



wwPDB EM Validation Summary Report ⓘ

Jun 22, 2026 – 07:35 PM EDT

PDB ID : 3J9Y / pdb_00003j9y
EMDB ID : EMD-6311
Title : Cryo-EM structure of tetracycline resistance protein TetM bound to a translating E.coli ribosome
Authors : Arenz, S.; Nguyen, F.; Beckmann, R.; Wilson, D.N.
Deposited on : 2015-03-23
Resolution : 3.90 Å(reported)
Based on initial model : 5AFI

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:

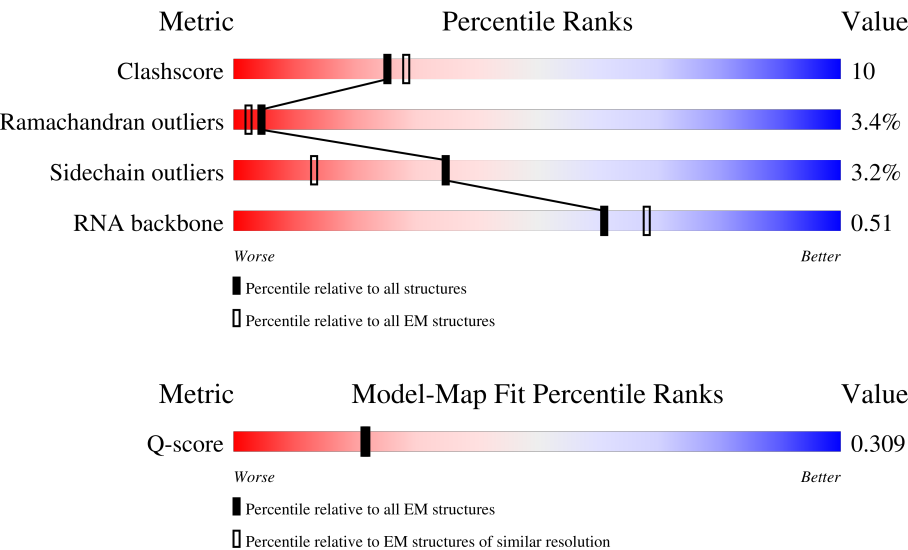
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1539	8% 58% 34% 8%
2	b	240	74% 57% 31% 9%
3	d	206	71% 66% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	e	167	
5	f	135	
6	h	130	
7	k	129	
8	l	124	
9	o	89	
10	p	82	
11	q	84	
12	r	75	
13	t	87	
14	u	71	
15	v	78	
16	x	11	
17	w	639	
18	c	233	
19	g	179	
20	i	130	
21	j	103	
22	m	118	
23	n	102	
24	s	92	
25	A	2903	
26	B	120	
27	C	273	
28	D	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	E	201	
30	F	179	
31	G	177	
32	H	149	
33	I	142	
34	J	142	
35	K	123	
36	L	144	
37	M	136	
38	N	127	
39	O	117	
40	P	115	
41	Q	118	
42	R	103	
43	S	110	
44	T	100	
45	U	104	
46	V	94	
47	W	85	
48	X	78	
49	Y	63	
50	Z	59	
51	0	57	
52	1	55	
53	2	46	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	3	65	
55	4	38	
56	5	165	
57	6	70	
58	7	69	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UR3	a	1498	-	-	X	-
1	MA6	a	1519	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148915 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	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	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S8.

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

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 8 is a protein called 30S ribosomal protein S12.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 15 is a RNA chain called P-site fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	77	FME	-	modified residue	GB 147949

- Molecule 16 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	9	Total	C	N	O	P		
			189	85	31	64	9	0	0

- Molecule 17 is a protein called Tetracycline resistance protein TetM.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	w	639	Total	C	N	O		
			2590	1308	640	642	0	0

- Molecule 18 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 19 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 21 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 22 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 23 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

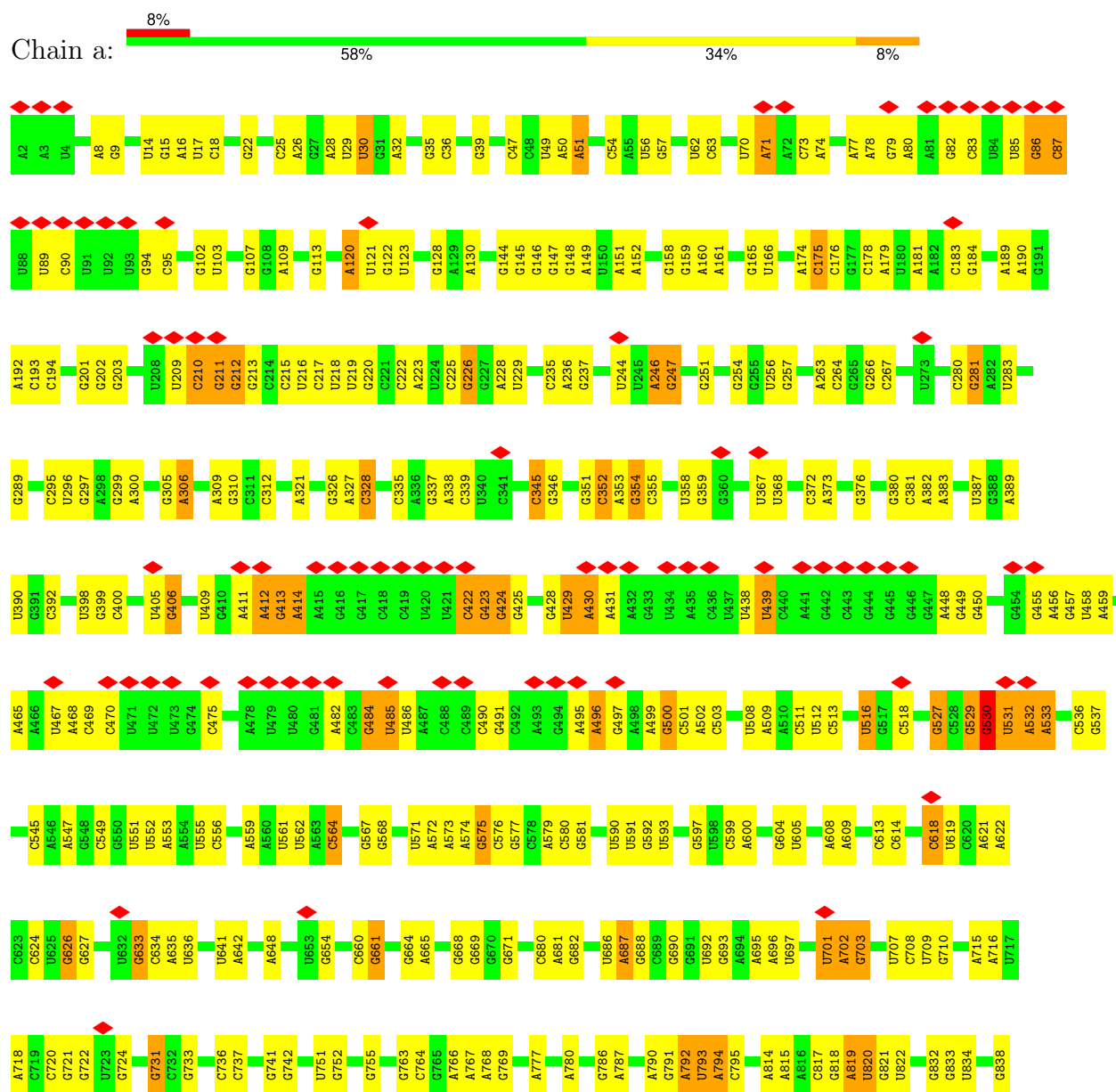
- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

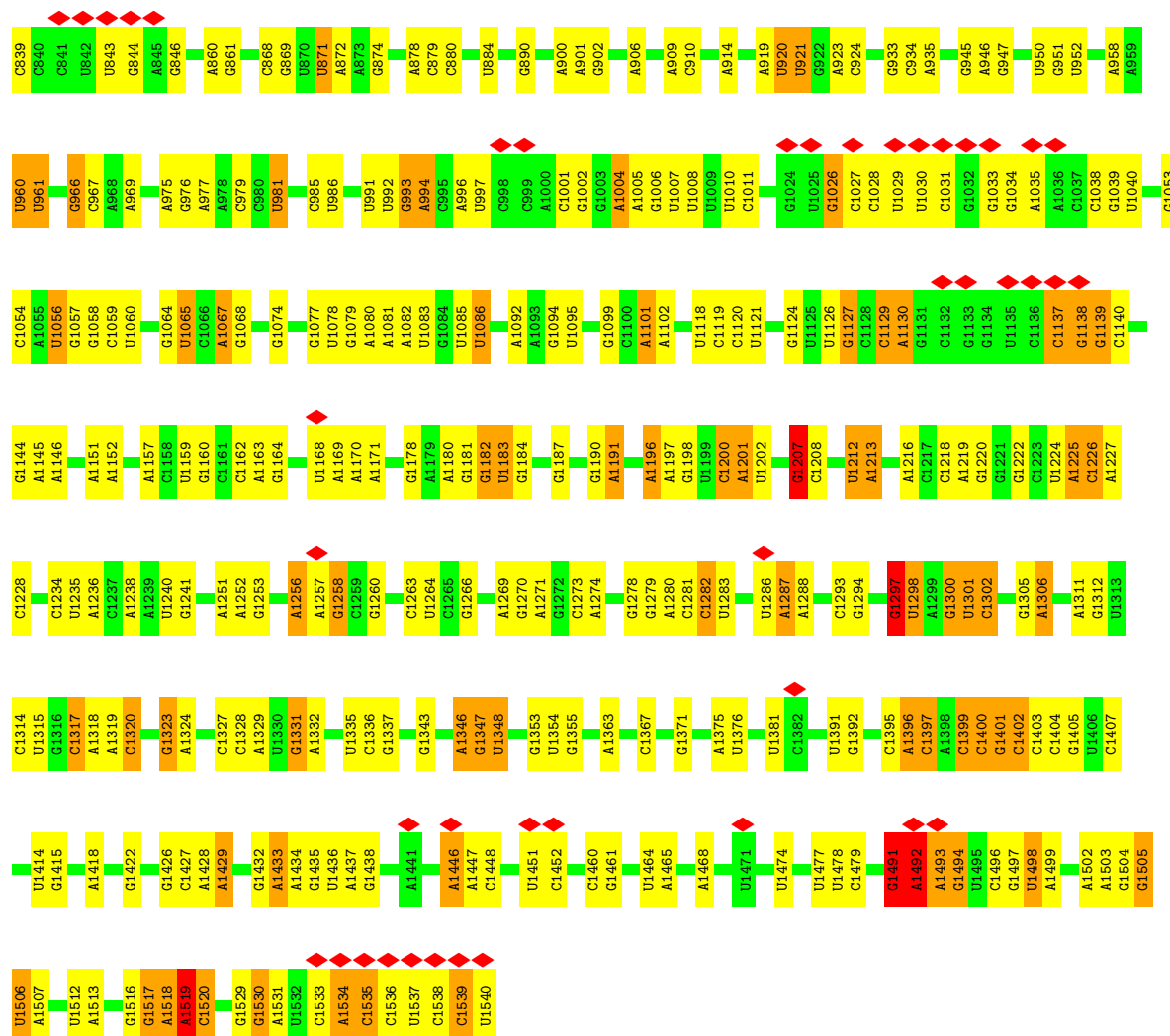
Mol	Chain	Residues	Atoms				AltConf	Trace
58	7	69	Total	C	N	O	0	0
			276	138	69	69		

3 Residue-property plots

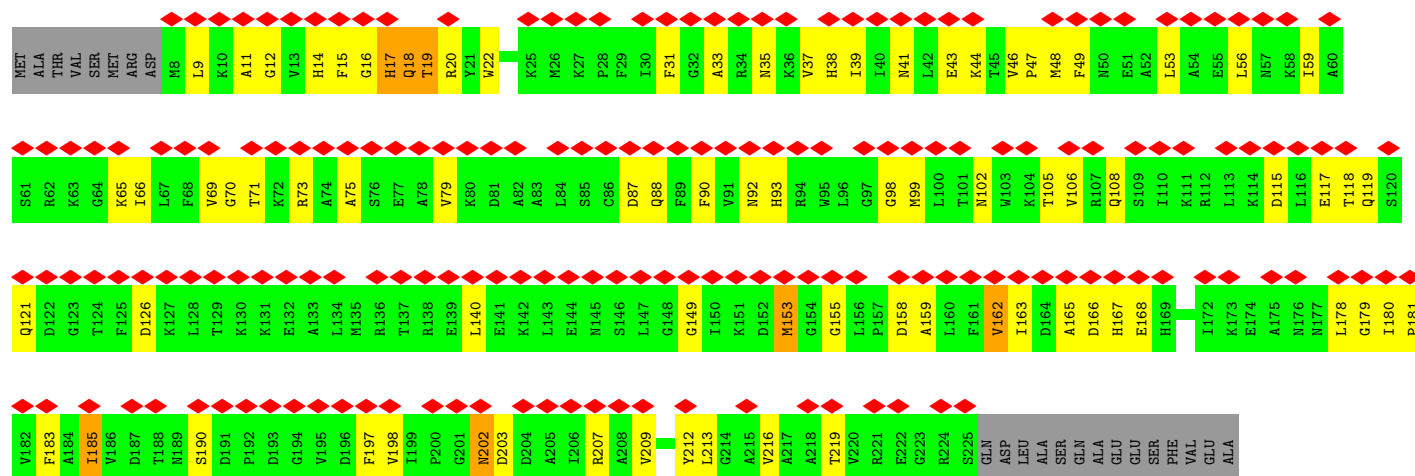
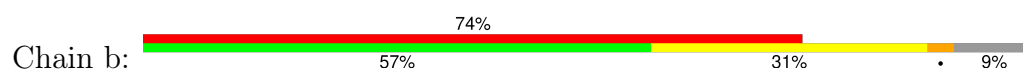
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

