



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:15 PM EST

PDB ID : 3J7Z  
EMDB ID : EMD-6057  
Title : Structure of the E. coli 50S subunit with ErmCL nascent chain  
Authors : Arenz, S.; Meydan, S.; Starosta, A.L.; Berninghausen, O.; Beckmann, R.;  
Vazquez-Laslop, N.; Wilson, D.N.  
Deposited on : 2014-08-27  
Resolution : 3.90 Å(reported)  
Based on initial model : 4KIX

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

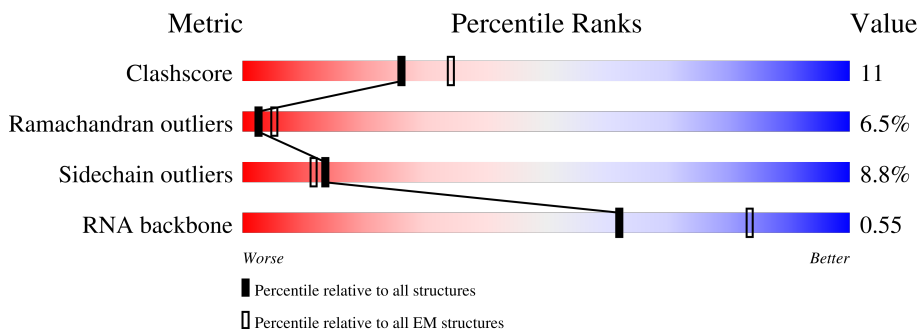
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	121	

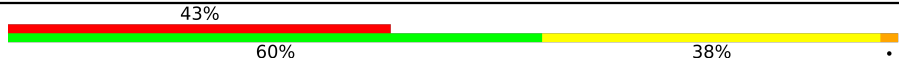


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Mol	Chain	Length	Quality of chain
8	7	3	100%
9	A	2903	9% 58% 30% 9% ..
10	B	118	20% 68% 25% 8%
11	C	273	17% 68% 27% ..
12	D	209	20% 66% 28% 5% .
13	E	201	35% 70% 25% ..
14	F	179	84% 66% 28% ...
15	G	177	41% 63% 28% 7% ..
16	H	149	24% 20% 11% . 66%
17	I	142	97% 51% 43% 6% .
18	J	142	13% 61% 29% 9% .
19	K	123	20% 54% 35% 8% ..
20	L	144	28% 70% 24% ...
21	M	136	9% 62% 30% 7% .
22	N	127	9% 62% 29% . 6%
23	O	117	38% 68% 27% ..
24	P	115	20% 66% 24% 7% ..
25	Q	118	15% 63% 31% 5% ..
26	R	103	23% 63% 34% .
27	S	110	15% 67% 25% 6% .
28	T	100	21% 55% 31% 6% . 7%
29	U	104	46% 61% 31% 6% ..
30	V	94	27% 79% 19% .
31	W	85	22% 32% 40% 20% . 7%
32	X	78	17% 71% 22% 5% ..

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Mol	Chain	Length	Quality of chain
33	Y	63	
34	Z	59	
35	a	19	

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 90700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	148	1117	705	196	209	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	30	227	144	33	47	3	0	0

- Molecule 8 is a RNA chain called P-tRNA CCA-end.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	3	58	28	11	17	2	0	0

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	2854	61274	27334	11279	19807	2854	0	0

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	118	2529	1126	464	821	118	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

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

- Molecule 18 is a protein called 50S ribosomal protein L13.

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

- Molecule 19 is a protein called 50S ribosomal protein L14.

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

- Molecule 20 is a protein called 50S ribosomal protein L15.

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

- Molecule 21 is a protein called 50S ribosomal protein L16.

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

- Molecule 22 is a protein called 50S ribosomal protein L17.

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

- Molecule 23 is a protein called 50S ribosomal protein L18.

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

- Molecule 24 is a protein called 50S ribosomal protein L19.

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

- Molecule 25 is a protein called 50S ribosomal protein L20.

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

- Molecule 26 is a protein called 50S ribosomal protein L21.

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

- Molecule 27 is a protein called 50S ribosomal protein L22.

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

- Molecule 28 is a protein called 50S ribosomal protein L23.



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

- Molecule 29 is a protein called 50S ribosomal protein L24.

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

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

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

- Molecule 33 is a protein called 50S ribosomal protein L29.

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

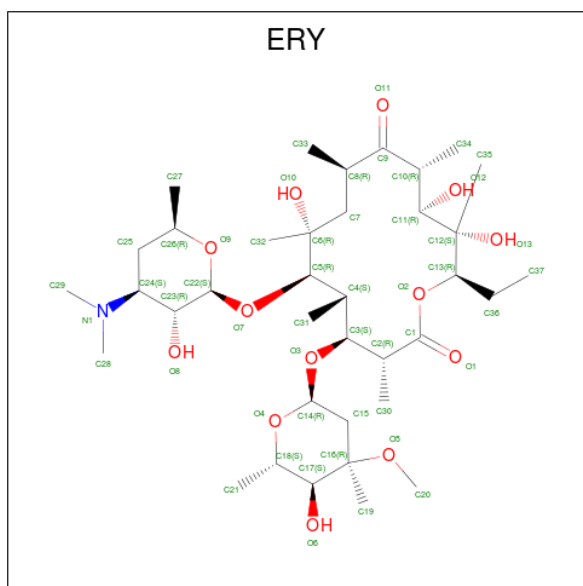
- Molecule 34 is a protein called 50S ribosomal protein L30.

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

- Molecule 35 is a protein called ErmCL nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	a	7	36	27	4	5	0	3

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).

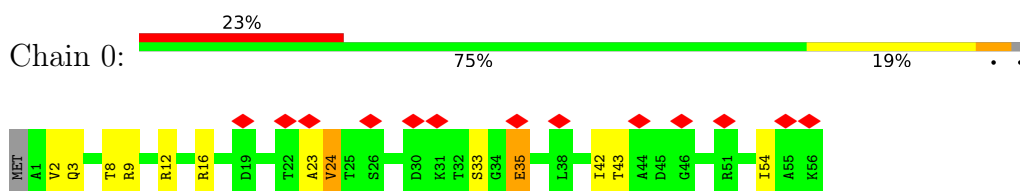


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
36	A	1	51	37	1	13	0

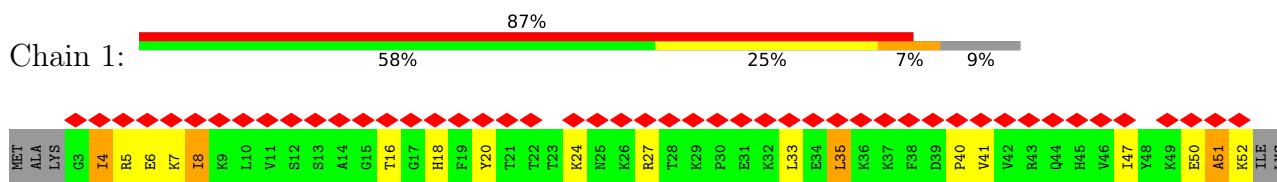
### 3 Residue-property plots [i](#)

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.

