



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:02 PM UTC

PDB ID : 4V5M / pdb_00004v5m
EMDB ID : EMD-1798
Title : tRNA tranlocation on the 70S ribosome: the pre-translocational translocation intermediate TI(PRE)
Authors : Ratje, A.H.; Loerke, J.; Mikolajka, A.; Bruenner, M.; Hildebrand, P.W.; Starosta, A.L.; Doenhoefer, A.; Connell, S.R.; Fucini, P.; Mielke, T.; Whitford, P.C.; Onuchic, J.N.; Yu, Y.; Sanbonmatsu, K.Y.; Hartmann, R.K.; Penczek, P.A.; Wilson, D.N.; Spahn, C.M.T.
Deposited on : 2010-10-01
Resolution : 7.80 Å(reported)
Based on initial models : 2WRI, 2WRJ

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)

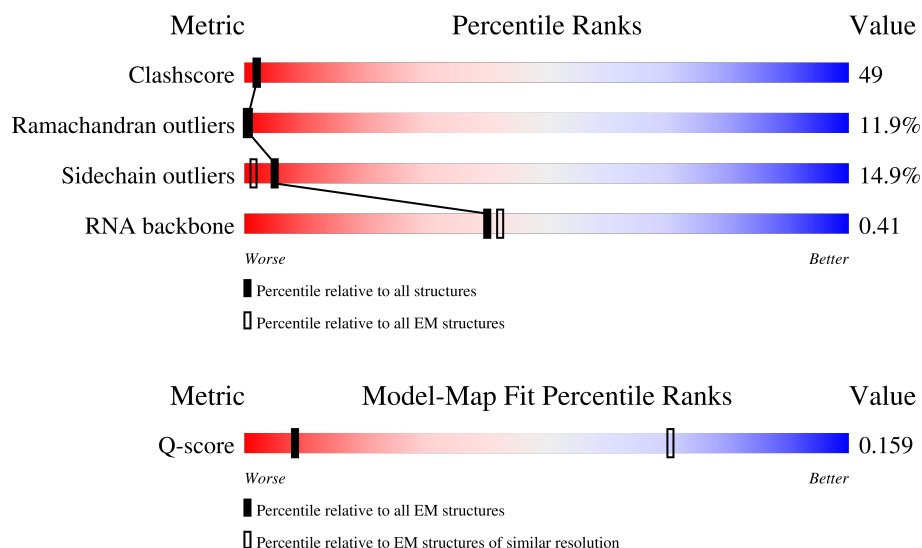
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	370 (7.30 - 8.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AA	1522	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	AB	256	
3	AC	239	
4	AD	209	
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	132	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	11	
24	AY	691	
25	B0	85	
26	B1	98	

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Mol	Chain	Length	Quality of chain
27	B2	72	
28	B3	60	
29	B4	71	
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BK	147	
44	BL	121	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	

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Mol	Chain	Length	Quality of chain
52	BU	118	
53	BV	101	
54	BW	113	
55	BX	96	
56	BY	110	
57	BZ	206	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 152777 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 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0
			32329	14390	5992	10444	1503		

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0
			987	611	205	169	2		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	70	Total	C	N	O	0	0
			574	367	112	95		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0
			629	403	114	110	2		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AU	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a RNA chain called TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0
			230	105	41	74	10		

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AY	666	Total	C	N	O	S	0	0
			5214	3316	892	988	18		

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0
			662	410	140	111	1		

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	93	Total	C	N	O	S	0	0
			731	460	145	125	1		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0
			598	370	121	106	1		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	59	Total	C	N	O	S	0	0
			467	298	90	78	1		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B4	57	Total	C	N	O	S	0	0
			450	285	77	83	5		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0
			459	288	90	76	5		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0
			433	270	88	71	4		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0
			418	257	104	55	2		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B8	63	Total	C	N	O	S	0	0
			507	326	101	78	2		

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0
			62474	27806	11681	20087	2900		

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0
			2551	1136	471	826	118		

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0
			1742	1101	319	319	3		

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0
			2145	1353	428	361	3		

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	204	Total	C	N	O	S	0	0
			1563	988	299	270	6		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	207	Total	C	N	O	S	0	0
			1623	1035	303	282	3		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0
			1474	942	268	260	4		

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	166	Total	C	N	O	S	0	0
			1268	803	237	227	1		

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	139	Total	C	N	O	S	0	0
			1025	653	181	186	5		

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BL	67	Total	C	N	O	0	0
			477	301	81	95		

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BN	138	Total	C	N	O	S	0	0
			1104	712	206	182	4		

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0
			1114	692	227	193	2		

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0
			1122	715	212	188	7		

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BR	117	Total	C	N	O	0	0
			960	599	202	159		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BS	98	Total	C	N	O	0	0
			770	486	154	130		

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BT	137	Total	C	N	O	S	0	0
			1141	710	234	196	1		

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0
			958	604	202	151	1		

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0
			896	563	176	155	2		

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	BX	92	Total	C	N	O	0	0
			725	471	131	123		

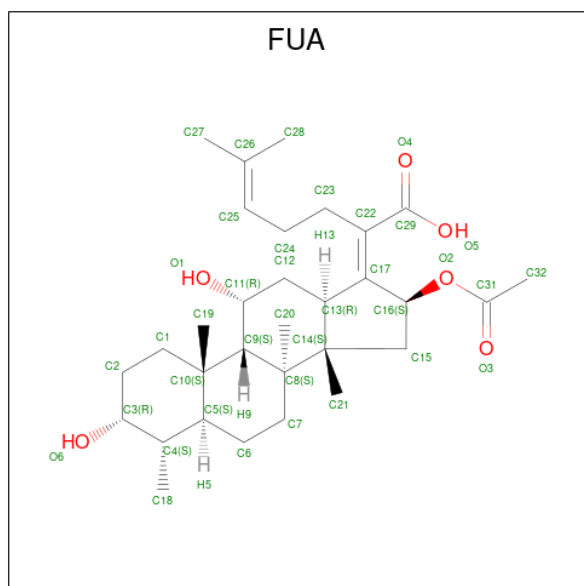
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BY	106	Total	C	N	O	S	0	0
			810	520	154	131	5		

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

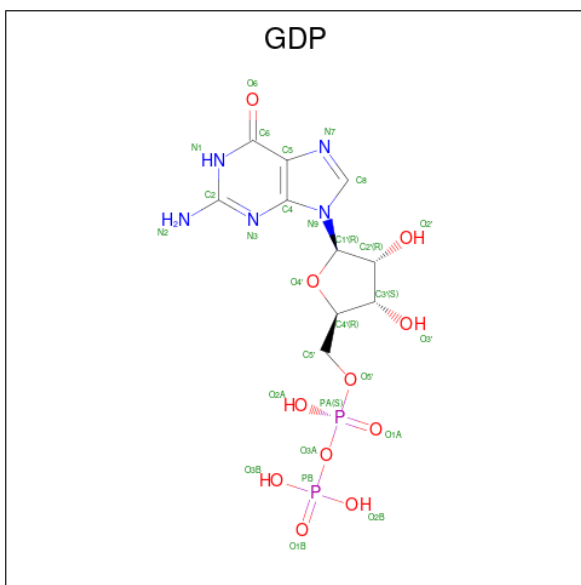
Mol	Chain	Residues	Atoms					AltConf	Trace
57	BZ	184	Total	C	N	O	S	0	0
			1467	936	261	268	2		

- Molecule 58 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$).



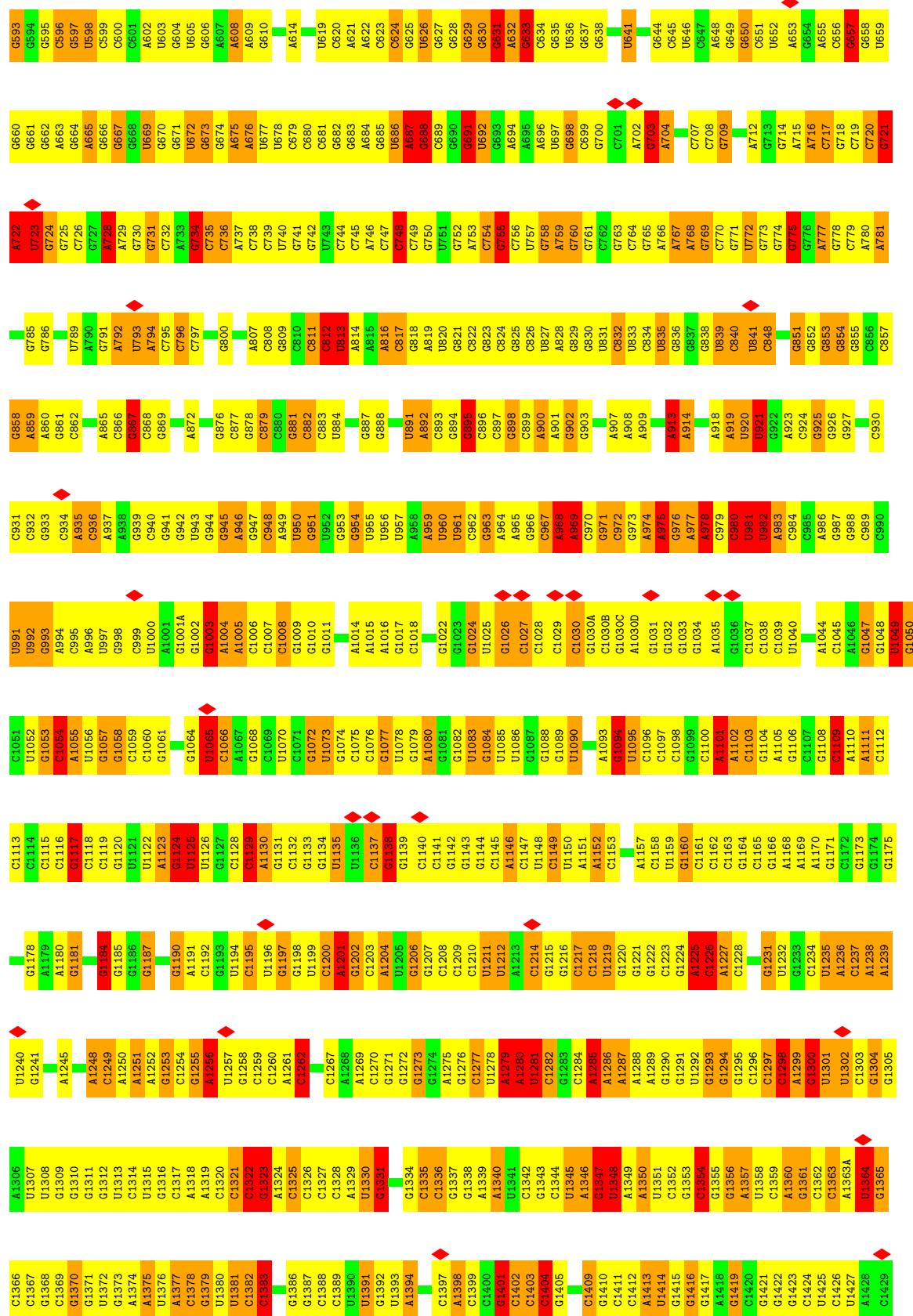
Mol	Chain	Residues	Atoms			AltConf
58	AY	1	Total	C	O	0
			37	31	6	

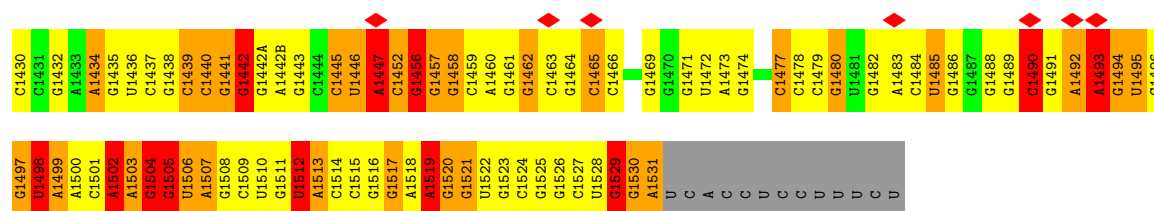
- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



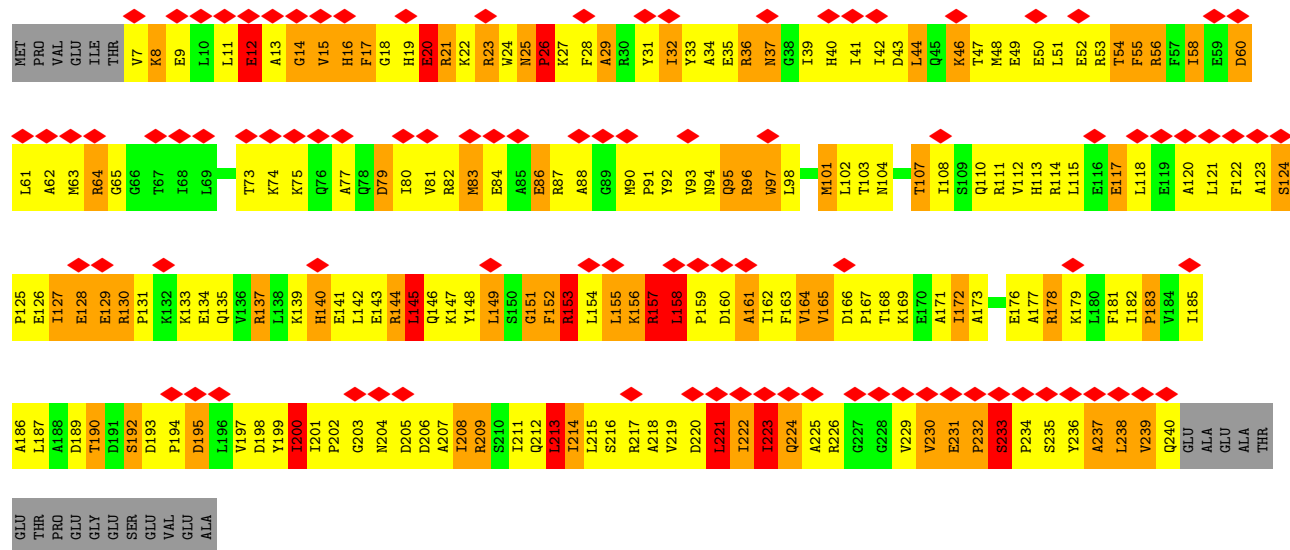
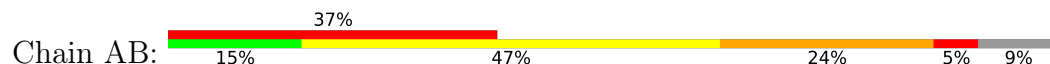
Mol	Chain	Residues	Atoms					AltConf
59	AY	1	Total	C	N	O	P	0
			28	10	5	11	2	



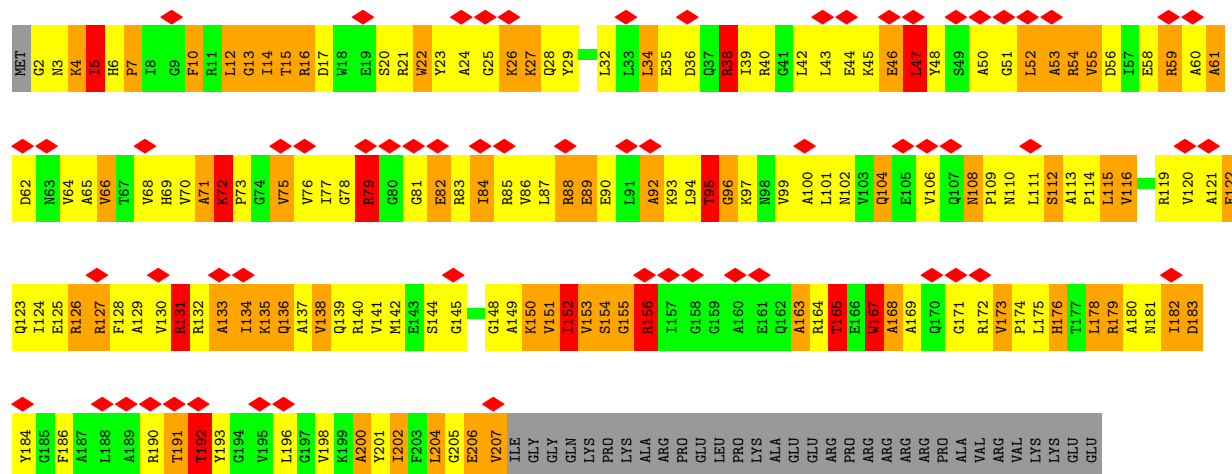
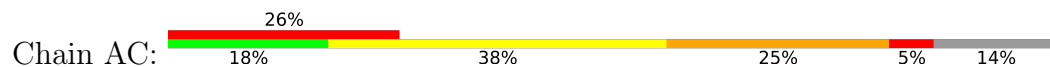