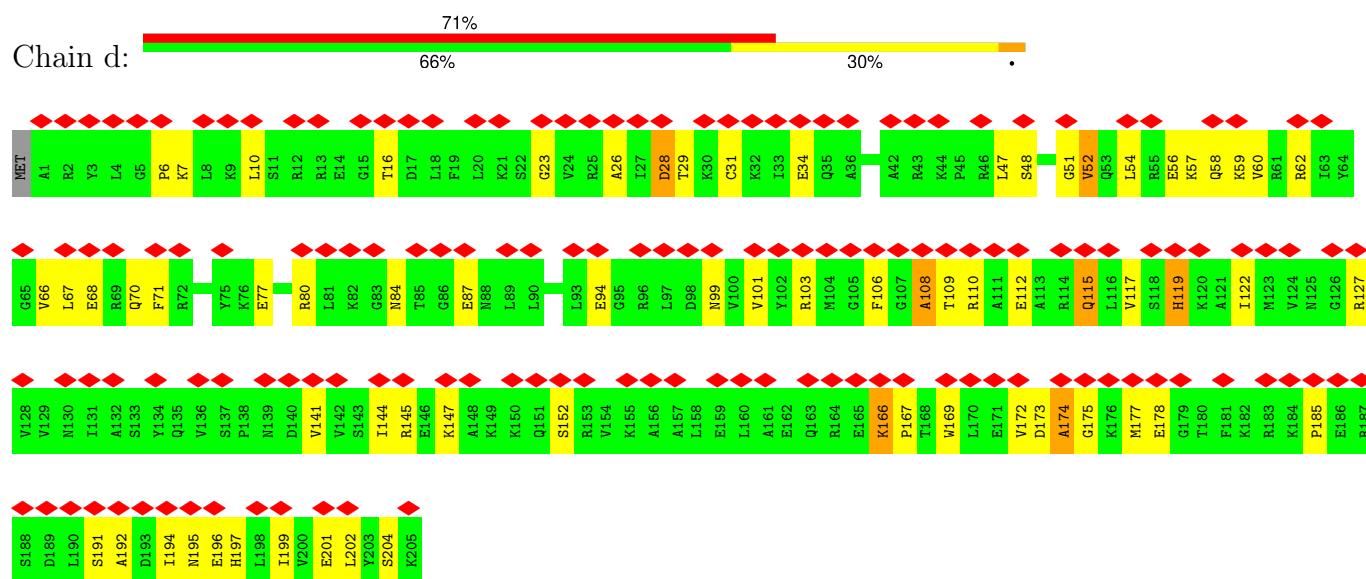




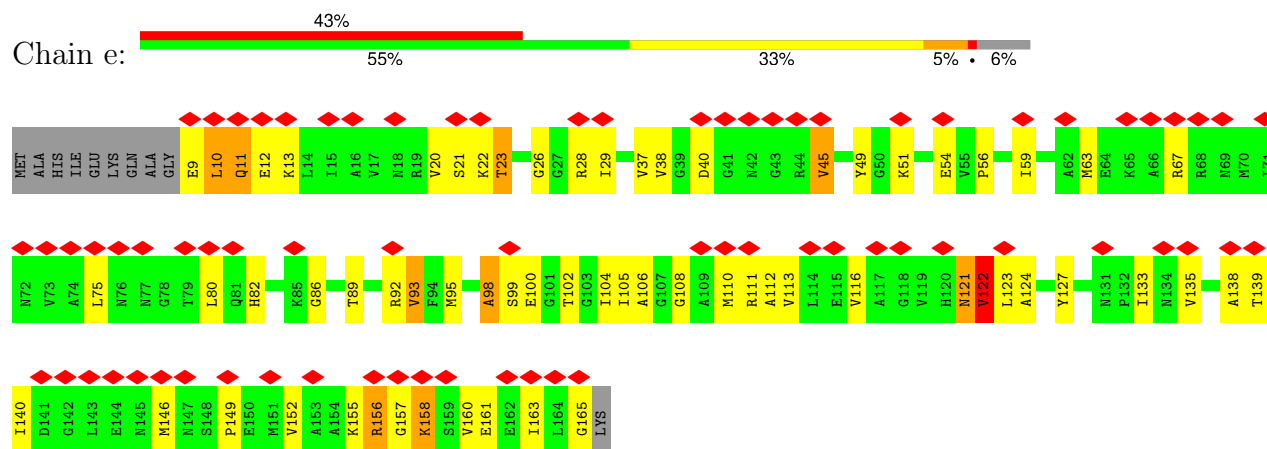
• Molecule 2: 30S ribosomal protein S2



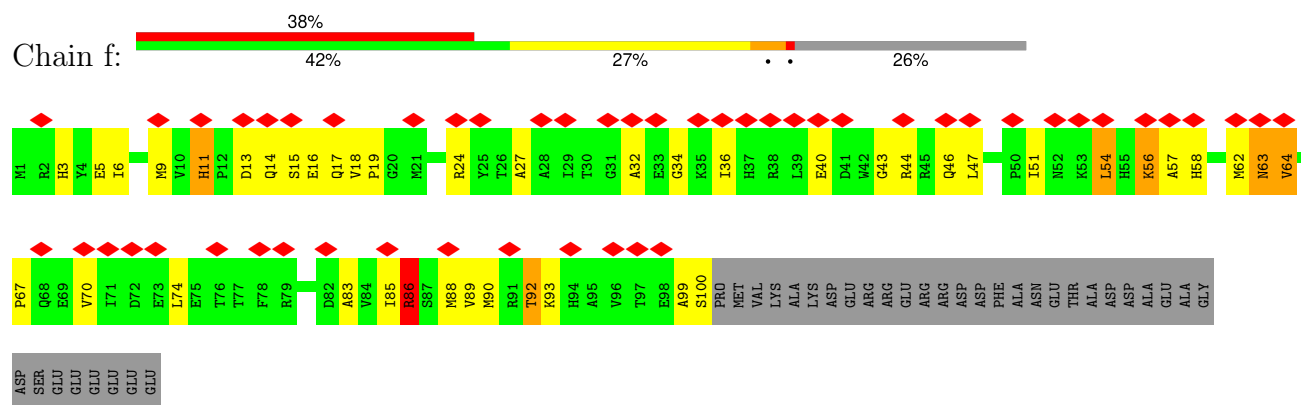
• Molecule 3: 30S ribosomal protein S4



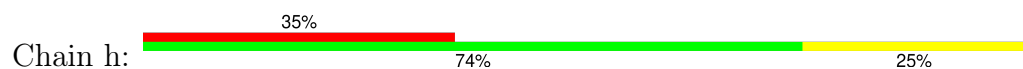
• Molecule 4: 30S ribosomal protein S5

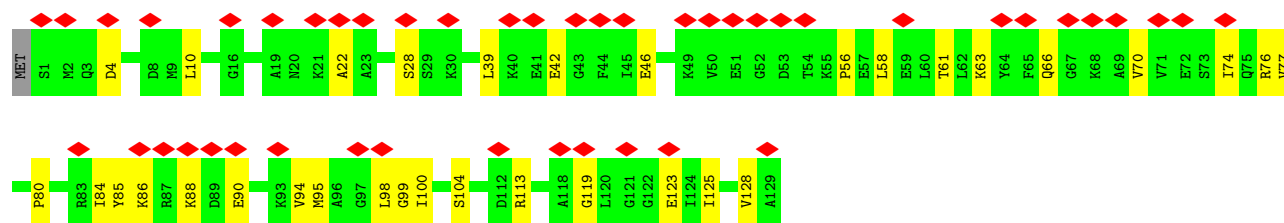


• Molecule 5: 30S ribosomal protein S6

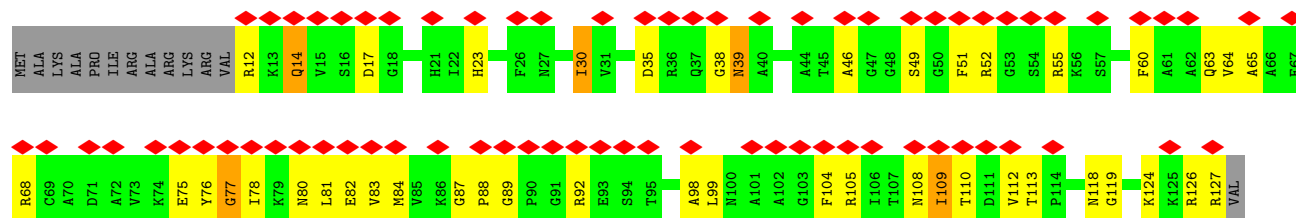


• Molecule 6: 30S ribosomal protein S8

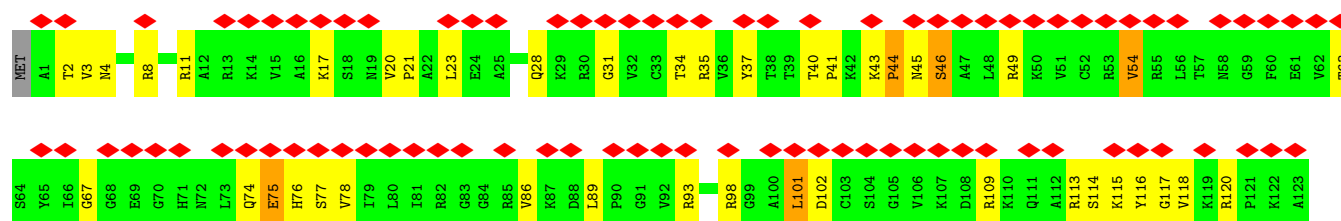




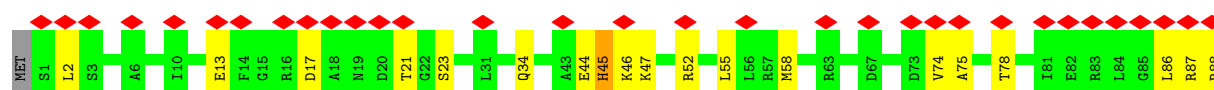
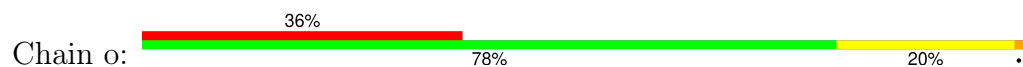
• Molecule 7: 30S ribosomal protein S11



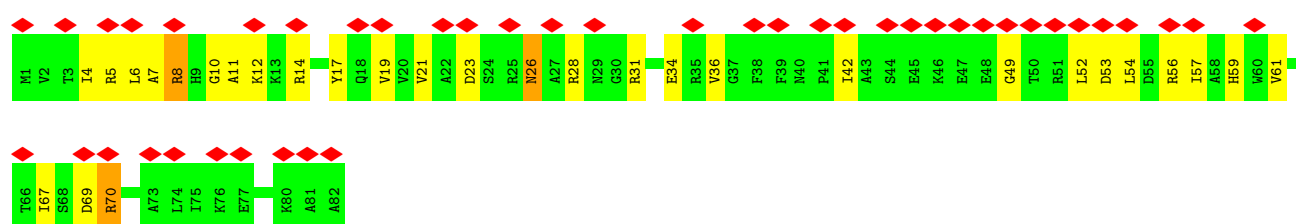
• Molecule 8: 30S ribosomal protein S12



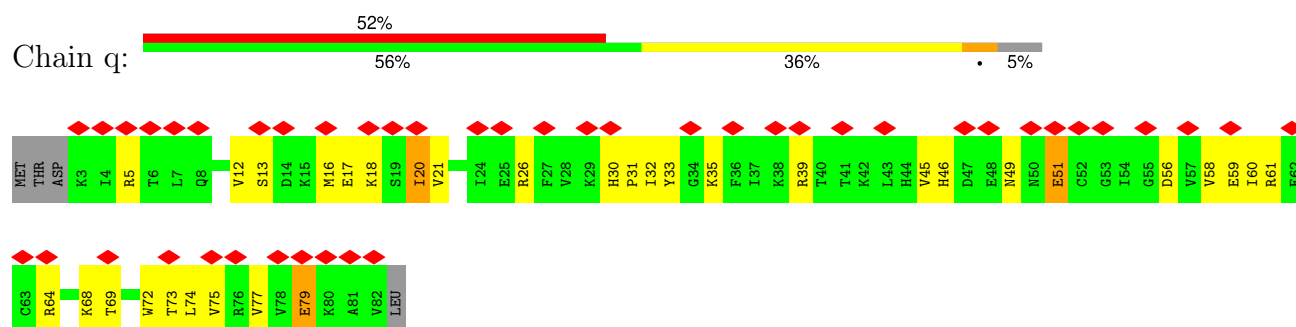
• Molecule 9: 30S ribosomal protein S15



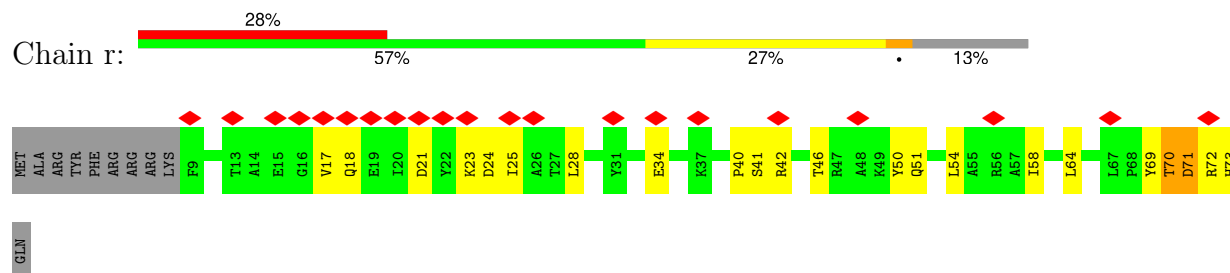
• Molecule 10: 30S ribosomal protein S16



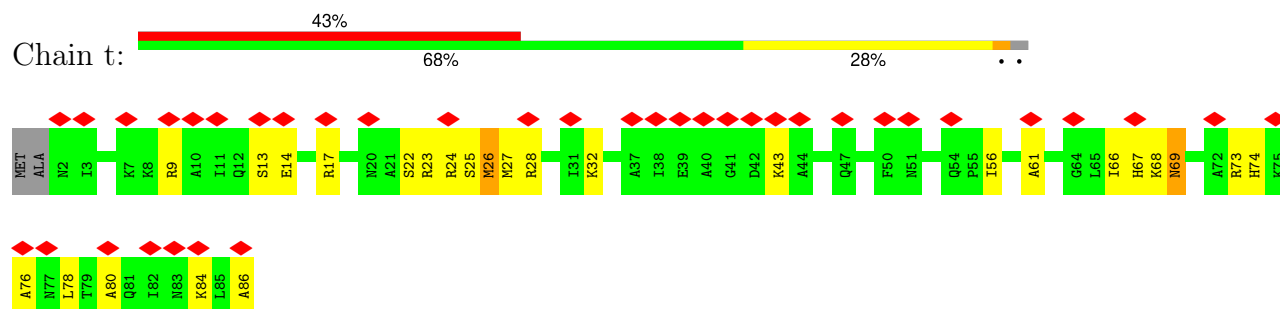
• Molecule 11: 30S ribosomal protein S17



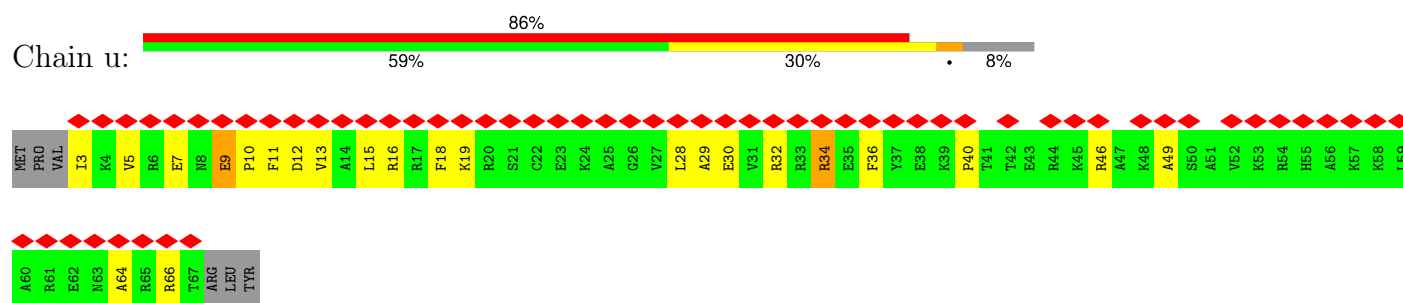
- Molecule 12: 30S ribosomal protein S18



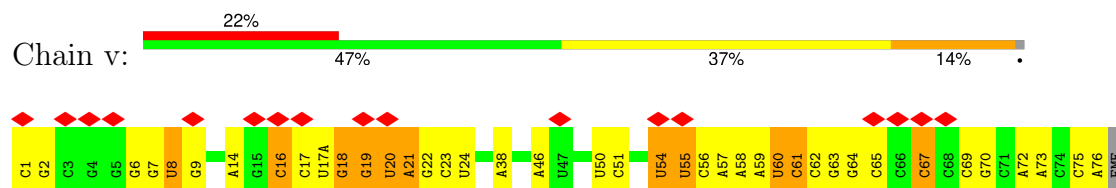
- Molecule 13: 30S ribosomal protein S20



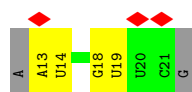
- Molecule 14: 30S ribosomal protein S21



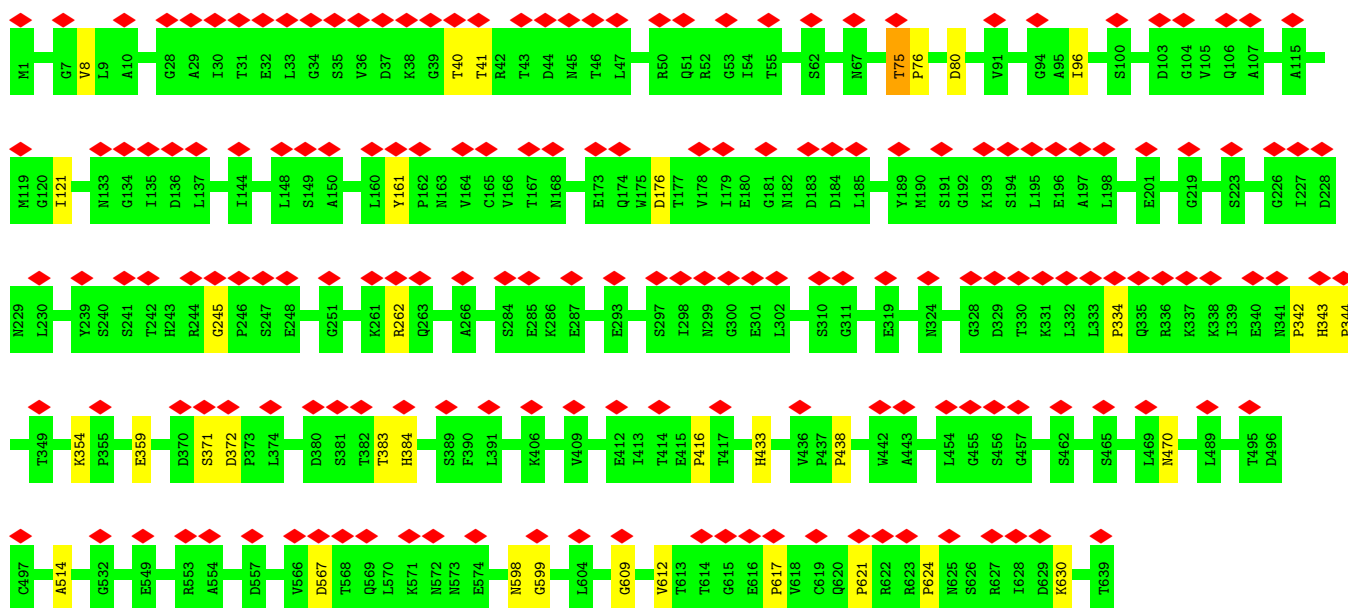
- Molecule 15: P-site fMet-tRNA^{fMet}



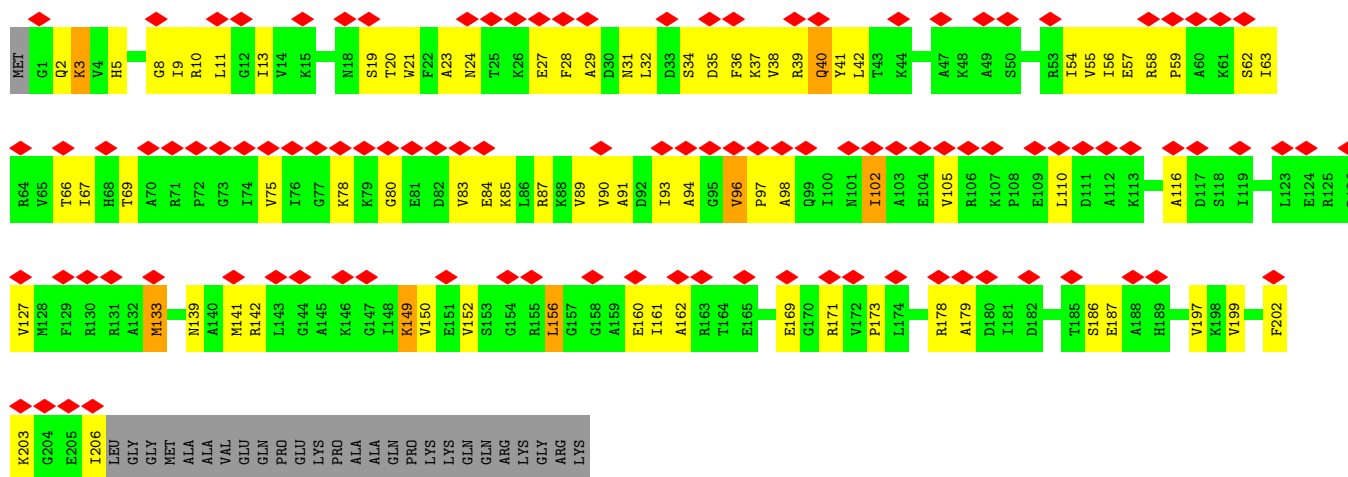
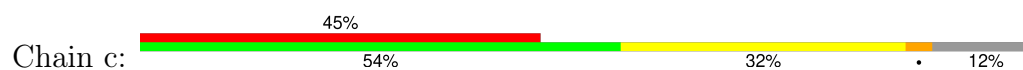
- Molecule 16: mRNA