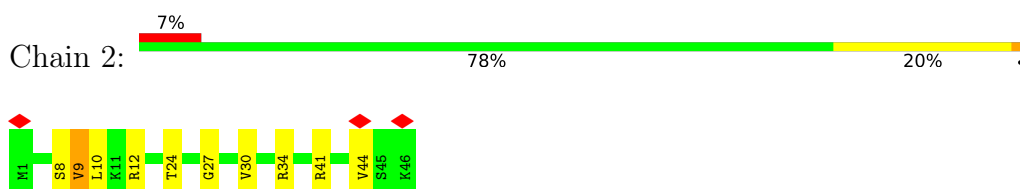
- Molecule 1: 50S ribosomal protein L32



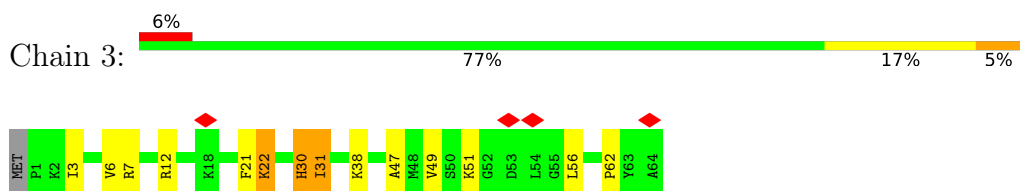
- Molecule 2: 50S ribosomal protein L33



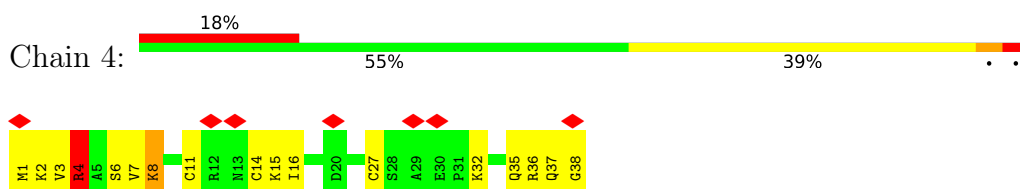
- Molecule 3: 50S ribosomal protein L34



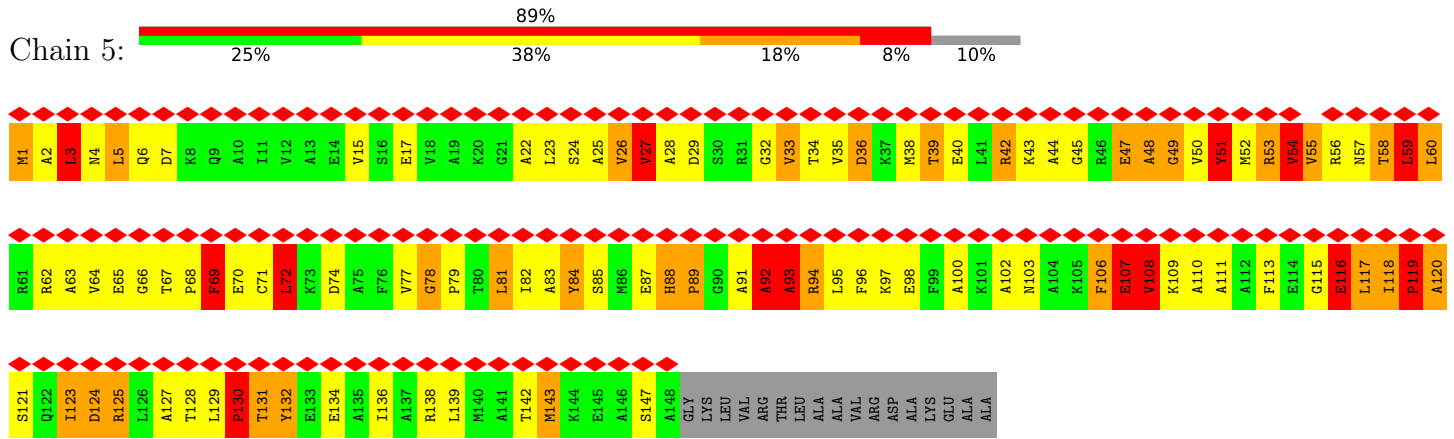
- Molecule 4: 50S ribosomal protein L35



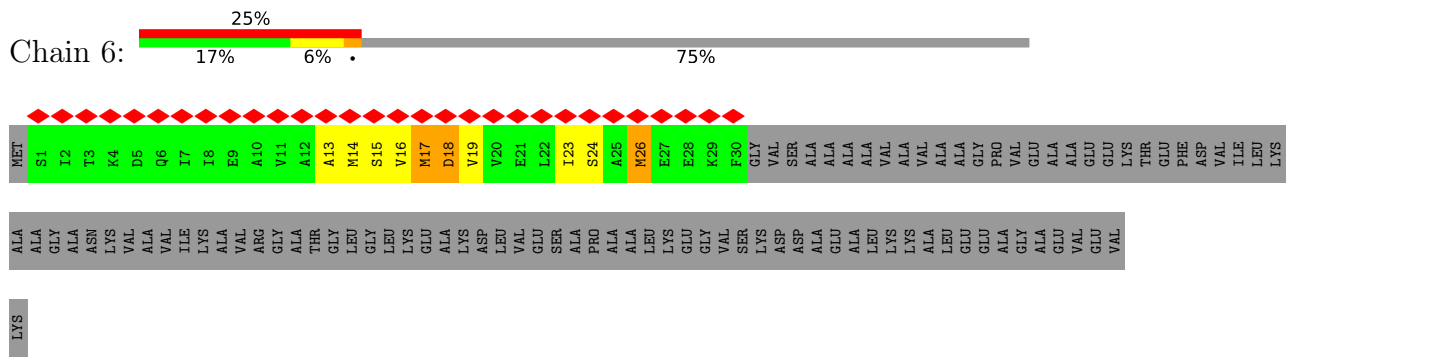
- Molecule 5: 50S ribosomal protein L36



• Molecule 6: 50S ribosomal protein L10



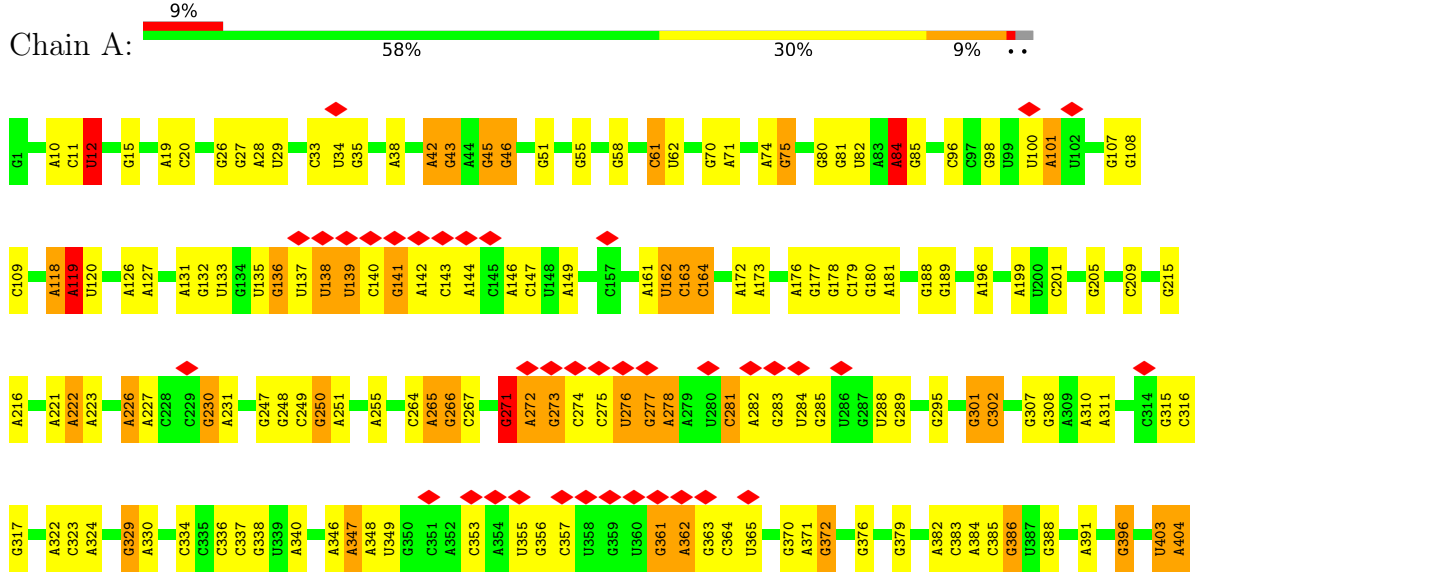
• Molecule 7: 50S ribosomal protein L7/L12