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

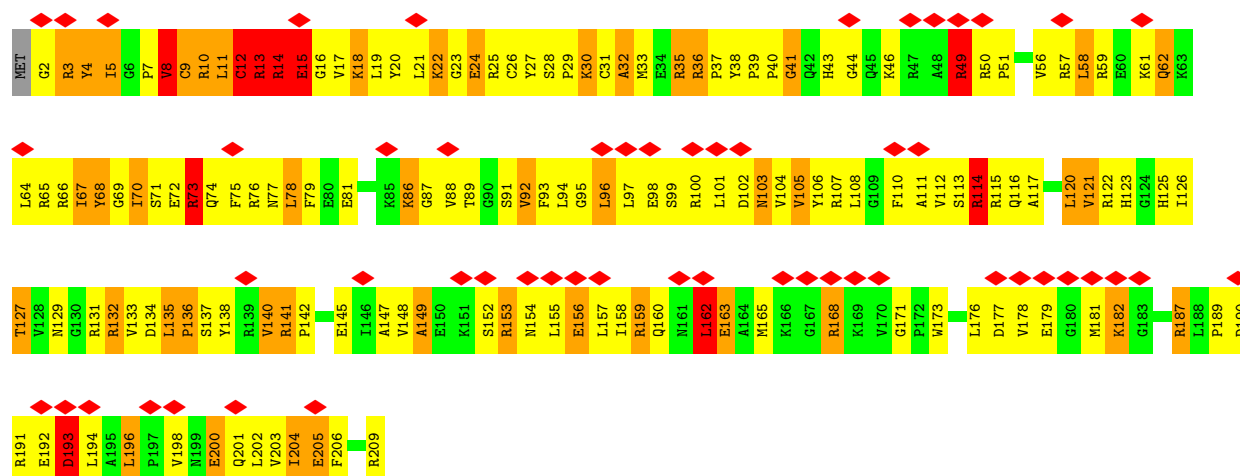


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

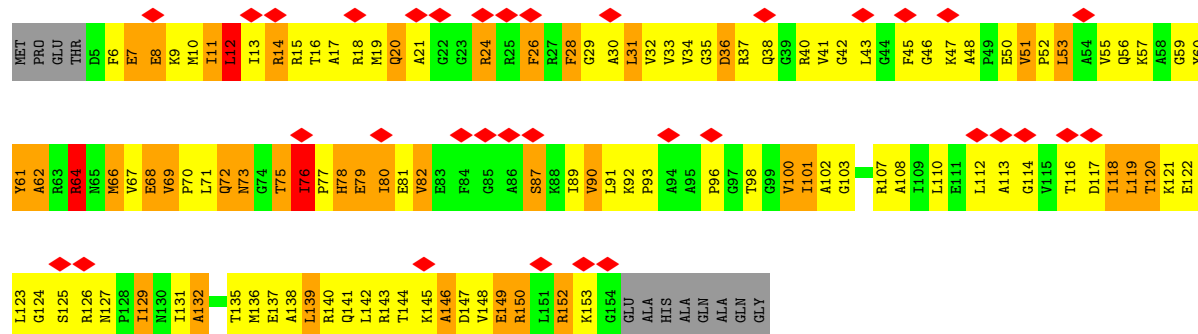
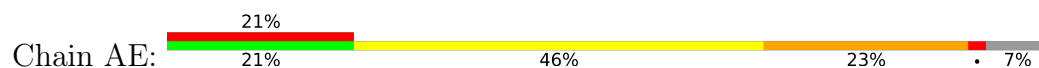


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

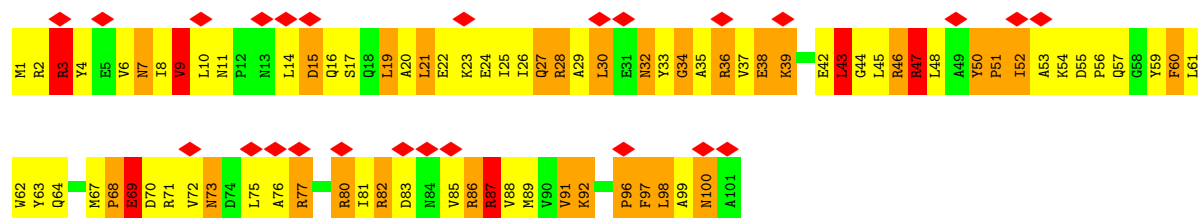
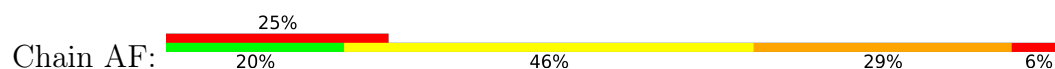




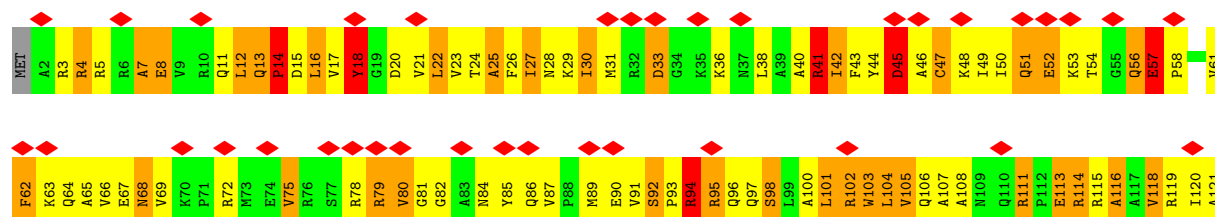
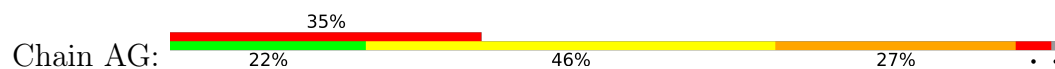
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

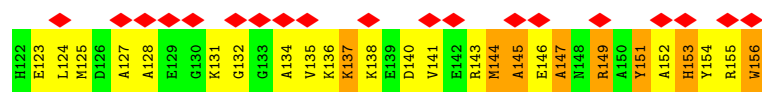


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

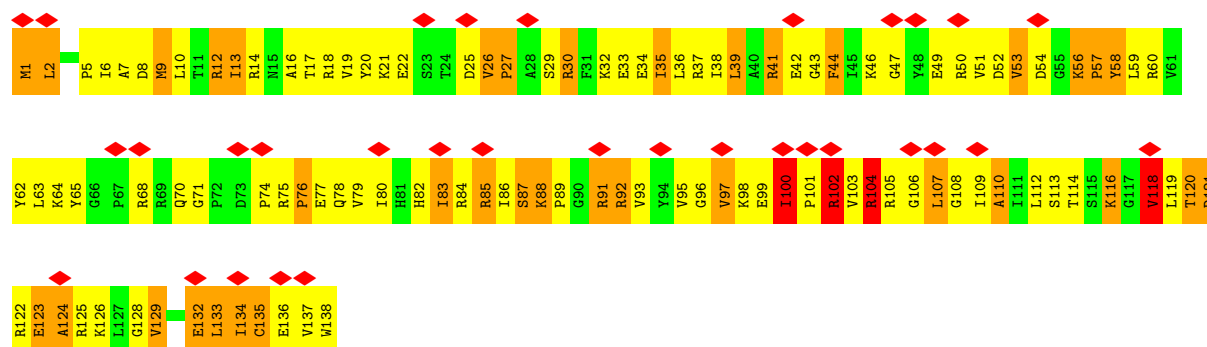
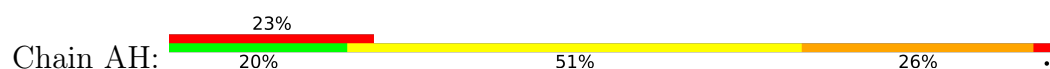


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

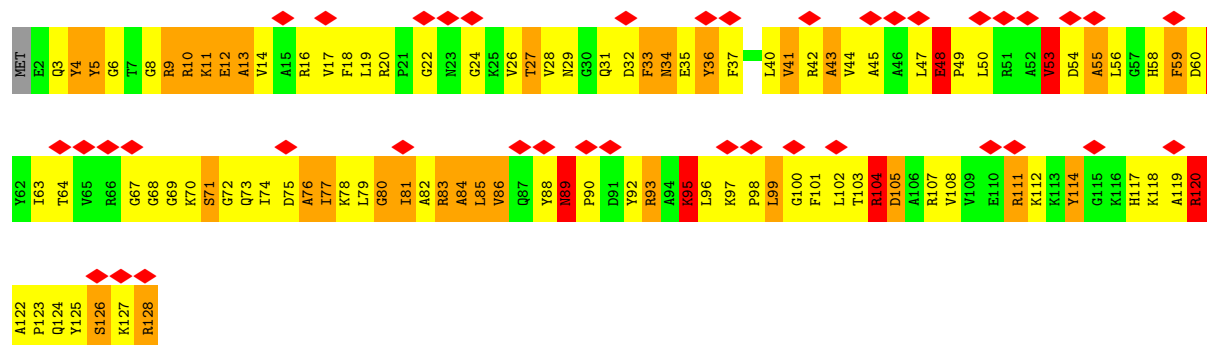
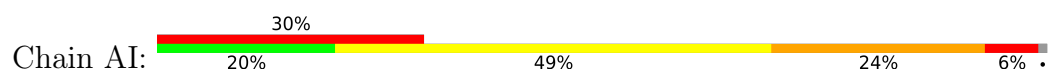




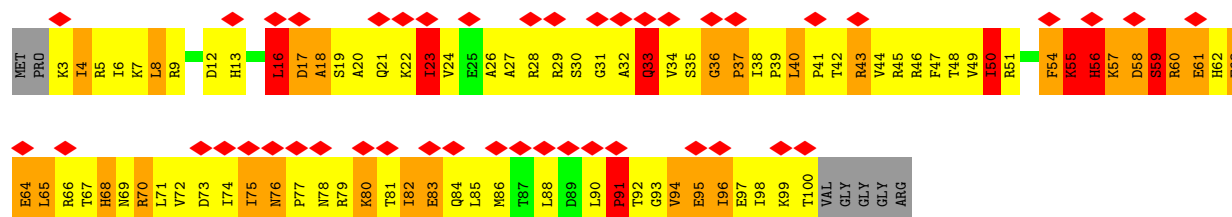
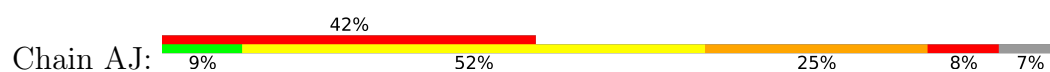
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

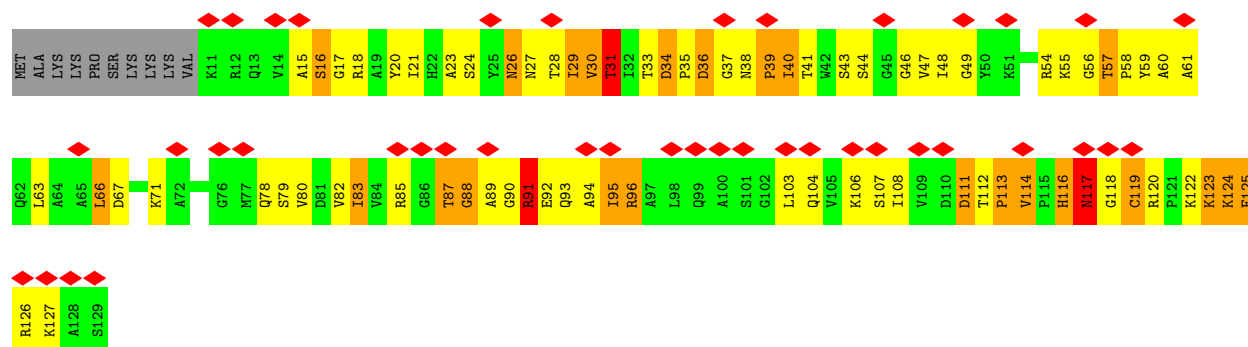


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

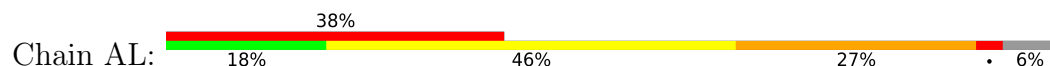


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

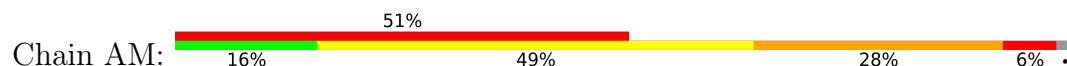




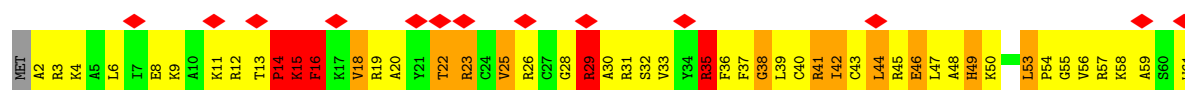
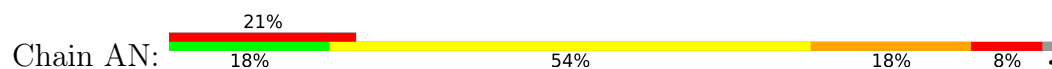
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



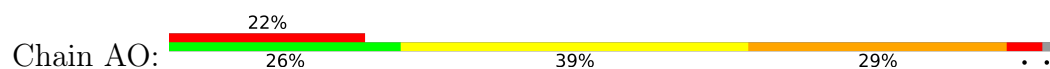
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

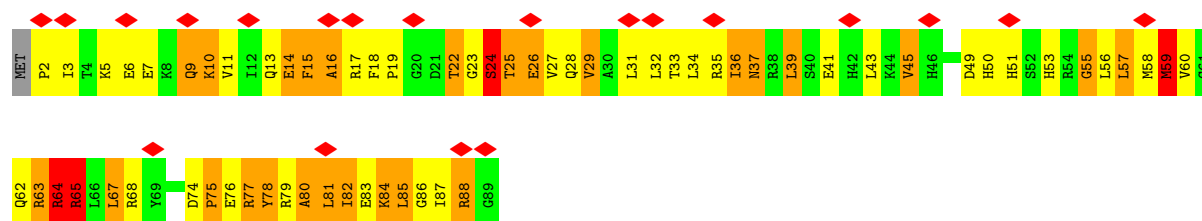


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

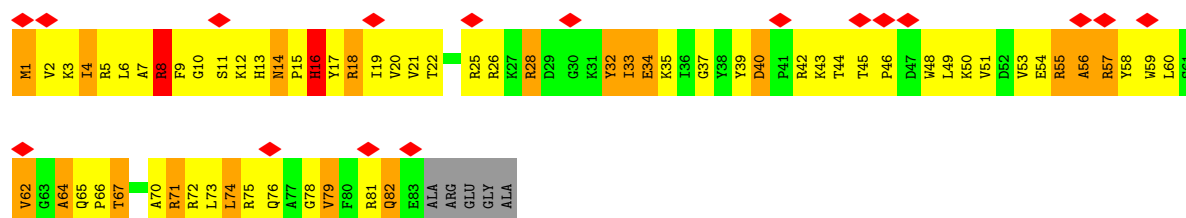
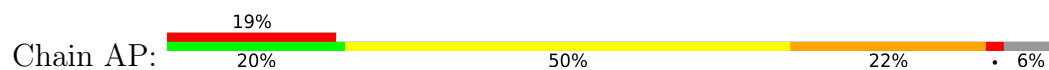