• Molecule 17: Tetracycline resistance protein TetM

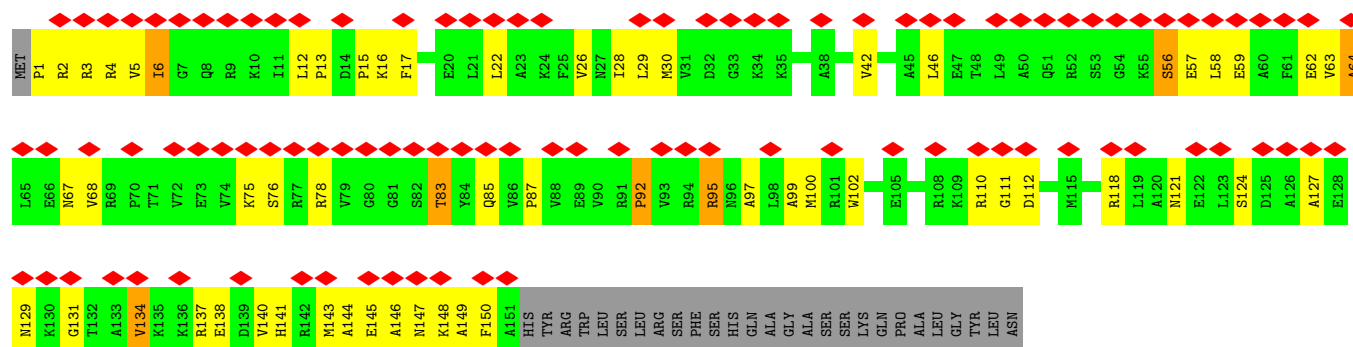


• Molecule 18: 30S ribosomal protein S3

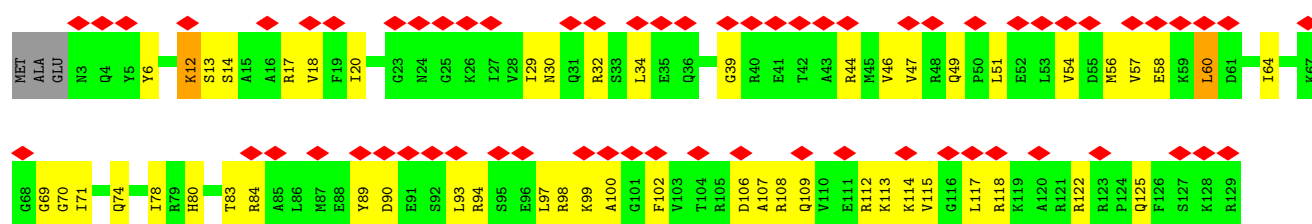


• Molecule 19: 30S ribosomal protein S7

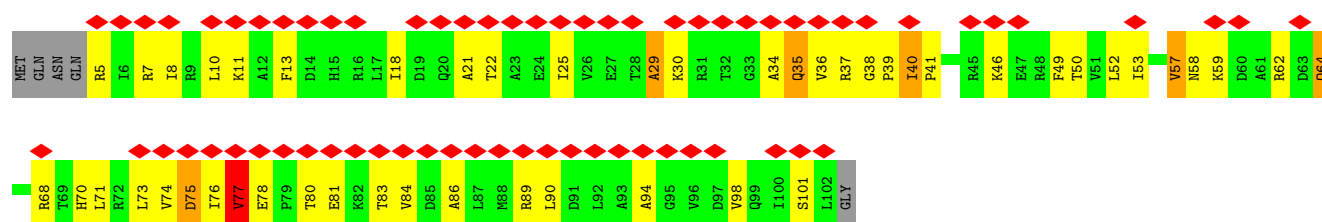




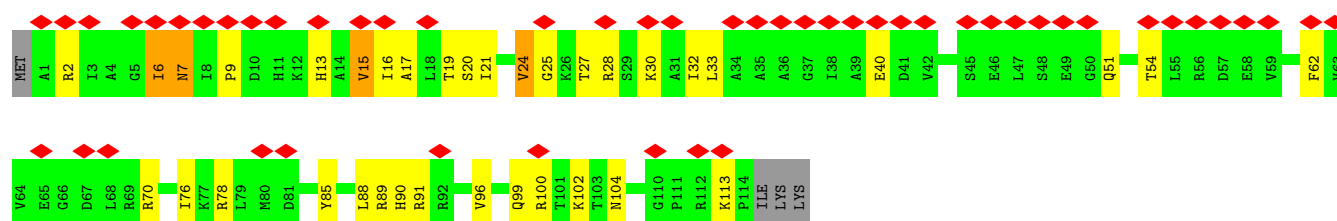
• Molecule 20: 30S ribosomal protein S9



• Molecule 21: 30S ribosomal protein S10

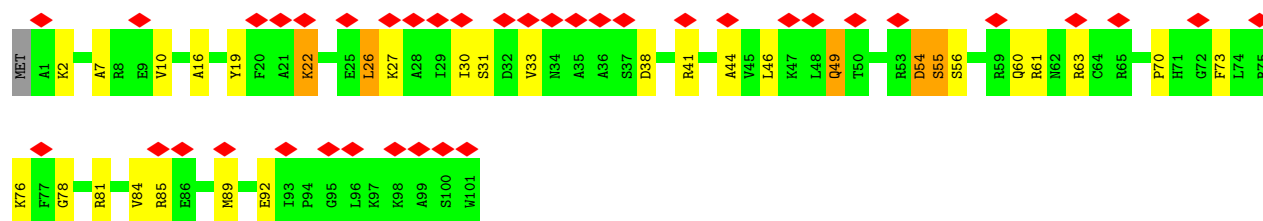


• Molecule 22: 30S ribosomal protein S13

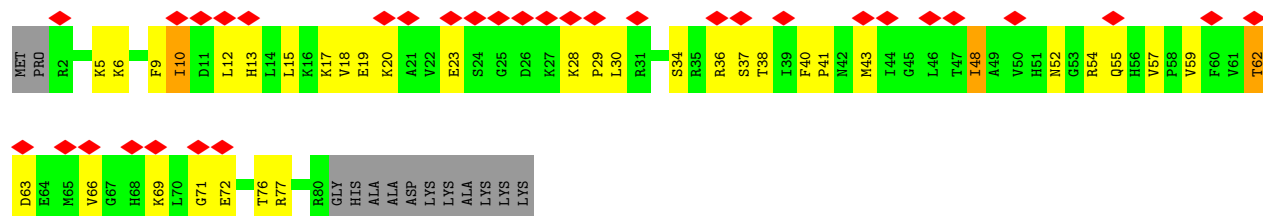


• Molecule 23: 30S ribosomal protein S14

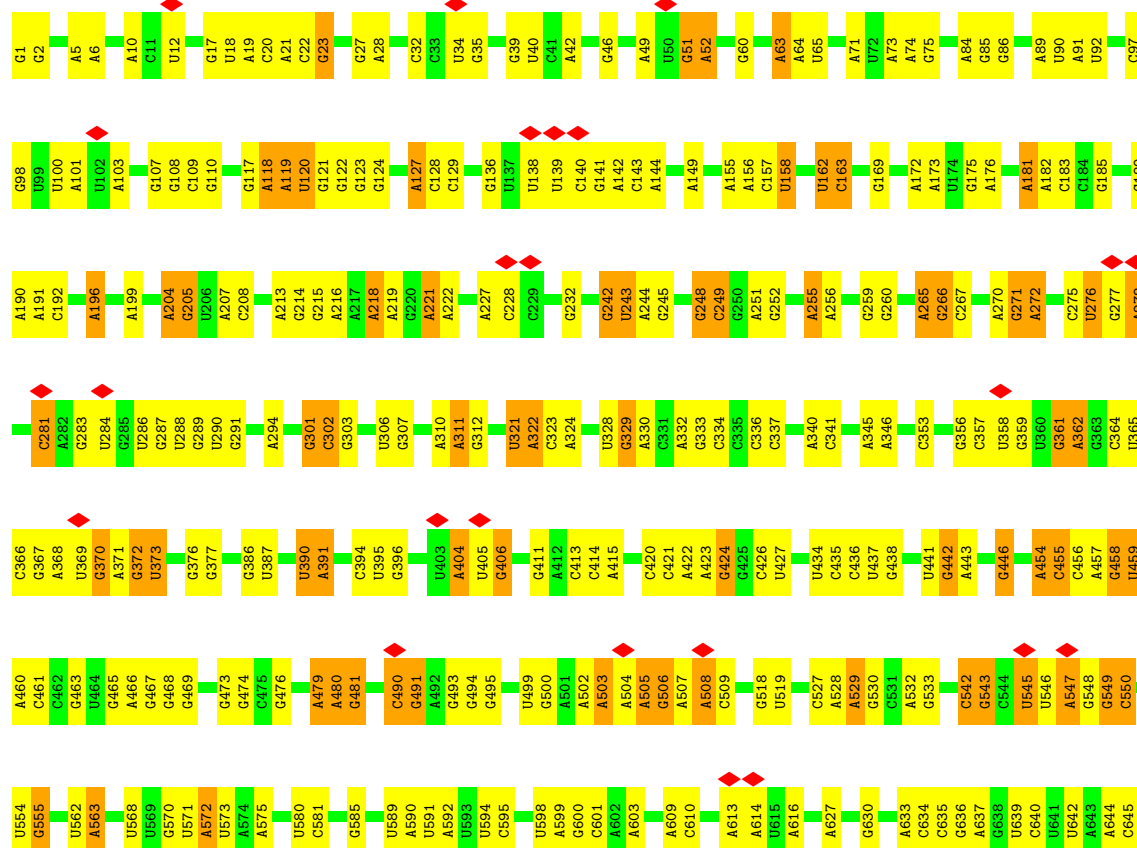


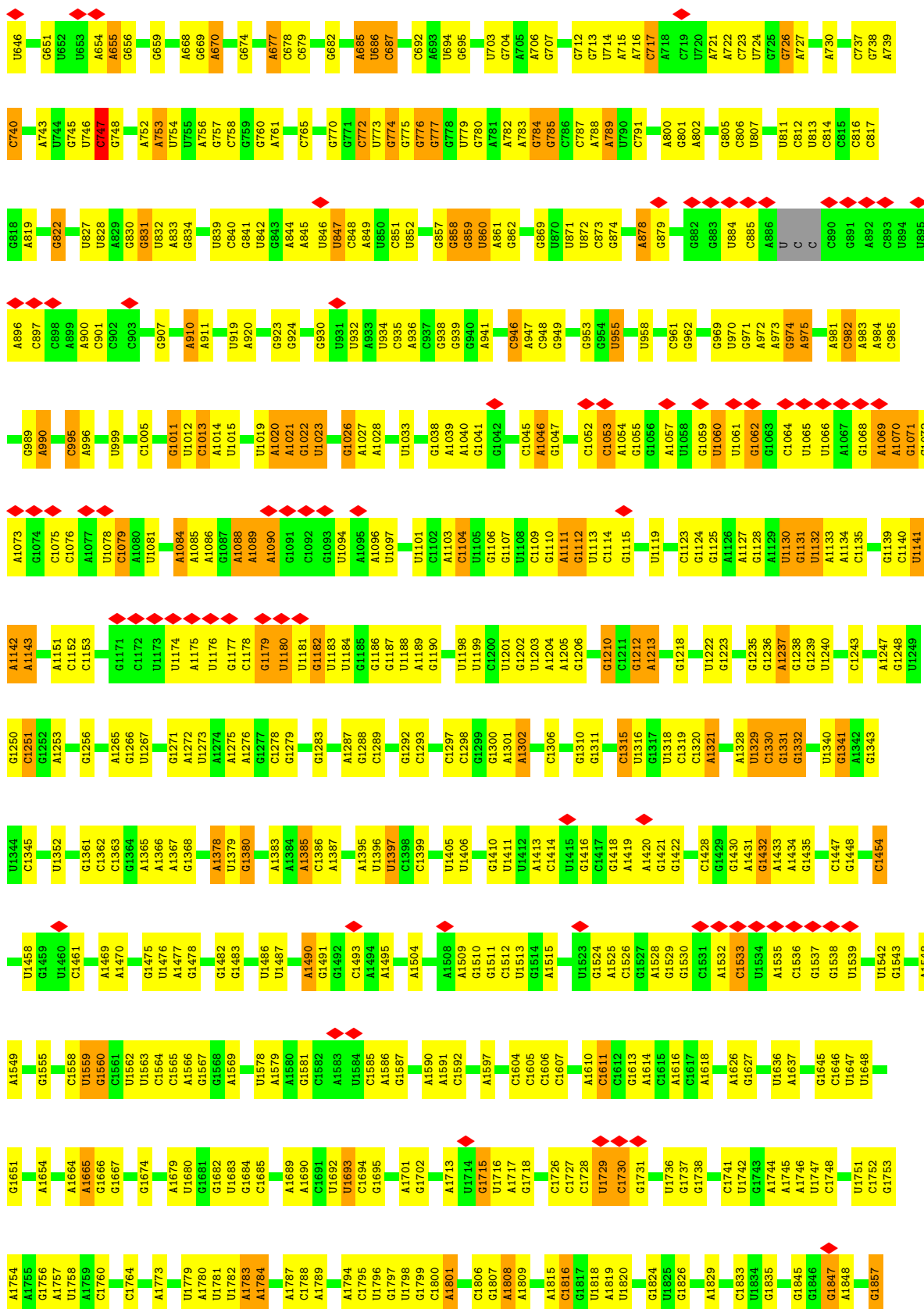


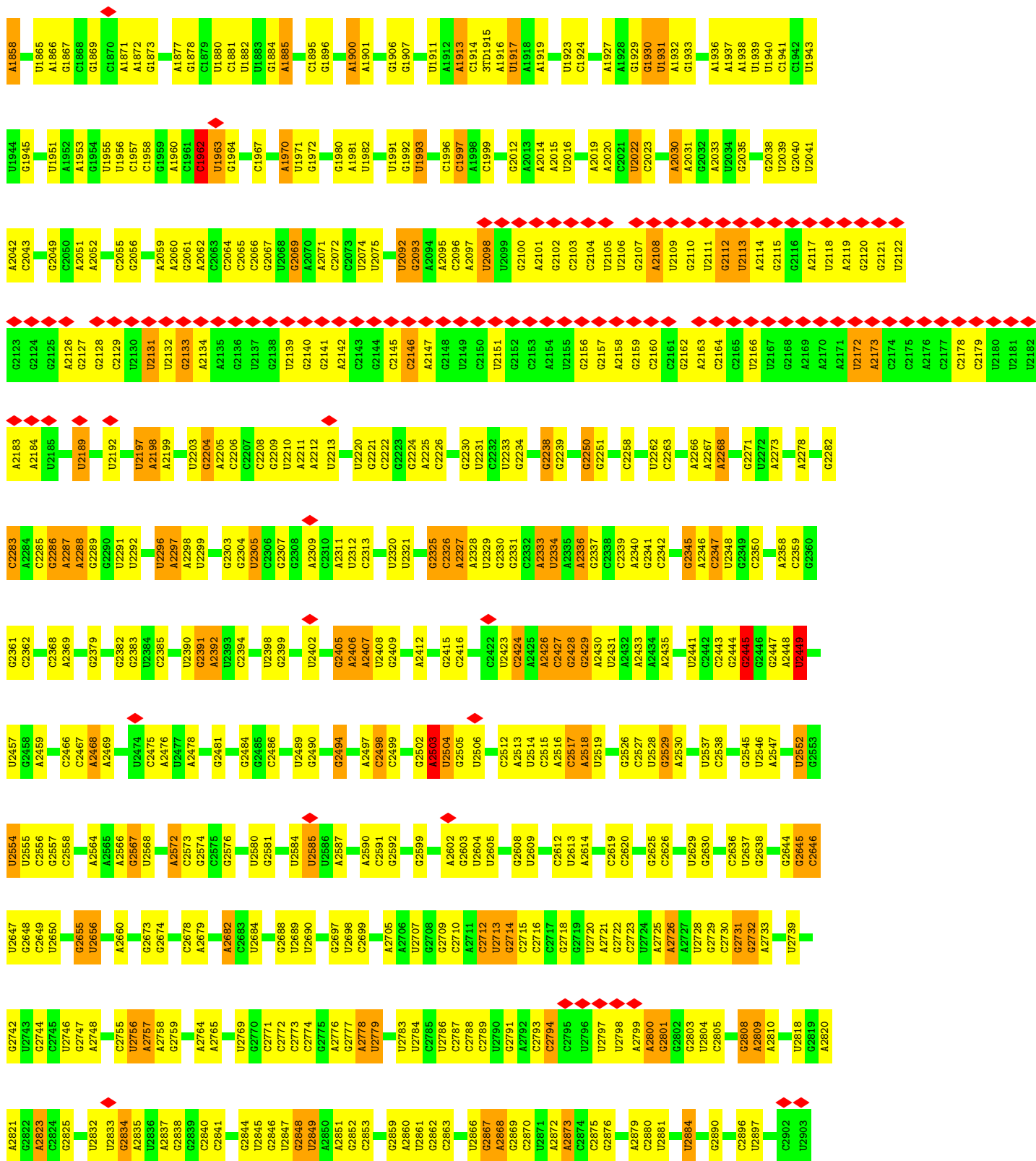
• Molecule 24: 30S ribosomal protein S19