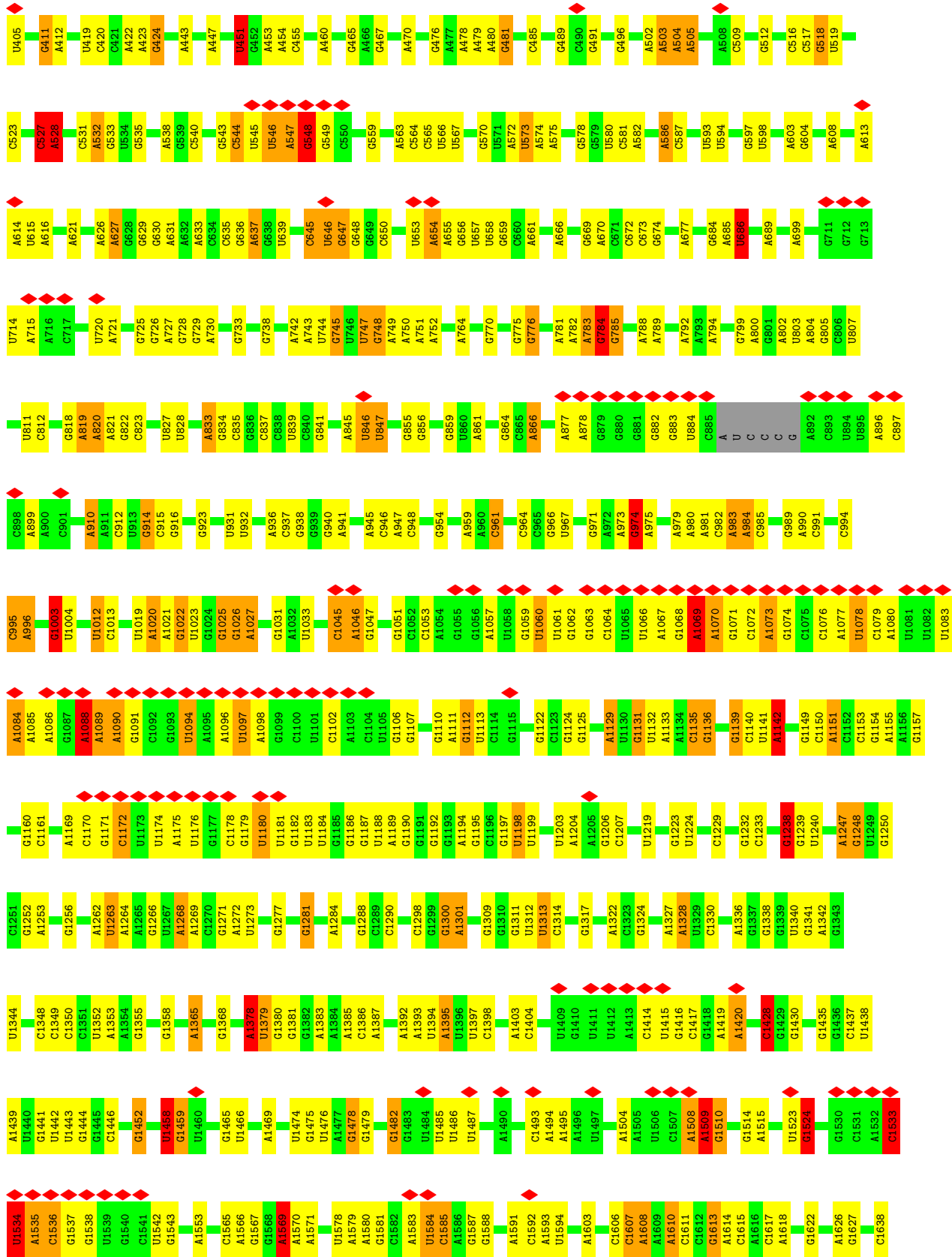


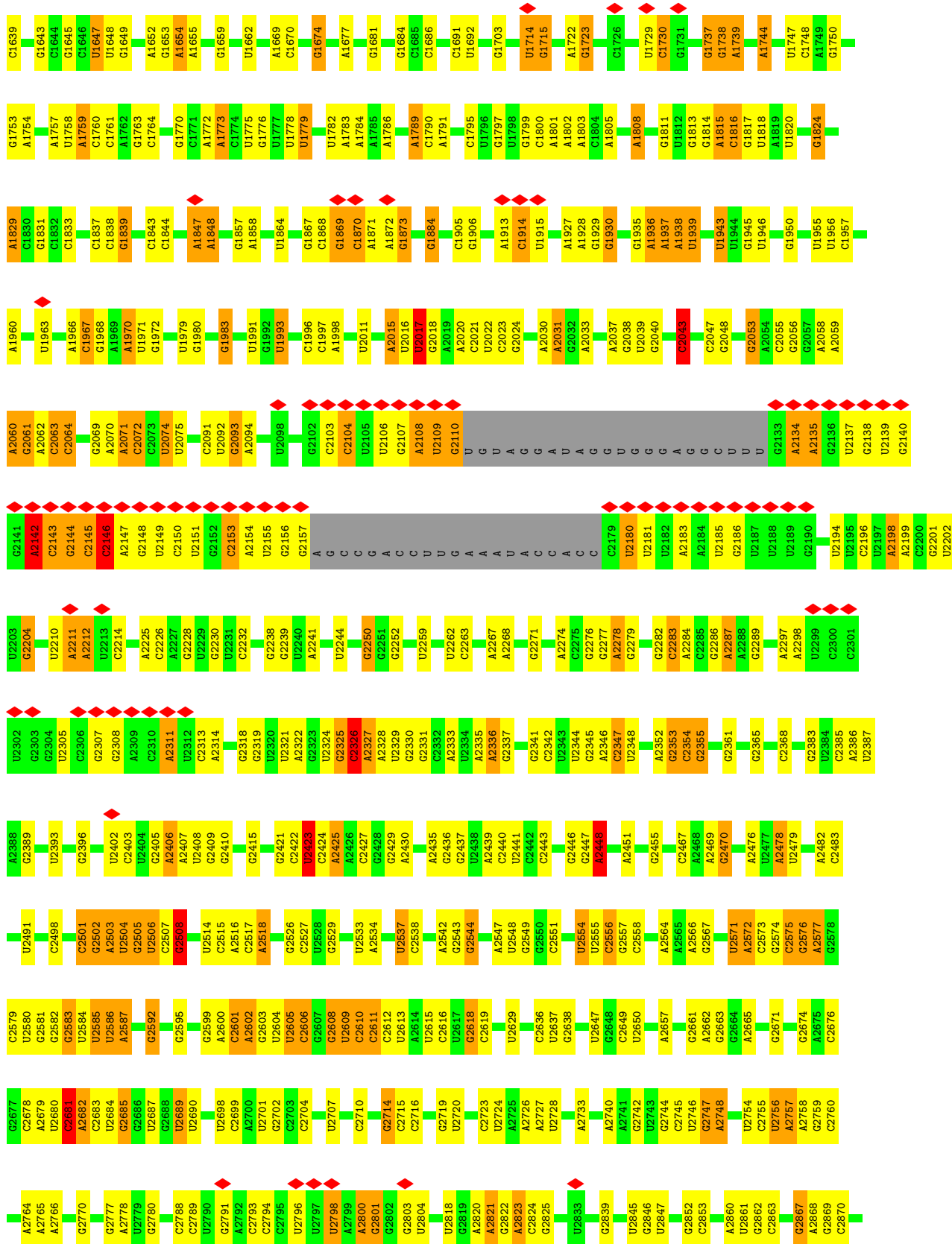
• Molecule 8: P-tRNA CCA-end

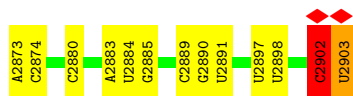


• Molecule 9: 23S rRNA

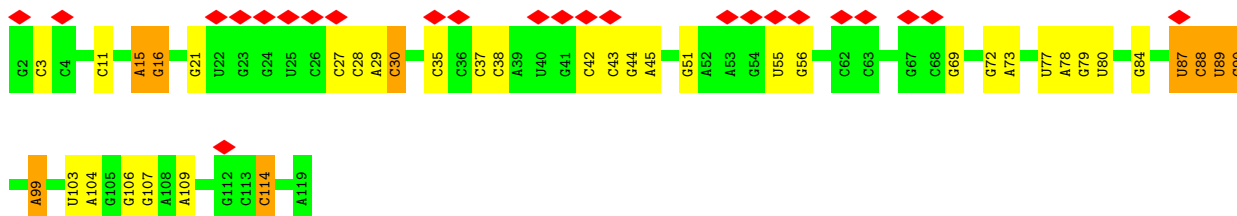




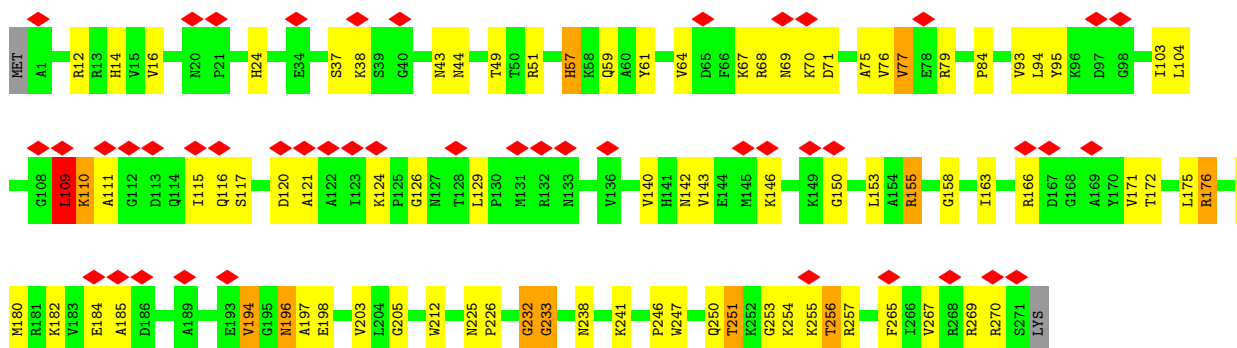




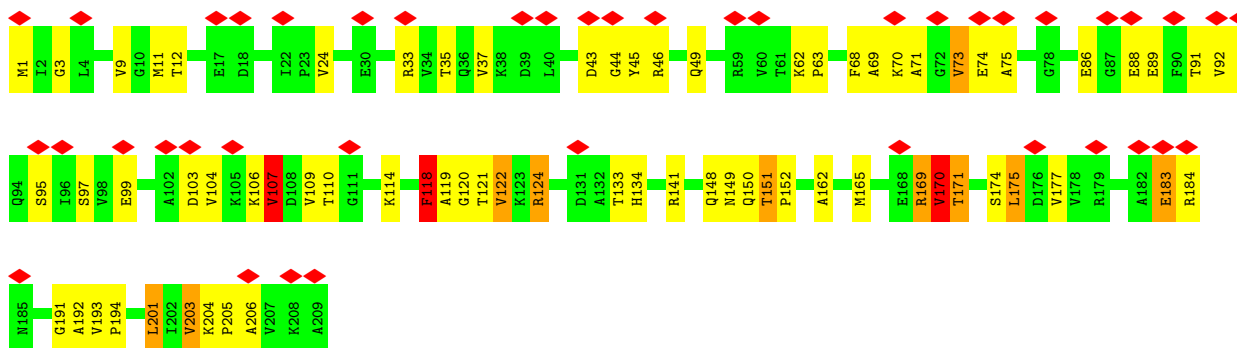
• Molecule 10: 5S rRNA



• Molecule 11: 50S ribosomal protein L2

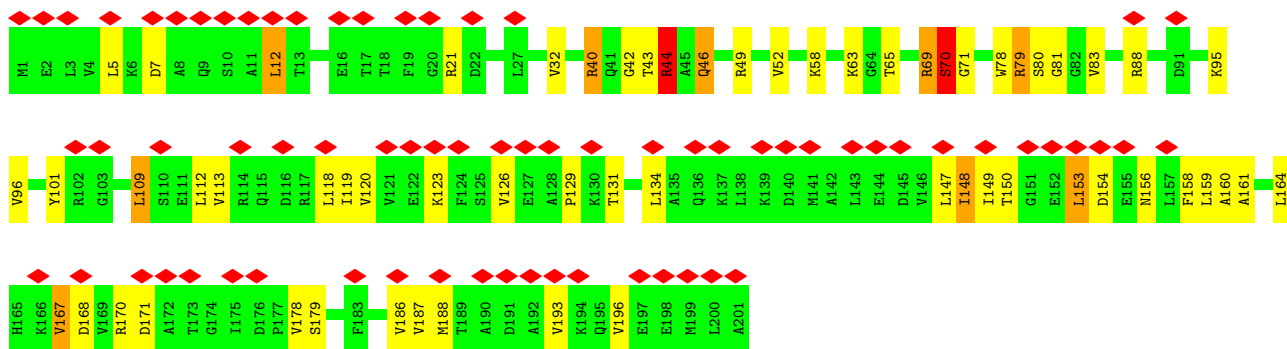


• Molecule 12: 50S ribosomal protein L3

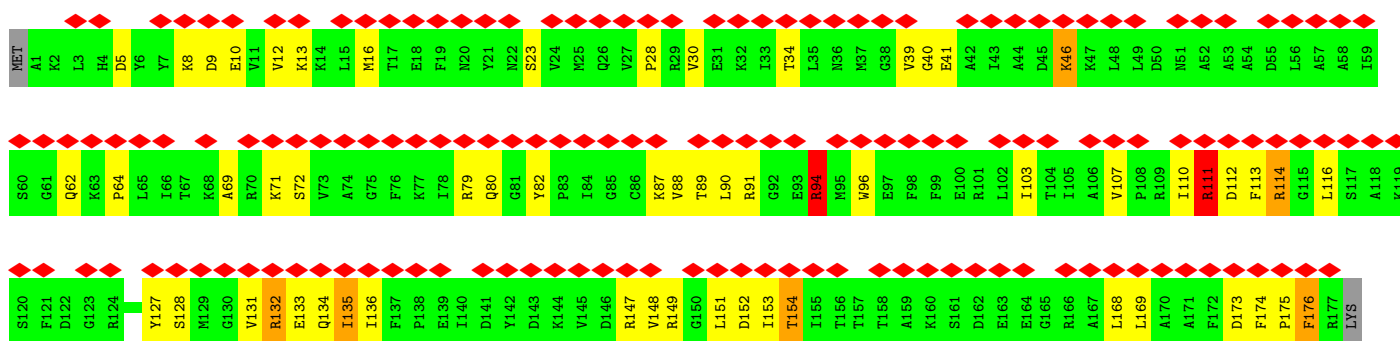
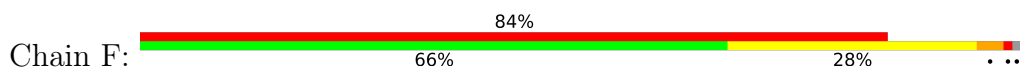


• Molecule 13: 50S ribosomal protein L4

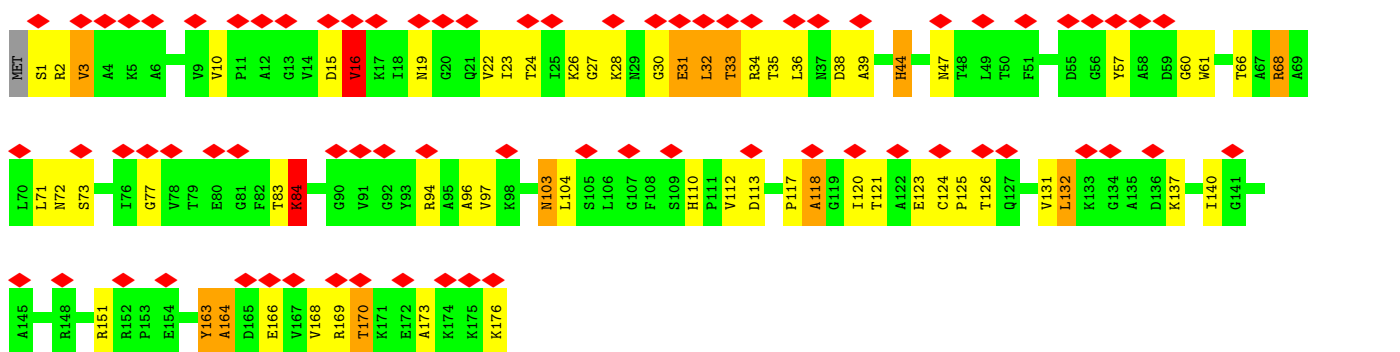
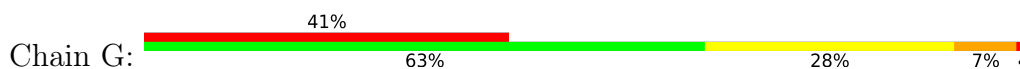