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

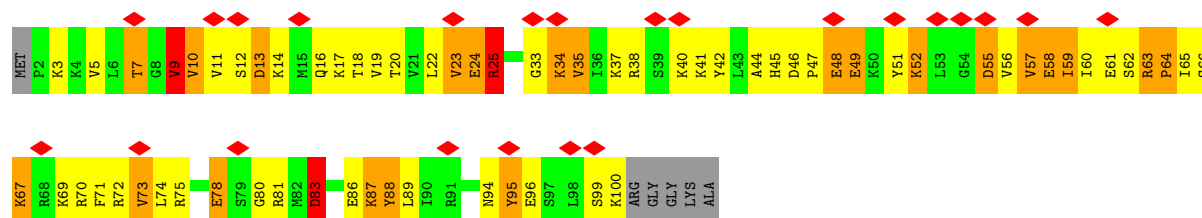




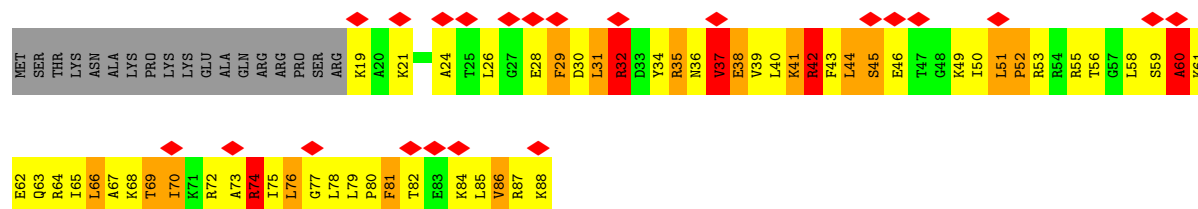
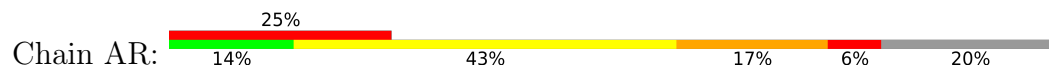
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



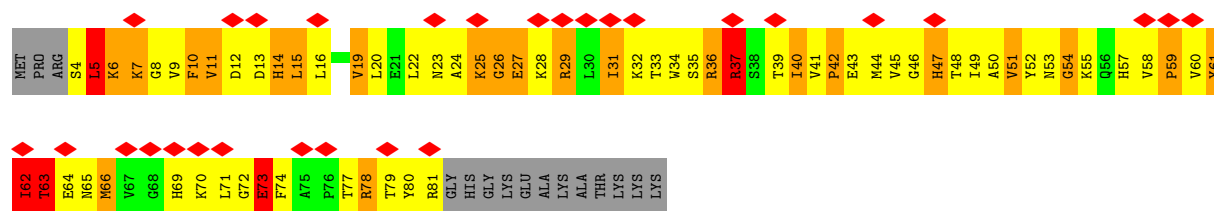
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

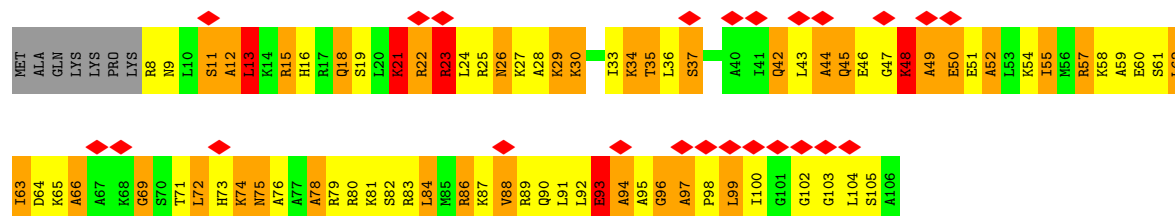


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

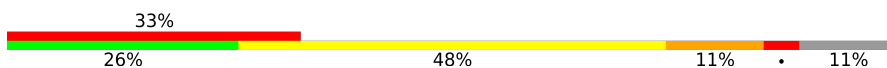


- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT: 



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU: 



- Molecule 22: TRNA

Chain AV: 



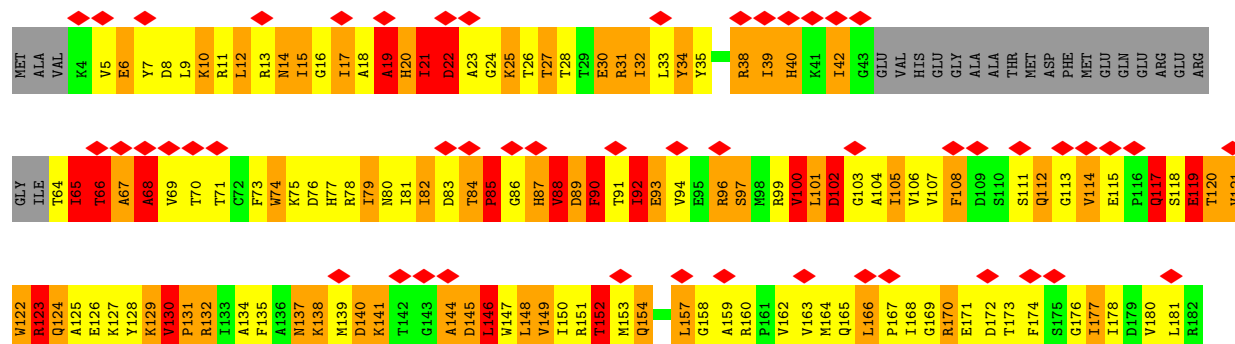
- Molecule 23: MRNA

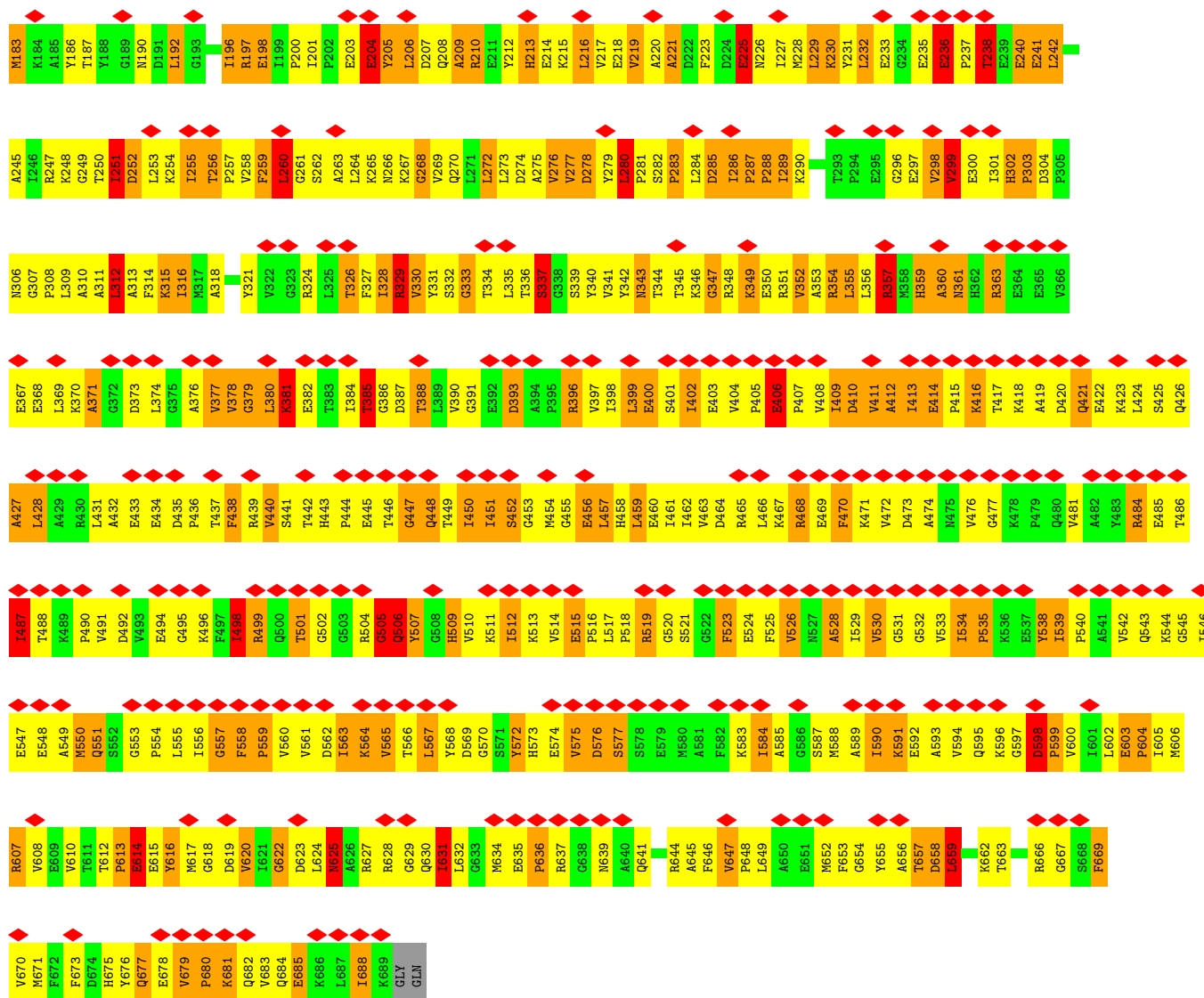
Chain AX: 



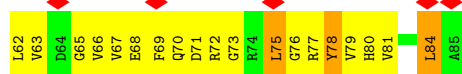
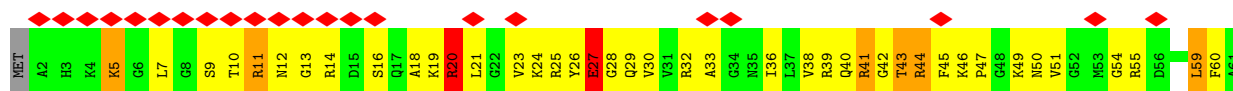
- Molecule 24: ELONGATION FACTOR G

Chain AY: 

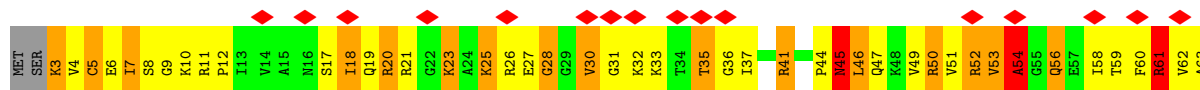
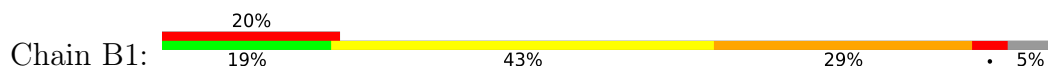


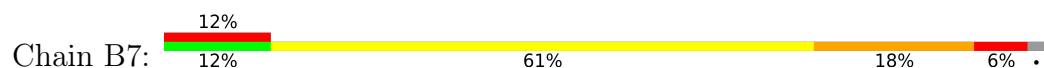


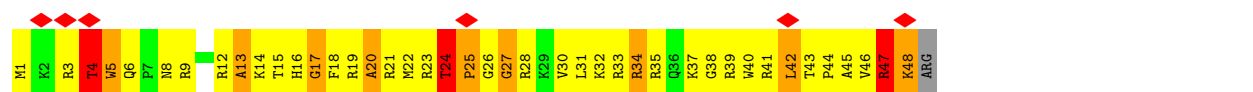
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



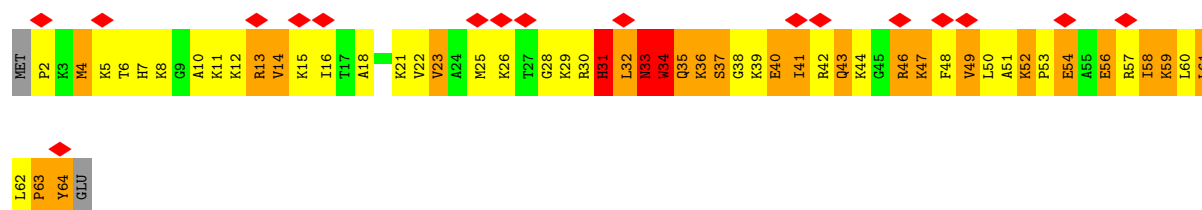
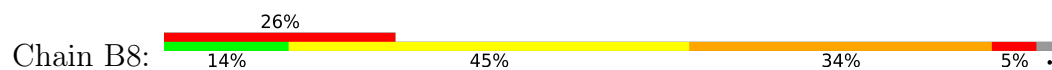
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



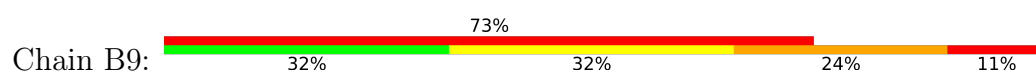




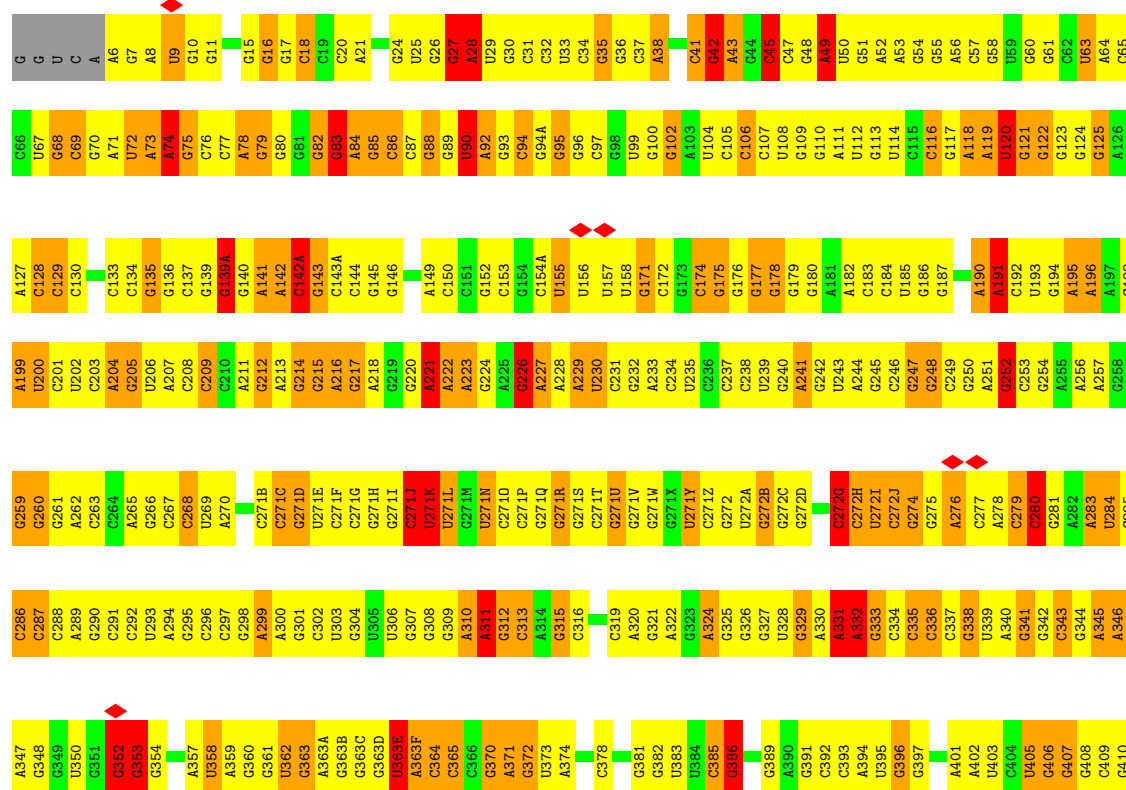
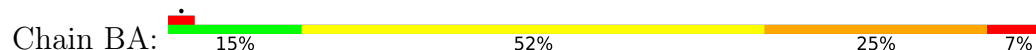
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

