84	0/1093	1.24	9/1460 (0.6%)
36	BN	0.89	0/973	1.43	19/1301 (1.5%)
37	BO	0.85	0/902	1.32	11/1209 (0.9%)
38	BP	0.85	0/929	1.42	13/1242 (1.0%)
39	BQ	0.86	0/960	1.33	14/1278 (1.1%)
40	BR	0.79	0/829	1.18	6/1107 (0.5%)
41	BS	0.76	0/864	1.20	8/1156 (0.7%)
42	BT	0.77	0/744	1.27	8/994 (0.8%)
43	BU	0.78	0/787	1.20	5/1051 (0.5%)
44	BV	0.75	0/766	1.17	6/1025 (0.6%)
45	BW	0.84	0/604	1.29	5/799 (0.6%)
46	BX	0.87	0/635	1.39	11/848 (1.3%)
47	BY	0.77	0/510	1.26	4/677 (0.6%)
48	BZ	0.84	0/453	1.29	5/605 (0.8%)
49	B0	0.85	0/450	1.33	7/599 (1.2%)
50	B1	0.77	0/417	1.21	4/556 (0.7%)
51	B2	0.98	0/380	1.49	10/498 (2.0%)
52	B3	0.76	0/513	1.16	4/676 (0.6%)
53	B4	0.86	0/303	1.39	5/397 (1.3%)
54	BA	1.91	1309/69796 (1.9%)	2.32	5106/108888 (4.7%)
55	BB	2.03	85/2800 (3.0%)	2.33	222/4367 (5.1%)
56	B5	0.71	0/1673	1.10	10/2255 (0.4%)
All	All	1.71	2216/160085 (1.4%)	2.09	8646/239402 (3.6%)

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	AC	0	2
8	AI	0	1
10	AK	0	1
21	AA	0	365
22	A1	0	10
23	A2	0	1
24	A3	0	14
25	BC	0	2
33	BK	0	1
34	BL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	666
55	BB	0	30
All	All	0	1094

The worst 5 of 2216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1044	C	C4-N4	-7.34	1.27	1.33
54	BA	2752	C	C4-N4	-7.31	1.27	1.33
24	A3	3	C	C4-N4	-7.23	1.27	1.33
21	AA	6	G	C6-N1	-7.22	1.34	1.39
21	AA	1479	C	C4-N4	-7.20	1.27	1.33

The worst 5 of 8646 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2510	C	N3-C2-O2	-15.56	111.01	121.90
54	BA	975	A	N1-C6-N6	-13.84	110.30	118.60
54	BA	479	A	N1-C6-N6	-13.45	110.53	118.60
21	AA	412	A	N1-C6-N6	-12.78	110.93	118.60
54	BA	900	A	N1-C6-N6	-12.71	110.97	118.60

There are no chirality outliers.

5 of 1094 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	6	G	Sidechain
2	AC	168	ARG	Sidechain
2	AC	172	VAL	Peptide
8	AI	124	PRO	Peptide
10	AK	115	ILE	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	AB	1708	0	1736	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	15886	9	0
22	A1	1627	0	798	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	801	1	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	3	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	2	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	1	0
51	B2	377	0	418	1	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	30186	21	0
55	BB	2504	0	1181	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	97702	45	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 0.

The worst 5 of 45 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)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.81	0.62
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
26:BD:154:LYS:HE3	26:BD:156:PHE:CE1	2.46	0.51
54:BA:931:U:C5	54:BA:1167:C:H1'	2.46	0.50
21:AA:5:U:H4'	21:AA:6:G:C6	2.46	0.50

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	AB	218/220 (99%)	195 (89%)	22 (10%)	1 (0%)	25	64
2	AC	205/208 (99%)	191 (93%)	12 (6%)	2 (1%)	13	49
3	AD	203/206 (98%)	185 (91%)	15 (7%)	3 (2%)	8	40
4	AE	150/152 (99%)	134 (89%)	9 (6%)	7 (5%)	2	16
5	AF	99/101 (98%)	86 (87%)	6 (6%)	7 (7%)	1	11
6	AG	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
7	AH	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
8	AI	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	3	21
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	1	15
10	AK	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	52
11	AL	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
12	AM	112/115 (97%)	98 (88%)	12 (11%)	2 (2%)	7	35
13	AN	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	13	49
14	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	11	44
15	AP	79/81 (98%)	68 (86%)	7 (9%)	4 (5%)	1	15
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	26
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	7	35
18	AS	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
19	AT	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	5	27
20	AU	51/53 (96%)	27 (53%)	14 (28%)	10 (20%)	0	2
25	BC	270/273 (99%)	238 (88%)	21 (8%)	11 (4%)	2	18
26	BD	207/209 (99%)	178 (86%)	18 (9%)	11 (5%)	1	15
27	BE	199/201 (99%)	177 (89%)	17 (8%)	5 (2%)	4	26
28	BF	176/179 (98%)	151 (86%)	21 (12%)	4 (2%)	5	28
29	BG	174/177 (98%)	152 (87%)	13 (8%)	9 (5%)	1	15
30	BH	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	9	41
31	BI	139/142 (98%)	125 (90%)	10 (7%)	4 (3%)	3	23
32	BJ	140/142 (99%)	125 (89%)	8 (6%)	7 (5%)	1	16
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	4	26
34	BL	141/144 (98%)	117 (83%)	12 (8%)	12 (8%)	0	9
35	BM	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	2	20
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	91 (81%)	15 (13%)	6 (5%)	1	15
39	BQ	115/118 (98%)	100 (87%)	15 (13%)	0	100	100
40	BR	101/103 (98%)	94 (93%)	3 (3%)	4 (4%)	2	18
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	6	32
42	BT	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	3	21
43	BU	101/104 (97%)	85 (84%)	12 (12%)	4 (4%)	2	18
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	65 (83%)	6 (8%)	7 (9%)	0	8
46	BX	75/79 (95%)	70 (93%)	3 (4%)	2 (3%)	4	25
47	BY	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	8	38
48	BZ	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	3	20
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	32
50	B1	50/52 (96%)	43 (86%)	3 (6%)	4 (8%)	1	9
51	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
52	B3	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3	21
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	9	41
All	All	5876/6008 (98%)	5249 (89%)	458 (8%)	169 (3%)	6	23