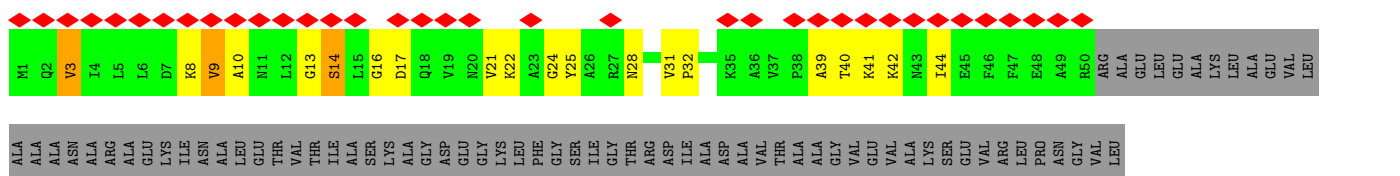
• Molecule 14: 50S ribosomal protein L5



• Molecule 15: 50S ribosomal protein L6



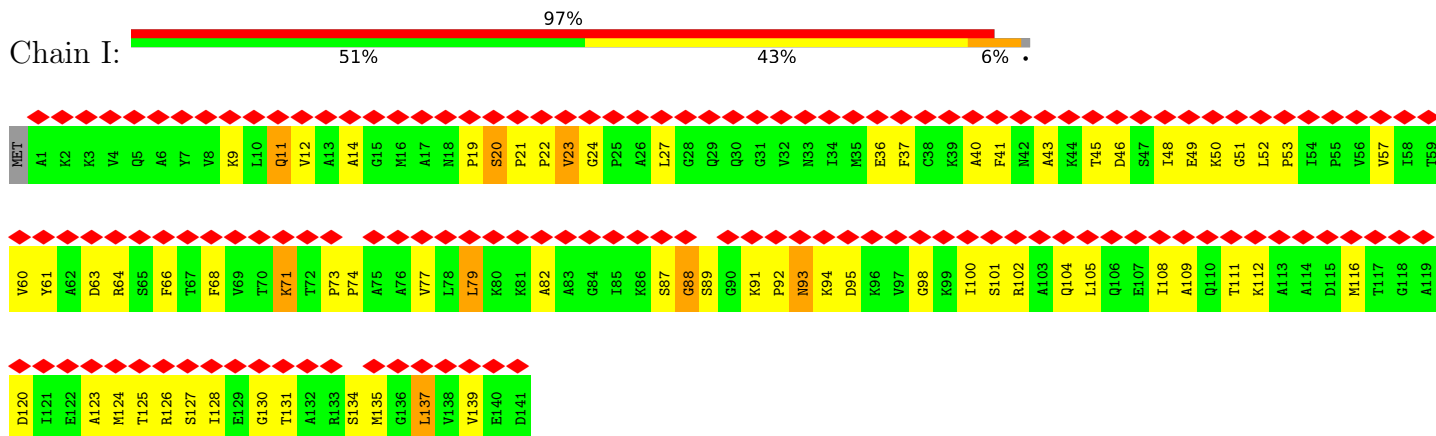
• Molecule 16: 50S ribosomal protein L9



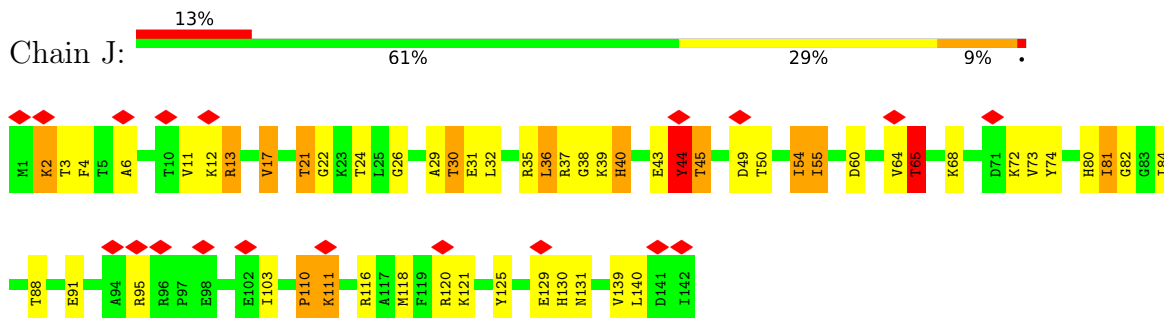


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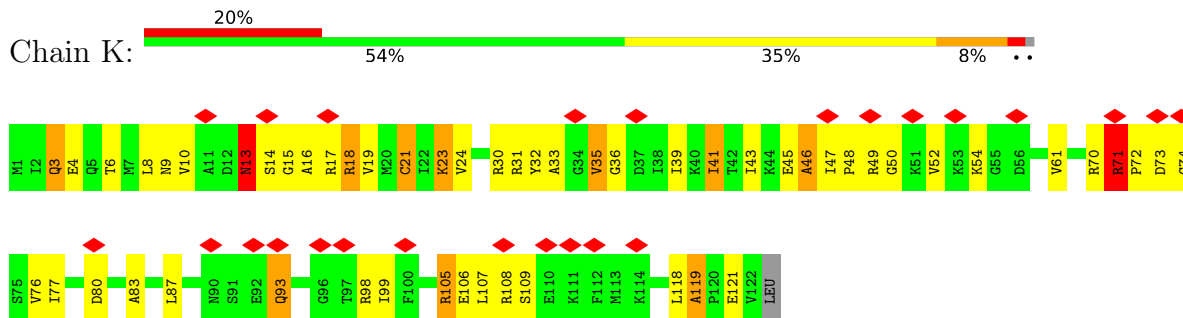
• Molecule 17: 50S ribosomal protein L11



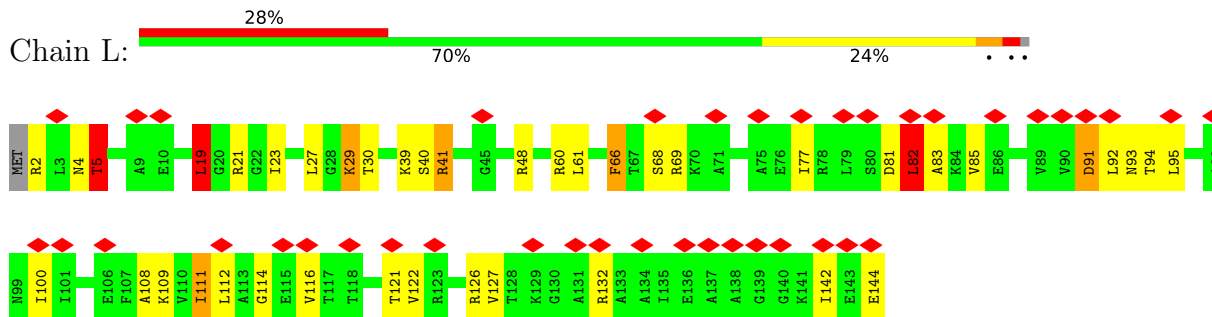
• Molecule 18: 50S ribosomal protein L13



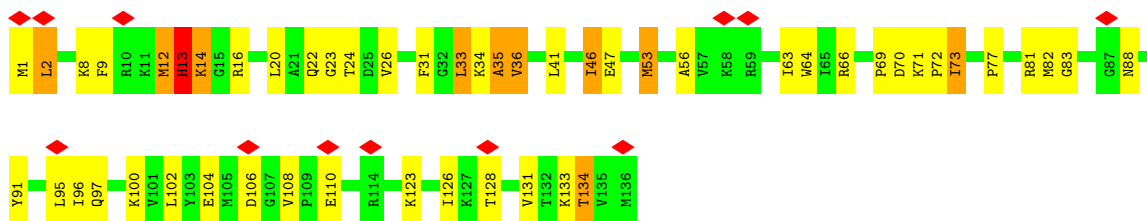
• Molecule 19: 50S ribosomal protein L14



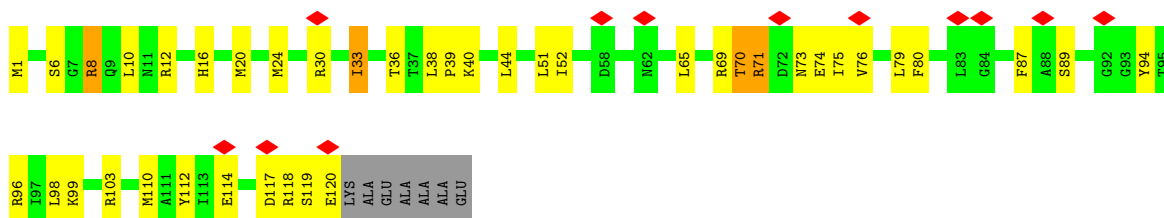
• Molecule 20: 50S ribosomal protein L15



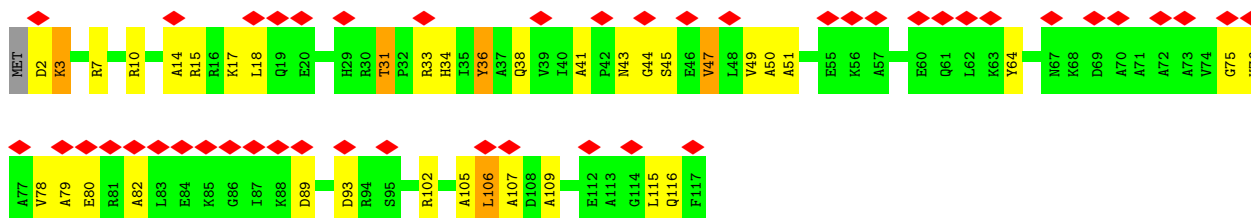
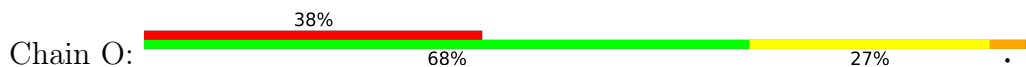
• Molecule 21: 50S ribosomal protein L16