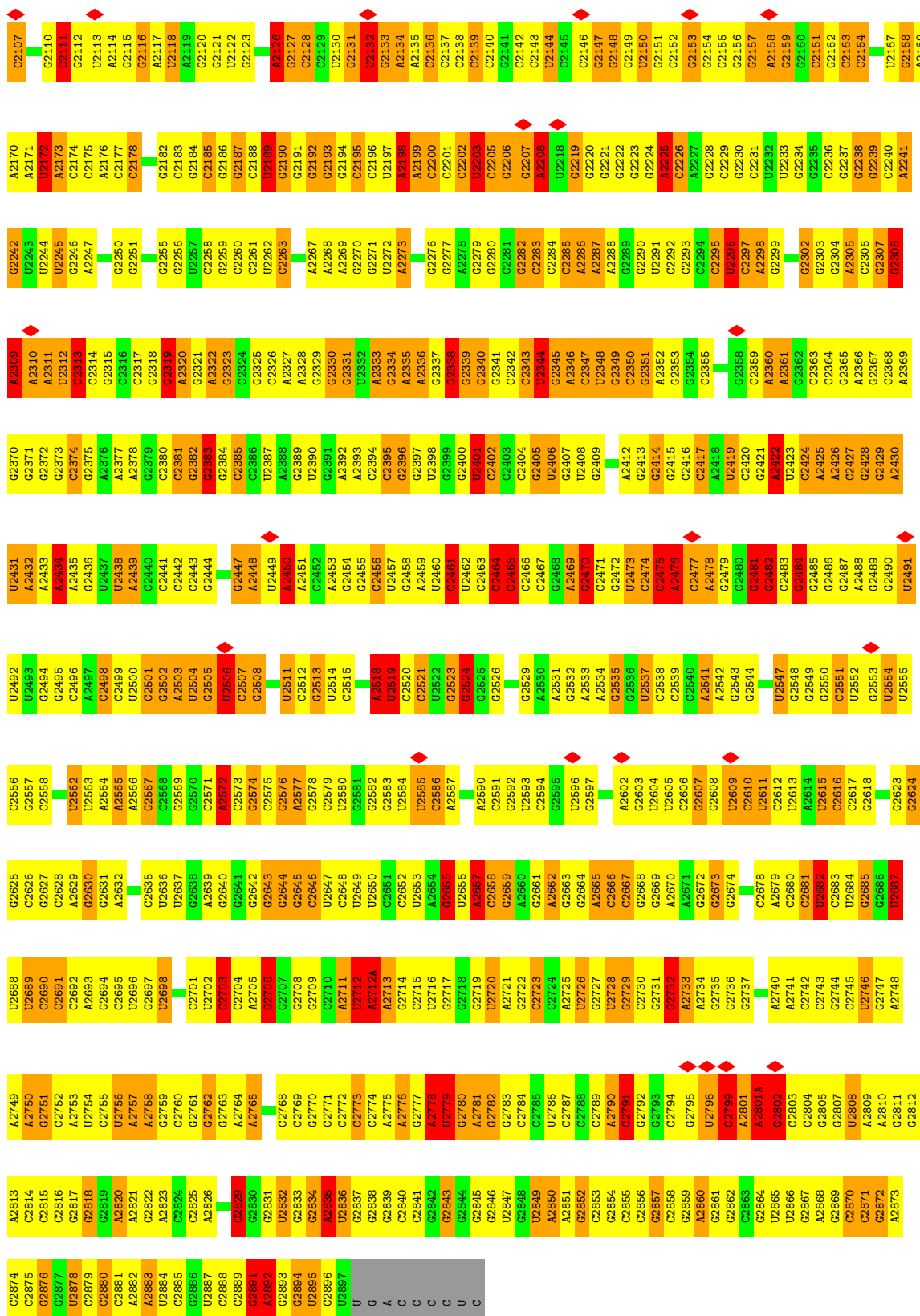


• Molecule 35: 23S RIBOSOMAL RNA



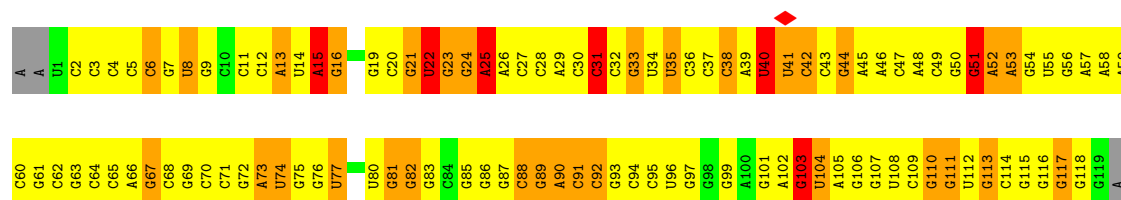




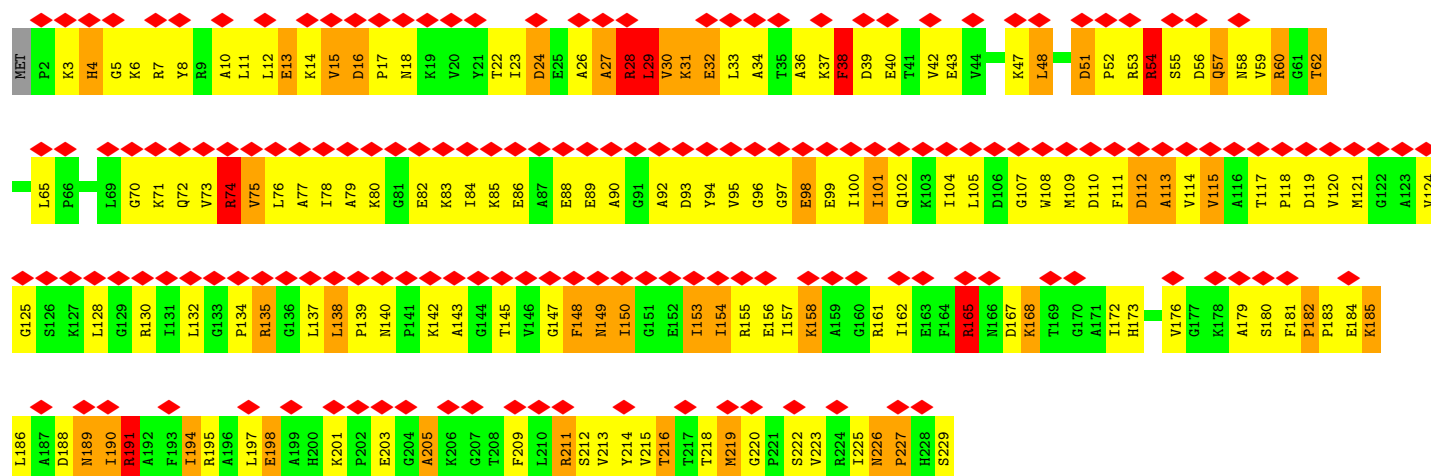
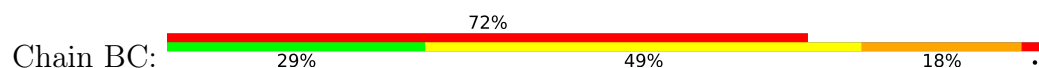


• Molecule 36: 5S RIBOSOMAL RNA

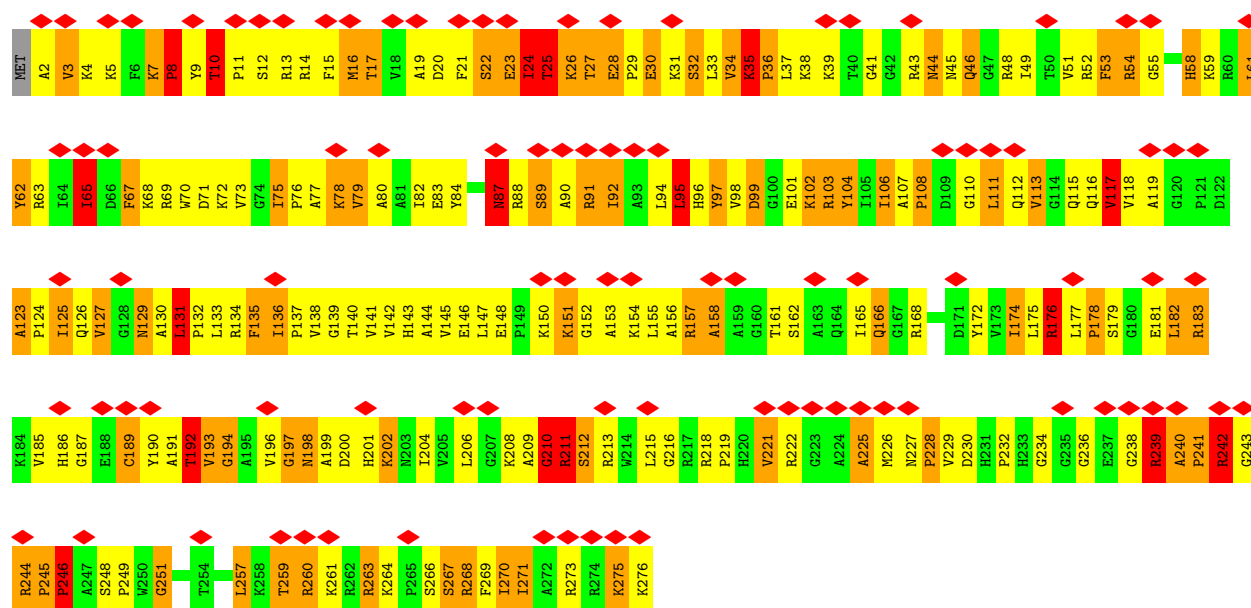
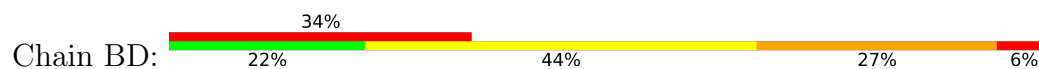
Chain BB: 8% 58% 25% 6%



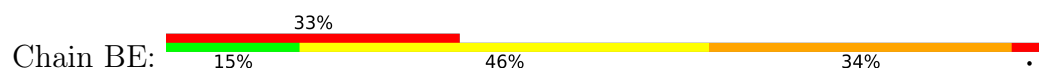
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

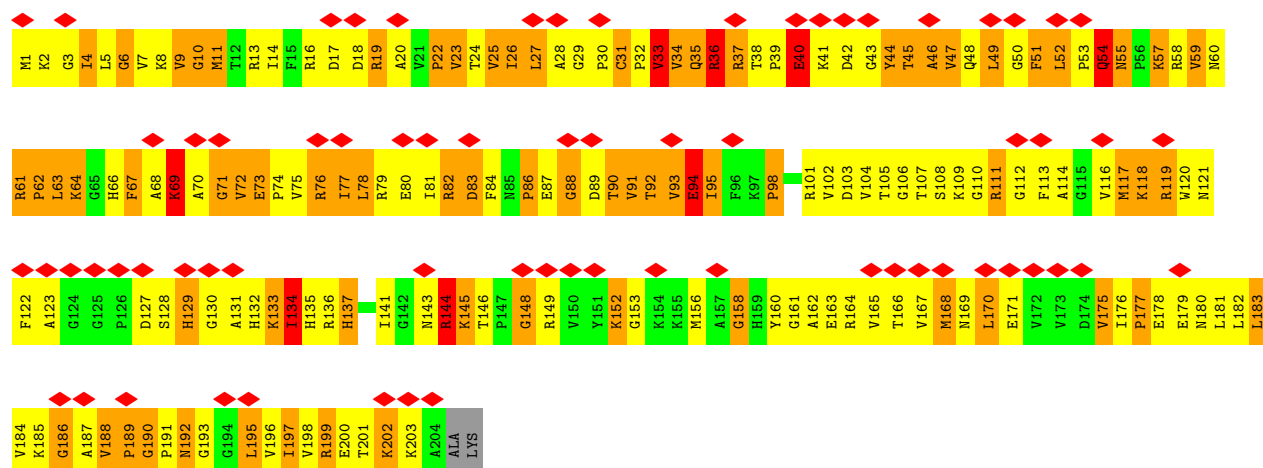


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

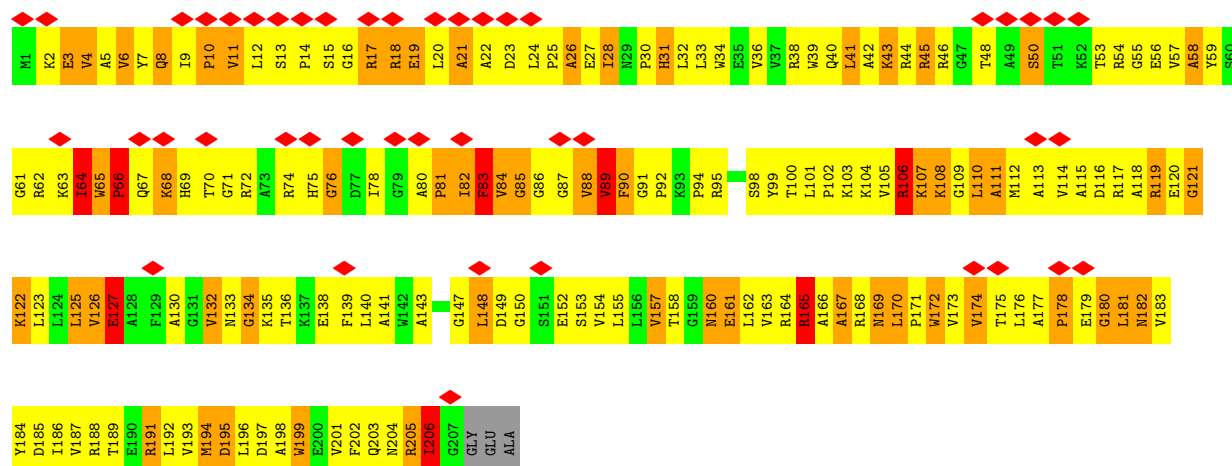
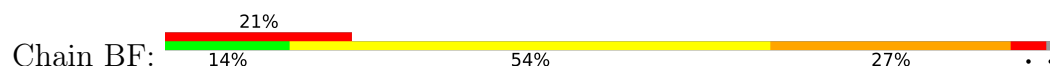


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

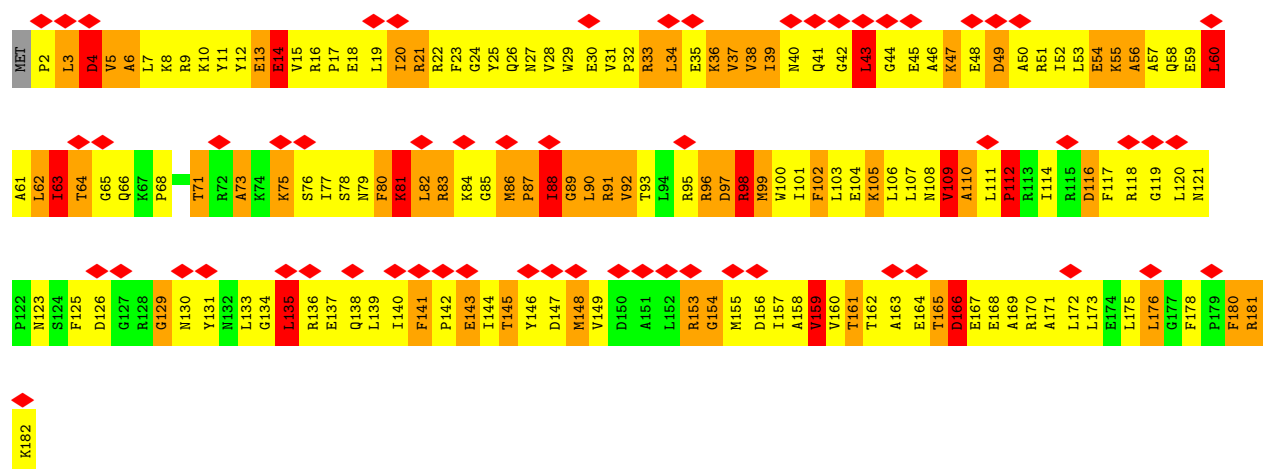
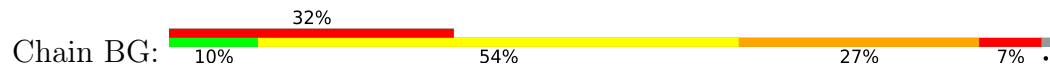




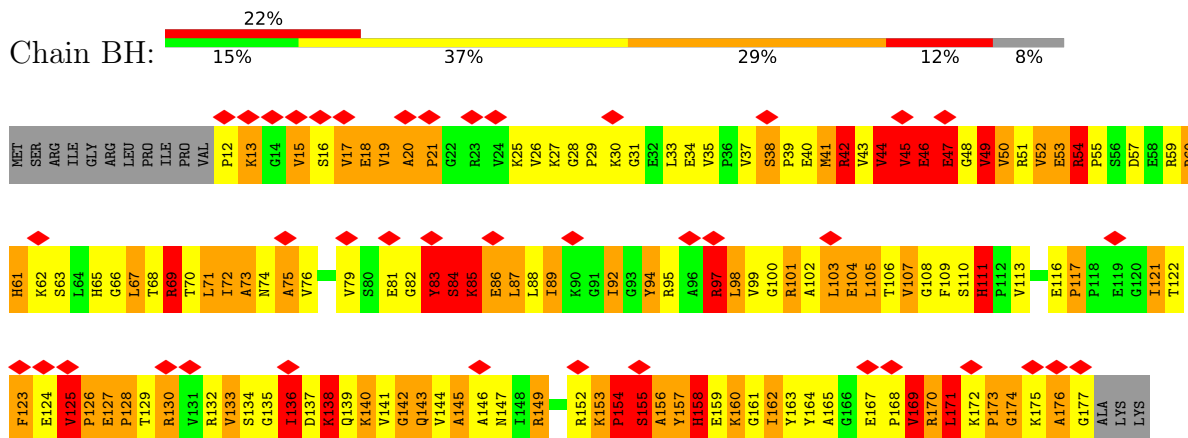
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