• Molecule 25: 23S ribosomal RNA

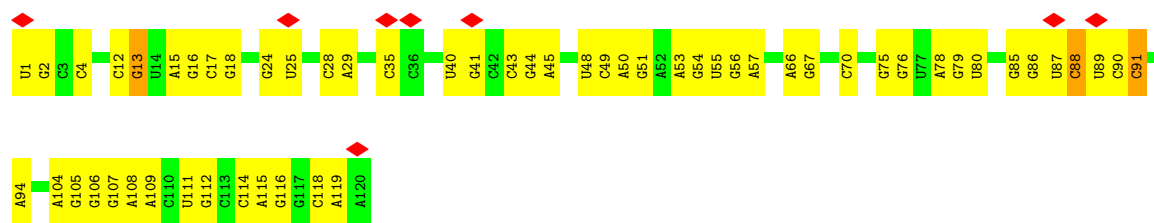




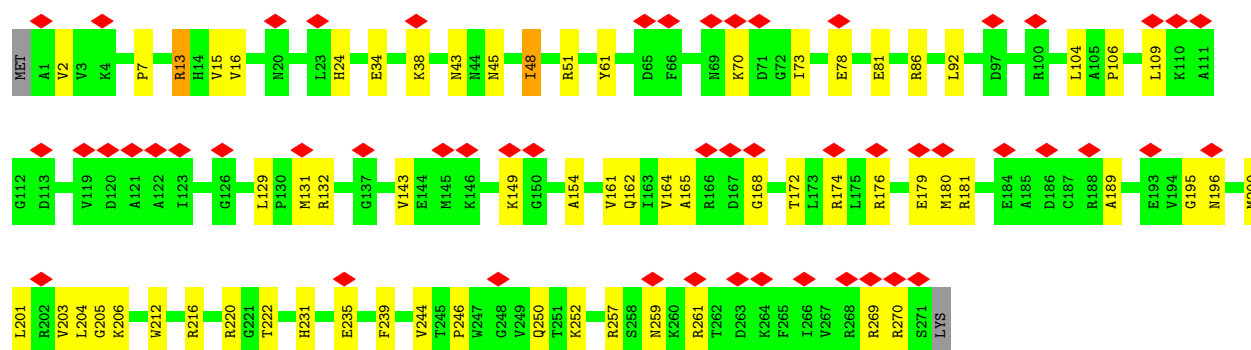
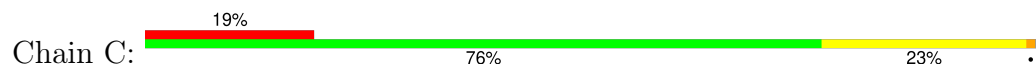


• Molecule 26: 5S ribosomal RNA

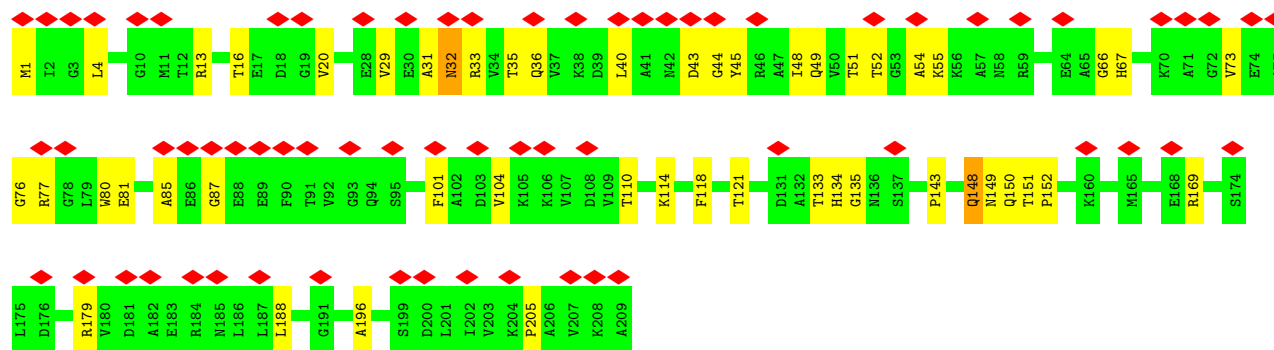
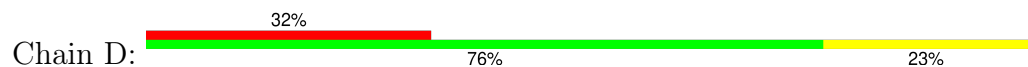




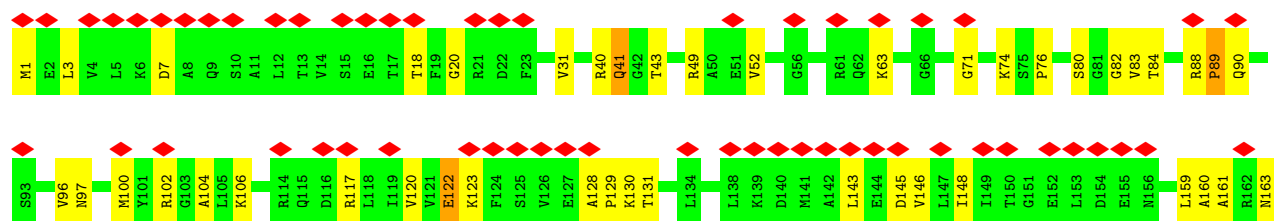
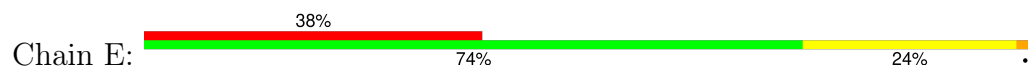
• Molecule 27: 50S ribosomal protein L2

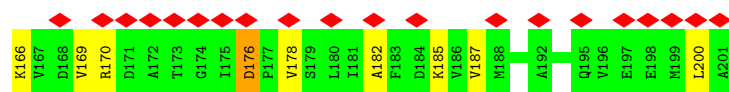


• Molecule 28: 50S ribosomal protein L3

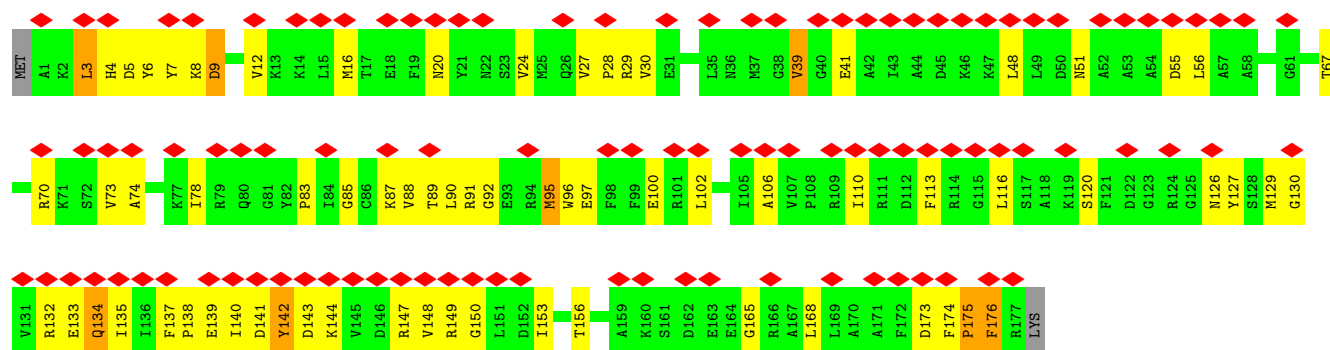


• Molecule 29: 50S ribosomal protein L4

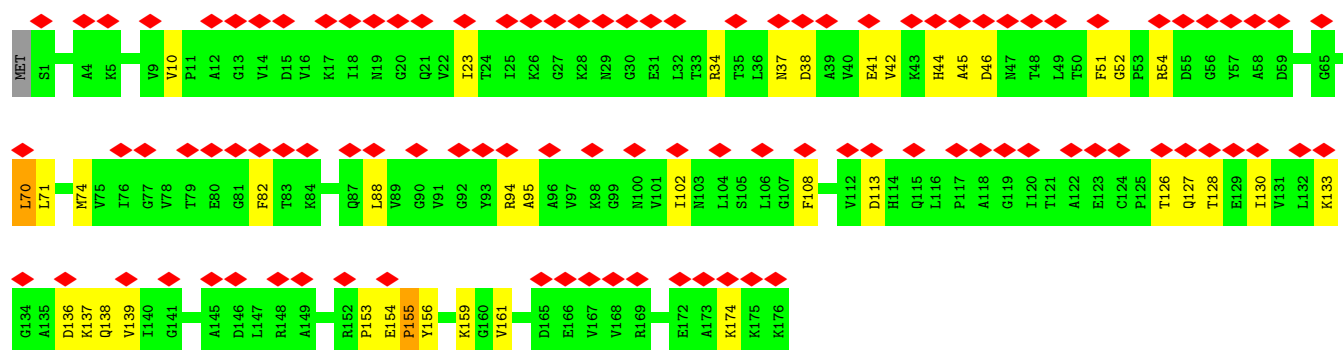
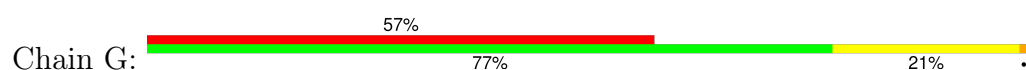




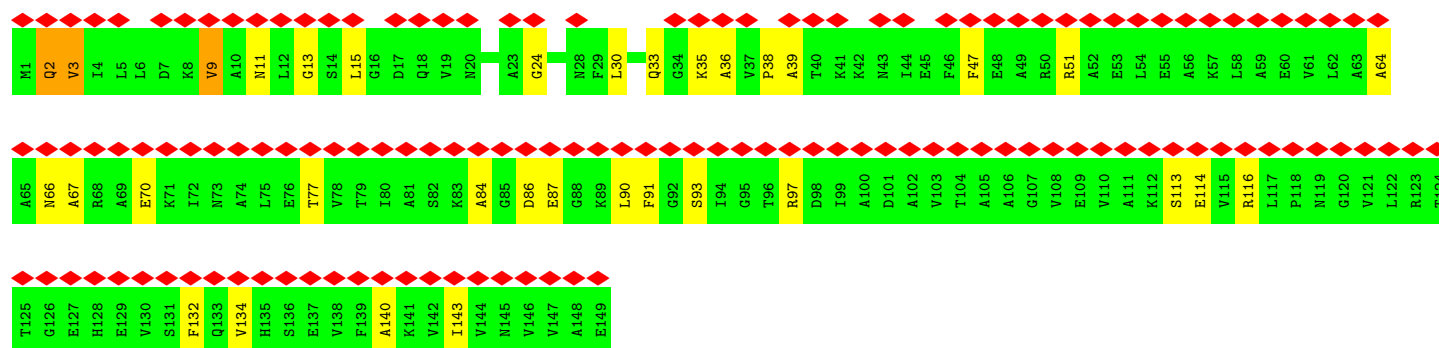
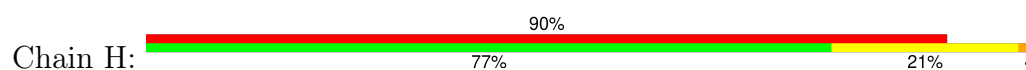
• Molecule 30: 50S ribosomal protein L5



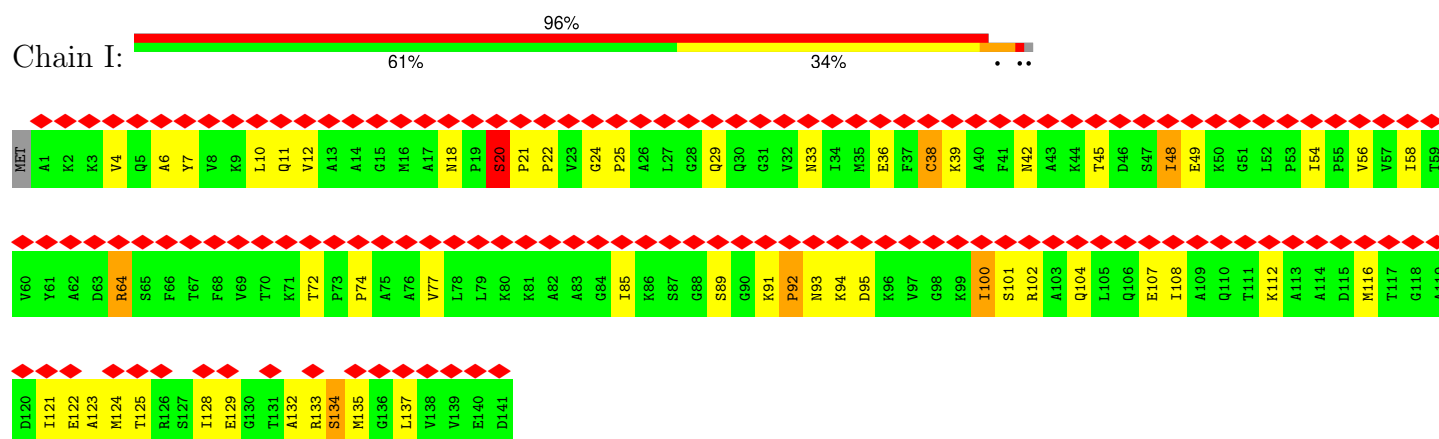
• Molecule 31: 50S ribosomal protein L6



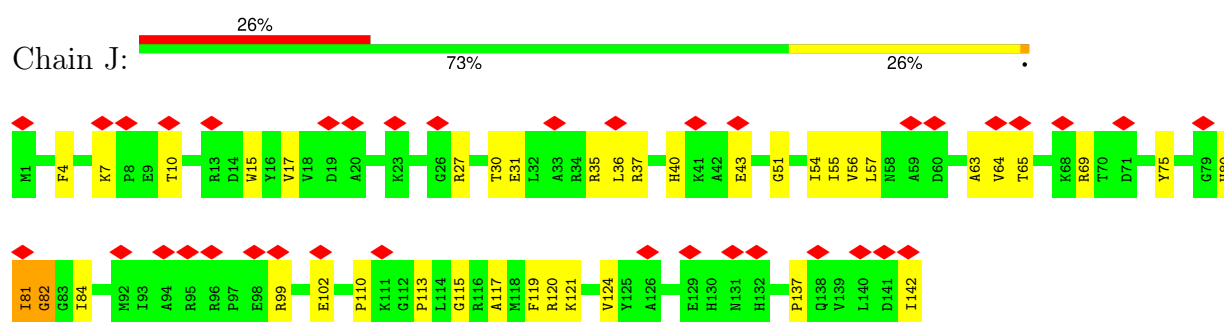
• Molecule 32: 50S ribosomal protein L9



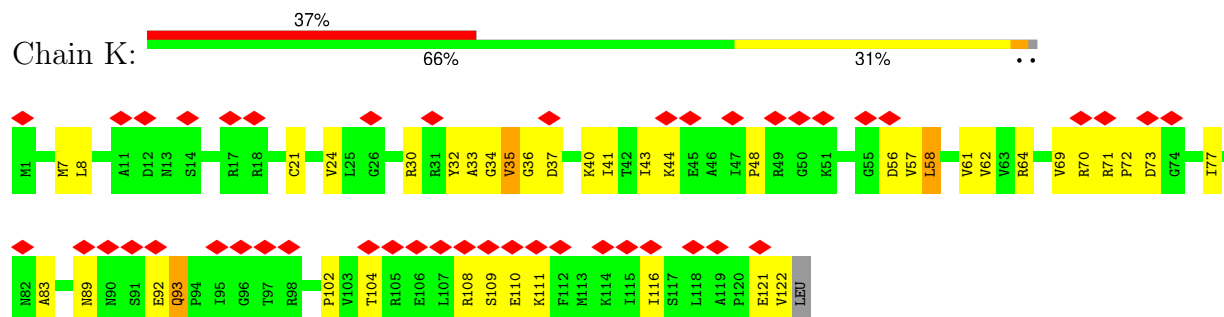
• Molecule 33: 50S ribosomal protein L11