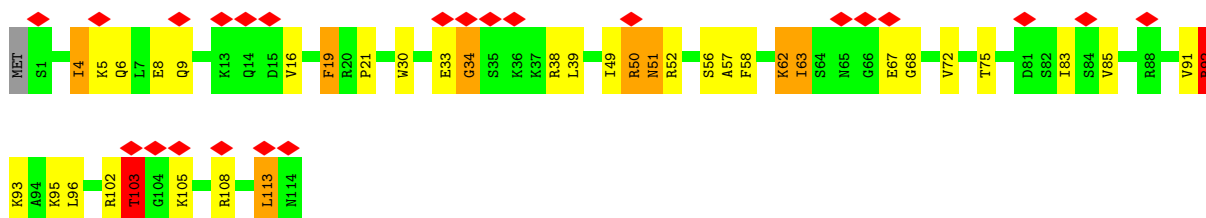
• Molecule 22: 50S ribosomal protein L17



• Molecule 23: 50S ribosomal protein L18

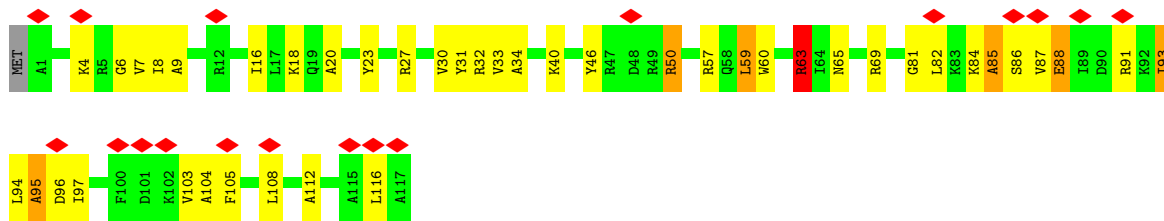


• Molecule 24: 50S ribosomal protein L19

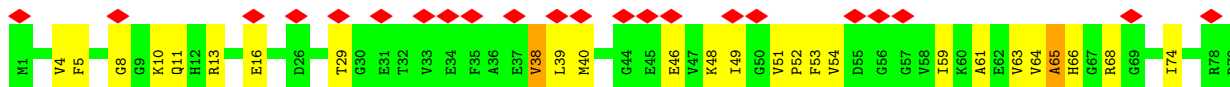


• Molecule 25: 50S ribosomal protein L20

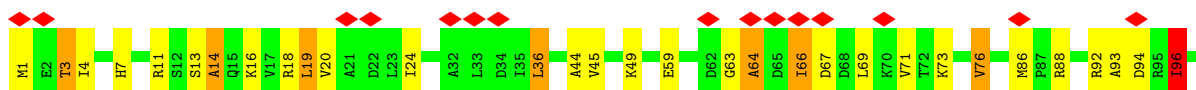




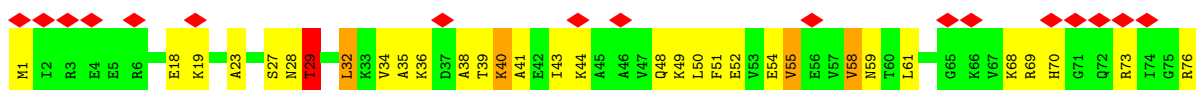
• Molecule 26: 50S ribosomal protein L21



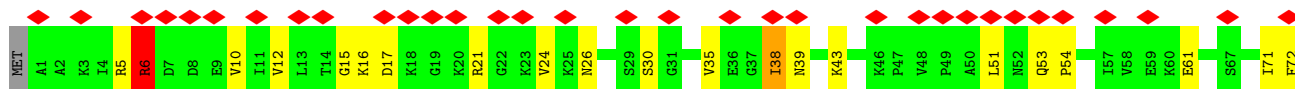
• Molecule 27: 50S ribosomal protein L22



• Molecule 28: 50S ribosomal protein L23

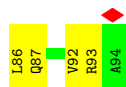
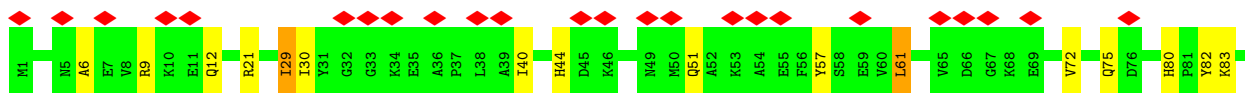
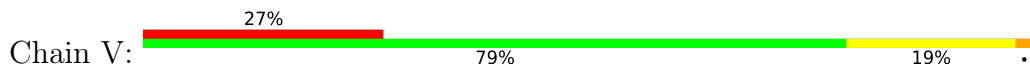


• Molecule 29: 50S ribosomal protein L24

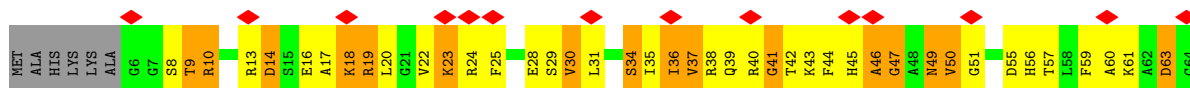




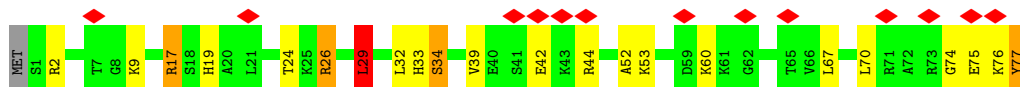
• Molecule 30: 50S ribosomal protein L25



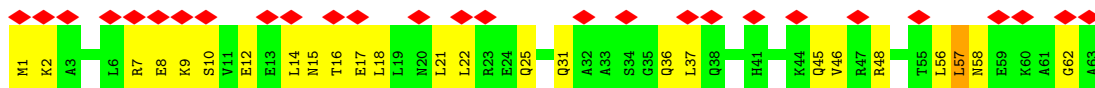
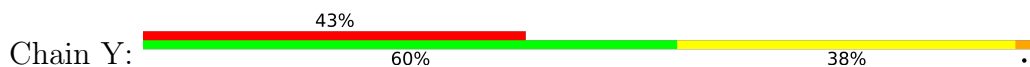
• Molecule 31: 50S ribosomal protein L27



• Molecule 32: 50S ribosomal protein L28



• Molecule 33: 50S ribosomal protein L29



• Molecule 34: 50S ribosomal protein L30



• Molecule 35: ErmCL nascent chain



MET	GLY	178	SER	184	THR	VAL	HIS	TYR	GLN	PRO	ASN	LYS	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269163	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 ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ( $\text{\AA}$ )	196.11601, 202.764, 255.94801	wwPDB
Map dimensions	177, 183, 231	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: ERY

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	0	0.54	0/450	0.70	0/599
2	1	0.53	0/416	0.74	0/554
3	2	0.53	0/380	0.70	0/498
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)
7	6	0.59	0/227	0.65	0/304
8	7	0.16	0/64	0.54	0/97
9	A	0.80	15/68626 (0.0%)	1.22	301/107056 (0.3%)
10	B	0.66	0/2828	1.10	2/4410 (0.0%)
11	C	0.54	0/2121	0.79	3/2852 (0.1%)
12	D	0.57	0/1586	0.77	1/2134 (0.0%)
13	E	0.53	0/1571	0.76	2/2113 (0.1%)
14	F	0.50	0/1434	0.71	1/1926 (0.1%)
15	G	0.55	0/1343	0.73	0/1816
16	H	0.53	0/389	0.73	0/523
17	I	0.62	0/1046	0.84	1/1410 (0.1%)
18	J	0.63	1/1152 (0.1%)	0.78	0/1551
19	K	0.65	1/947 (0.1%)	0.77	0/1268
20	L	0.56	0/1054	0.79	2/1403 (0.1%)
21	M	0.61	0/1093	0.77	0/1460
22	N	0.51	0/973	0.68	0/1301
23	O	0.46	0/902	0.70	0/1209
24	P	0.52	0/929	0.78	1/1242 (0.1%)
25	Q	0.62	0/960	0.71	1/1278 (0.1%)
26	R	0.61	1/829 (0.1%)	0.76	0/1107
27	S	0.54	0/864	0.73	0/1156
28	T	0.55	0/744	0.85	1/994 (0.1%)
29	U	0.56	0/787	0.78	0/1051
30	V	0.48	0/766	0.67	1/1025 (0.1%)
31	W	0.69	0/603	1.00	1/797 (0.1%)
32	X	0.50	0/635	0.79	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Y	0.46	0/510	0.75	0/677
34	Z	0.54	0/453	0.84	1/605 (0.2%)
35	a	0.86	0/32	1.43	1/40 (2.5%)
All	All	0.74	18/98661 (0.0%)	1.12	347/147901 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	5	0	1
11	C	0	1
12	D	0	1
18	J	0	1
19	K	0	1
All	All	0	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	984	A	N9-C4	-8.36	1.32	1.37
9	A	528	A	N9-C4	-6.60	1.33	1.37
9	A	1142	A	N9-C4	-6.51	1.33	1.37
9	A	783	A	N9-C4	-6.27	1.34	1.37
9	A	1569	A	N9-C4	-6.16	1.34	1.37

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1073	A	N1-C6-N6	-20.00	106.60	118.60
9	A	1073	A	C5-C6-N6	14.06	134.95	123.70
9	A	2053	G	N1-C6-O6	13.89	128.23	119.90
9	A	984	A	C2-N3-C4	-12.15	104.53	110.60
9	A	961	C	O5'-P-OP2	-11.75	95.12	105.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide

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Mol	Chain	Res	Type	Group
11	C	233	GLY	Peptide
12	D	9	VAL	Peptide
18	J	110	PRO	Peptide
19	K	71	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	16	0
2	1	409	0	440	15	0
3	2	377	0	418	5	0
4	3	504	0	574	10	0
5	4	302	0	340	14	0
6	5	1117	0	1155	123	0
7	6	227	0	237	6	0
8	7	58	0	33	12	0
9	A	61274	0	30817	801	0
10	B	2529	0	1281	20	0
11	C	2082	0	2157	54	0
12	D	1565	0	1616	52	0
13	E	1552	0	1619	40	0
14	F	1410	0	1447	44	0
15	G	1323	0	1374	37	0
16	H	384	0	405	12	0
17	I	1032	0	1088	53	0
18	J	1129	0	1162	50	0
19	K	938	0	1012	40	0
20	L	1045	0	1117	37	0
21	M	1074	0	1157	29	0
22	N	960	0	1000	30	0
23	O	892	0	923	21	0
24	P	917	0	965	38	0
25	Q	947	0	1022	52	0
26	R	816	0	839	35	0
27	S	857	0	922	28	0
28	T	738	0	807	33	0
29	U	779	0	834	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	753	0	780	12	0
31	W	596	0	610	80	0
32	X	625	0	655	18	0
33	Y	509	0	543	13	0
34	Z	449	0	491	15	0
35	a	36	0	34	0	0
36	A	51	0	67	8	0
All	All	90700	0	60402	1640	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1640 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)
9:A:912:C:OP1	21:M:8:LYS:NZ	1.79	1.15
9:A:2062:A:N6	36:A:9000:ERY:H273	1.64	1.13
9:A:2061:G:OP2	13:E:63:LYS:NZ	1.88	1.06
6:5:71:CYS:HB3	6:5:117:LEU:HD12	1.33	1.04
9:A:2579:C:H2'	9:A:2580:U:H5'	1.40	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	16
2	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	19
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	14
6	5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	2
7	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3	29
11	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	21
12	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	18
13	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2	23
14	F	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	6	38
15	G	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	0	10
16	H	48/149 (32%)	29 (60%)	14 (29%)	5 (10%)	0	9
17	I	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	19
18	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	19
19	K	120/123 (98%)	95 (79%)	15 (12%)	10 (8%)	1	14
20	L	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3	30
21	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	14
22	N	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	19	57
23	O	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	17	54
24	P	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	15
25	Q	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	30
26	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4	33
27	S	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	25
28	T	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	8
29	U	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	10
30	V	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
31	W	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	2
32	X	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	3	27
33	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	19
34	Z	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	3	29
35	a	1/19 (5%)	1 (100%)	0	0	100	100
All	All	3385/3714 (91%)	2613 (77%)	553 (16%)	219 (6%)	2	19