• Molecule 41: 50S RIBOSOMAL PROTEIN L5



- Molecule 42: 50S RIBOSOMAL PROTEIN L6

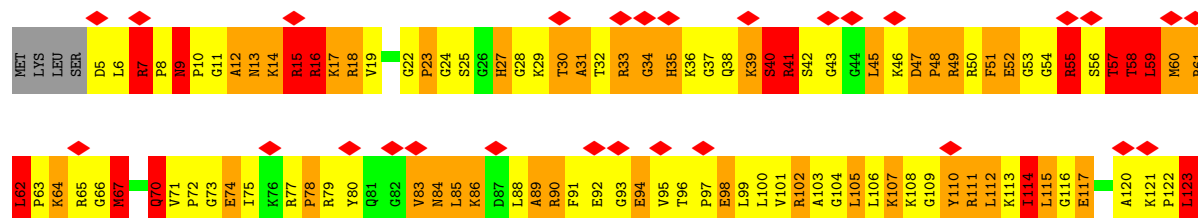




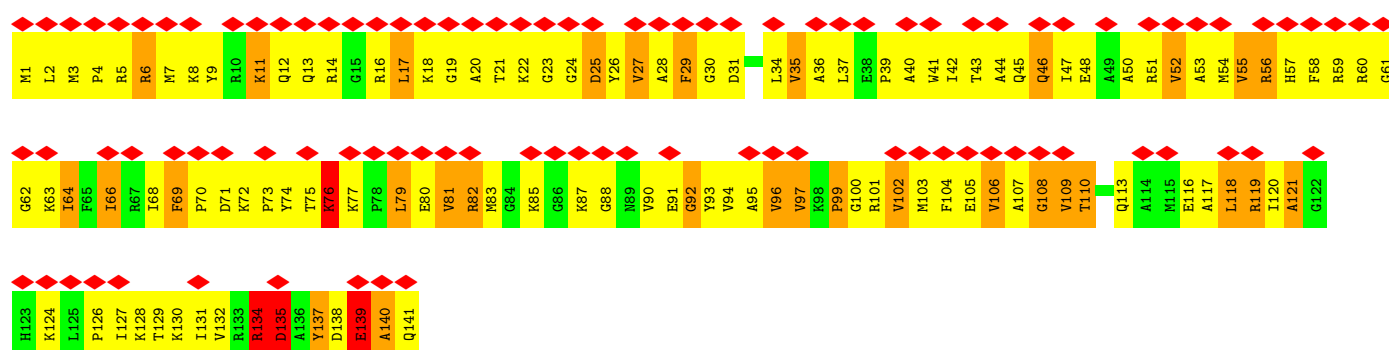
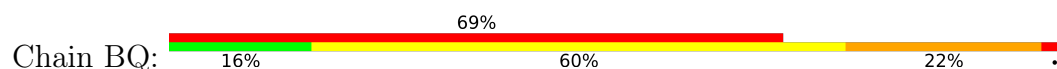
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



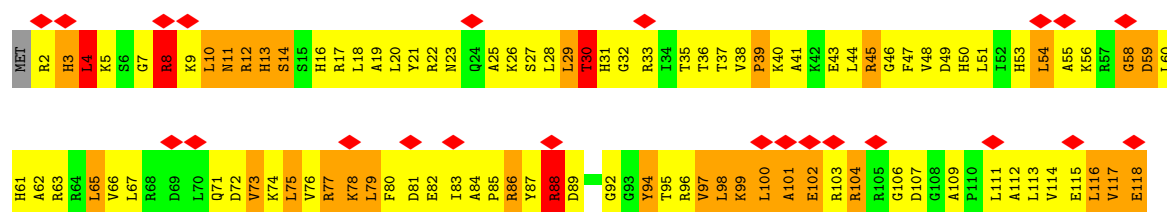
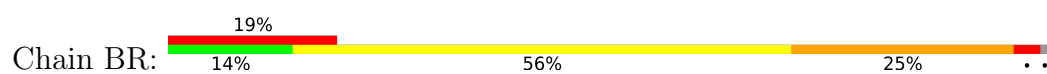
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



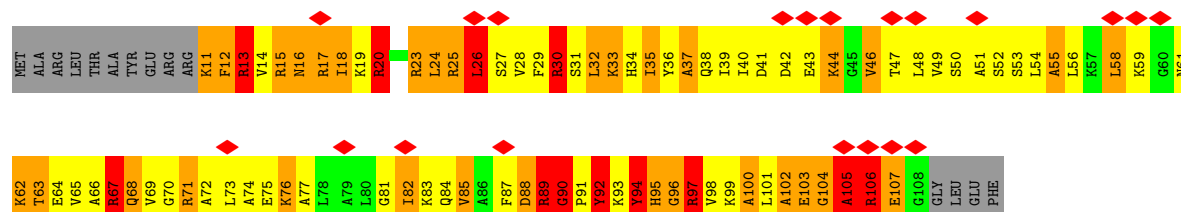
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



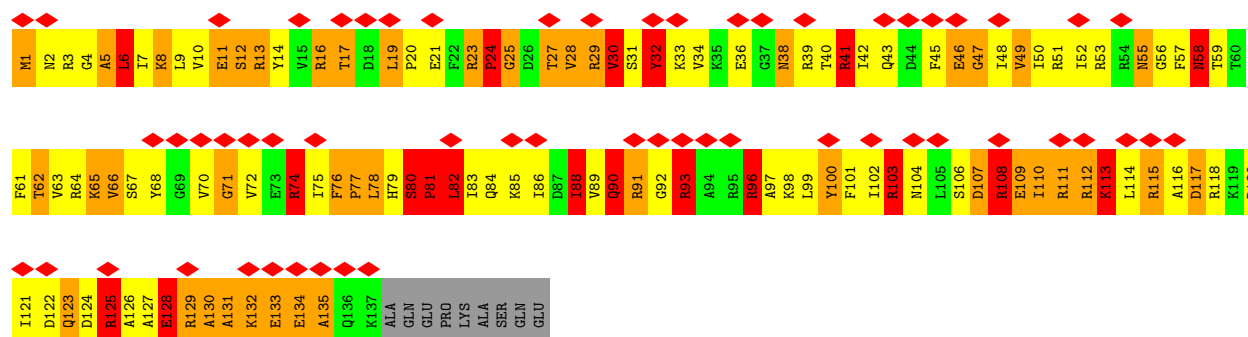
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



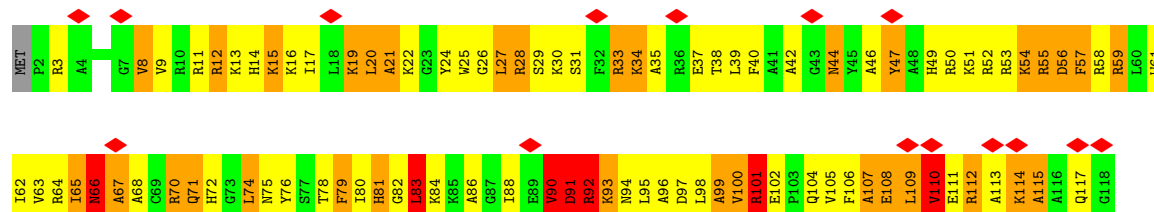
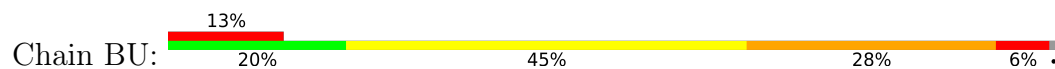
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



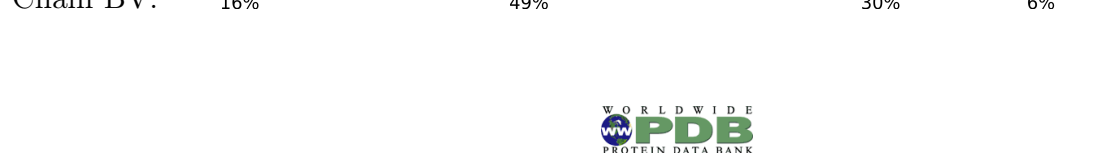
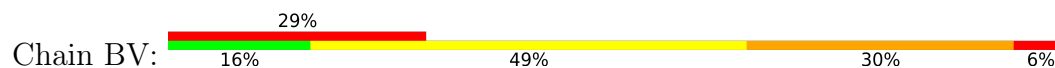
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L20



• Molecule 53: 50S RIBOSOMAL PROTEIN L21





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	13410.900	Depositor
Minimum map value	-6356.590	Depositor
Average map value	213.063	Depositor
Map value standard deviation	916.721	Depositor
Recommended contour level	3000	Depositor
Map size ($\text{\AA}$)	378, 378, 378	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.26, 1.26, 1.26	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AA	1.60	91/36190 (0.3%)	1.40	307/56486 (0.5%)
2	AB	1.90	24/1935 (1.2%)	1.88	43/2609 (1.6%)
3	AC	2.06	30/1636 (1.8%)	1.87	49/2205 (2.2%)
4	AD	1.86	21/1733 (1.2%)	1.80	28/2318 (1.2%)
5	AE	1.98	23/1162 (2.0%)	1.97	24/1564 (1.5%)
6	AF	1.84	10/856 (1.2%)	1.88	22/1154 (1.9%)
7	AG	1.87	15/1276 (1.2%)	1.83	24/1709 (1.4%)
8	AH	2.00	23/1136 (2.0%)	1.98	32/1527 (2.1%)
9	AI	1.94	11/1029 (1.1%)	2.41	21/1379 (1.5%)
10	AJ	1.90	9/807 (1.1%)	1.81	13/1085 (1.2%)
11	AK	1.97	15/900 (1.7%)	1.81	10/1213 (0.8%)
12	AL	1.96	11/986 (1.1%)	1.96	20/1320 (1.5%)
13	AM	1.86	10/998 (1.0%)	1.88	25/1336 (1.9%)
14	AN	2.00	12/501 (2.4%)	1.86	5/664 (0.8%)
15	AO	1.89	10/745 (1.3%)	1.85	10/992 (1.0%)
16	AP	1.83	8/716 (1.1%)	1.71	8/963 (0.8%)
17	AQ	1.92	8/836 (1.0%)	1.80	13/1117 (1.2%)
18	AR	1.89	5/579 (0.9%)	1.82	13/768 (1.7%)
19	AS	1.69	5/642 (0.8%)	1.68	2/865 (0.2%)
20	AT	1.88	10/765 (1.3%)	1.83	15/1007 (1.5%)
21	AU	1.67	2/212 (0.9%)	1.85	2/277 (0.7%)
22	AV	1.60	6/1832 (0.3%)	1.46	17/2855 (0.6%)
23	AX	1.61	2/257 (0.8%)	1.57	2/398 (0.5%)
24	AY	1.76	45/5312 (0.8%)	1.87	139/7193 (1.9%)
25	B0	1.74	5/671 (0.7%)	1.70	5/892 (0.6%)
26	B1	1.80	9/738 (1.2%)	1.78	10/981 (1.0%)
27	B2	1.68	1/600 (0.2%)	1.95	25/793 (3.2%)
28	B3	1.89	5/472 (1.1%)	1.86	9/634 (1.4%)
29	B4	1.67	4/460 (0.9%)	2.19	18/621 (2.9%)
30	B5	1.81	2/473 (0.4%)	1.87	10/639 (1.6%)
31	B6	1.76	0/440	2.10	20/586 (3.4%)
32	B7	1.88	5/426 (1.2%)	1.89	9/561 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	1.76	4/515 (0.8%)	1.92	15/679 (2.2%)
34	B9	1.82	5/310 (1.6%)	1.84	4/407 (1.0%)
35	BA	1.57	140/69972 (0.2%)	1.39	572/109237 (0.5%)
36	BB	1.57	4/2853 (0.1%)	1.36	24/4451 (0.5%)
37	BC	1.86	20/1774 (1.1%)	1.78	29/2391 (1.2%)
38	BD	1.87	28/2195 (1.3%)	1.91	50/2955 (1.7%)
39	BE	1.85	18/1596 (1.1%)	1.93	43/2153 (2.0%)
40	BF	1.84	10/1658 (0.6%)	1.91	39/2244 (1.7%)
41	BG	1.79	13/1499 (0.9%)	2.33	40/2016 (2.0%)
42	BH	1.74	12/1292 (0.9%)	1.86	33/1744 (1.9%)
43	BK	1.68	6/1044 (0.6%)	1.76	16/1416 (1.1%)
44	BL	1.42	2/478 (0.4%)	1.86	8/640 (1.2%)
45	BN	1.80	9/1131 (0.8%)	1.93	24/1525 (1.6%)
46	BO	1.94	15/943 (1.6%)	1.87	21/1269 (1.7%)
47	BP	1.77	7/1131 (0.6%)	1.95	34/1504 (2.3%)
48	BQ	1.85	13/1143 (1.1%)	1.76	16/1527 (1.0%)
49	BR	1.77	8/974 (0.8%)	1.83	21/1302 (1.6%)
50	BS	1.76	9/778 (1.2%)	1.89	26/1036 (2.5%)
51	BT	1.86	16/1155 (1.4%)	1.98	38/1542 (2.5%)
52	BU	1.87	16/975 (1.6%)	1.87	19/1297 (1.5%)
53	BV	1.77	10/790 (1.3%)	1.78	13/1057 (1.2%)
54	BW	1.78	7/907 (0.8%)	1.80	18/1216 (1.5%)
55	BX	1.83	10/739 (1.4%)	1.84	15/993 (1.5%)
56	BY	1.65	9/823 (1.1%)	1.79	11/1098 (1.0%)
57	BZ	1.78	12/1499 (0.8%)	1.83	29/2035 (1.4%)
All	All	1.67	840/165495 (0.5%)	1.56	2108/246445 (0.9%)

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
1	AA	0	107
2	AB	0	5
3	AC	0	3
4	AD	0	3
5	AE	0	4
6	AF	0	6
7	AG	0	6
8	AH	0	4
9	AI	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	AJ	0	2
11	AK	0	2
12	AL	0	3
13	AM	0	3
14	AN	0	2
15	AO	0	3
16	AP	0	6
17	AQ	0	3
18	AR	0	3
19	AS	0	3
20	AT	0	2
21	AU	0	3
22	AV	0	5
23	AX	0	1
24	AY	0	13
25	B0	0	1
26	B1	0	3
27	B2	0	6
28	B3	0	2
29	B4	0	3
30	B5	0	2
31	B6	0	3
32	B7	0	1
33	B8	0	2
34	B9	0	2
35	BA	1	152
36	BB	0	6
37	BC	0	6
38	BD	0	2
39	BE	0	3
40	BF	0	3
41	BG	0	5
42	BH	0	8
43	BK	0	3
45	BN	0	3
46	BO	0	3
47	BP	0	5
48	BQ	0	3
49	BR	0	2
50	BS	0	6
51	BT	0	6
52	BU	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	BV	0	2
54	BW	0	4
55	BX	0	2
56	BY	0	3
57	BZ	0	4
All	All	1	457

The worst 5 of 840 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	BG	112	PRO	C-N	13.96	1.53	1.33
9	AI	53	VAL	C-N	12.03	1.50	1.33
9	AI	104	ARG	C-N	11.92	1.50	1.33
3	AC	204	LEU	CA-C	10.06	1.57	1.52
3	AC	167	TRP	CA-C	-9.99	1.48	1.53

The worst 5 of 2108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BG	112	PRO	O-C-N	-48.13	57.66	122.64
9	AI	53	VAL	O-C-N	-46.64	64.27	122.57
9	AI	104	ARG	O-C-N	-36.45	74.11	122.59
41	BG	112	PRO	CA-C-N	-24.58	84.00	122.59
41	BG	112	PRO	C-N-CA	-24.58	84.00	122.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1992	G	C3'

5 of 457 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	106	C	Sidechain
1	AA	108	G	Sidechain
1	AA	30	U	Sidechain
1	AA	5	U	Sidechain
1	AA	69	G	Sidechain

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	AA	32329	0	16041	1546	0
2	AB	1900	0	1951	260	0
3	AC	1612	0	1677	220	0
4	AD	1703	0	1767	213	0
5	AE	1146	0	1207	148	0
6	AF	843	0	857	99	0
7	AG	1257	0	1296	128	0
8	AH	1116	0	1177	124	0
9	AI	1010	0	1037	151	0
10	AJ	794	0	840	195	0
11	AK	885	0	904	94	0
12	AL	970	0	1057	147	0
13	AM	987	0	1059	145	0
14	AN	492	0	533	77	0
15	AO	734	0	771	78	0
16	AP	700	0	720	86	0
17	AQ	823	0	891	72	0
18	AR	574	0	644	82	0
19	AS	629	0	652	122	0
20	AT	763	0	861	119	0
21	AU	208	0	221	29	0
22	AV	1640	0	831	100	0
23	AX	230	0	114	17	0
24	AY	5214	0	5288	826	0
25	B0	662	0	688	94	0
26	B1	731	0	808	117	0
27	B2	598	0	653	104	0
28	B3	467	0	523	55	0
29	B4	450	0	449	98	0
30	B5	459	0	480	104	0
31	B6	433	0	461	154	0
32	B7	418	0	467	60	0
33	B8	507	0	576	107	0
34	B9	307	0	338	36	0
35	BA	62474	0	31032	3288	0
36	BB	2551	0	1281	164	0
37	BC	1742	0	1798	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	316	0
39	BE	1563	0	1629	259	0
40	BF	1623	0	1677	294	0
41	BG	1474	0	1535	301	0
42	BH	1268	0	1337	235	0
43	BK	1025	0	1066	182	0
44	BL	477	0	509	15	0
45	BN	1104	0	1180	207	0
46	BO	933	0	996	132	0
47	BP	1114	0	1187	302	0
48	BQ	1122	0	1179	173	0
49	BR	960	0	1021	166	0
50	BS	770	0	832	179	0
51	BT	1141	0	1202	239	0
52	BU	958	0	1015	183	0
53	BV	779	0	852	157	0
54	BW	896	0	953	109	0
55	BX	725	0	778	98	0
56	BY	810	0	901	193	0
57	BZ	1467	0	1492	238	0
58	AY	37	0	47	12	0
59	AY	28	0	12	7	0
All	All	152777	0	105584	12557	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 49.