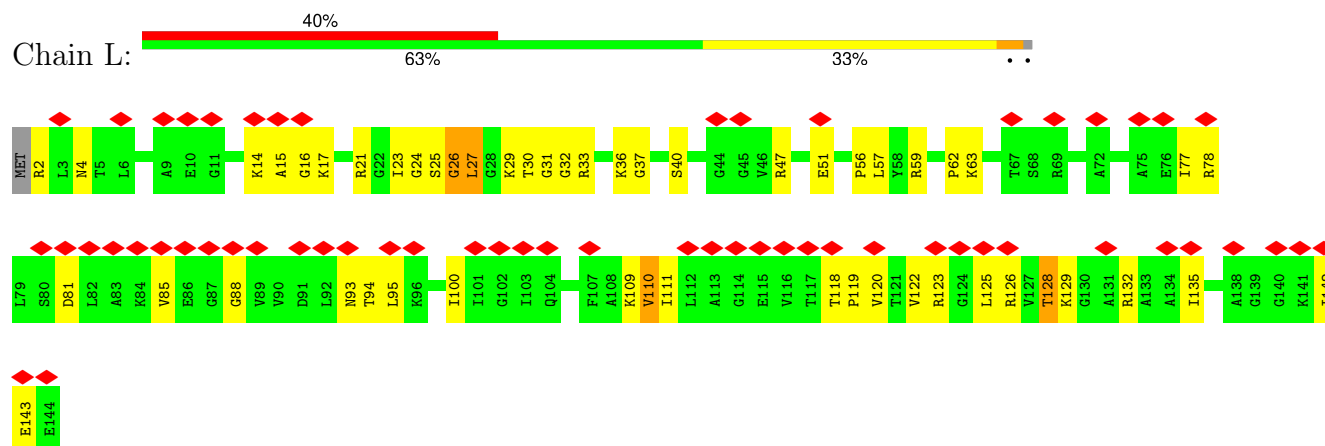
• Molecule 34: 50S ribosomal protein L13



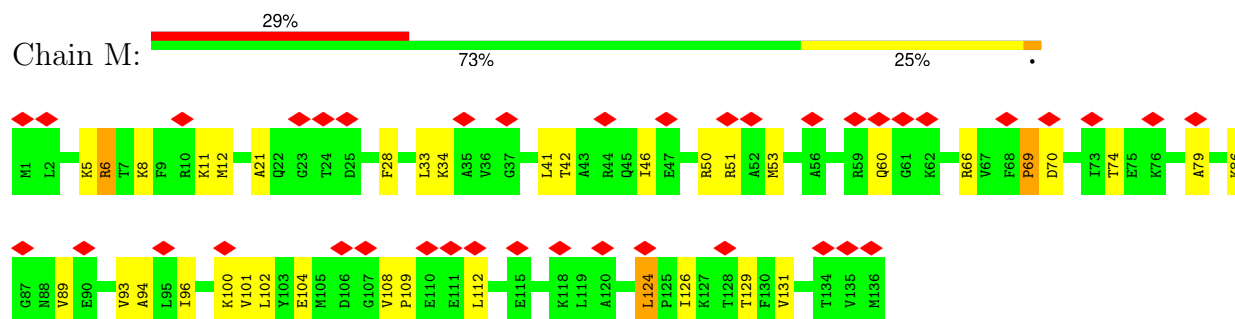
• Molecule 35: 50S ribosomal protein L14



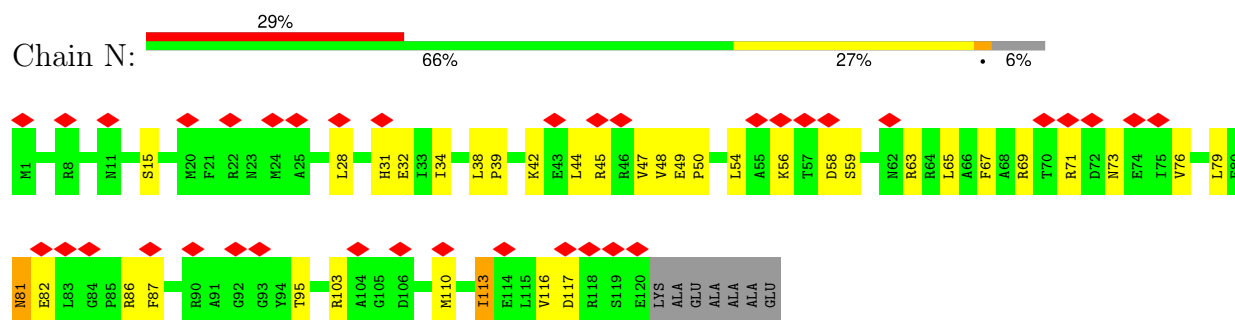
• Molecule 36: 50S ribosomal protein L15



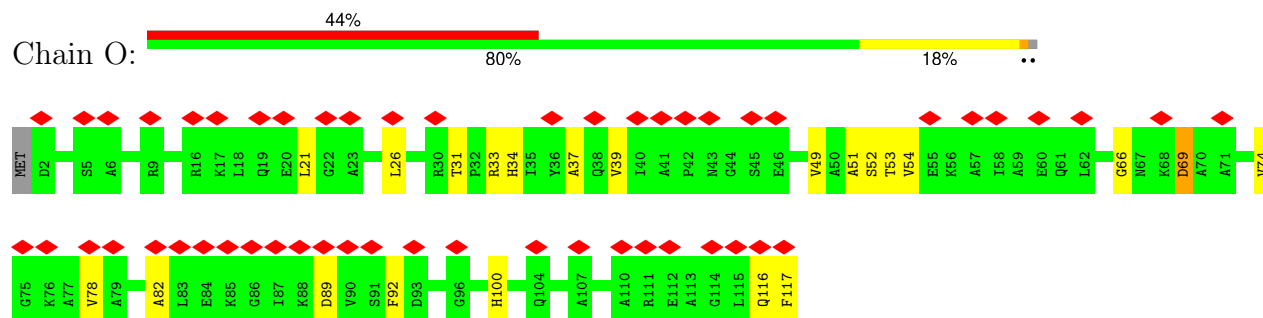
- Molecule 37: 50S ribosomal protein L16



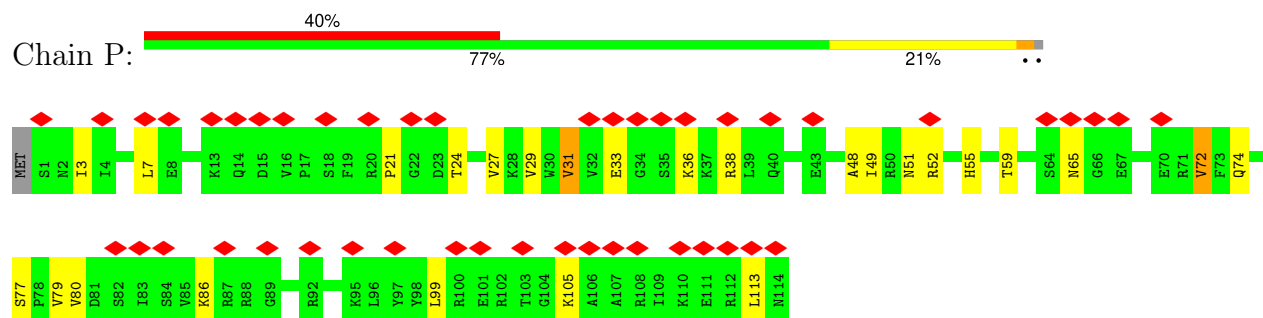
- Molecule 38: 50S ribosomal protein L17



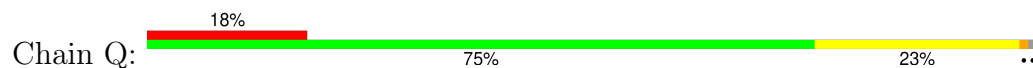
- Molecule 39: 50S ribosomal protein L18

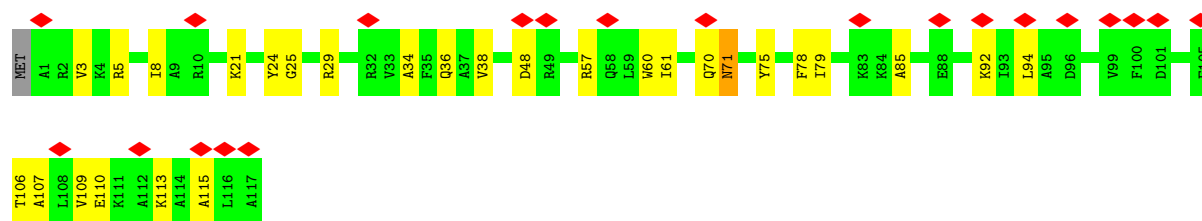


- Molecule 40: 50S ribosomal protein L19

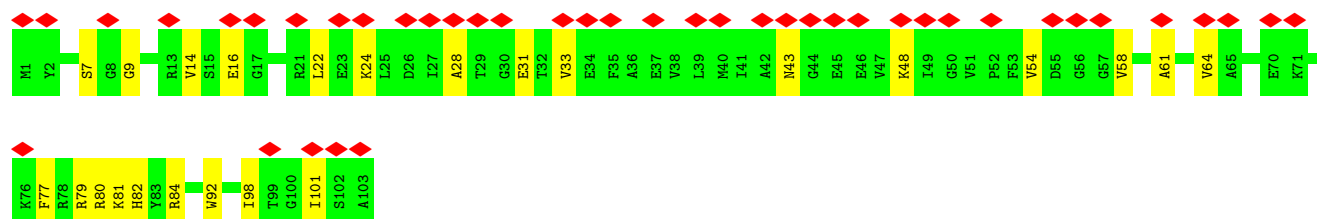
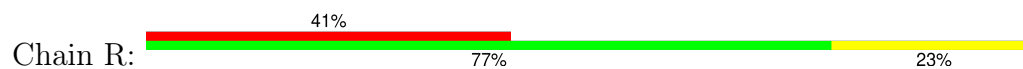


- Molecule 41: 50S ribosomal protein L20

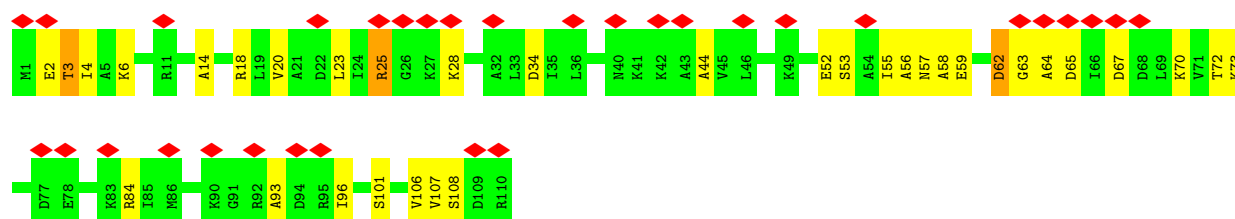




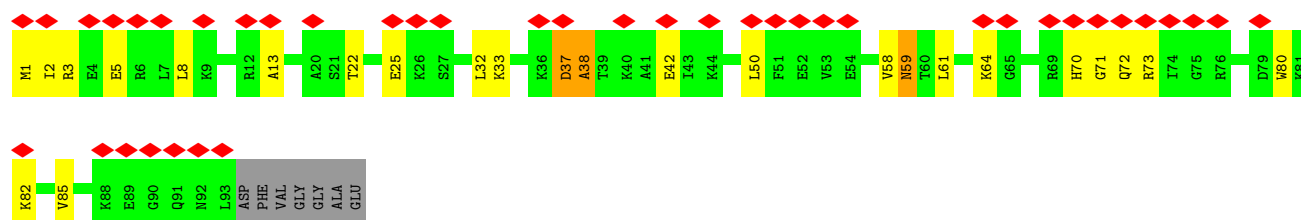
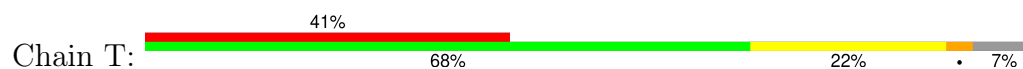
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22

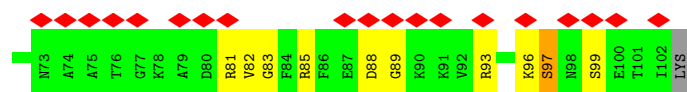


- Molecule 44: 50S ribosomal protein L23

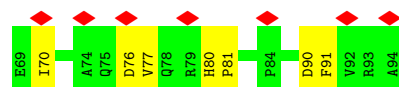
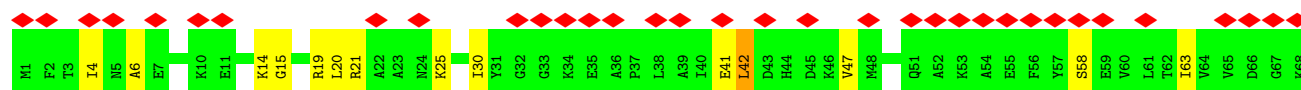
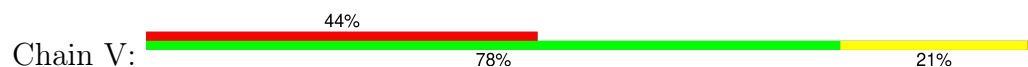


- Molecule 45: 50S ribosomal protein L24

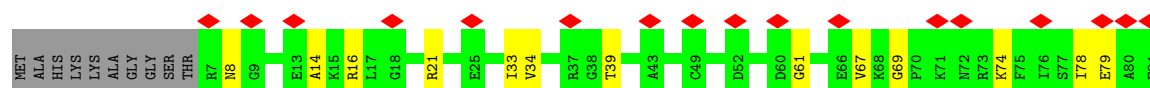
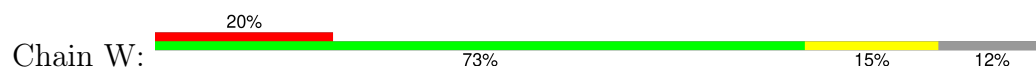




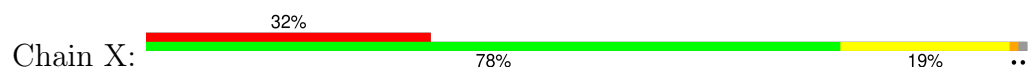
- Molecule 46: 50S ribosomal protein L25



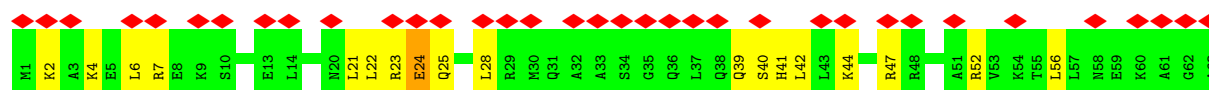
- Molecule 47: 50S ribosomal protein L27



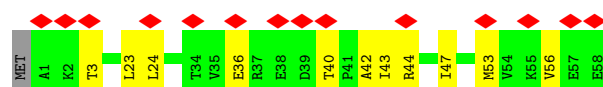
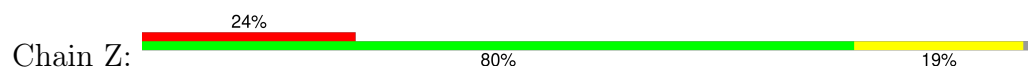
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29

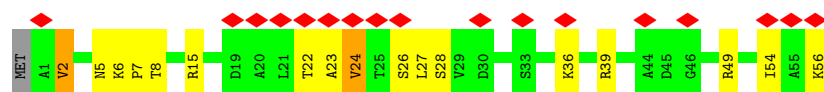


- Molecule 50: 50S ribosomal protein L30

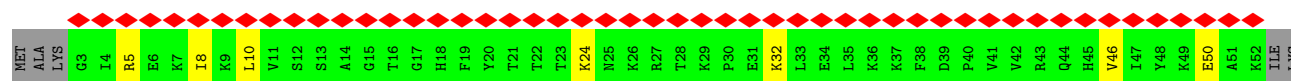
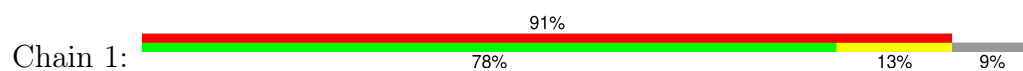


- Molecule 51: 50S ribosomal protein L32

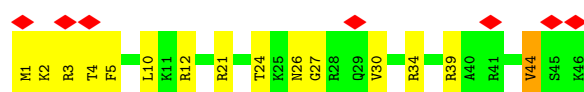




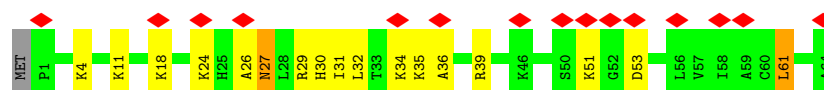
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



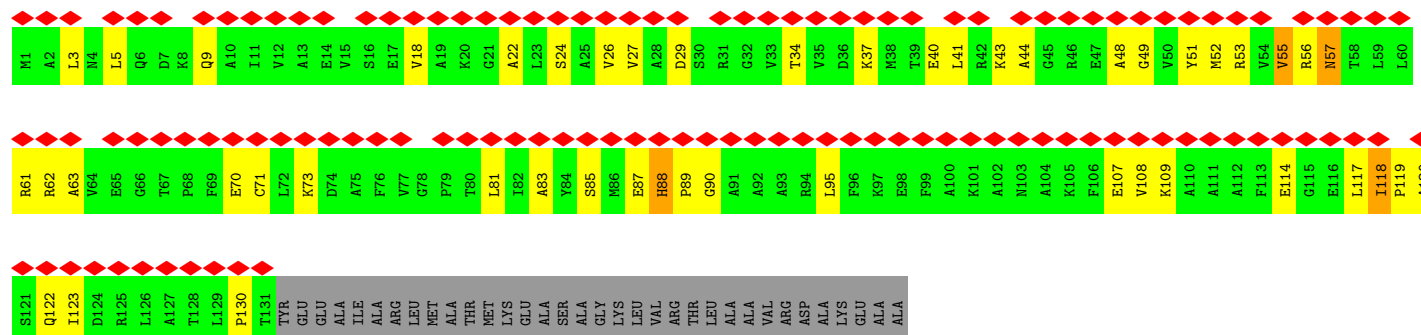
- Molecule 54: 50S ribosomal protein L35