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
8	AI	44	ARG
16	AQ	80	LYS
20	AU	6	ARG
20	AU	9	GLU

### 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	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	56	72
2	AC	170/171 (99%)	167 (98%)	3 (2%)	54	71
3	AD	172/173 (99%)	168 (98%)	4 (2%)	45	64
4	AE	113/113 (100%)	110 (97%)	3 (3%)	40	58
5	AF	87/87 (100%)	86 (99%)	1 (1%)	70	80
6	AG	123/123 (100%)	123 (100%)	0	100	100
7	AH	104/105 (99%)	102 (98%)	2 (2%)	52	69
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	82 (95%)	4 (5%)	22	44
10	AK	90/90 (100%)	88 (98%)	2 (2%)	47	65
11	AL	103/104 (99%)	102 (99%)	1 (1%)	73	82
12	AM	91/92 (99%)	88 (97%)	3 (3%)	33	52
13	AN	83/84 (99%)	81 (98%)	2 (2%)	44	62
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	48	66
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	62 (95%)	3 (5%)	23	44
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	38	57
26	BD	164/164 (100%)	161 (98%)	3 (2%)	54	71
27	BE	165/165 (100%)	163 (99%)	2 (1%)	67	78
28	BF	149/150 (99%)	148 (99%)	1 (1%)	81	87
29	BG	137/138 (99%)	134 (98%)	3 (2%)	47	65
30	BH	114/114 (100%)	113 (99%)	1 (1%)	75	83
31	BI	109/110 (99%)	106 (97%)	3 (3%)	38	57
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	56	72
33	BK	103/103 (100%)	99 (96%)	4 (4%)	27	48
34	BL	102/103 (99%)	101 (99%)	1 (1%)	73	82
35	BM	109/109 (100%)	106 (97%)	3 (3%)	38	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	73	82
37	BO	86/87 (99%)	85 (99%)	1 (1%)	67	78
38	BP	99/100 (99%)	95 (96%)	4 (4%)	27	47
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	70	80
40	BR	84/84 (100%)	83 (99%)	1 (1%)	67	78
41	BS	93/93 (100%)	90 (97%)	3 (3%)	34	53
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	76 (97%)	2 (3%)	41	59
45	BW	59/59 (100%)	55 (93%)	4 (7%)	13	34
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	45 (96%)	2 (4%)	25	46
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	41	59
52	B3	51/52 (98%)	50 (98%)	1 (2%)	50	68
53	B4	34/34 (100%)	33 (97%)	1 (3%)	37	56
56	B5	173/181 (96%)	170 (98%)	3 (2%)	56	72
All	All	4842/4870 (99%)	4756 (98%)	86 (2%)	54	71

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BL	46	VAL
41	BS	15	GLN
35	BM	97	GLN
38	BP	67	GLU
45	BW	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
18	AS	56	HIS

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Mol	Chain	Res	Type
26	BD	134	HIS
32	BJ	77	HIS
13	AN	62	ASN
1	AB	145	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	250 (16%)	72 (4%)
22	A1	73/76 (96%)	8 (10%)	6 (8%)
23	A2	14/15 (93%)	3 (21%)	1 (7%)
24	A3	76/77 (98%)	9 (11%)	6 (7%)
54	BA	2902/2903 (99%)	460 (15%)	132 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4710/4722 (99%)	747 (15%)	220 (4%)

5 of 747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	651	G
54	BA	1300	G
55	BB	57	A
54	BA	2494	G
54	BA	675	A

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

11 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
24	4SU	A3	8	24	18,21,22	1.70	3 (16%)	25,30,33	0.84	1 (4%)
24	OMC	A3	33	24	19,22,23	0.95	0	25,31,34	1.18	2 (8%)
22	CM0	A1	34	22,23	21,26,27	1.49	2 (9%)	26,37,40	1.36	3 (11%)
22	PSU	A1	55	22	18,21,22	1.01	1 (5%)	21,30,33	1.39	2 (9%)
24	5MU	A3	55	24	19,22,23	0.91	0	27,32,35	1.55	4 (14%)
24	H2U	A3	21	24	18,21,22	1.40	2 (11%)	19,30,33	1.14	3 (15%)
22	4SU	A1	7	22	18,21,22	1.58	2 (11%)	25,30,33	1.13	2 (8%)
22	7MG	A1	46	22	23,26,27	4.17	2 (8%)	27,39,42	1.59	3 (11%)
22	6MZ	A1	37	22	17,25,26	0.96	1 (5%)	15,36,39	1.81	2 (13%)
22	5MU	A1	54	22	19,22,23	0.80	0	27,32,35	1.62	6 (22%)
24	PSU	A3	56	24	18,21,22	1.05	1 (5%)	21,30,33	1.67	4 (19%)