5 of 219 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	47/48 (98%)	46 (98%)	1 (2%)	53 73
2	1	45/49 (92%)	42 (93%)	3 (7%)	16 46
3	2	38/38 (100%)	35 (92%)	3 (8%)	12 41
4	3	51/52 (98%)	46 (90%)	5 (10%)	8 31
5	4	34/34 (100%)	31 (91%)	3 (9%)	10 37
6	5	112/123 (91%)	93 (83%)	19 (17%)	2 14
7	6	26/85 (31%)	22 (85%)	4 (15%)	2 17
11	C	216/218 (99%)	202 (94%)	14 (6%)	17 46
12	D	164/164 (100%)	151 (92%)	13 (8%)	12 41
13	E	165/165 (100%)	146 (88%)	19 (12%)	5 26
14	F	148/150 (99%)	138 (93%)	10 (7%)	16 45
15	G	137/138 (99%)	122 (89%)	15 (11%)	6 28
16	H	40/114 (35%)	39 (98%)	1 (2%)	47 69
17	I	109/110 (99%)	105 (96%)	4 (4%)	34 60
18	J	116/116 (100%)	100 (86%)	16 (14%)	3 21
19	K	103/104 (99%)	92 (89%)	11 (11%)	6 29
20	L	102/103 (99%)	95 (93%)	7 (7%)	15 45
21	M	109/109 (100%)	93 (85%)	16 (15%)	3 19
22	N	100/103 (97%)	93 (93%)	7 (7%)	15 44
23	O	86/87 (99%)	78 (91%)	8 (9%)	9 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	P	99/100 (99%)	91 (92%)	8 (8%)	11	40
25	Q	89/90 (99%)	81 (91%)	8 (9%)	9	36
26	R	84/84 (100%)	78 (93%)	6 (7%)	14	44
27	S	93/93 (100%)	84 (90%)	9 (10%)	8	32
28	T	80/84 (95%)	77 (96%)	3 (4%)	33	59
29	U	83/85 (98%)	76 (92%)	7 (8%)	11	39
30	V	78/78 (100%)	75 (96%)	3 (4%)	33	59
31	W	59/63 (94%)	53 (90%)	6 (10%)	7	30
32	X	67/68 (98%)	61 (91%)	6 (9%)	9	36
33	Y	55/55 (100%)	52 (94%)	3 (6%)	21	51
34	Z	48/49 (98%)	40 (83%)	8 (17%)	2	15
35	a	4/18 (22%)	4 (100%)	0	100	100
All	All	2787/2977 (94%)	2541 (91%)	246 (9%)	13	37

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	J	17	VAL
30	V	61	LEU
20	L	82	LEU
29	U	92	VAL
33	Y	16	THR

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

Mol	Chain	Res	Type
30	V	44	HIS
30	V	80	HIS
33	Y	41	HIS
14	F	26	GLN
4	3	30	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	117/118 (99%)	17 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	7	1/3 (33%)	0	0
9	A	2850/2903 (98%)	466 (16%)	43 (1%)
All	All	2968/3024 (98%)	483 (16%)	43 (1%)

5 of 483 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	12	U
9	A	15	G
9	A	34	U
9	A	35	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1847	A
9	A	2326	C
9	A	1870	C
9	A	2142	A
9	A	2503	A

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
36	ERY	A	9000	-	53,53,53	0.79	1 (1%)	82,82,82	1.66	19 (23%)

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
36	ERY	A	9000	-	-	7/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.32	1.59	1.55

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C25-C24-C23	-5.02	102.73	109.97
36	A	9000	ERY	O7-C5-C6	-4.80	100.47	106.39
36	A	9000	ERY	O2-C1-O1	-3.59	117.24	123.94
36	A	9000	ERY	C3-C2-C1	-3.46	102.94	110.01
36	A	9000	ERY	C27-C26-C25	-3.15	108.46	113.40

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

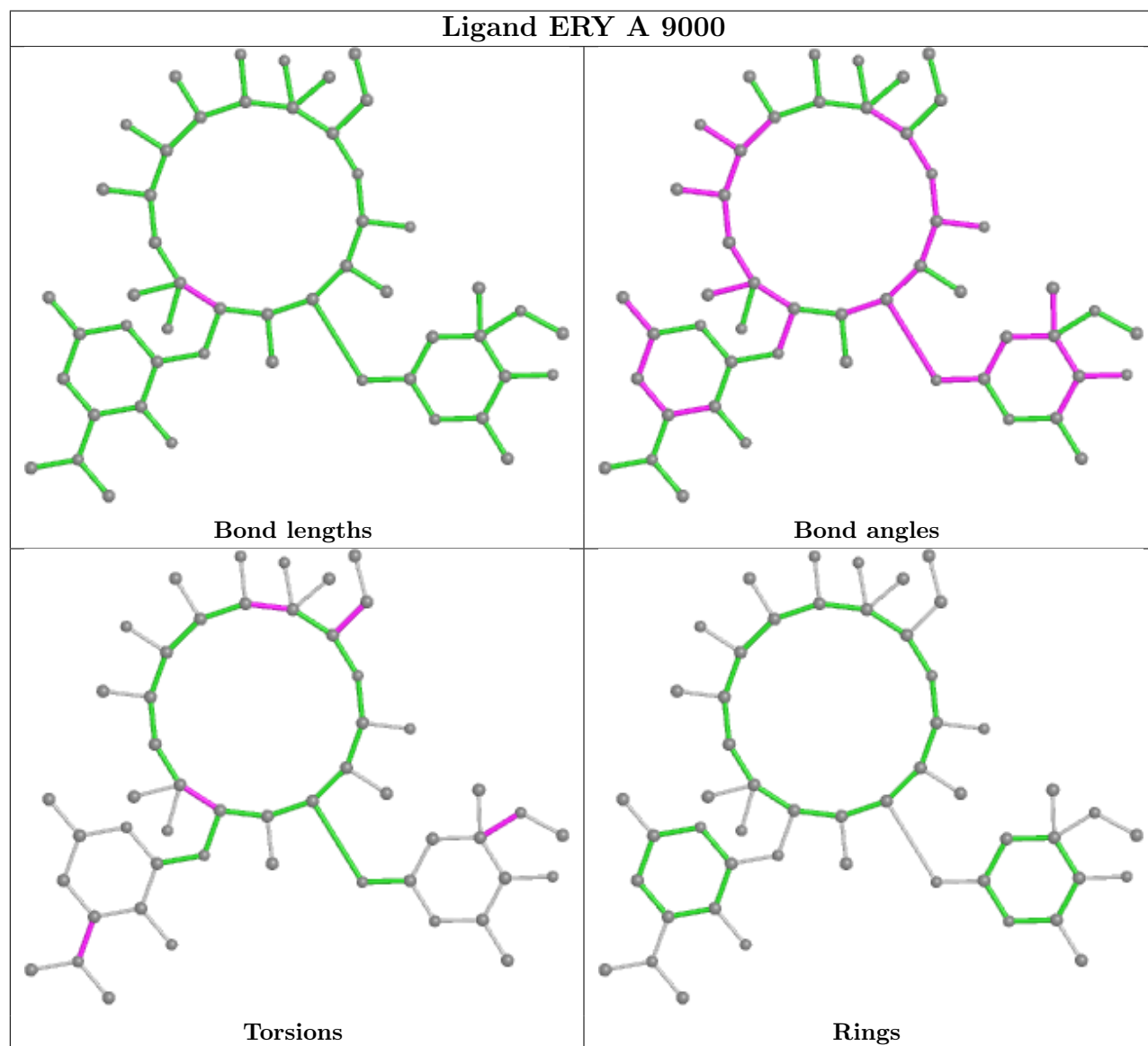
Mol	Chain	Res	Type	Atoms
36	A	9000	ERY	C15-C16-O5-C20
36	A	9000	ERY	C19-C16-O5-C20
36	A	9000	ERY	C10-C11-C12-O13
36	A	9000	ERY	C25-C24-N1-C28
36	A	9000	ERY	C4-C5-C6-C32

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	ERY	8	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.

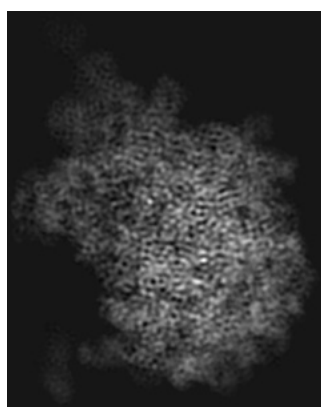
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6057. These allow visual inspection of the internal detail of the map and identification of artifacts.

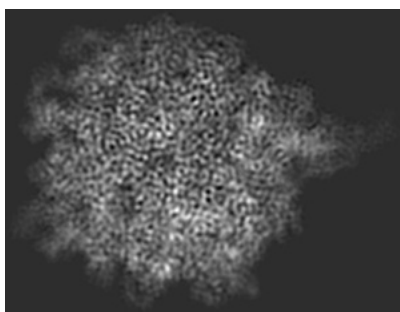
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

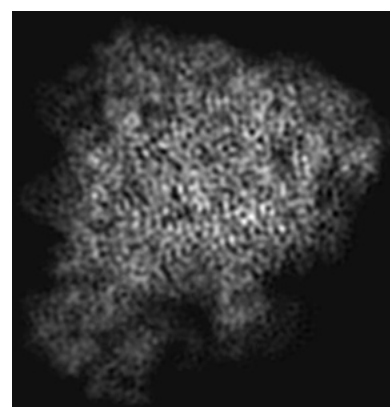
#### 6.1.1 Primary map



X



Y

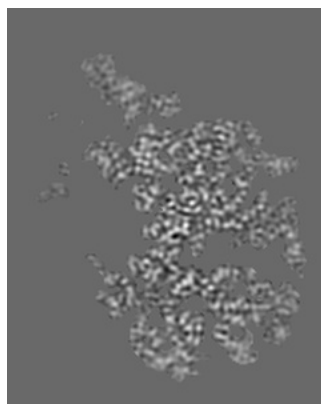


Z

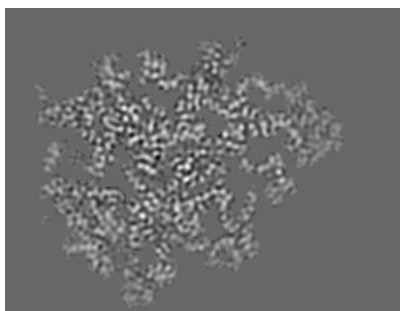
The images above show the map projected in three orthogonal directions.