The worst 5 of 12557 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:509:A:H5'	1:AA:510:A:OP2	1.26	1.30
24:AY:496:LYS:HE2	24:AY:498:ILE:CD1	1.66	1.25
53:BV:15:GLU:HB3	53:BV:16:PRO:HD2	1.23	1.20
24:AY:550:MET:HE3	24:AY:563:ILE:HD11	1.24	1.19
41:BG:63:ILE:HA	41:BG:143:GLU:HG3	1.22	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	AB	232/256 (91%)	146 (63%)	55 (24%)	31 (13%)	0	4
3	AC	204/239 (85%)	129 (63%)	58 (28%)	17 (8%)	0	9
4	AD	206/209 (99%)	133 (65%)	52 (25%)	21 (10%)	0	7
5	AE	148/162 (91%)	116 (78%)	27 (18%)	5 (3%)	3	21
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	1	13
7	AG	153/156 (98%)	107 (70%)	34 (22%)	12 (8%)	1	10
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	1	15
9	AI	125/128 (98%)	84 (67%)	26 (21%)	15 (12%)	0	4
10	AJ	96/105 (91%)	64 (67%)	19 (20%)	13 (14%)	0	4
11	AK	117/129 (91%)	93 (80%)	18 (15%)	6 (5%)	1	15
12	AL	122/132 (92%)	81 (66%)	26 (21%)	15 (12%)	0	4
13	AM	122/126 (97%)	77 (63%)	25 (20%)	20 (16%)	0	2
14	AN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	11
15	AO	86/89 (97%)	53 (62%)	25 (29%)	8 (9%)	0	8
16	AP	81/88 (92%)	58 (72%)	19 (24%)	4 (5%)	1	16
17	AQ	97/105 (92%)	76 (78%)	16 (16%)	5 (5%)	1	15
18	AR	68/88 (77%)	51 (75%)	11 (16%)	6 (9%)	0	8
19	AS	76/93 (82%)	39 (51%)	20 (26%)	17 (22%)	0	1
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0	3
21	AU	22/27 (82%)	14 (64%)	6 (27%)	2 (9%)	0	8
24	AY	662/691 (96%)	442 (67%)	135 (20%)	85 (13%)	0	4
25	B0	82/85 (96%)	64 (78%)	16 (20%)	2 (2%)	4	27
26	B1	91/98 (93%)	60 (66%)	20 (22%)	11 (12%)	0	4
27	B2	69/72 (96%)	34 (49%)	22 (32%)	13 (19%)	0	2
28	B3	57/60 (95%)	41 (72%)	12 (21%)	4 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	55/71 (78%)	25 (46%)	16 (29%)	14 (26%)	0	1
30	B5	57/60 (95%)	40 (70%)	6 (10%)	11 (19%)	0	2
31	B6	48/54 (89%)	22 (46%)	10 (21%)	16 (33%)	0	0
32	B7	46/49 (94%)	35 (76%)	9 (20%)	2 (4%)	2	17
33	B8	61/65 (94%)	35 (57%)	17 (28%)	9 (15%)	0	3
34	B9	35/37 (95%)	23 (66%)	8 (23%)	4 (11%)	0	5
37	BC	226/229 (99%)	173 (76%)	42 (19%)	11 (5%)	1	16
38	BD	273/276 (99%)	185 (68%)	55 (20%)	33 (12%)	0	4
39	BE	202/206 (98%)	121 (60%)	49 (24%)	32 (16%)	0	2
40	BF	205/210 (98%)	134 (65%)	44 (22%)	27 (13%)	0	4
41	BG	179/182 (98%)	113 (63%)	44 (25%)	22 (12%)	0	4
42	BH	164/180 (91%)	89 (54%)	37 (23%)	38 (23%)	0	1
43	BK	137/147 (93%)	89 (65%)	36 (26%)	12 (9%)	0	8
44	BL	65/121 (54%)	56 (86%)	9 (14%)	0	100	100
45	BN	136/140 (97%)	89 (65%)	31 (23%)	16 (12%)	0	4
46	BO	120/122 (98%)	94 (78%)	17 (14%)	9 (8%)	1	10
47	BP	144/150 (96%)	75 (52%)	44 (31%)	25 (17%)	0	2
48	BQ	139/141 (99%)	104 (75%)	28 (20%)	7 (5%)	1	16
49	BR	115/118 (98%)	79 (69%)	24 (21%)	12 (10%)	0	6
50	BS	96/112 (86%)	43 (45%)	34 (35%)	19 (20%)	0	2
51	BT	135/146 (92%)	76 (56%)	34 (25%)	25 (18%)	0	2
52	BU	115/118 (98%)	70 (61%)	33 (29%)	12 (10%)	0	6
53	BV	99/101 (98%)	67 (68%)	15 (15%)	17 (17%)	0	2
54	BW	111/113 (98%)	80 (72%)	18 (16%)	13 (12%)	0	4
55	BX	90/96 (94%)	62 (69%)	23 (26%)	5 (6%)	1	14
56	BY	104/110 (94%)	45 (43%)	35 (34%)	24 (23%)	0	1
57	BZ	182/206 (88%)	108 (59%)	41 (22%)	33 (18%)	0	2
All	All	6645/7104 (94%)	4378 (66%)	1475 (22%)	792 (12%)	1	4

5 of 792 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	13	ALA

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Mol	Chain	Res	Type
2	AB	20	GLU
2	AB	95	GLN
2	AB	190	THR
2	AB	195	ASP

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	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	5	18
3	AC	160/188 (85%)	136 (85%)	24 (15%)	3	12
4	AD	180/181 (99%)	158 (88%)	22 (12%)	5	17
5	AE	115/123 (94%)	99 (86%)	16 (14%)	3	14
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	17
7	AG	126/127 (99%)	109 (86%)	17 (14%)	4	14
8	AH	119/119 (100%)	105 (88%)	14 (12%)	5	18
9	AI	98/99 (99%)	89 (91%)	9 (9%)	8	27
10	AJ	88/92 (96%)	74 (84%)	14 (16%)	2	11
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	24
12	AL	104/109 (95%)	92 (88%)	12 (12%)	5	18
13	AM	99/101 (98%)	86 (87%)	13 (13%)	4	15
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	17
15	AO	79/80 (99%)	67 (85%)	12 (15%)	3	12
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	24
17	AQ	94/97 (97%)	83 (88%)	11 (12%)	5	18
18	AR	61/77 (79%)	56 (92%)	5 (8%)	10	31
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	13
20	AT	76/82 (93%)	66 (87%)	10 (13%)	4	15
21	AU	19/22 (86%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AY	563/582 (97%)	472 (84%)	91 (16%)	2	11
25	B0	66/67 (98%)	57 (86%)	9 (14%)	3	14
26	B1	78/83 (94%)	63 (81%)	15 (19%)	1	8
27	B2	66/67 (98%)	58 (88%)	8 (12%)	5	17
28	B3	51/52 (98%)	44 (86%)	7 (14%)	3	14
29	B4	51/63 (81%)	35 (69%)	16 (31%)	0	2
30	B5	51/52 (98%)	46 (90%)	5 (10%)	7	24
31	B6	49/52 (94%)	35 (71%)	14 (29%)	0	2
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	17
33	B8	53/55 (96%)	47 (89%)	6 (11%)	5	19
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	5
37	BC	180/181 (99%)	158 (88%)	22 (12%)	5	17
38	BD	217/218 (100%)	178 (82%)	39 (18%)	2	9
39	BE	165/166 (99%)	136 (82%)	29 (18%)	2	9
40	BF	165/166 (99%)	149 (90%)	16 (10%)	8	24
41	BG	155/156 (99%)	131 (84%)	24 (16%)	2	12
42	BH	136/148 (92%)	111 (82%)	25 (18%)	1	8
43	BK	104/111 (94%)	88 (85%)	16 (15%)	2	12
44	BL	46/85 (54%)	41 (89%)	5 (11%)	6	21
45	BN	117/119 (98%)	96 (82%)	21 (18%)	2	9
46	BO	100/100 (100%)	85 (85%)	15 (15%)	3	12
47	BP	112/116 (97%)	86 (77%)	26 (23%)	1	5
48	BQ	111/111 (100%)	93 (84%)	18 (16%)	2	11
49	BR	100/101 (99%)	86 (86%)	14 (14%)	3	13
50	BS	77/88 (88%)	66 (86%)	11 (14%)	3	13
51	BT	120/127 (94%)	95 (79%)	25 (21%)	1	6
52	BU	92/94 (98%)	84 (91%)	8 (9%)	9	29
53	BV	82/82 (100%)	67 (82%)	15 (18%)	2	8
54	BW	91/92 (99%)	78 (86%)	13 (14%)	3	13
55	BX	74/78 (95%)	61 (82%)	13 (18%)	2	9
56	BY	87/91 (96%)	72 (83%)	15 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	BZ	162/179 (90%)	132 (82%)	30 (18%)	1 8
All	All	5586/5868 (95%)	4756 (85%)	830 (15%)	5 12

5 of 830 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BD	67	PHE
42	BH	94	TYR
56	BY	102	CYS
38	BD	176	ARG
38	BD	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
38	BD	112	GLN
43	BK	30	HIS
38	BD	164	GLN
39	BE	180	ASN
47	BP	9	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	280 (18%)	47 (3%)
22	AV	76/77 (98%)	17 (22%)	0
23	AX	10/11 (90%)	5 (50%)	0
35	BA	2900/2915 (99%)	635 (21%)	77 (2%)
36	BB	118/122 (96%)	27 (22%)	2 (1%)
All	All	4607/4647 (99%)	964 (20%)	126 (2%)

5 of 964 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	332	A
35	BA	2425	A
35	BA	1020	A
35	BA	2422	A
35	BA	2779	U

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
59	GDP	AY	702	-	29,30,30	1.34	5 (17%)	45,47,47	1.86	10 (22%)
58	FUA	AY	701	-	39,40,40	2.15	12 (30%)	50,64,64	1.91	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	AY	702	-	-	2/16/32/32	0/3/3/3
58	FUA	AY	701	-	-	6/16/92/92	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	701	FUA	C23-C22	-5.46	1.37	1.51
58	AY	701	FUA	C15-C14	-4.28	1.46	1.54
58	AY	701	FUA	C23-C24	-4.28	1.39	1.53
58	AY	701	FUA	C19-C10	-4.03	1.47	1.54
58	AY	701	FUA	C29-C22	3.92	1.53	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	701	FUA	C8-C9-C10	-6.33	109.63	116.42
59	AY	702	GDP	C2-N3-C4	4.80	120.56	112.30
59	AY	702	GDP	C5-C4-N3	-4.63	121.02	128.39
58	AY	701	FUA	C6-C5-C10	-4.58	106.16	111.66
58	AY	701	FUA	C24-C23-C22	4.30	121.88	112.72

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AY	701	FUA	C13-C17-C22-C23
58	AY	701	FUA	C13-C17-C22-C29
59	AY	702	GDP	C5'-O5'-PA-O3A
59	AY	702	GDP	C5'-O5'-PA-O1A
58	AY	701	FUA	C32-C31-O2-C16

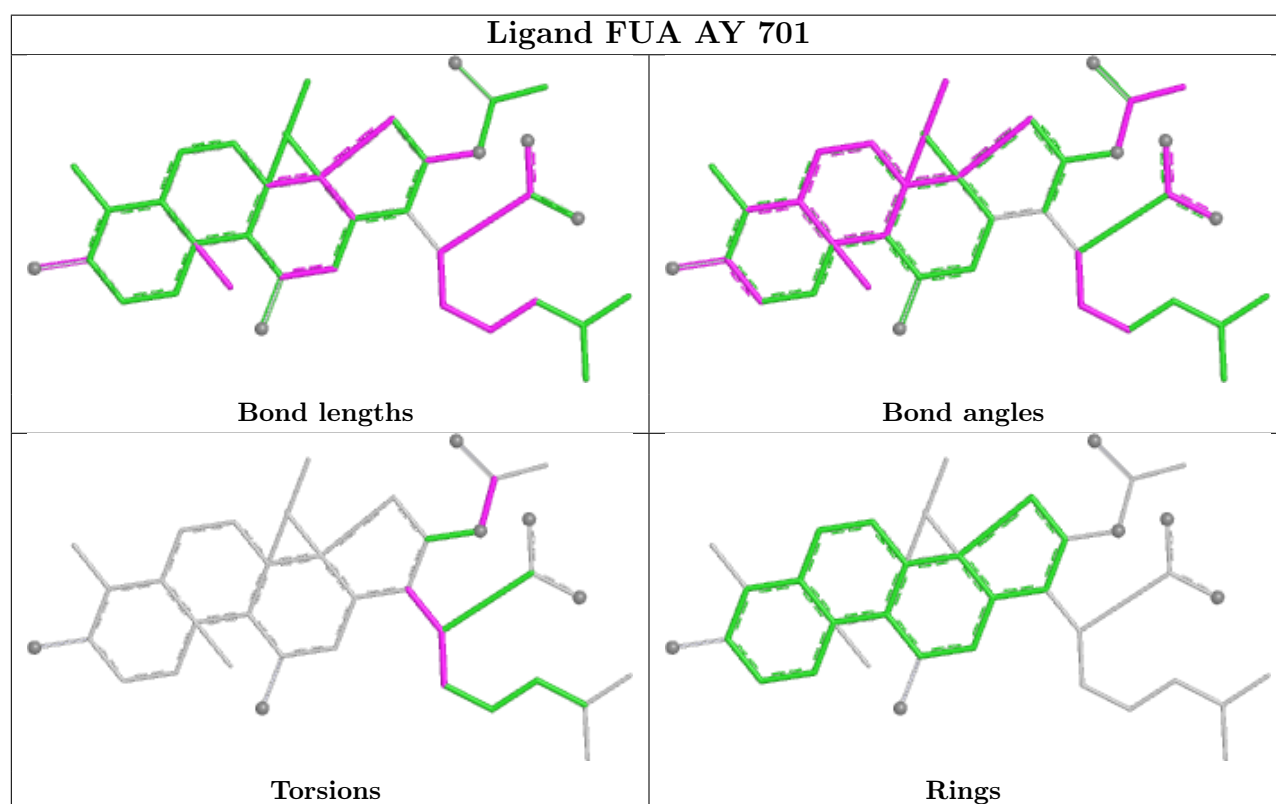
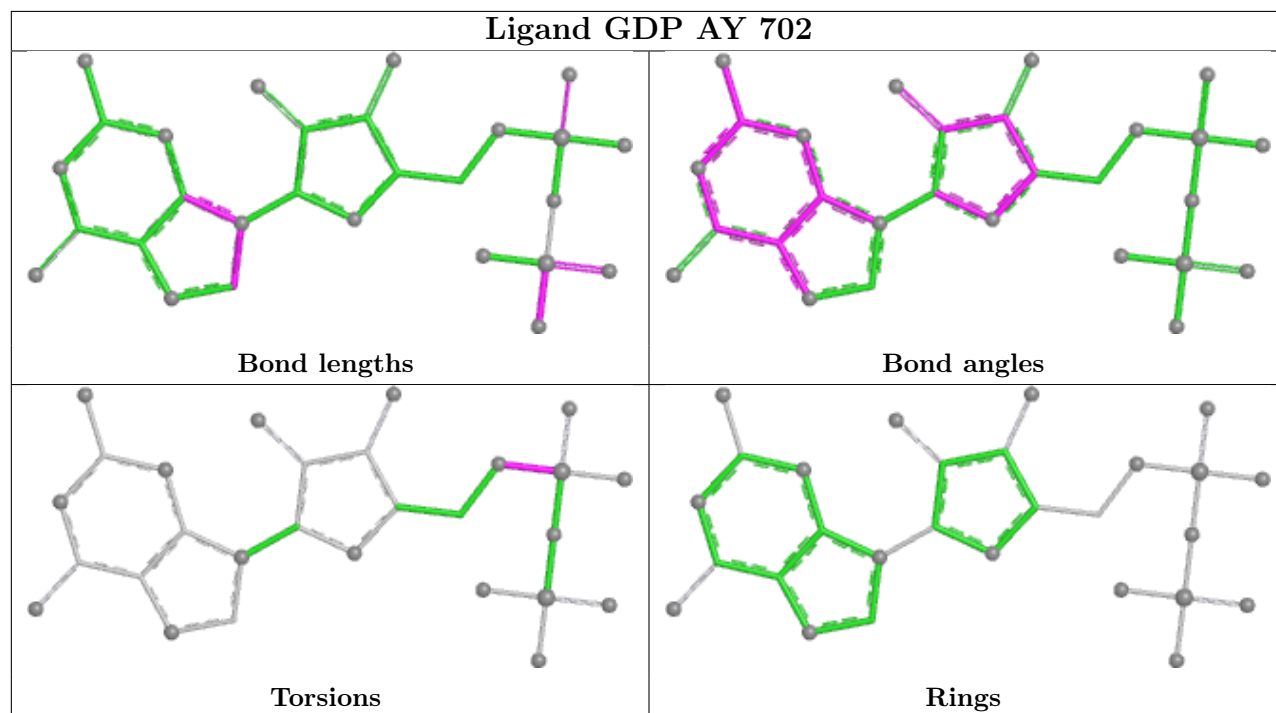
There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	702	GDP	7	0
58	AY	701	FUA	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