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
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
22	CM0	A1	34	22,23	-	2/12/30/31	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-19.48	1.33	1.45
24	A3	8	4SU	C5-C4	-5.69	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	34	CM0	O5-C5	-5.14	1.24	1.36
22	A1	7	4SU	C5-C4	-5.08	1.36	1.42
24	A3	21	H2U	C2-N3	-3.66	1.31	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	6.40	112.43	103.37
22	A1	37	6MZ	C9-N6-C6	5.01	127.49	122.85
22	A1	55	PSU	C6-C5-C4	4.17	120.99	118.17
22	A1	34	CM0	C7-O5-C5	4.14	122.76	117.48
22	A1	54	5MU	C5M-C5-C6	-4.12	117.27	122.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	46	7MG	C3'-C4'-C5'-O5'

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](#)

2 ligands 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	$\# Z  > 2$
58	FME	BA	3001	57	8,9,10	0.74	0	8,9,11	1.05	0
57	VAL	A1	101	22,58	4,6,7	0.80	0	6,7,9	1.10	1 (16%)

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
58	FME	BA	3001	57	-	1/7/9/11	-
57	VAL	A1	101	22,58	-	0/5/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-2.67	117.91	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

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](#)

There are no chain breaks in this entry.



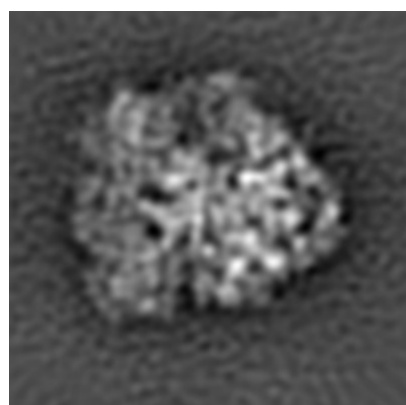
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2472. These allow visual inspection of the internal detail of the map and identification of artifacts.

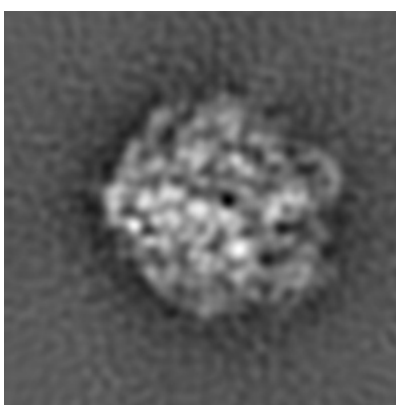
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

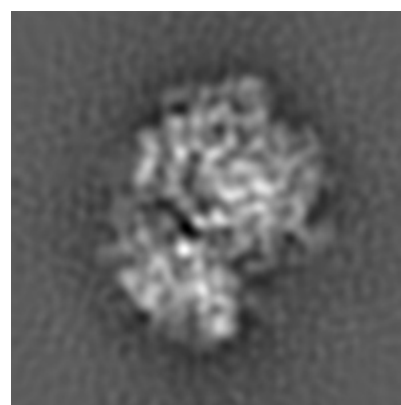
#### 6.1.1 Primary map



X



Y

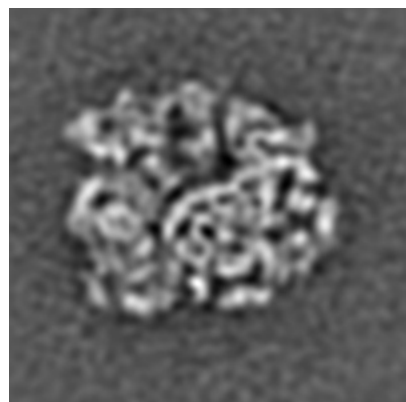


Z

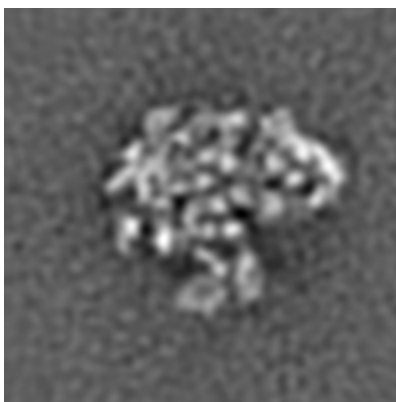
The images above show the map projected in three orthogonal directions.

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

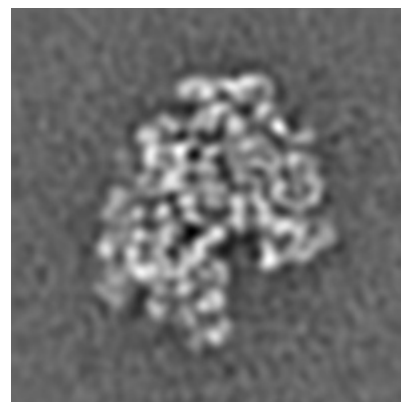
#### 6.2.1 Primary map



X Index: 64



Y Index: 64

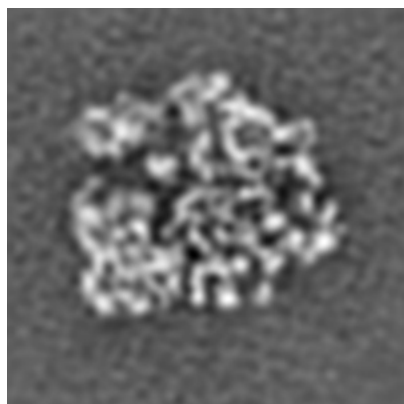


Z Index: 64

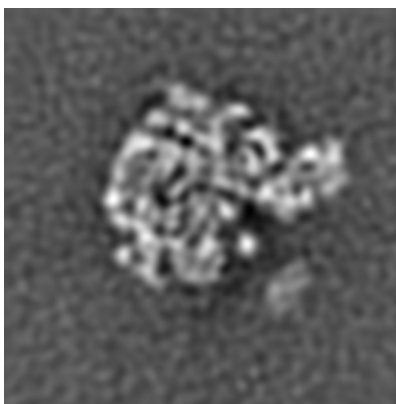
The images above show central slices of the map in three orthogonal directions.