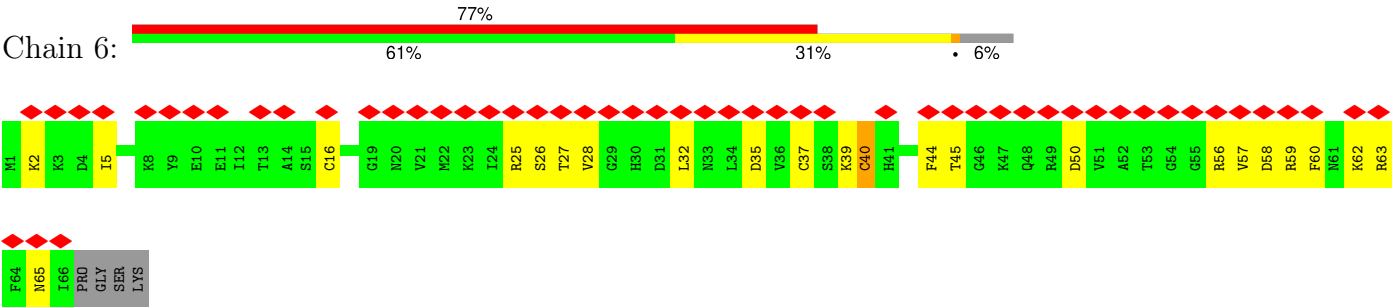
- Molecule 55: 50S ribosomal protein L36



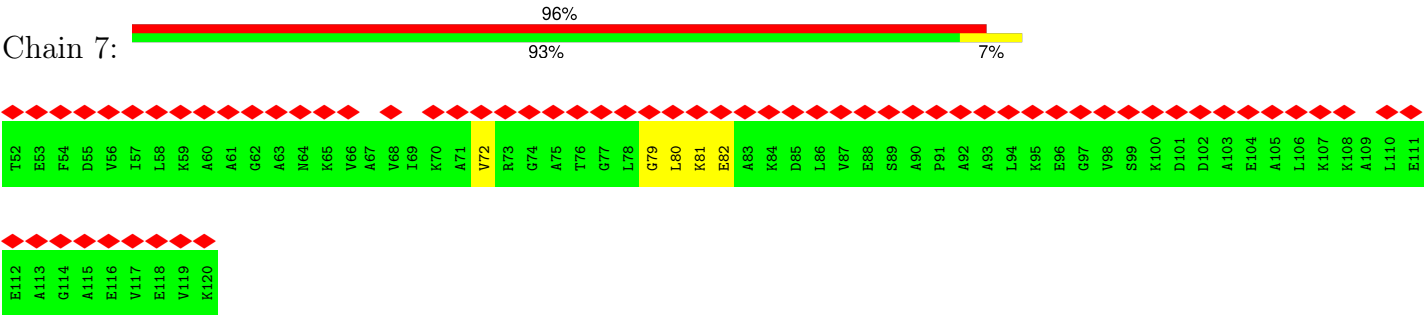
- Molecule 56: 50S ribosomal protein L10



- Molecule 57: 50S ribosomal protein L31



• Molecule 58: 50S ribosomal protein L7/L12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size ($\text{\AA}$)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.108, 1.108, 1.108	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MA6, PSU, 5MU, OMG, OMC, H2U, 4SU, 7MG, 5MC, 2MG, 1MG, 6MZ, 4OC, 2MA, OMU, 3TD

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	a	0.20	0/36701	0.33	6/57246 (0.0%)
2	b	0.40	0/1735	0.76	1/2338 (0.0%)
3	d	0.34	0/1665	0.79	0/2227
4	e	0.41	0/1154	0.79	1/1554 (0.1%)
5	f	0.45	0/835	0.85	3/1128 (0.3%)
6	h	0.35	0/989	0.77	0/1326
7	k	0.37	0/885	0.84	2/1195 (0.2%)
8	l	0.36	0/969	0.80	1/1300 (0.1%)
9	o	0.44	0/722	0.72	0/964
10	p	0.43	0/659	0.84	0/884
11	q	0.33	0/657	0.79	0/881
12	r	0.35	0/511	0.71	0/689
13	t	0.50	0/671	0.82	1/888 (0.1%)
14	u	0.39	0/500	0.77	0/668
15	v	0.22	1/1747 (0.1%)	0.33	0/2721
16	x	0.45	1/210 (0.5%)	0.25	0/324
17	w	0.31	0/2594	0.96	12/3251 (0.4%)
18	c	0.43	0/1651	0.76	0/2225
19	g	0.50	1/1195 (0.1%)	0.85	0/1602
20	i	0.35	0/1034	0.75	0/1375
21	j	0.51	0/796	0.88	2/1077 (0.2%)
22	m	0.50	0/892	0.85	0/1193
23	n	0.33	0/811	0.75	0/1081
24	s	0.35	0/652	0.73	0/877
25	A	0.23	1/69174 (0.0%)	0.34	0/107910
26	B	0.17	0/2876	0.32	0/4483
27	C	0.42	0/2121	0.82	0/2852
28	D	0.45	0/1586	0.83	1/2134 (0.0%)
29	E	0.33	0/1571	0.70	2/2113 (0.1%)
30	F	0.40	0/1434	0.78	0/1926
31	G	0.47	0/1343	0.84	1/1816 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	H	0.34	0/1122	0.73	0/1515
33	I	0.38	0/1046	0.79	2/1410 (0.1%)
34	J	0.36	0/1152	0.73	0/1551
35	K	0.36	0/947	0.72	0/1268
36	L	0.35	0/1054	0.77	1/1403 (0.1%)
37	M	0.40	0/1093	0.77	2/1460 (0.1%)
38	N	0.36	0/973	0.76	0/1301
39	O	0.41	0/902	0.74	0/1209
40	P	0.34	0/929	0.75	0/1242
41	Q	0.40	0/960	0.77	0/1278
42	R	0.43	0/829	0.82	1/1107 (0.1%)
43	S	0.37	0/864	0.83	1/1156 (0.1%)
44	T	0.35	0/744	0.79	0/994
45	U	0.47	1/787 (0.1%)	0.78	1/1051 (0.1%)
46	V	0.37	0/766	0.78	0/1025
47	W	0.39	0/582	0.83	2/769 (0.3%)
48	X	0.34	0/635	0.69	0/848
49	Y	0.43	0/510	0.73	0/677
50	Z	0.31	0/453	0.67	0/605
51	0	0.32	0/450	0.72	0/599
52	1	0.34	0/416	0.74	0/554
53	2	0.35	0/380	0.79	0/498
54	3	0.33	0/513	0.80	2/676 (0.3%)
55	4	0.33	0/303	0.77	0/397
56	5	0.38	0/1001	0.79	0/1350
57	6	0.45	0/531	0.89	0/709
58	7	0.55	0/275	1.17	0/342
All	All	0.29	5/160557 (0.0%)	0.51	45/239242 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	U	41	VAL	C-O	6.54	1.31	1.24
19	g	92	PRO	C-O	5.79	1.31	1.24
16	x	14	U	C1'-N1	5.74	1.57	1.48
25	A	2552	OMU	O3'-P	5.48	1.61	1.56
15	v	8	4SU	O3'-P	5.19	1.61	1.56

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1491	G	C4'-C3'-O3'	8.84	126.26	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	w	121	ILE	CA-C-N	8.79	128.84	119.78
17	w	121	ILE	C-N-CA	8.79	128.84	119.78
1	a	530	G	P-O5'-C5'	-7.37	109.85	120.90
1	a	529	G	O3'-P-O5'	-7.22	93.17	104.00

There are no chirality outliers.

There are no planarity outliers.

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	a	33029	0	16642	620	0
2	b	1704	0	1732	48	0
3	d	1643	0	1710	46	0
4	e	1141	0	1169	91	0
5	f	817	0	808	35	0
6	h	979	0	1034	16	0
7	k	869	0	878	43	0
8	l	955	0	1019	42	0
9	o	714	0	737	21	0
10	p	649	0	666	23	0
11	q	648	0	691	27	0
12	r	504	0	502	13	0
13	t	665	0	714	18	0
14	u	495	0	486	17	0
15	v	1644	0	840	28	0
16	x	189	0	96	8	0
17	w	2590	0	731	18	0
18	c	1624	0	1699	56	0
19	g	1181	0	1240	47	0
20	i	1022	0	1070	30	0
21	j	786	0	828	36	0
22	m	883	0	944	40	0
23	n	799	0	841	20	0
24	s	637	0	665	43	0
25	A	62276	0	31346	829	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	2572	0	1302	27	0
27	C	2082	0	2157	42	0
28	D	1565	0	1616	35	0
29	E	1552	0	1619	32	0
30	F	1410	0	1447	49	0
31	G	1323	0	1374	23	0
32	H	1111	0	1148	27	0
33	I	1032	0	1088	37	0
34	J	1129	0	1162	31	0
35	K	938	0	1012	25	0
36	L	1045	0	1117	35	0
37	M	1074	0	1157	22	0
38	N	960	0	1000	26	0
39	O	892	0	923	12	0
40	P	917	0	965	28	0
41	Q	947	0	1022	21	0
42	R	816	0	839	15	0
43	S	857	0	922	22	0
44	T	738	0	807	19	0
45	U	779	0	834	16	0
46	V	753	0	780	13	0
47	W	575	0	592	8	0
48	X	625	0	655	12	0
49	Y	509	0	543	10	0
50	Z	449	0	491	7	0
51	0	444	0	461	14	0
52	1	409	0	440	4	0
53	2	377	0	418	20	0
54	3	504	0	574	17	0
55	4	302	0	343	12	0
56	5	988	0	1025	34	0
57	6	522	0	524	48	0
58	7	276	0	79	2	0
All	All	148915	0	99524	2538	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 10.

The worst 5 of 2538 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:a:1081:A:H5'	4:e:22:LYS:CG	1.27	1.58
1:a:1399:C:H4'	1:a:1400:C:C5'	1.31	1.54
1:a:1081:A:C5'	4:e:22:LYS:HG3	1.44	1.44
1:a:1081:A:H5'	4:e:22:LYS:CD	1.42	1.43
1:a:518:C:C5	1:a:530:G:H5'	1.54	1.41

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	
2	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	2	19
3	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	1	18
4	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	1	16
5	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	15
6	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	4	29
7	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	1	17
8	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	2	20
9	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	1	16
10	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	29
11	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	15
12	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	11
13	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	4	29
14	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	11
17	w	637/639 (100%)	562 (88%)	51 (8%)	24 (4%)	2	21
18	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	12	45
19	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1	15
21	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1	15
22	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	2	19
23	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	1	17
24	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
27	C	269/273 (98%)	242 (90%)	22 (8%)	5 (2%)	6	33
28	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	12	45
29	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	3	23
30	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3	24
31	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	3	26
32	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4	28
33	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	15
34	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	38
35	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	4	29
36	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	12
37	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	5	31
38	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	4	29
39	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	14	47
40	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	14	47
41	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
42	R	101/103 (98%)	81 (80%)	18 (18%)	2 (2%)	6	32
43	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	1	16
44	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	3	24
45	U	100/104 (96%)	81 (81%)	16 (16%)	3 (3%)	3	26
46	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	5	31
47	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	9	38
48	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	9	40
49	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7	36
50	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	33
52	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	7	36
55	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
56	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	1	17
57	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	7	36
58	7	67/69 (97%)	58 (87%)	8 (12%)	1 (2%)	8	37
All	All	6551/6928 (95%)	5610 (86%)	716 (11%)	225 (3%)	4	24

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	e	122	VAL
5	f	63	ASN
10	p	8	ARG
11	q	79	GLU
12	r	17	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/198 (91%)	173 (96%)	7 (4%)	28	52
3	d	172/173 (99%)	166 (96%)	6 (4%)	32	54
4	e	114/126 (90%)	104 (91%)	10 (9%)	9	32
5	f	87/116 (75%)	82 (94%)	5 (6%)	18	44
6	h	104/105 (99%)	103 (99%)	1 (1%)	68	75
7	k	89/99 (90%)	86 (97%)	3 (3%)	32	55
8	l	103/104 (99%)	99 (96%)	4 (4%)	28	52
9	o	76/77 (99%)	75 (99%)	1 (1%)	61	71
10	p	65/65 (100%)	61 (94%)	4 (6%)	16	43
11	q	74/78 (95%)	72 (97%)	2 (3%)	39	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	r	48/65 (74%)	47 (98%)	1 (2%)	47	65
13	t	65/66 (98%)	63 (97%)	2 (3%)	35	57
14	u	44/61 (72%)	44 (100%)	0	100	100
17	w	6/576 (1%)	6 (100%)	0	100	100
18	c	170/190 (90%)	159 (94%)	11 (6%)	15	42
19	g	124/147 (84%)	119 (96%)	5 (4%)	28	51
20	i	105/107 (98%)	103 (98%)	2 (2%)	50	66
21	j	86/90 (96%)	82 (95%)	4 (5%)	23	48
22	m	92/96 (96%)	88 (96%)	4 (4%)	26	49
23	n	79/84 (94%)	75 (95%)	4 (5%)	21	46
24	s	70/79 (89%)	65 (93%)	5 (7%)	13	40
27	C	216/218 (99%)	210 (97%)	6 (3%)	38	59
28	D	164/164 (100%)	163 (99%)	1 (1%)	78	80
29	E	165/165 (100%)	161 (98%)	4 (2%)	43	63
30	F	148/150 (99%)	138 (93%)	10 (7%)	14	41
31	G	137/138 (99%)	136 (99%)	1 (1%)	76	78
32	H	114/114 (100%)	114 (100%)	0	100	100
33	I	109/110 (99%)	103 (94%)	6 (6%)	19	45
34	J	116/116 (100%)	114 (98%)	2 (2%)	53	68
35	K	103/104 (99%)	98 (95%)	5 (5%)	22	47
36	L	102/103 (99%)	100 (98%)	2 (2%)	48	65
37	M	109/109 (100%)	108 (99%)	1 (1%)	70	75
38	N	100/103 (97%)	97 (97%)	3 (3%)	36	57
39	O	86/87 (99%)	84 (98%)	2 (2%)	44	63
40	P	99/100 (99%)	94 (95%)	5 (5%)	21	46
41	Q	89/90 (99%)	85 (96%)	4 (4%)	24	49
42	R	84/84 (100%)	82 (98%)	2 (2%)	43	63
43	S	93/93 (100%)	90 (97%)	3 (3%)	34	56
44	T	80/84 (95%)	78 (98%)	2 (2%)	42	62
45	U	83/85 (98%)	81 (98%)	2 (2%)	43	63
46	V	78/78 (100%)	77 (99%)	1 (1%)	61	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	W	57/63 (90%)	56 (98%)	1 (2%)	51	67
48	X	67/68 (98%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	54 (98%)	1 (2%)	51	67
50	Z	48/49 (98%)	48 (100%)	0	100	100
51	0	47/48 (98%)	45 (96%)	2 (4%)	26	49
52	1	45/49 (92%)	44 (98%)	1 (2%)	45	64
53	2	38/38 (100%)	37 (97%)	1 (3%)	40	60
54	3	51/52 (98%)	50 (98%)	1 (2%)	48	65
55	4	34/34 (100%)	33 (97%)	1 (3%)	37	58
56	5	100/123 (81%)	97 (97%)	3 (3%)	36	57
57	6	59/62 (95%)	58 (98%)	1 (2%)	53	68
All	All	4829/5638 (86%)	4674 (97%)	155 (3%)	35	56

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	K	73	ASP
47	W	67	VAL
38	N	15	SER
41	Q	48	ASP
55	4	17	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
45	U	65	GLN
46	V	75	GLN
53	2	26	ASN
22	m	90	HIS
22	m	7	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	256 (16%)	0
15	v	76/78 (97%)	18 (23%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	x	8/11 (72%)	0	0
25	A	2898/2903 (99%)	549 (18%)	91 (3%)
26	B	119/120 (99%)	18 (15%)	4 (3%)
All	All	4639/4651 (99%)	841 (18%)	95 (2%)

5 of 841 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A

5 of 95 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1378	A
25	A	2210	U
25	A	1432	G
25	A	1857	G
25	A	2326	C