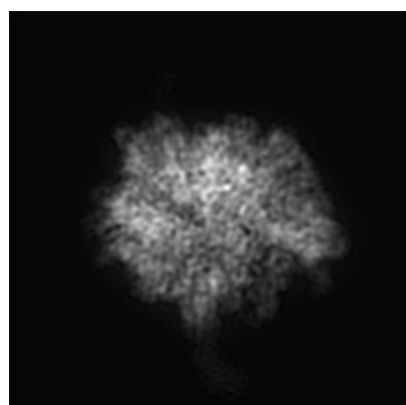
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1798. These allow visual inspection of the internal detail of the map and identification of artifacts.

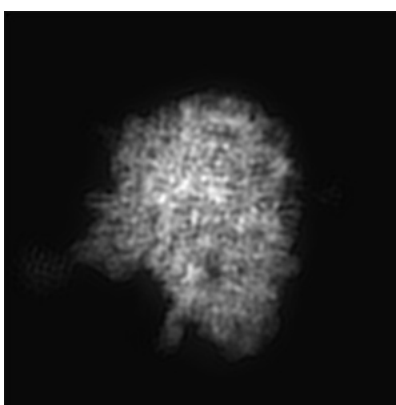
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

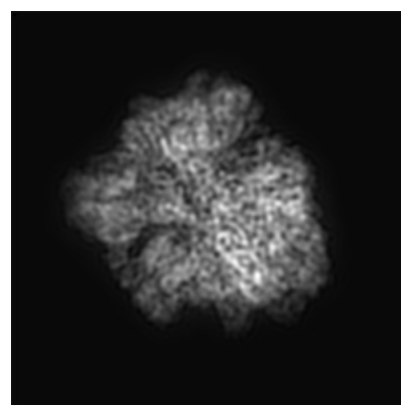
6.1.1 Primary map



X



Y

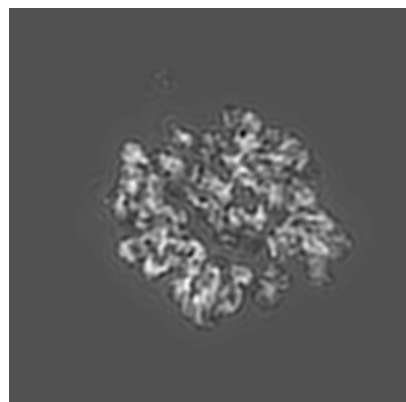


Z

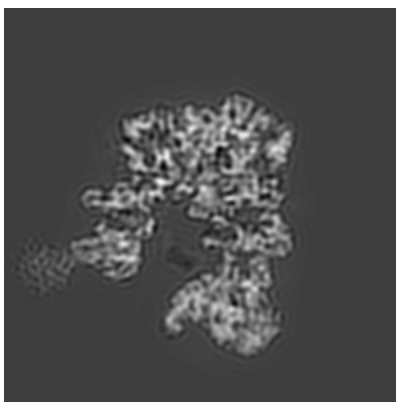
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

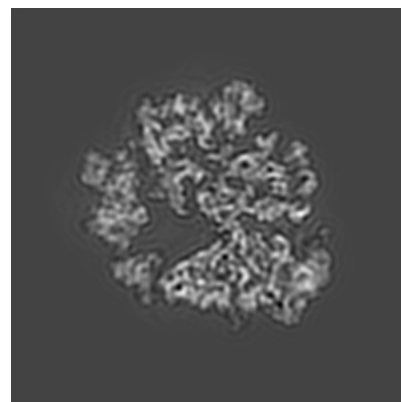
6.2.1 Primary map



X Index: 150



Y Index: 150

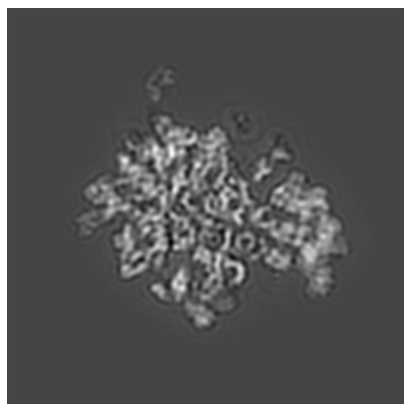


Z Index: 150

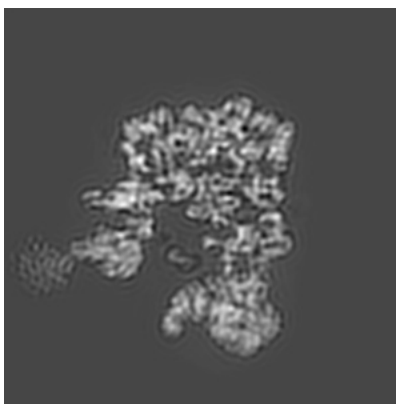
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

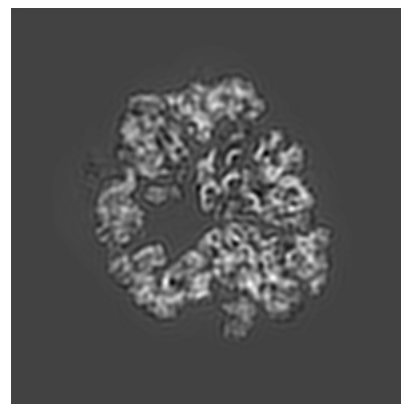
6.3.1 Primary map



X Index: 162



Y Index: 152

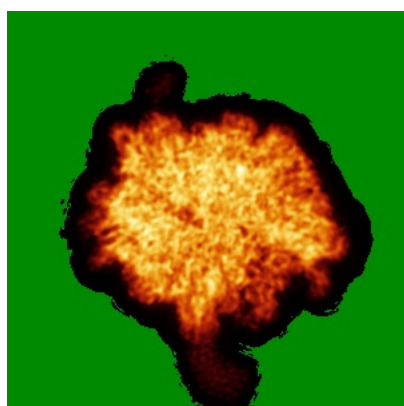


Z Index: 142

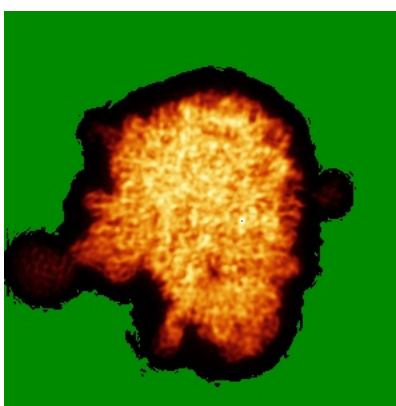
The images above show the largest variance slices of the map in three orthogonal directions.

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

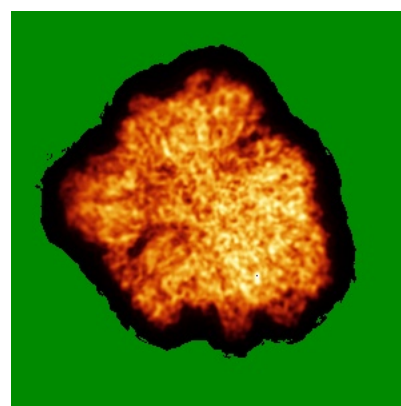
6.4.1 Primary map



X



Y



Z

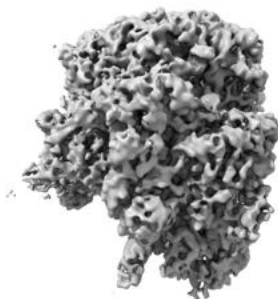
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3000.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

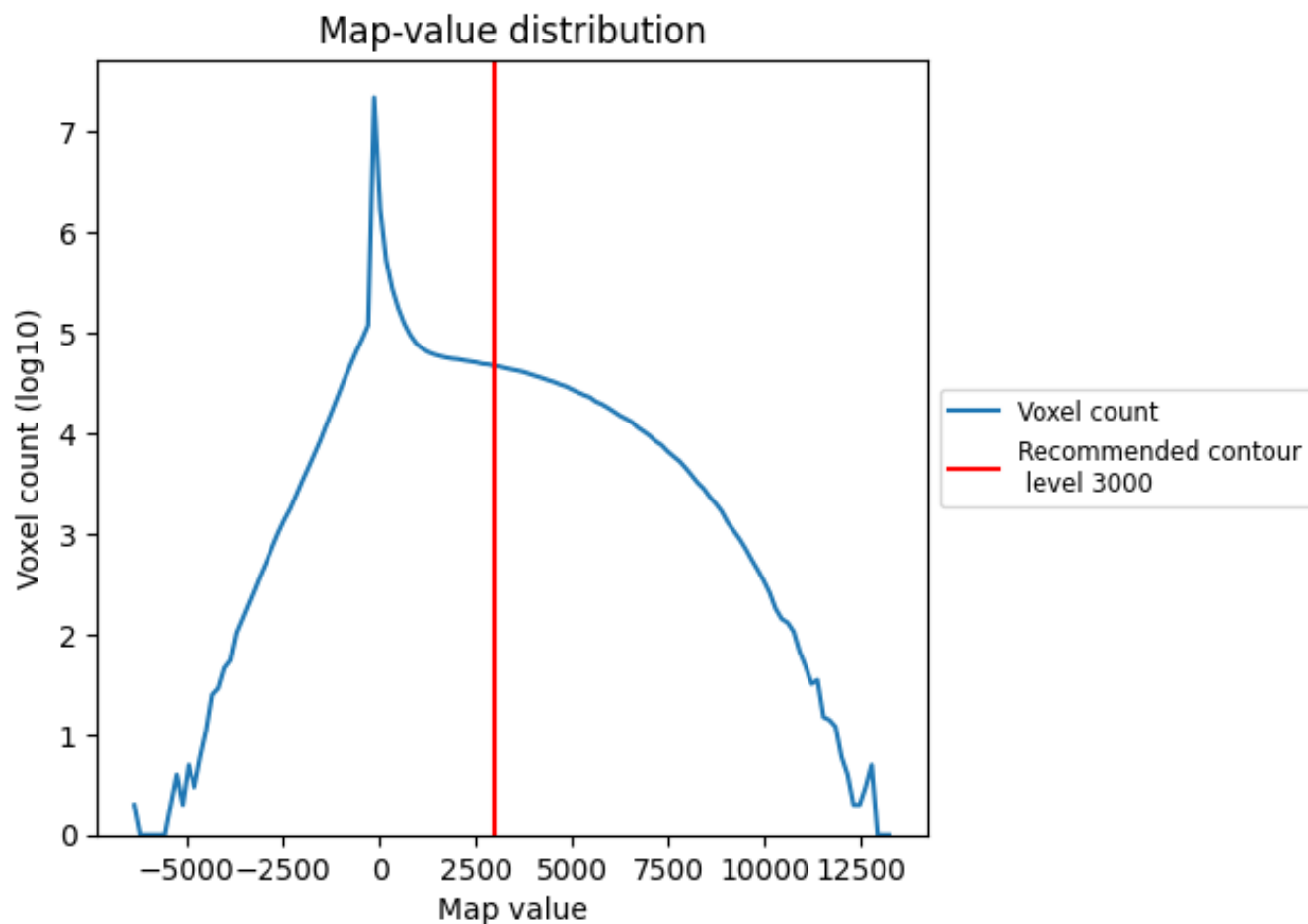
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

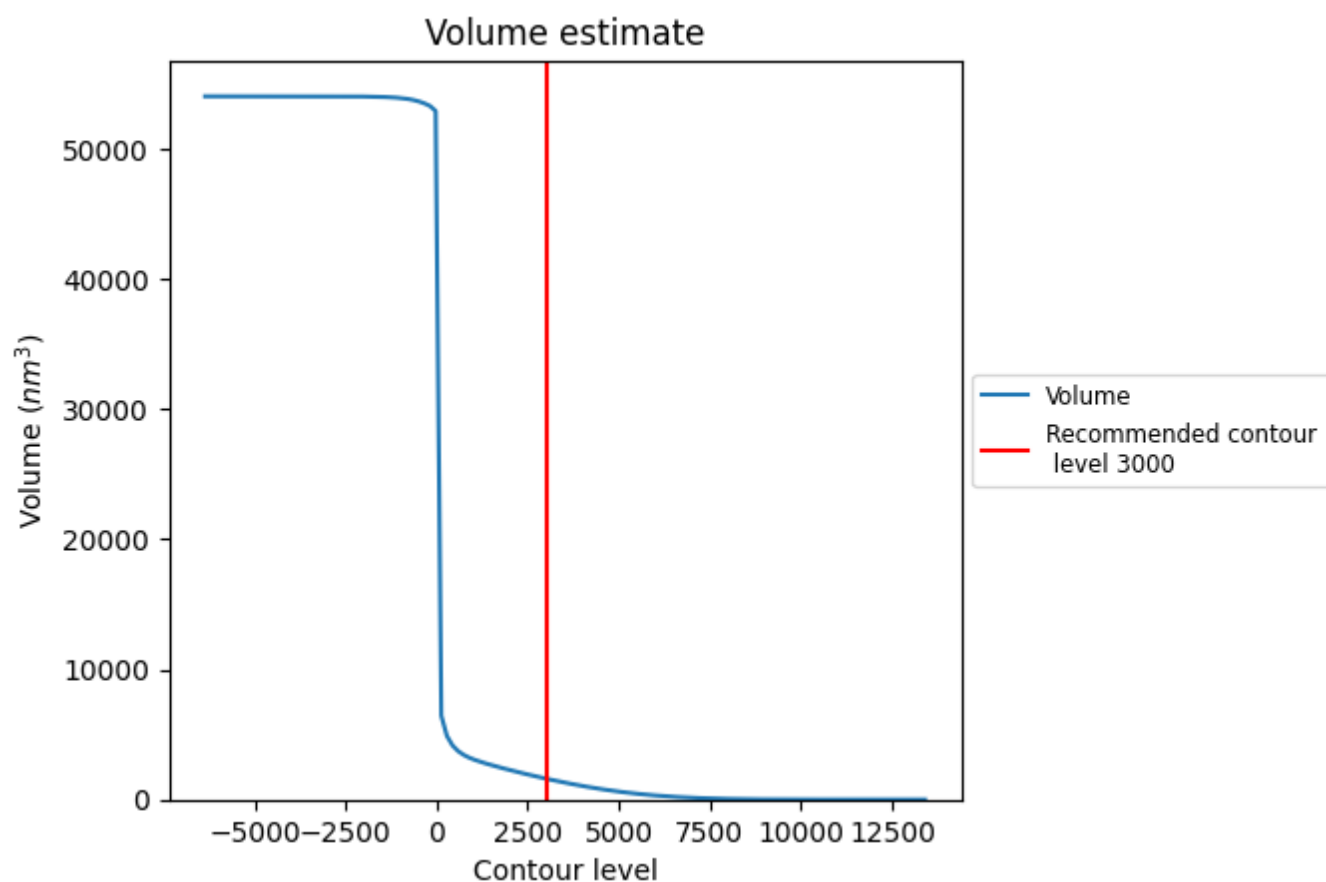
This section contains the results of statistical analysis of the map.