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

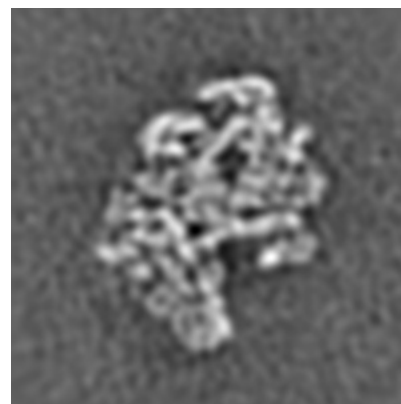
### 6.3.1 Primary map



X Index: 67



Y Index: 71

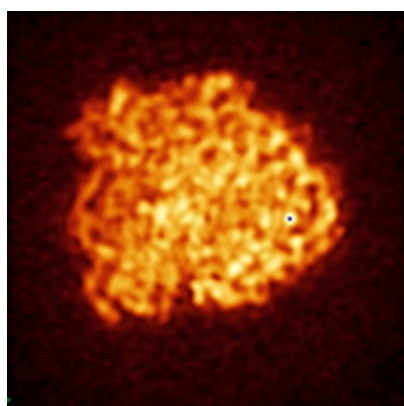


Z Index: 61

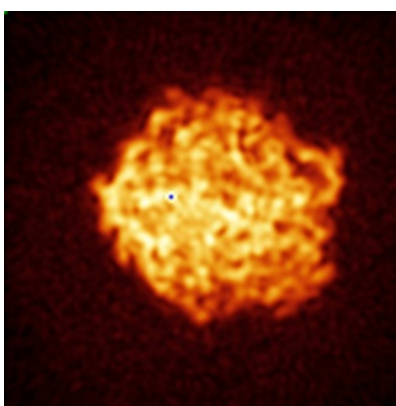
The images above show the largest variance slices of the map in three orthogonal directions.