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

39 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	$\# Z > 2$
25	5MU	A	1939	25	19,22,23	1.36	4 (21%)	27,32,35	2.28	6 (22%)
1	2MG	a	1207	1	23,26,27	1.26	4 (17%)	33,38,41	2.25	8 (24%)
25	2MA	A	2503	25	22,25,26	1.46	5 (22%)	32,37,40	2.31	9 (28%)
15	PSU	v	55	15	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
25	5MC	A	747	25	19,22,23	1.54	3 (15%)	26,32,35	1.38	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	A	2580	25	18,21,22	1.43	3 (16%)	21,30,33	2.20	4 (19%)
1	2MG	a	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.31	8 (24%)
25	OMC	A	2498	25	19,22,23	0.81	1 (5%)	25,31,34	0.88	0
25	PSU	A	955	25	18,21,22	1.43	4 (22%)	21,30,33	2.17	4 (19%)
25	6MZ	A	2030	25	22,25,26	1.61	5 (22%)	29,36,39	2.26	10 (34%)
1	2MG	a	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.14	7 (21%)
25	2MG	A	1835	25	23,26,27	1.30	4 (17%)	33,38,41	2.24	8 (24%)
25	PSU	A	1917	25	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
25	2MG	A	2445	25	23,26,27	1.33	4 (17%)	33,38,41	1.96	6 (18%)
15	5MU	v	54	15	19,22,23	1.39	5 (26%)	27,32,35	2.25	5 (18%)
25	PSU	A	2605	25	18,21,22	1.43	3 (16%)	21,30,33	1.97	5 (23%)
1	UR3	a	1498	1	19,22,23	0.93	0	26,32,35	1.94	4 (15%)
1	4OC	a	1402	1	20,23,24	1.66	4 (20%)	25,32,35	2.45	10 (40%)
15	H2U	v	20	15	18,21,22	0.92	2 (11%)	19,30,33	1.04	2 (10%)
25	6MZ	A	1618	25	22,25,26	1.68	5 (22%)	29,36,39	2.31	9 (31%)
25	PSU	A	2604	25	18,21,22	1.38	3 (16%)	21,30,33	2.06	5 (23%)
25	H2U	A	2449	25	18,21,22	0.91	2 (11%)	19,30,33	1.10	2 (10%)
25	5MC	A	1962	25	19,22,23	1.59	3 (15%)	26,32,35	1.10	2 (7%)
25	PSU	A	1911	25	18,21,22	1.34	2 (11%)	21,30,33	2.12	4 (19%)
25	PSU	A	2457	25	18,21,22	1.36	3 (16%)	21,30,33	2.22	4 (19%)
25	PSU	A	2504	25	18,21,22	1.36	2 (11%)	21,30,33	1.96	3 (14%)
25	3TD	A	1915	25	19,22,23	1.35	3 (15%)	23,32,35	2.08	4 (17%)
25	OMU	A	2552	25	19,22,23	1.23	3 (15%)	25,31,34	2.28	7 (28%)
1	5MC	a	967	1	19,22,23	1.52	2 (10%)	26,32,35	1.08	2 (7%)
15	4SU	v	8	15	18,21,22	1.79	4 (22%)	25,30,33	2.37	6 (24%)
25	1MG	A	745	25	23,26,27	1.20	1 (4%)	33,39,42	1.86	7 (21%)
1	7MG	a	527	1	23,26,27	1.33	4 (17%)	27,39,42	2.57	7 (25%)
25	7MG	A	2069	25	23,26,27	1.37	4 (17%)	27,39,42	2.63	7 (25%)
1	MA6	a	1518	1	23,26,27	1.66	5 (21%)	33,38,41	2.26	9 (27%)
1	PSU	a	516	1	18,21,22	1.47	4 (22%)	21,30,33	2.29	5 (23%)
25	OMG	A	2251	15,25	23,26,27	1.26	3 (13%)	32,38,41	1.81	5 (15%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
1	MA6	a	1519	1	23,26,27	1.51	5 (21%)	33,38,41	2.35	13 (39%)
25	PSU	A	746	25	18,21,22	1.34	2 (11%)	21,30,33	1.97	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
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	2/9/27/28	0/3/3/3
25	2MA	A	2503	25	-	2/7/25/26	0/3/3/3
15	PSU	v	55	15	-	2/7/25/26	0/2/2/2
25	5MC	A	747	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/9/27/28	0/3/3/3
25	OMC	A	2498	25	-	1/9/27/28	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	2MG	A	2445	25	-	2/9/27/28	0/3/3/3
15	5MU	v	54	15	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	3/9/29/30	0/2/2/2
15	H2U	v	20	15	-	1/7/38/39	0/2/2/2
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	5MC	A	1962	25	-	1/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	2/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	3/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	2/9/27/28	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
15	4SU	v	8	15	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
1	7MG	a	527	1	-	3/7/37/38	0/3/3/3
25	7MG	A	2069	25	-	0/7/37/38	0/3/3/3
1	MA6	a	1518	1	-	6/11/29/30	0/3/3/3
1	PSU	a	516	1	-	2/7/25/26	0/2/2/2
25	OMG	A	2251	15,25	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	2/11/29/30	0/3/3/3
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1618	6MZ	C5-C4	5.74	1.49	1.39
25	A	1962	5MC	C5-C4	5.60	1.48	1.44
1	a	1407	5MC	C5-C4	5.44	1.48	1.44
25	A	747	5MC	C5-C4	5.36	1.48	1.44
25	A	2030	6MZ	C5-C4	5.33	1.48	1.39

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2069	7MG	N9-C4-N3	8.76	138.30	125.46
1	a	527	7MG	N9-C4-N3	8.73	138.26	125.46
1	a	966	2MG	C2-N3-C4	7.57	121.47	112.00
1	a	1207	2MG	C2-N3-C4	7.51	121.39	112.00
25	A	2503	2MA	C5-C4-N3	-7.38	119.40	127.18

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1402	4OC	C1'-C2'-O2'-CM2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10

There are no ring outliers.

17 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1207	2MG	2	0
25	A	2503	2MA	1	0
15	v	55	PSU	1	0
25	A	747	5MC	1	0
25	A	955	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	2030	6MZ	2	0
25	A	1917	PSU	1	0
25	A	2445	2MG	1	0
15	v	54	5MU	1	0
1	a	1498	UR3	7	0
1	a	1402	4OC	6	0
25	A	2449	H2U	1	0
25	A	1962	5MC	1	0
25	A	2552	OMU	1	0
1	a	1518	MA6	6	0
1	a	516	PSU	1	0
1	a	1519	MA6	13	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

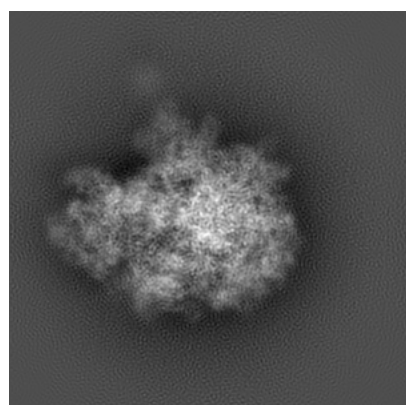
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6311. These allow visual inspection of the internal detail of the map and identification of artifacts.

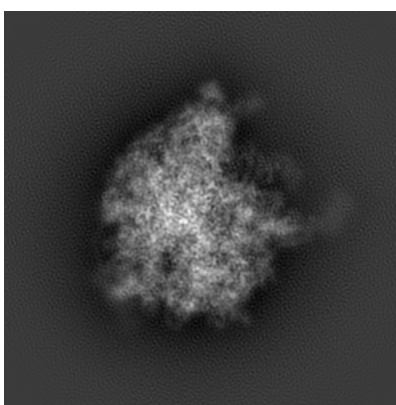
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

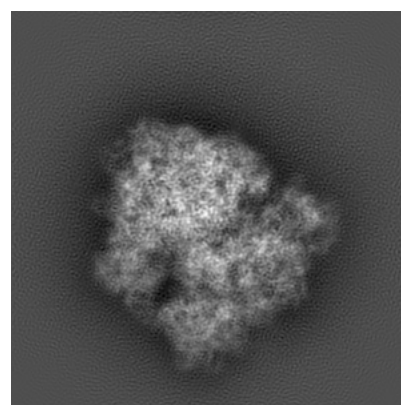
6.1.1 Primary map



X



Y

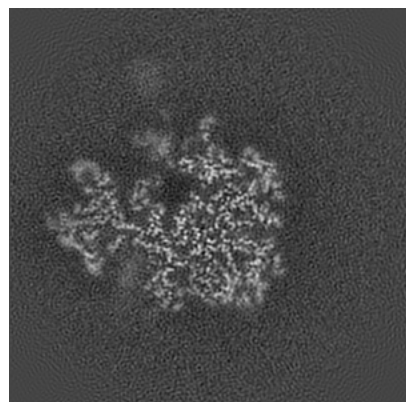


Z

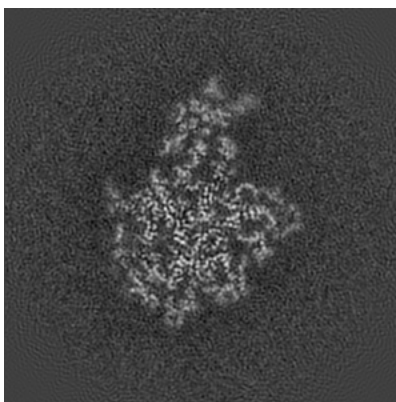
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

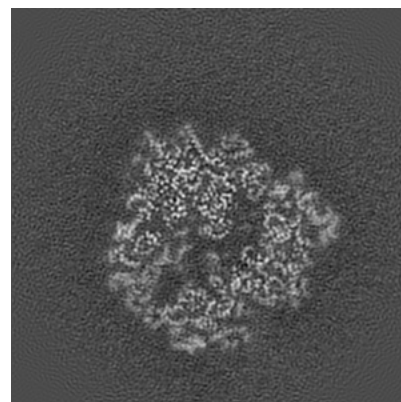
6.2.1 Primary map



X Index: 184



Y Index: 184

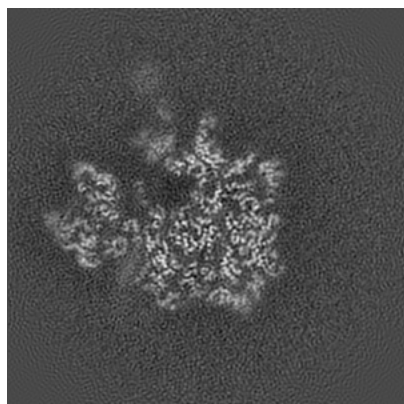


Z Index: 184

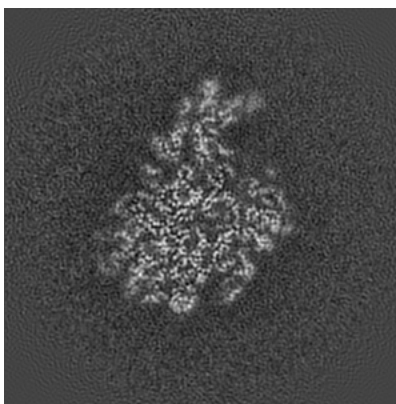
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

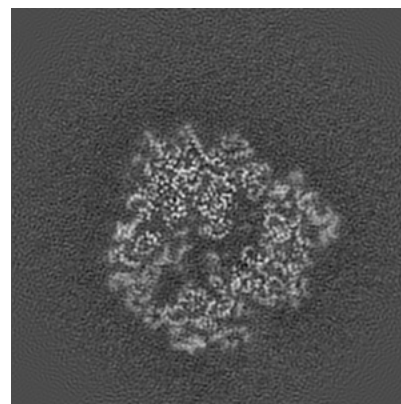
6.3.1 Primary map



X Index: 180



Y Index: 176

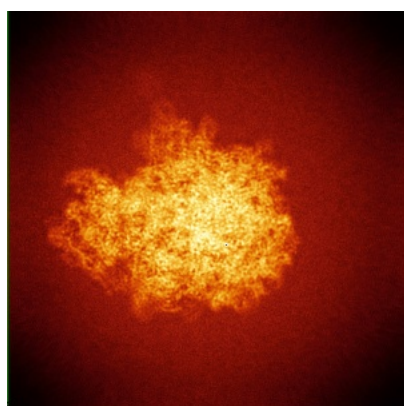


Z Index: 184

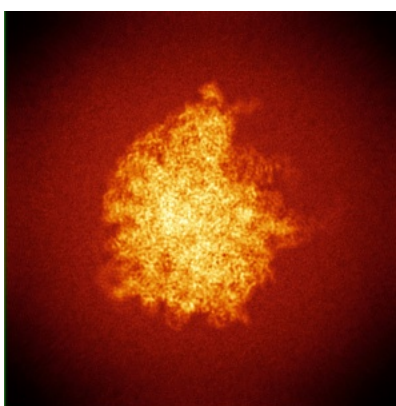
The images above show the largest variance slices of the map in three orthogonal directions.

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

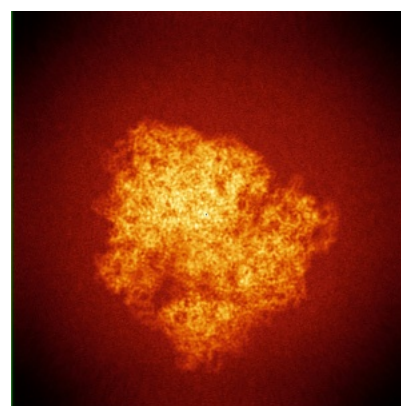
6.4.1 Primary map



X



Y

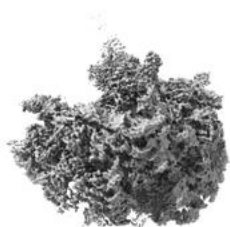


Z

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](#)

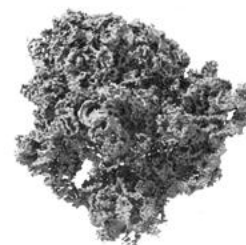
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

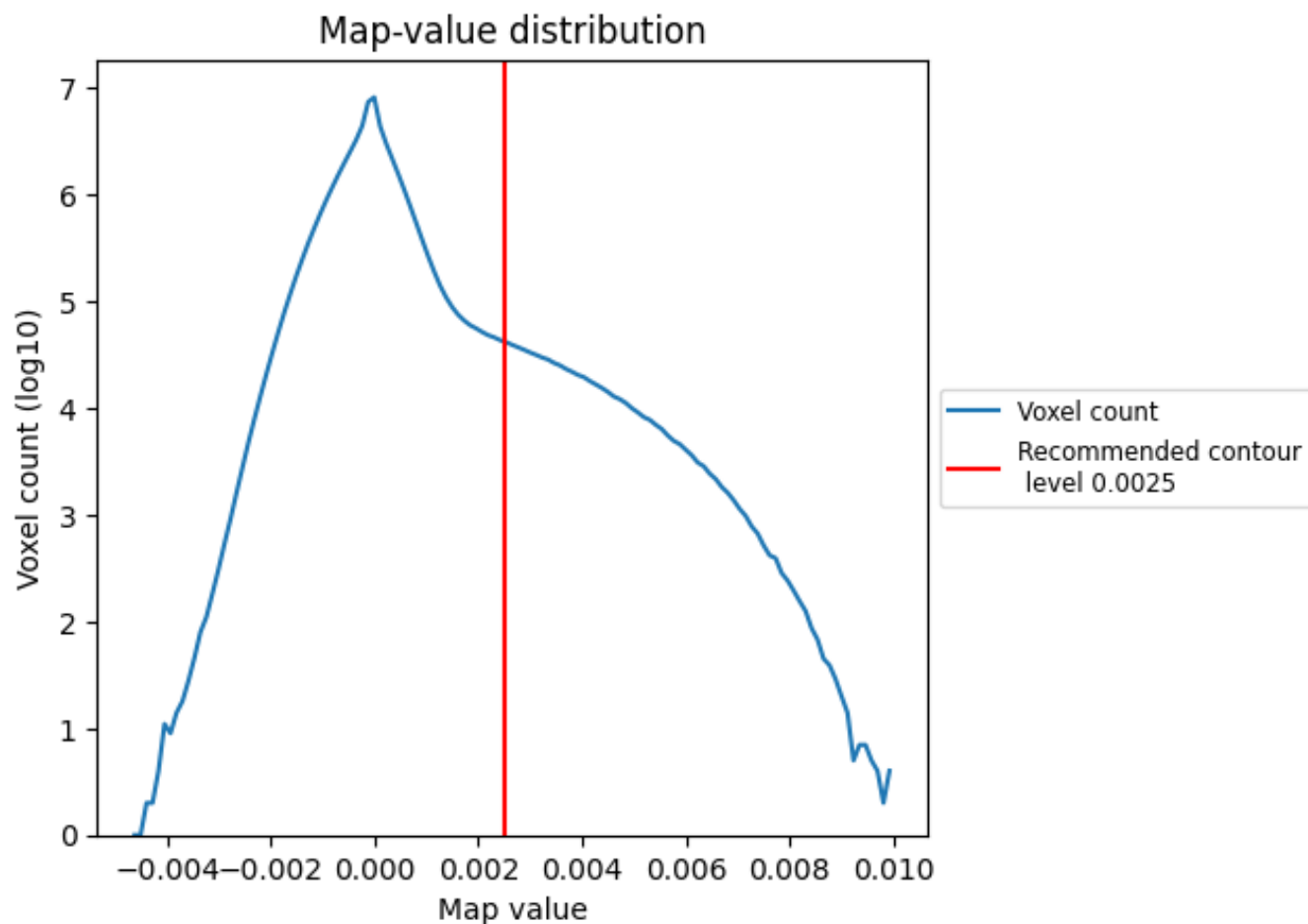
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

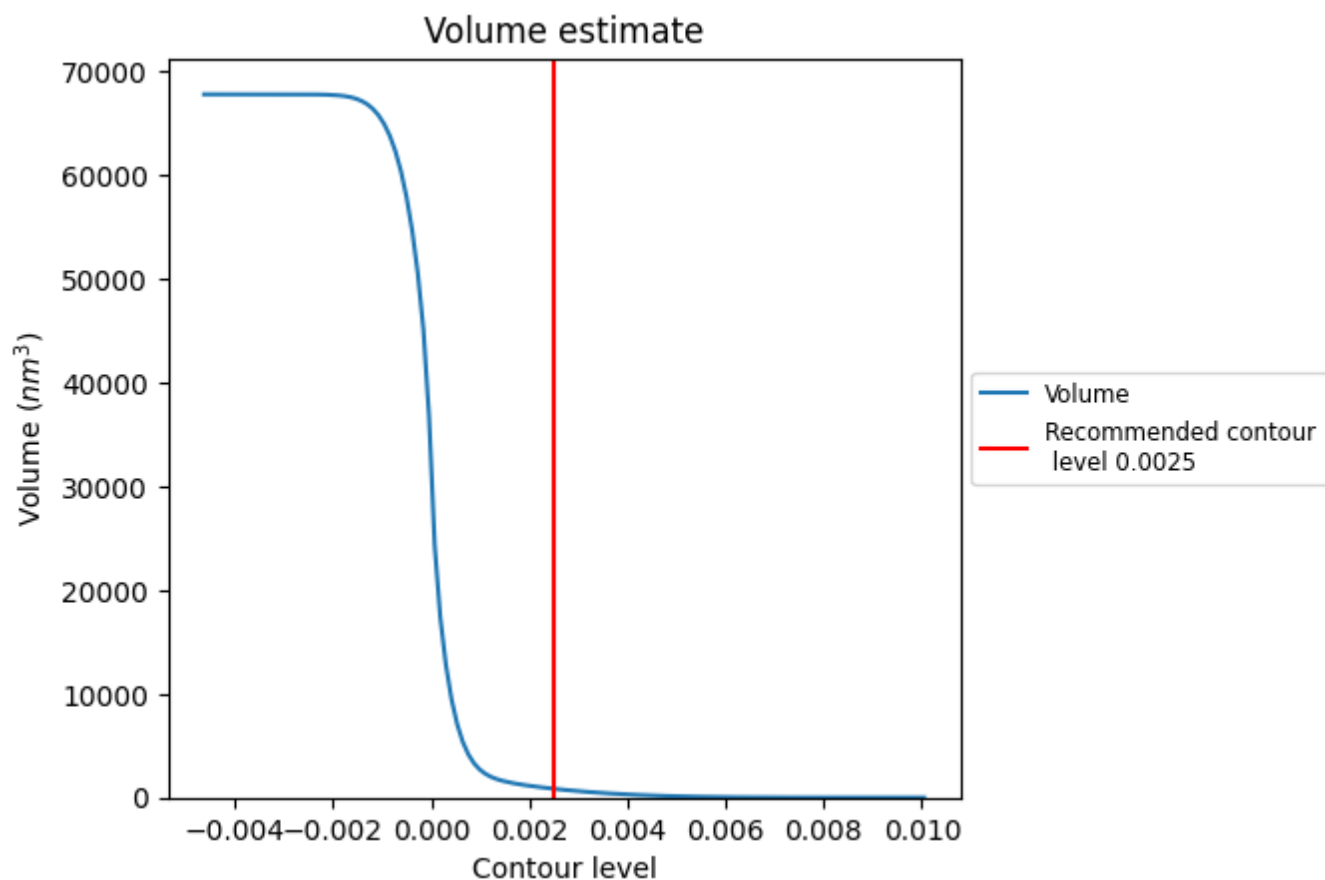
This section contains the results of statistical analysis of the map.