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

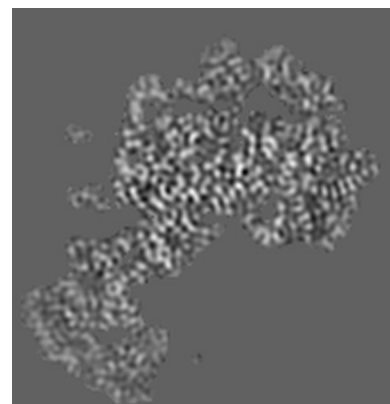
#### 6.2.1 Primary map



X Index: 88



Y Index: 91

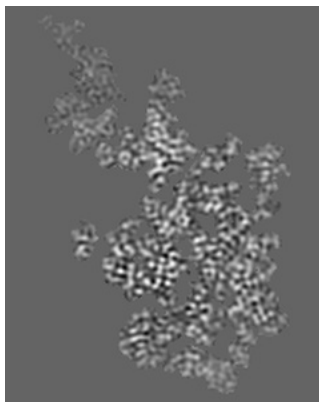


Z Index: 115

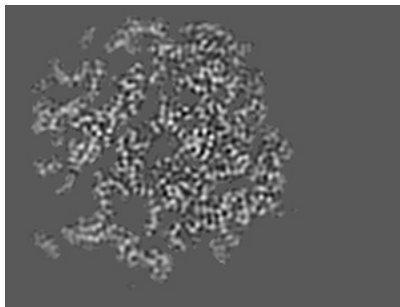
The images above show central slices of the map in three orthogonal directions.

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

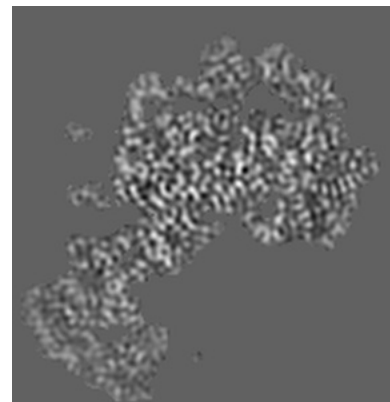
### 6.3.1 Primary map



X Index: 109



Y Index: 110



Z Index: 115

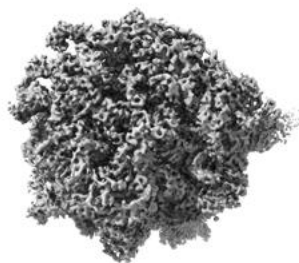
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

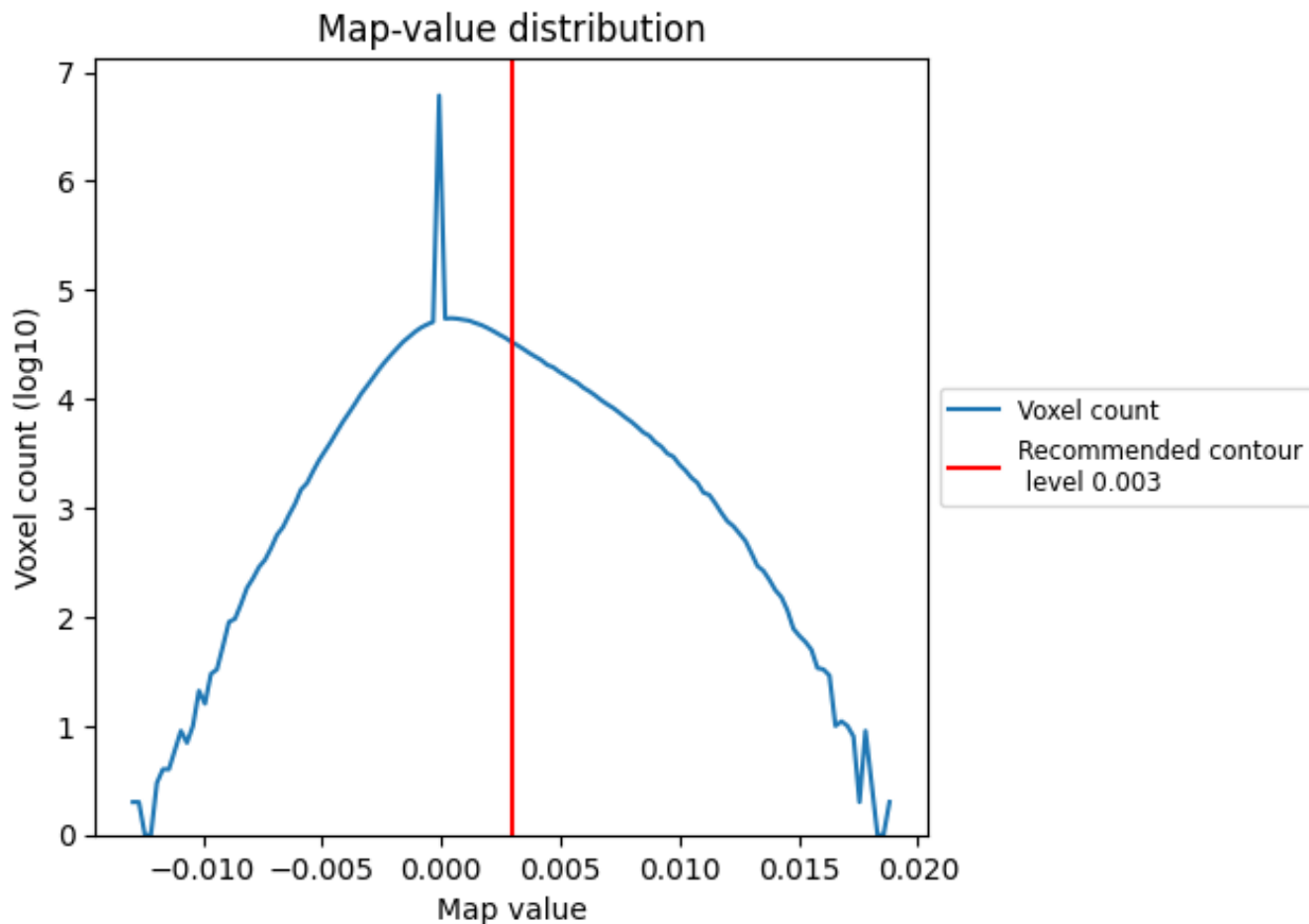
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

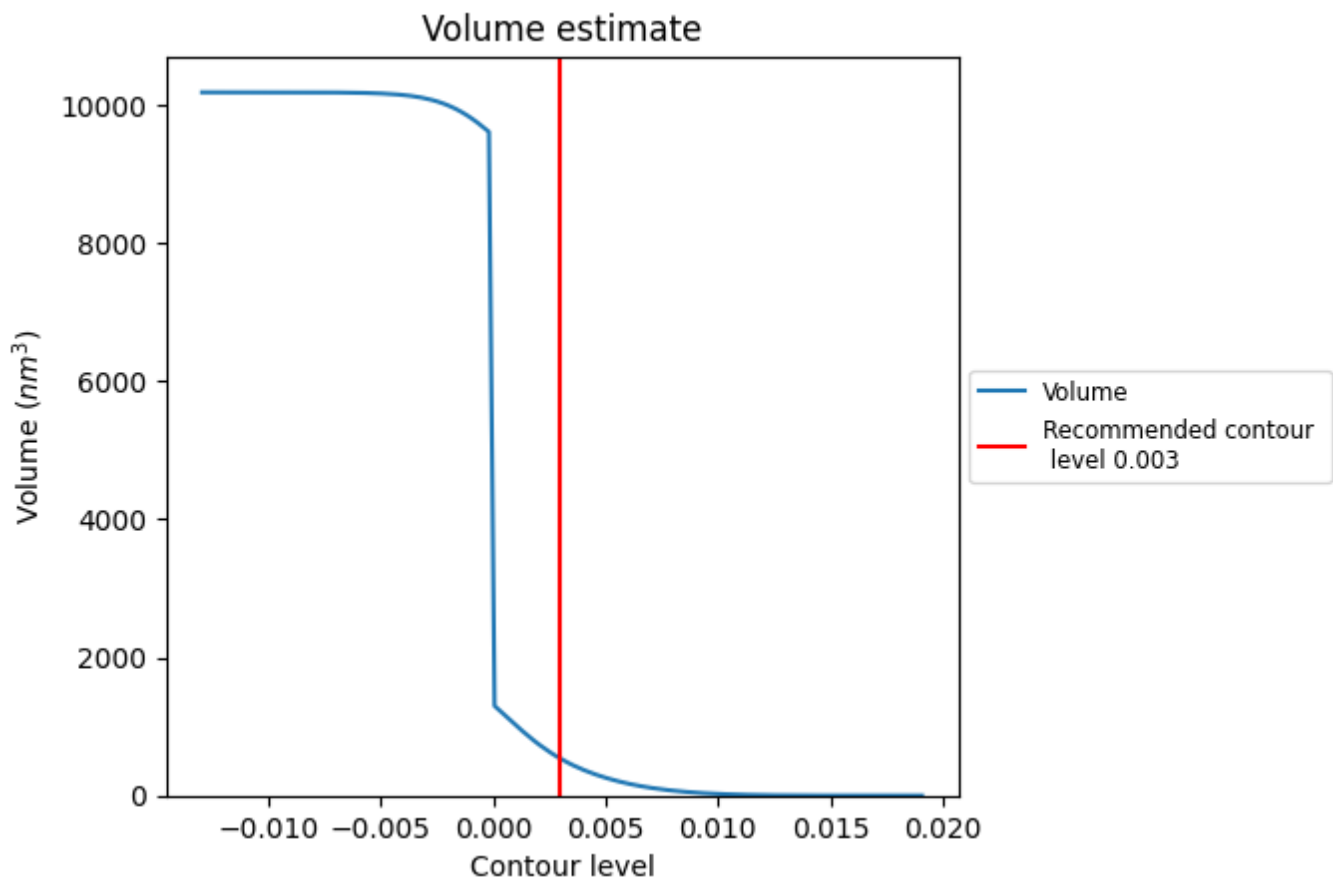
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm<sup>3</sup>; this corresponds to an approximate mass of 483 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