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

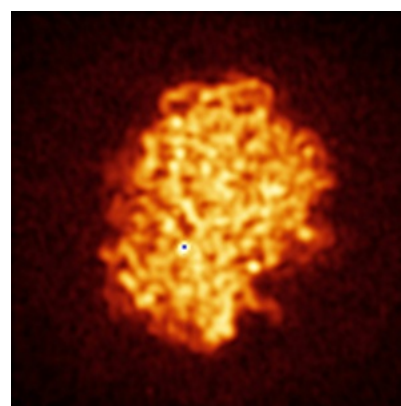
### 6.4.1 Primary map



X



Y

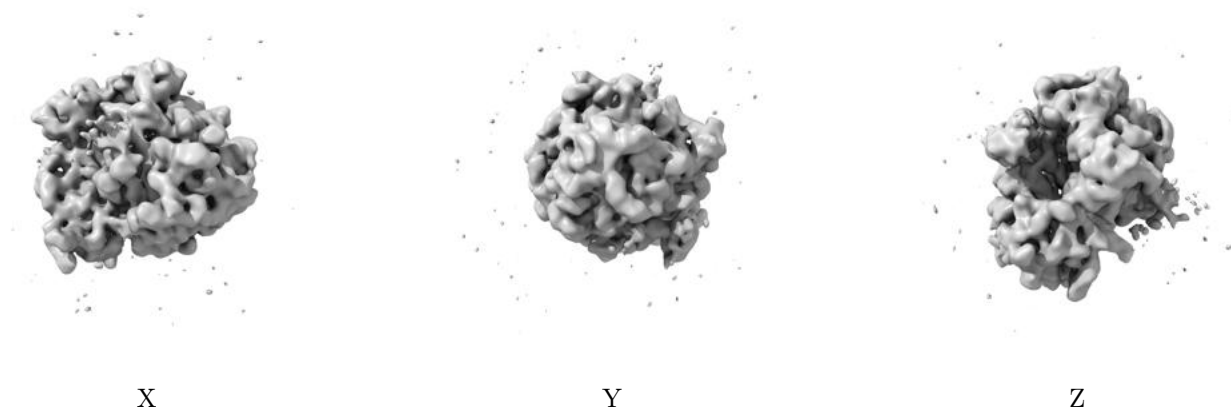


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

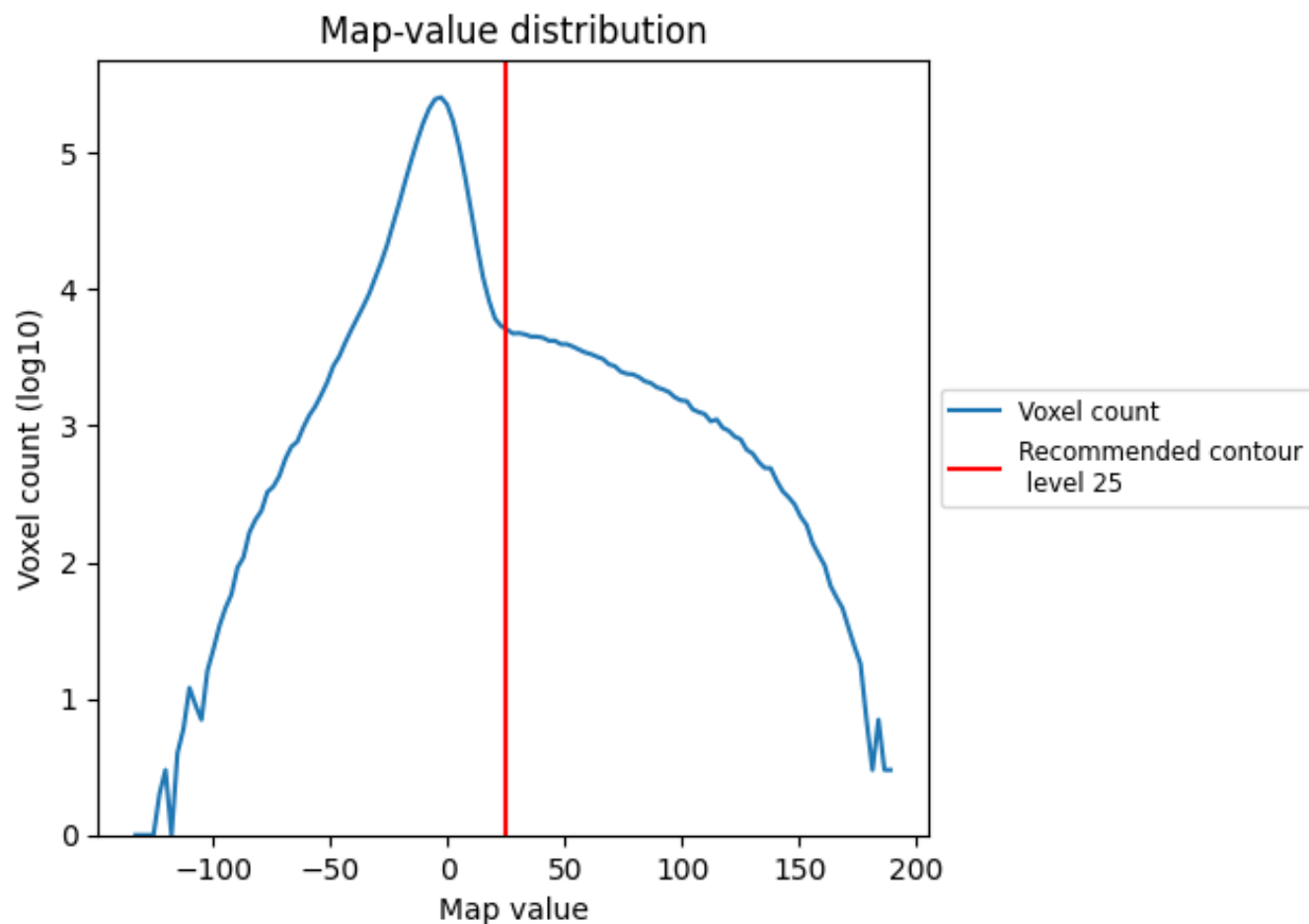
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

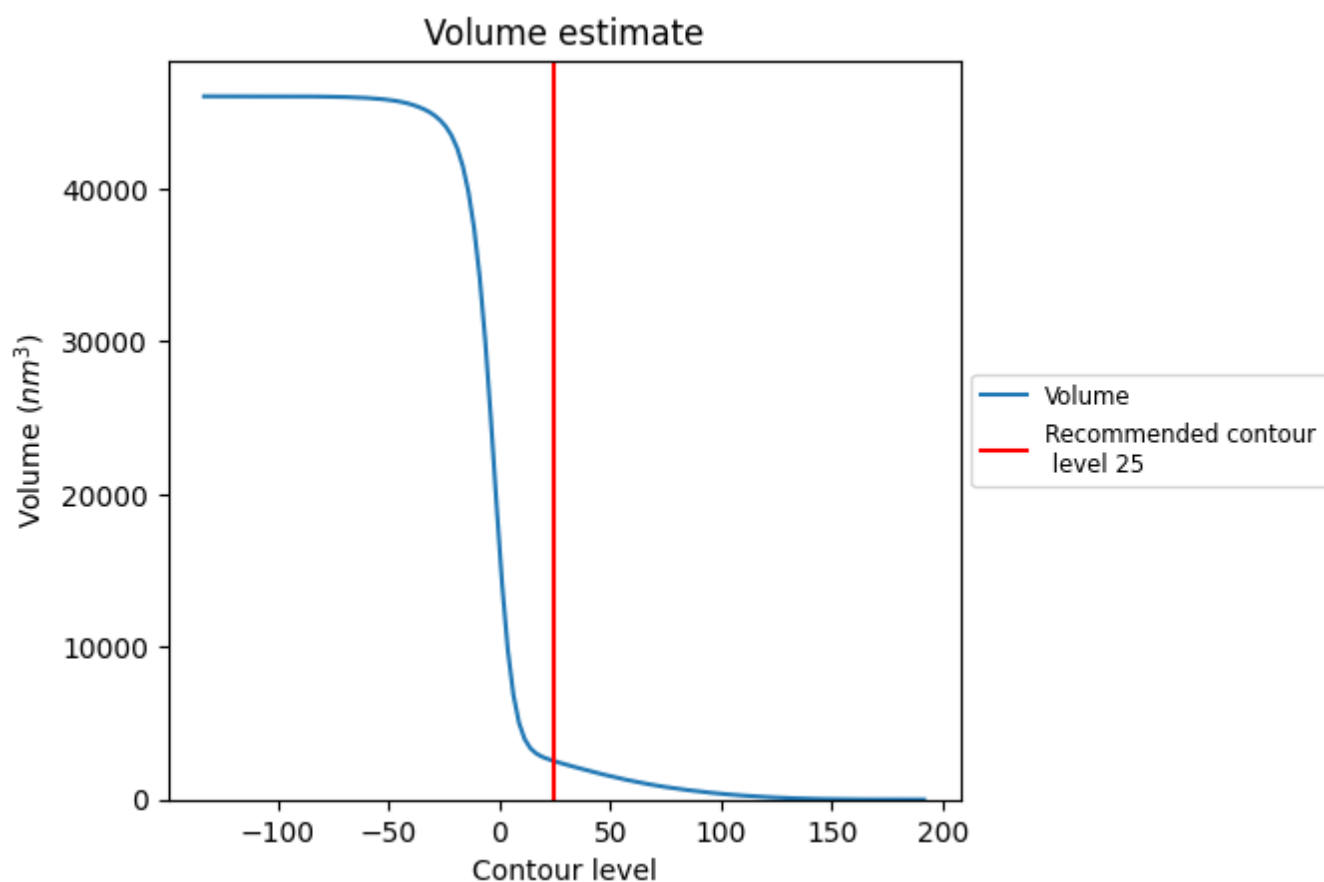
This section contains the results of statistical analysis of the map.