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.

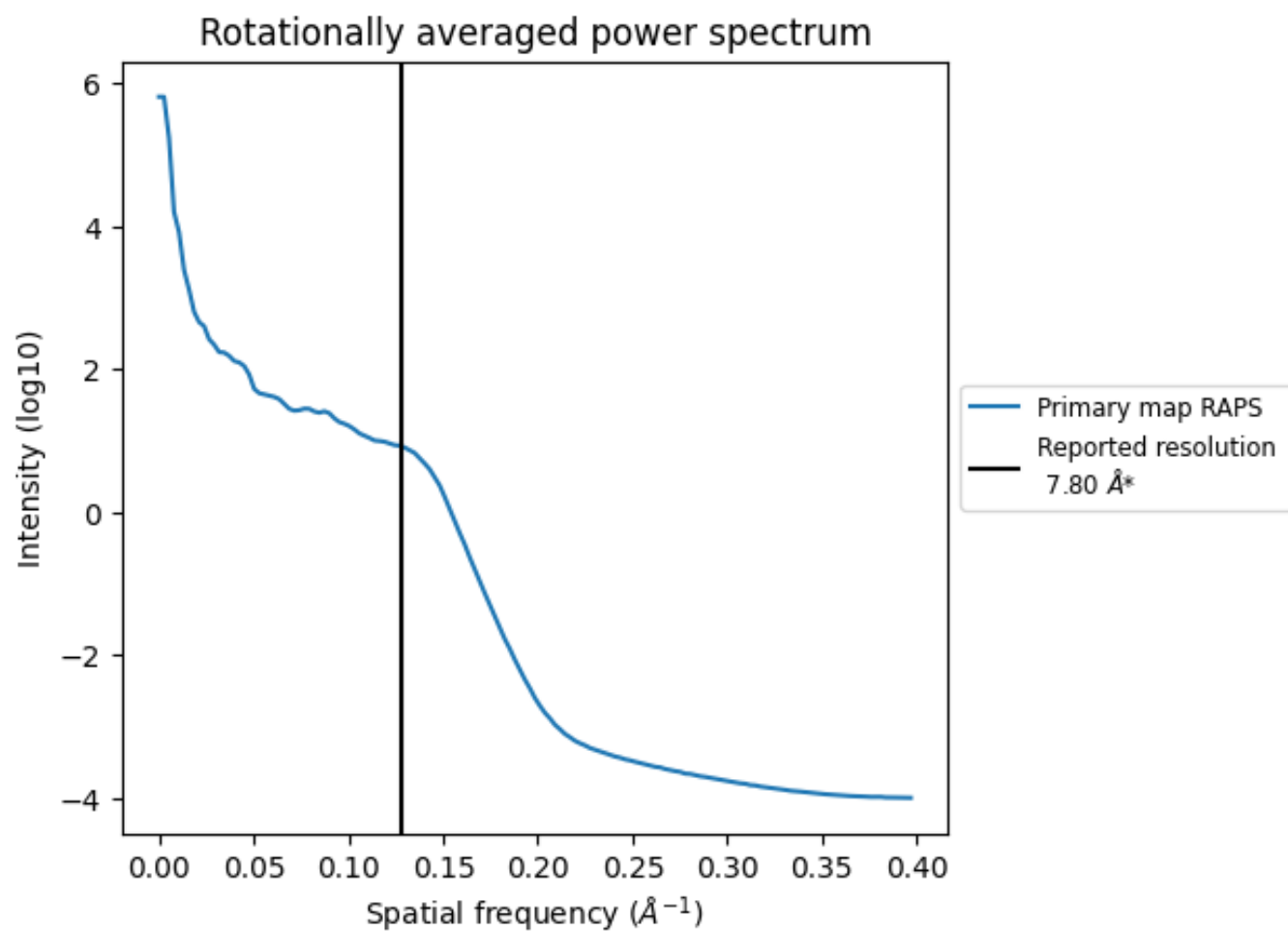
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1609 nm³; this corresponds to an approximate mass of 1453 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 0.128 Å⁻¹

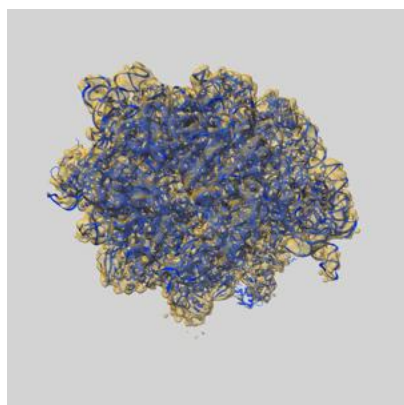
8 Fourier-Shell correlation

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

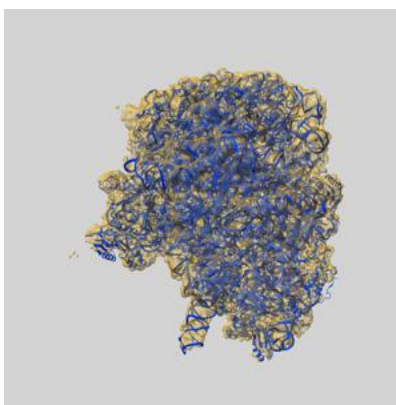
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1798 and PDB model 4V5M. Per-residue inclusion information can be found in section 3 on page 16.

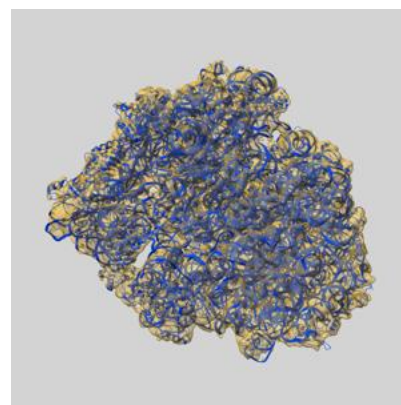
9.1 Map-model overlay [i](#)



X



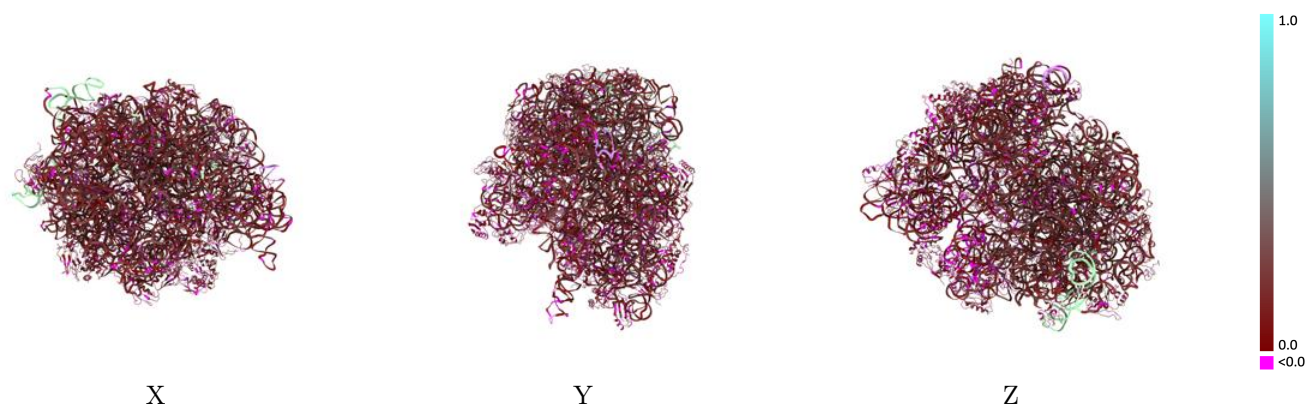
Y



Z

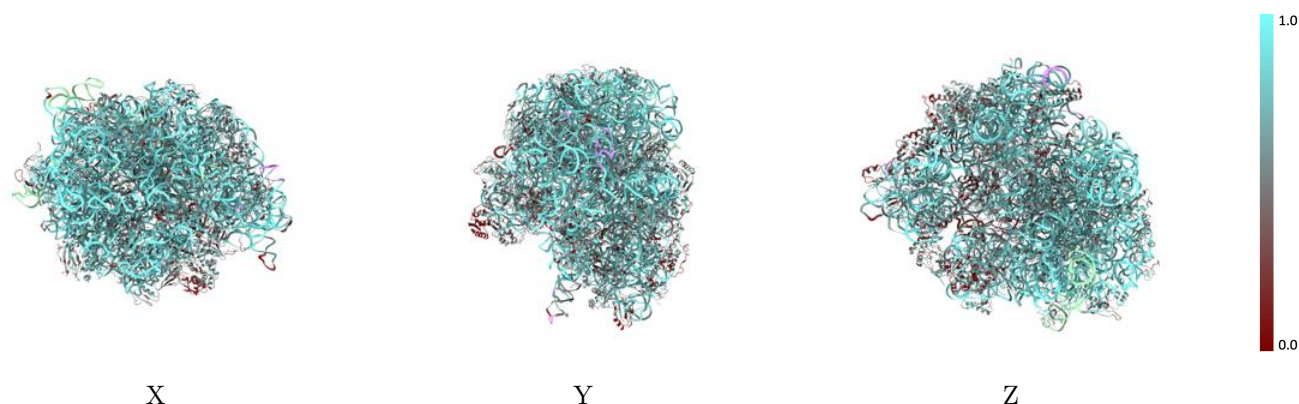
The images above show the 3D surface view of the map at the recommended contour level 3000.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



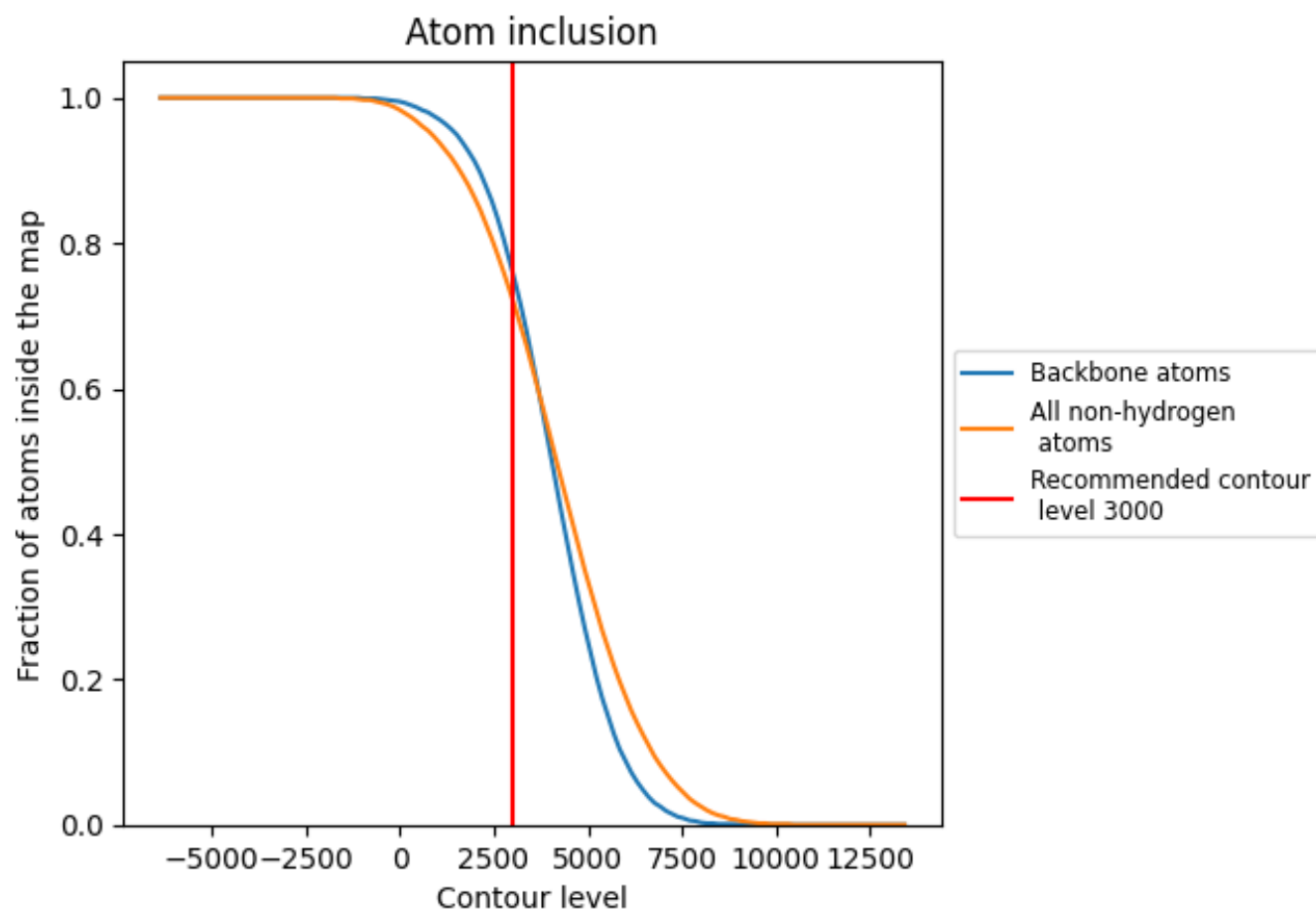
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3000).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (3000) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.1590
AA	 0.8290	 0.1700
AB	 0.4670	 0.1320
AC	 0.5500	 0.1360
AD	 0.5930	 0.1270
AE	 0.5820	 0.1350
AF	 0.5400	 0.1510
AG	 0.4980	 0.1130
AH	 0.5840	 0.1400
AI	 0.5860	 0.0960
AJ	 0.4570	 0.0840
AK	 0.5290	 0.1310
AL	 0.4580	 0.1200
AM	 0.4250	 0.0790
AN	 0.5970	 0.1230
AO	 0.5990	 0.1410
AP	 0.6300	 0.1120
AQ	 0.5510	 0.1200
AR	 0.5230	 0.1210
AS	 0.5220	 0.0840
AT	 0.5600	 0.1220
AU	 0.4760	 0.0650
AV	 0.6490	 0.1350
AX	 0.2700	 0.0910
AY	 0.4490	 0.1190
B0	 0.5200	 0.0990
B1	 0.5770	 0.1340
B2	 0.6330	 0.1500
B3	 0.6040	 0.1520
B4	 0.3880	 0.1080
B5	 0.6000	 0.1540
B6	 0.5940	 0.0930
B7	 0.6160	 0.1230
B8	 0.5530	 0.1240
B9	 0.2820	 0.0620



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Chain	Atom inclusion	Q-score
BA	 0.8410	 0.1880
BB	 0.8680	 0.1790
BC	 0.2520	 0.0480
BD	 0.5130	 0.1240
BE	 0.5330	 0.1270
BF	 0.6150	 0.1380
BG	 0.5160	 0.0980
BH	 0.5730	 0.1330
BK	 0.3590	 0.0890
BL	 0.0590	 0.0440
BN	 0.5870	 0.1450
BO	 0.3680	 0.1210
BP	 0.5850	 0.1430
BQ	 0.2790	 0.0930
BR	 0.6000	 0.1370
BS	 0.6620	 0.1480
BT	 0.4780	 0.1260
BU	 0.6310	 0.1220
BV	 0.5540	 0.1420
BW	 0.6050	 0.1280
BX	 0.6140	 0.1420
BY	 0.4970	 0.1340
BZ	 0.4570	 0.0750