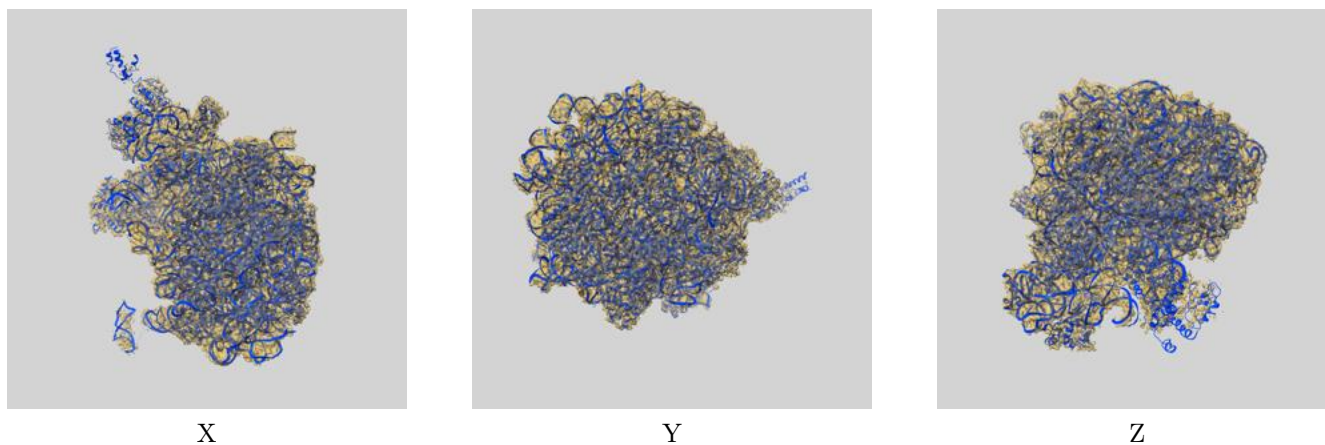
## 8 Fourier-Shell correlation

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-6057 and PDB model 3J7Z. Per-residue inclusion information can be found in section 3 on page 11.

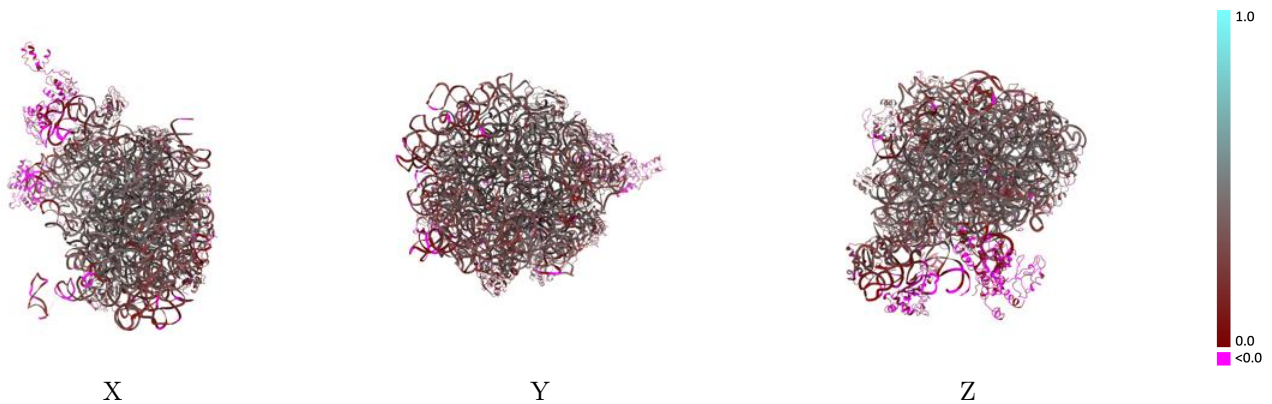
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.003 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.

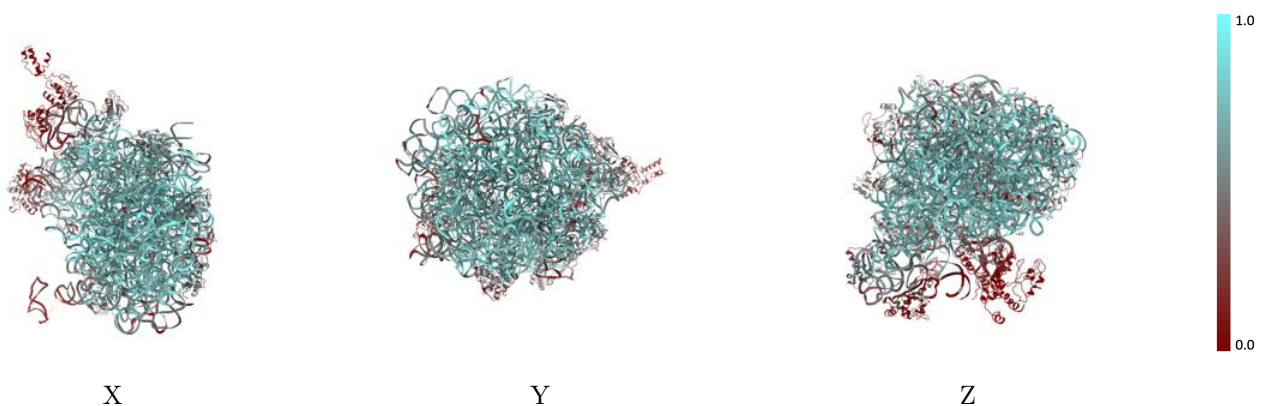


## 9.2 Q-score mapped to coordinate model [i](#)



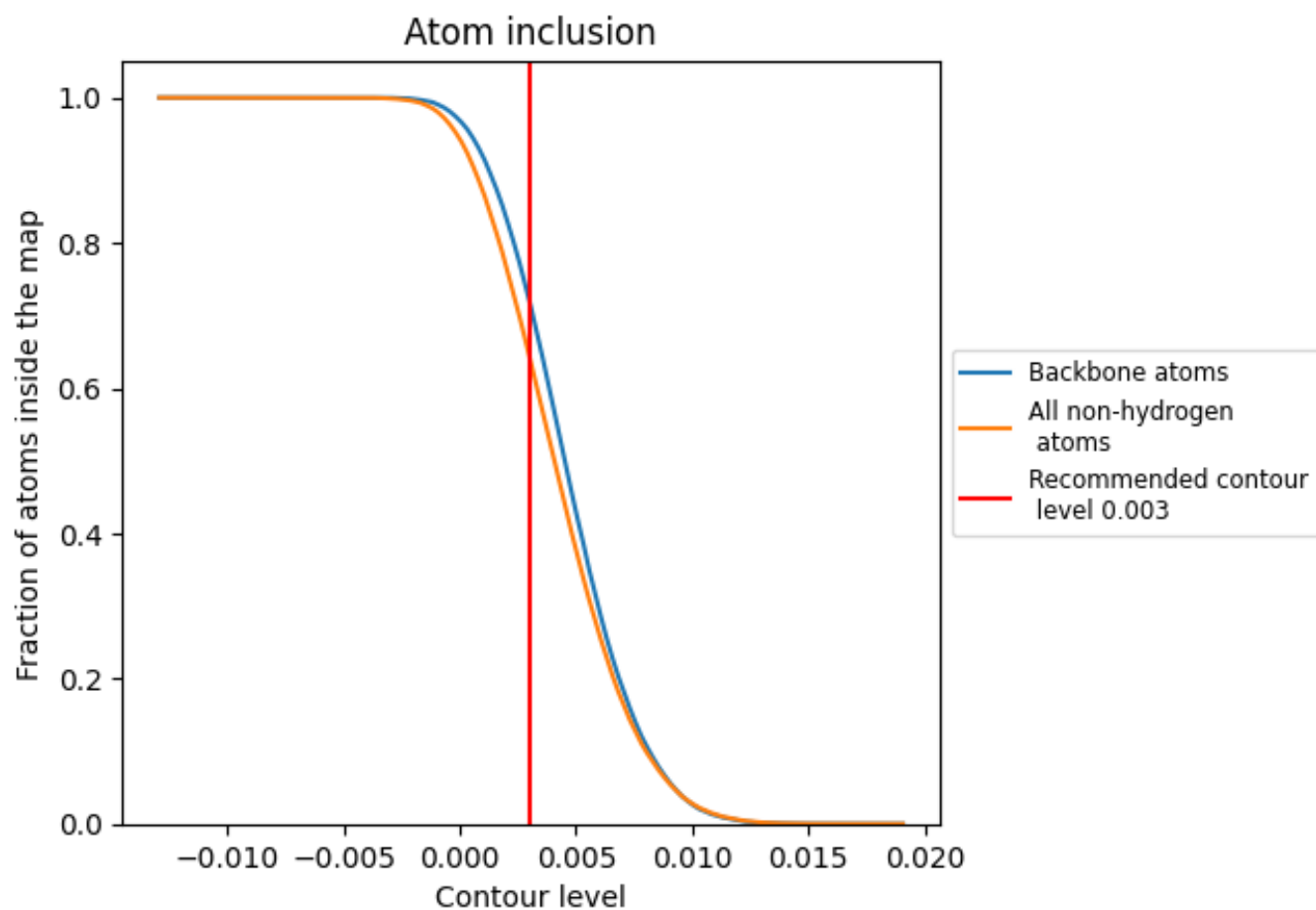
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6425	 0.3120
0	 0.5958	 0.3310
1	 0.1097	 0.1330
2	 0.6535	 0.3740
3	 0.6660	 0.4030
4	 0.6473	 0.3940
5	 0.0740	 0.0490
6	 0.0088	 0.0340
7	 0.8621	 0.4460
A	 0.7115	 0.3290
B	 0.5931	 0.2290
C	 0.6126	 0.3460
D	 0.5865	 0.3600
E	 0.5033	 0.2980
F	 0.1770	 -0.0030
G	 0.4433	 0.2540
H	 0.2770	 0.2090
I	 0.0548	 -0.0030
J	 0.5936	 0.3350
K	 0.5838	 0.3730
L	 0.5354	 0.3210
M	 0.6046	 0.3730
N	 0.6399	 0.3690
O	 0.4762	 0.2560
P	 0.5732	 0.3430
Q	 0.6388	 0.3450
R	 0.5383	 0.3170
S	 0.5885	 0.3470
T	 0.5222	 0.2860
U	 0.4302	 0.2430
V	 0.5081	 0.3020
W	 0.5793	 0.3410
X	 0.5973	 0.3600
Y	 0.4406	 0.2310
Z	 0.5721	 0.3550
a	 0.6667	 0.4460