### 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.

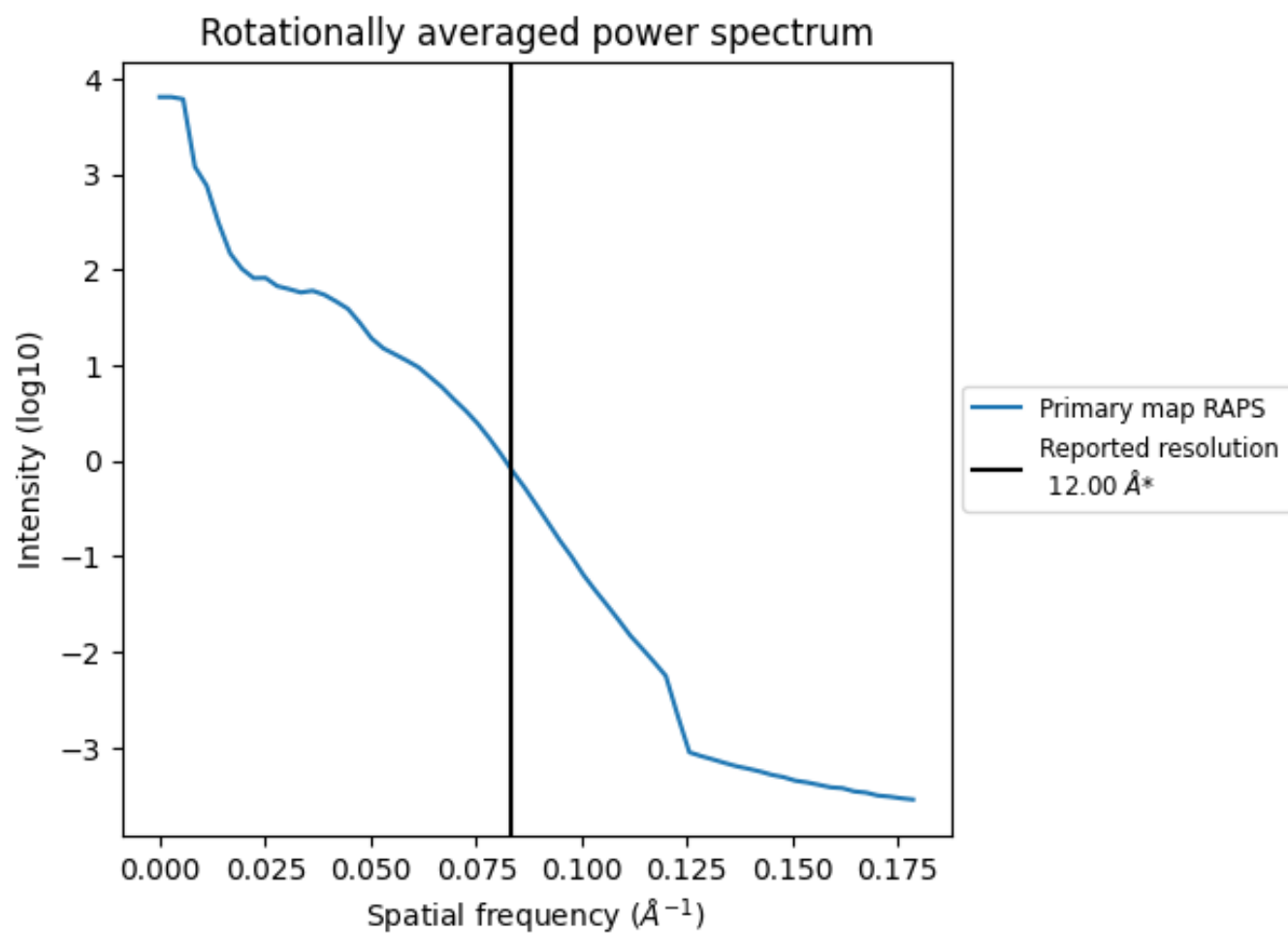
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2507 nm<sup>3</sup>; this corresponds to an approximate mass of 2264 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.083 Å<sup>-1</sup>

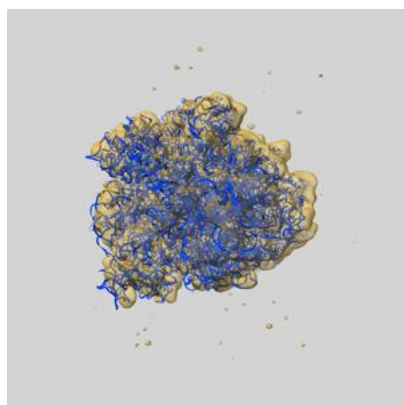
## 8 Fourier-Shell correlation

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

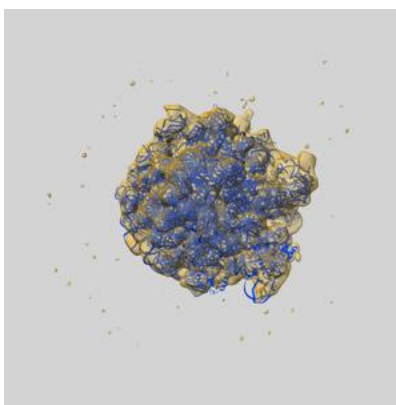
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2472 and PDB model 4V6Z. Per-residue inclusion information can be found in section [3](#) on page [17](#).