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.

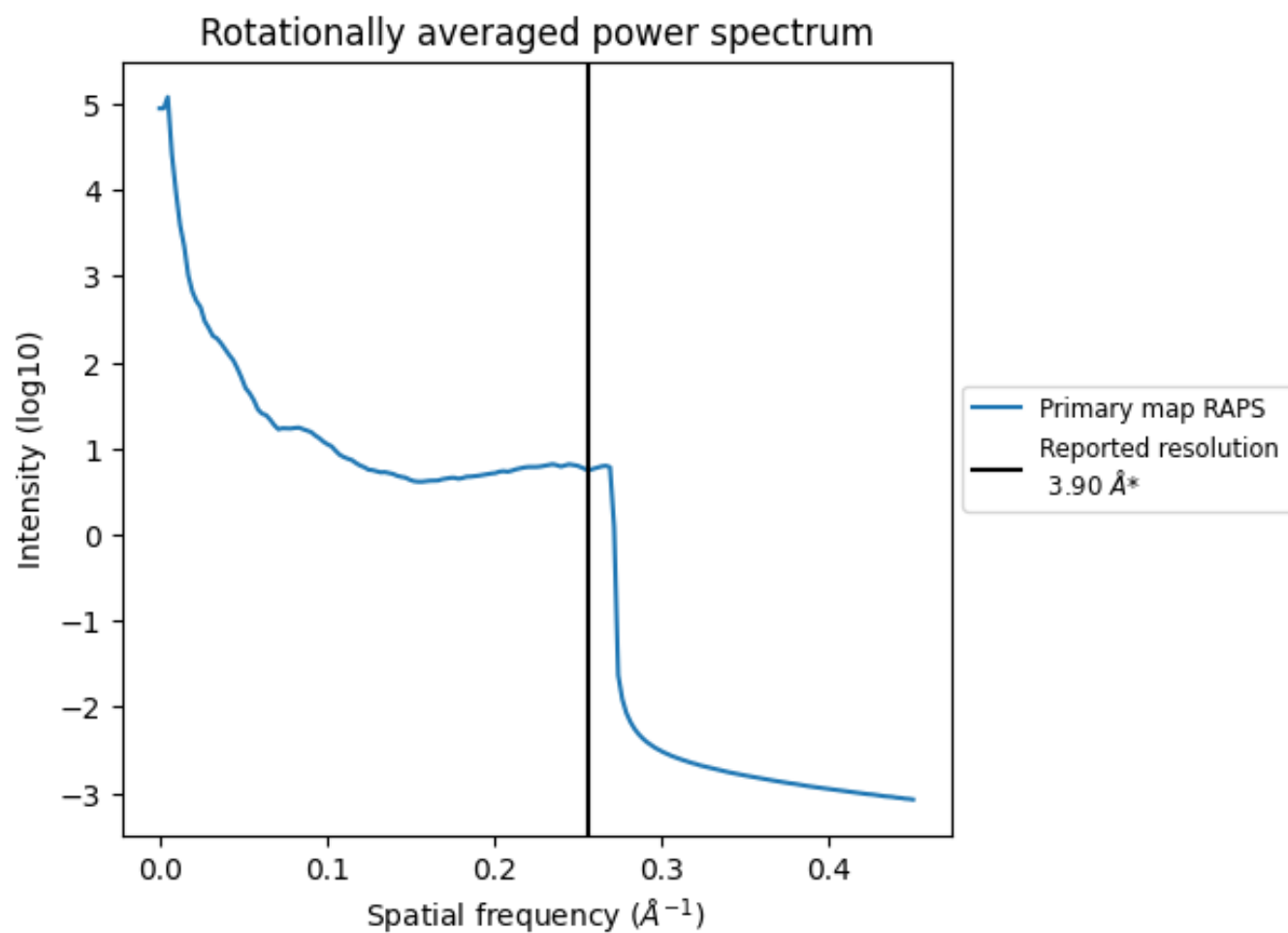
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 847 nm³; this corresponds to an approximate mass of 765 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 0.256 Å⁻¹

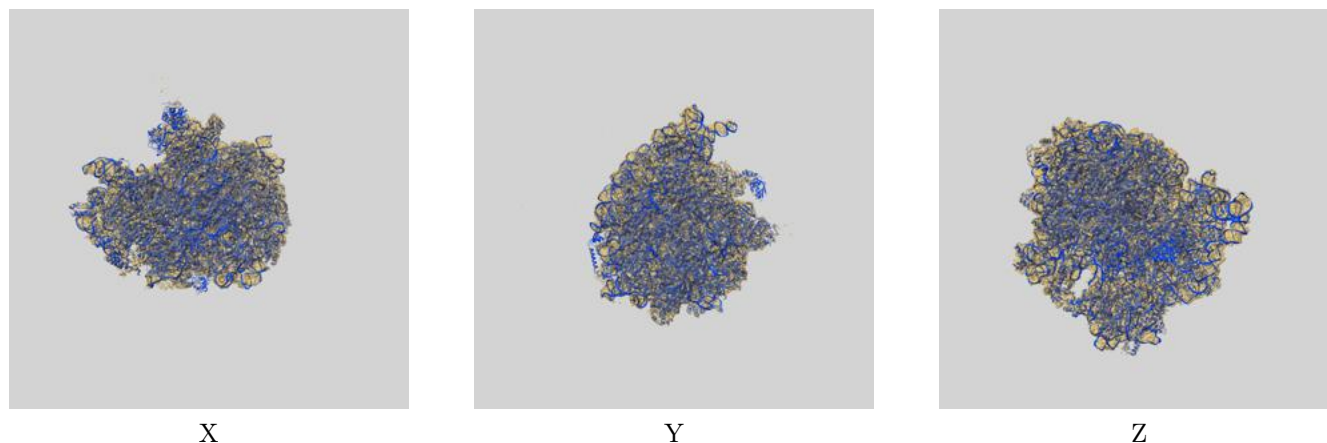
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

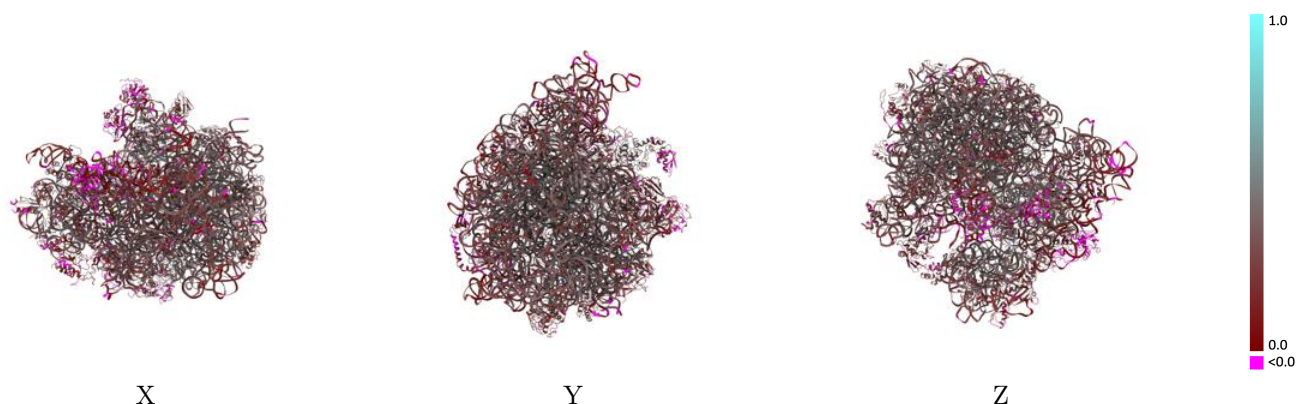
This section contains information regarding the fit between EMDB map EMD-6311 and PDB model 3J9Y. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



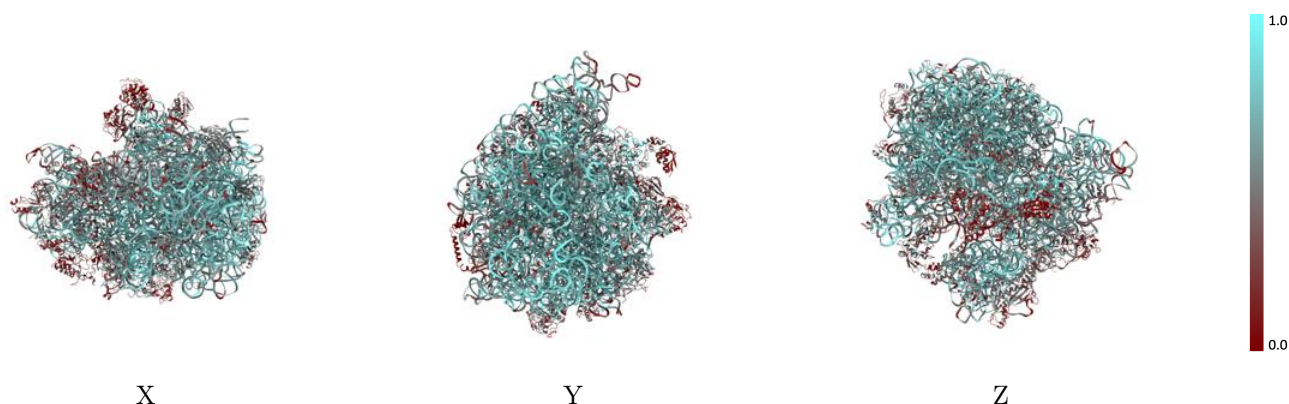
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



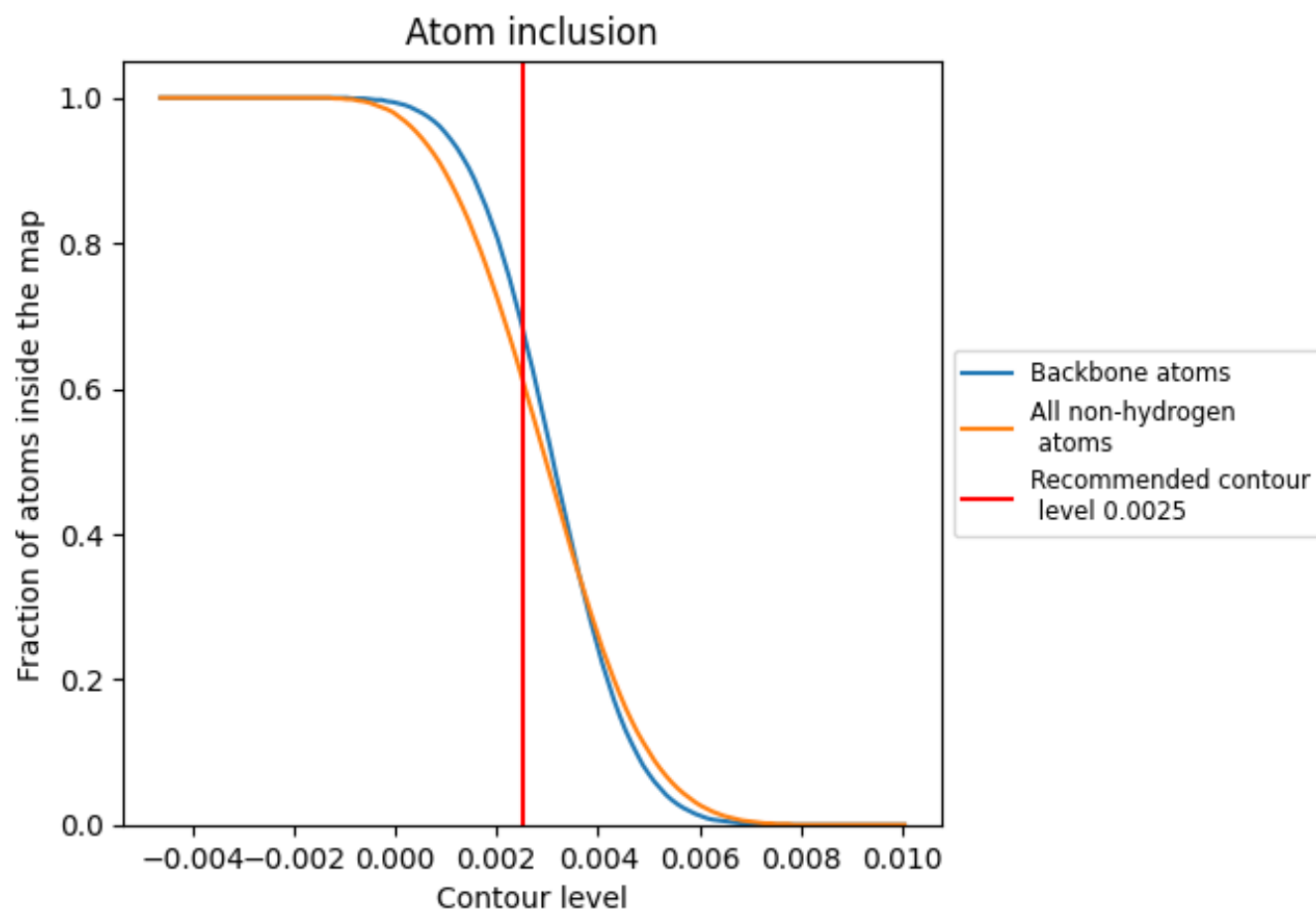
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6150	 0.3090
0	 0.5280	 0.3330
1	 0.0200	 0.2110
2	 0.5780	 0.3730
3	 0.5460	 0.3920
4	 0.5720	 0.3390
5	 0.0880	 0.0610
6	 0.2270	 0.1460
7	 0.0470	 0.0810
A	 0.7370	 0.3470
B	 0.7080	 0.3020
C	 0.5580	 0.3710
D	 0.4880	 0.3260
E	 0.4470	 0.2970
F	 0.3660	 0.2340
G	 0.3460	 0.2370
H	 0.0880	 0.1440
I	 0.0690	 0.0950
J	 0.5090	 0.3230
K	 0.4640	 0.3460
L	 0.4600	 0.3160
M	 0.4870	 0.3640
N	 0.5350	 0.3520
O	 0.4440	 0.2670
P	 0.4530	 0.3140
Q	 0.5680	 0.3550
R	 0.4450	 0.3010
S	 0.4930	 0.3260
T	 0.4270	 0.3070
U	 0.3650	 0.2580
V	 0.4340	 0.2890
W	 0.5210	 0.3530
X	 0.4920	 0.3440
Y	 0.3960	 0.2170
Z	 0.4830	 0.3330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.6890	 0.3000
b	 0.2410	 0.1730
c	 0.4090	 0.2980
d	 0.2640	 0.0730
e	 0.4230	 0.2640
f	 0.4080	 0.2110
g	 0.3330	 0.2490
h	 0.4580	 0.2970
i	 0.3890	 0.2650
j	 0.3020	 0.2490
k	 0.3500	 0.1950
l	 0.2940	 0.1340
m	 0.4230	 0.2770
n	 0.4530	 0.3180
o	 0.4840	 0.2870
p	 0.3960	 0.1970
q	 0.3830	 0.2310
r	 0.4760	 0.3050
s	 0.4330	 0.2790
t	 0.4430	 0.2380
u	 0.1390	 0.1780
v	 0.5560	 0.2840
w	 0.5710	 0.3570
x	 0.5180	 0.2760