



## wwPDB EM Validation Summary Report ⓘ

Feb 13, 2024 – 04:06 PM EST

PDB ID : 3J9Z  
EMDB ID : EMD-6315  
Title : Activation of GTP Hydrolysis in mRNA-tRNA Translocation by Elongation Factor G  
Authors : Li, W.; Liu, Z.; Koripella, R.K.; Langlois, R.; Sanyal, S.; Frank, J.  
Deposited on : 2015-03-27  
Resolution : 3.60 Å(reported)  
Based on initial model : 3J0U

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:

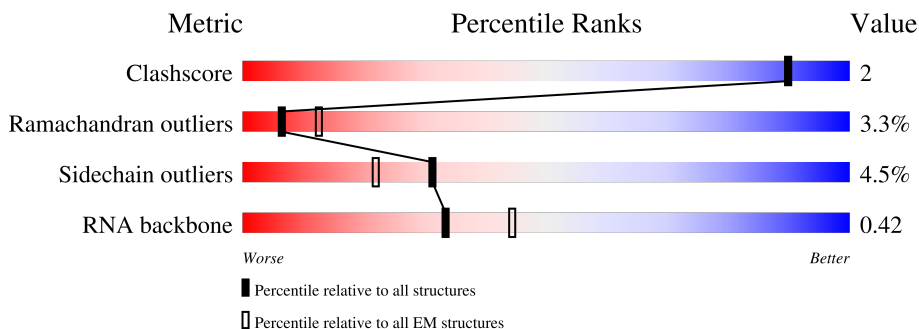
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.60 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.






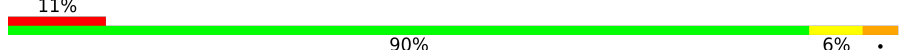

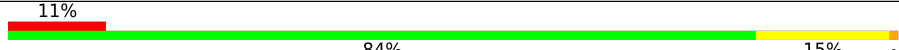
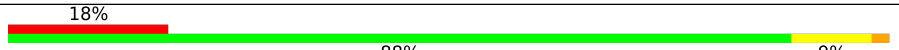
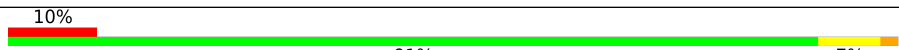
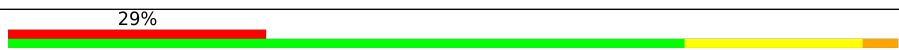

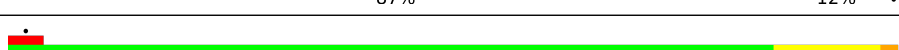
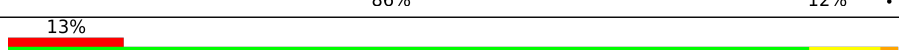
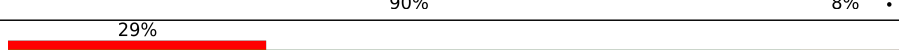
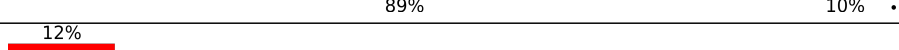
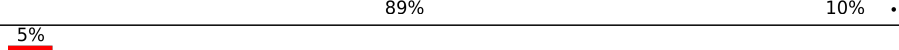
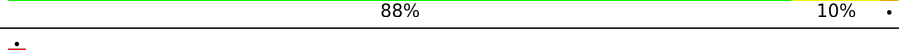


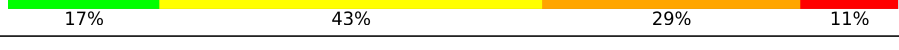


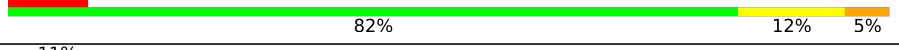
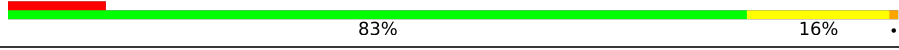


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	SA	1542	
2	S6	77	
3	S7	74	
4	SJ	103	
5	SK	128	
6	SL	123	
7	SM	117	

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Mol	Chain	Length	Quality of chain
8	SN	100	
9	SO	88	
10	SP	82	
11	SQ	83	
12	SR	74	
13	SS	91	
14	SB	240	
15	ST	86	
16	SU	70	
17	SC	232	
18	SD	205	
19	SE	166	
20	SF	135	
21	SG	178	
22	SH	129	
23	SI	129	
24	S1	702	
25	LA	2904	
26	LB	120	
27	LC	234	
28	LM	114	
29	LN	272	
30	LO	117	
31	LP	103	
32	LQ	110	