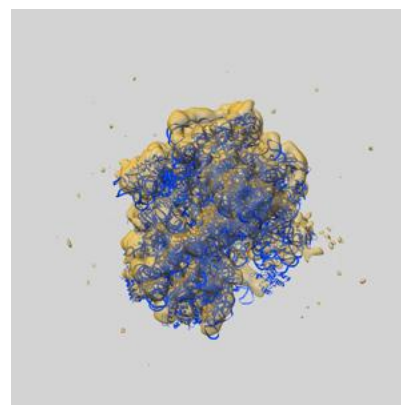
### 9.1 Map-model overlay [i](#)



X



Y

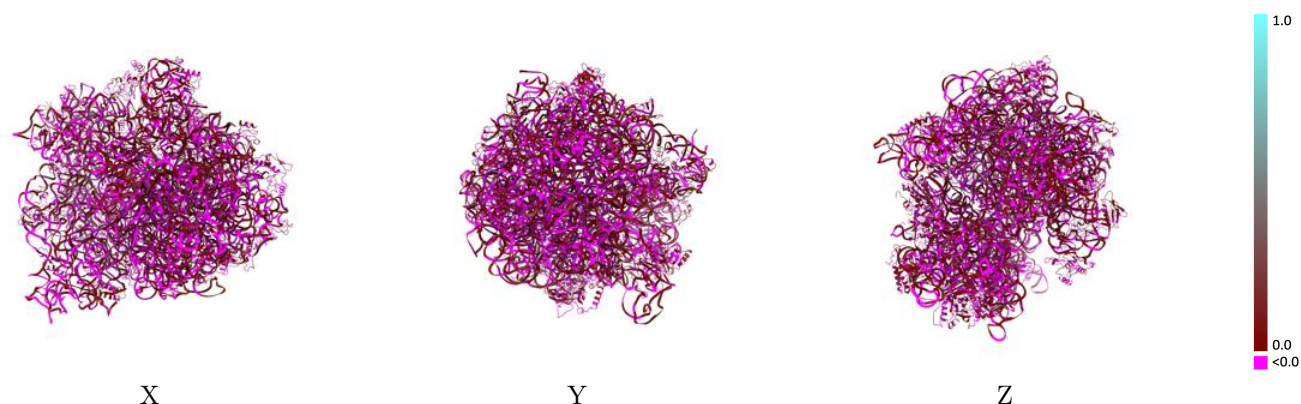


Z

The images above show the 3D surface view of the map at the recommended contour level 25.0 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.

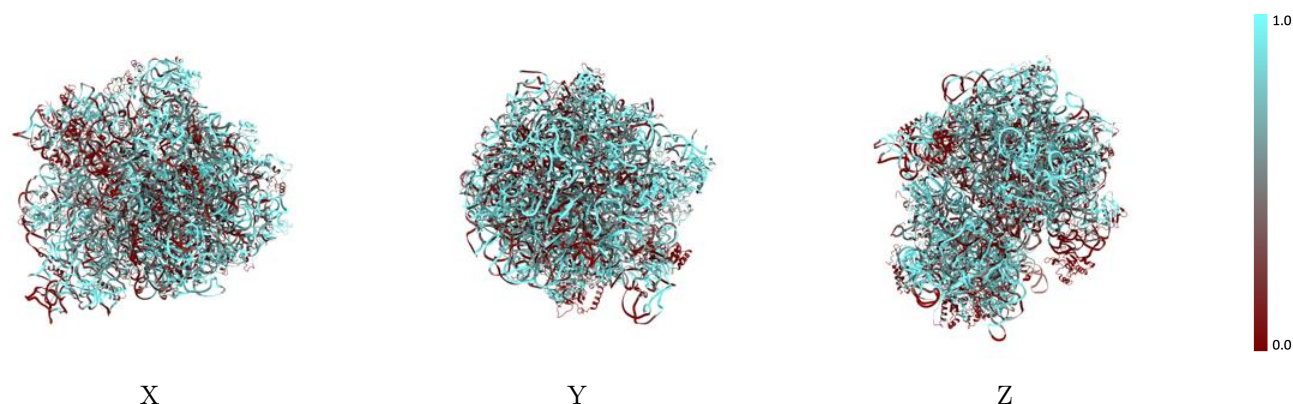


## 9.2 Q-score mapped to coordinate model [i](#)



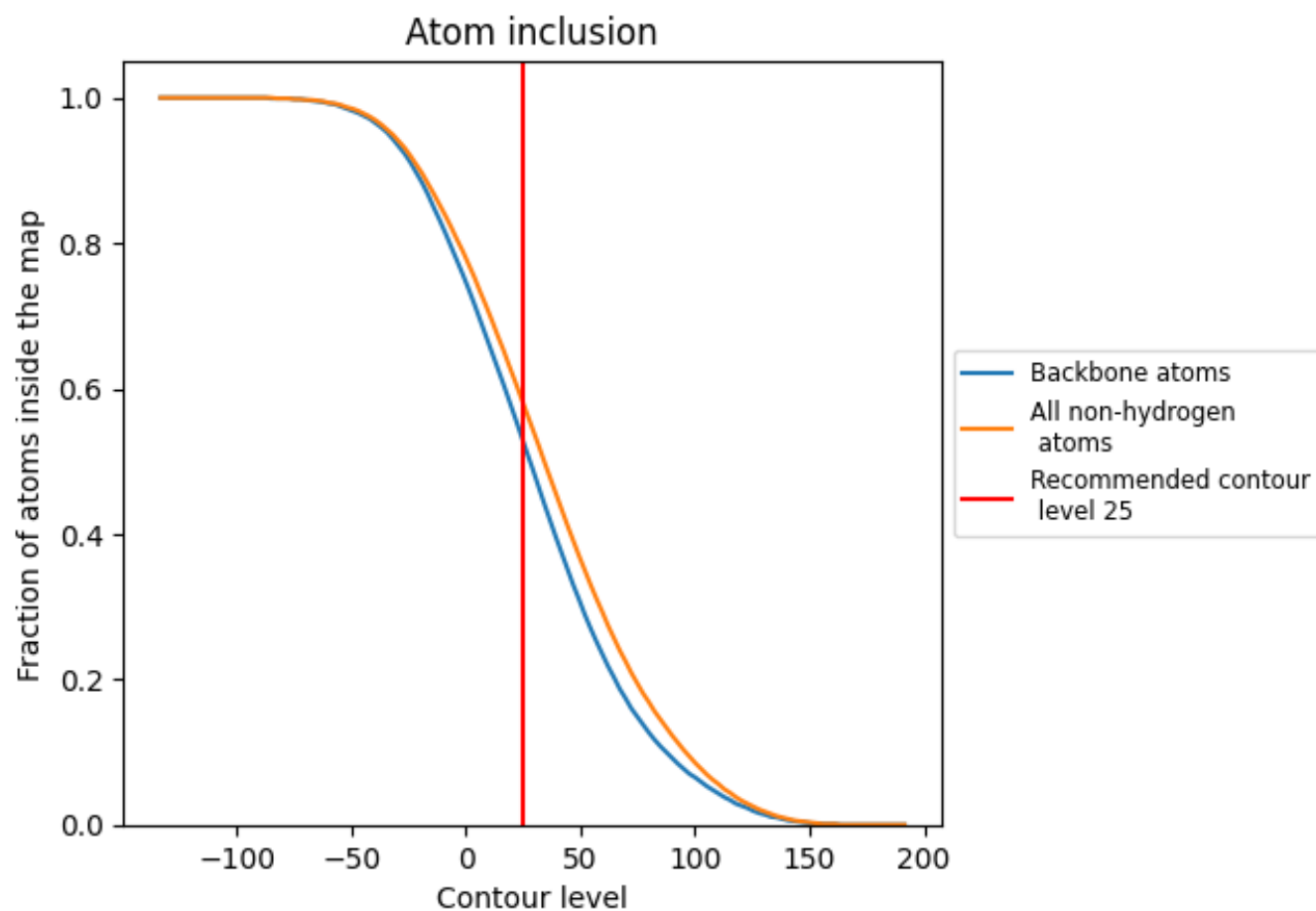
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 58% 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 (25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5810	 0.0150
A1	 0.5160	 0.0210
A2	 0.4760	 -0.0030
A3	 0.3830	 -0.0050
AA	 0.6610	 0.0230
AB	 0.4760	 0.0520
AC	 0.5210	 0.0080
AD	 0.4340	 0.0110
AE	 0.5200	 0.0300
AF	 0.7140	 0.0380
AG	 0.5950	 0.0120
AH	 0.5110	 0.0070
AI	 0.7070	 0.0030
AJ	 0.4240	 0.0020
AK	 0.6720	 0.0330
AL	 0.6300	 0.0140
AM	 0.6530	 0.0320
AN	 0.3420	 -0.0380
AO	 0.7130	 0.0190
AP	 0.4340	 0.0050
AQ	 0.5450	 0.0230
AR	 0.5810	 0.0020
AS	 0.6650	 0.0190
AT	 0.7030	 0.0010
AU	 0.5820	 0.0460
B0	 0.7100	 0.0380
B1	 0.5120	 0.0350
B2	 0.4170	 -0.0450
B3	 0.4130	 -0.0030
B4	 0.5100	 -0.0030
B5	 0.3460	 -0.0020
BA	 0.5880	 0.0150
BB	 0.7180	 0.0320
BC	 0.4310	 -0.0150
BD	 0.4710	 0.0100



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Chain	Atom inclusion	Q-score
BE	 0.5910	 -0.0060
BF	 0.5840	 0.0210
BG	 0.4590	 0.0220
BH	 0.2250	 0.0250
BI	 0.0000	 -0.0030
BJ	 0.4790	 -0.0040
BK	 0.4540	 0.0030
BL	 0.6080	 -0.0140
BM	 0.4260	 0.0170
BN	 0.5740	 -0.0180
BO	 0.8410	 0.0280
BP	 0.4290	 -0.0060
BQ	 0.5300	 -0.0060
BR	 0.6140	 -0.0070
BS	 0.4800	 0.0010
BT	 0.6280	 -0.0100
BU	 0.5690	 0.0050
BV	 0.6310	 0.0560
BW	 0.6220	 0.0220
BX	 0.4460	 -0.0480
BY	 0.5490	 0.0070
BZ	 0.4460	 0.0020