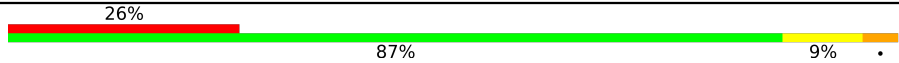
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Mol	Chain	Length	Quality of chain
33	LR	100	13% 86% 14%
34	LS	103	85% 12%
35	LT	94	90% 7%
36	LU	84	10% 70% 24% 5%
37	LV	77	88% 10%
38	LD	164	41% 93% 7%
39	LW	63	21% 87% 10%
40	LX	209	7% 83% 12%
41	LY	58	91% 5%
42	L1	56	80% 18%
43	L2	54	9% 96%
44	L3	46	13% 76% 15% 7%
45	L4	64	91% 8%
46	L5	38	92% 5%
47	L6	201	5% 87% 11%
48	LE	141	13% 91% 8%
49	L7	178	75% 21%
50	L8	176	6% 88% 11%
51	L9	149	36% 87% 12%
52	LF	142	85% 13%
53	LG	123	11% 82% 16%
54	LH	144	84% 13%
55	LI	136	91% 7%
56	LJ	127	12% 80% 17%
57	LK	117	85% 15%

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Mol	Chain	Length	Quality of chain
58	LZ	70	

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
59	GTP	S1	801	-	-	X	-

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 156714 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
			Total	C	N	O	P		
1	SA	1542	33076	14754	6064	10717	1541	0	0

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	S6	77	1639	732	297	534	76	0	0

- Molecule 3 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	S7	74	1577	704	282	518	73	0	0

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SJ	103	825	514	158	151	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SK	128	965	595	196	171	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S12.

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

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SM	117	910	564	183	160	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SO	88	716	440	146	129	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SQ	83	672	425	124	120	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SR	74	626	395	123	107	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SS	91	727	464	139	122	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SB	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 15 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	ST	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 16 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 17 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SC	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 18 is a protein called 30S ribosomal protein S4.

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

- Molecule 19 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SE	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 20 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SF	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 21 is a protein called 30S ribosomal protein S7.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SG	178	1400	874	269	253	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S8.

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

- Molecule 23 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SI	129	1036	642	208	183	3	0	0

- Molecule 24 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S1	702	5431	3420	938	1048	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	91	ALA	HIS	engineered mutation	UNP P0A6M8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	LA	2904	62333	27808	11464	20158	2903	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	1618	U	A	conflict	GB 33357927
LA	2030	C	A	conflict	GB 33357927

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	LB	120	2566	1144	468	835	119	0	0

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LC	234	1733	1081	315	330	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LN	272	2092	1294	425	366	7	0	0

- Molecule 30 is a protein called 50S ribosomal protein L20.

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

- Molecule 31 is a protein called 50S ribosomal protein L21.

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

- Molecule 32 is a protein called 50S ribosomal protein L22.

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

- Molecule 33 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LR	100	787	496	146	143	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LS	103	789	498	148	143		0	0

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LU	84	634	391	129	113	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L28.

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

- Molecule 38 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LD	164	1233	776	220	231	6	0	0

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L3.

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

- Molecule 41 is a protein called 50S ribosomal protein L30.

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

- Molecule 42 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 43 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	L2	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 44 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 45 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 46 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 47 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	L6	201	1552	974	283	290	5	0	0

- Molecule 48 is a protein called 50S ribosomal protein L11.

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

- Molecule 49 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	L7	178	1420	905	251	258	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	L8	176	1323	832	243	246	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	L9	149	1111	699	197	214	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L13.

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

- Molecule 53 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	LG	123	947	593	181	167	6	0	0

- Molecule 54 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LH	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 55 is a protein called 50S ribosomal protein L16.

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

- Molecule 56 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LJ	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

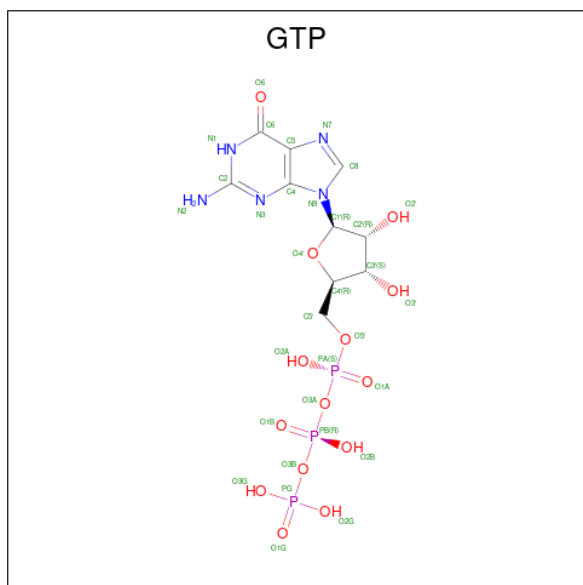
- Molecule 57 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LK	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LZ	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

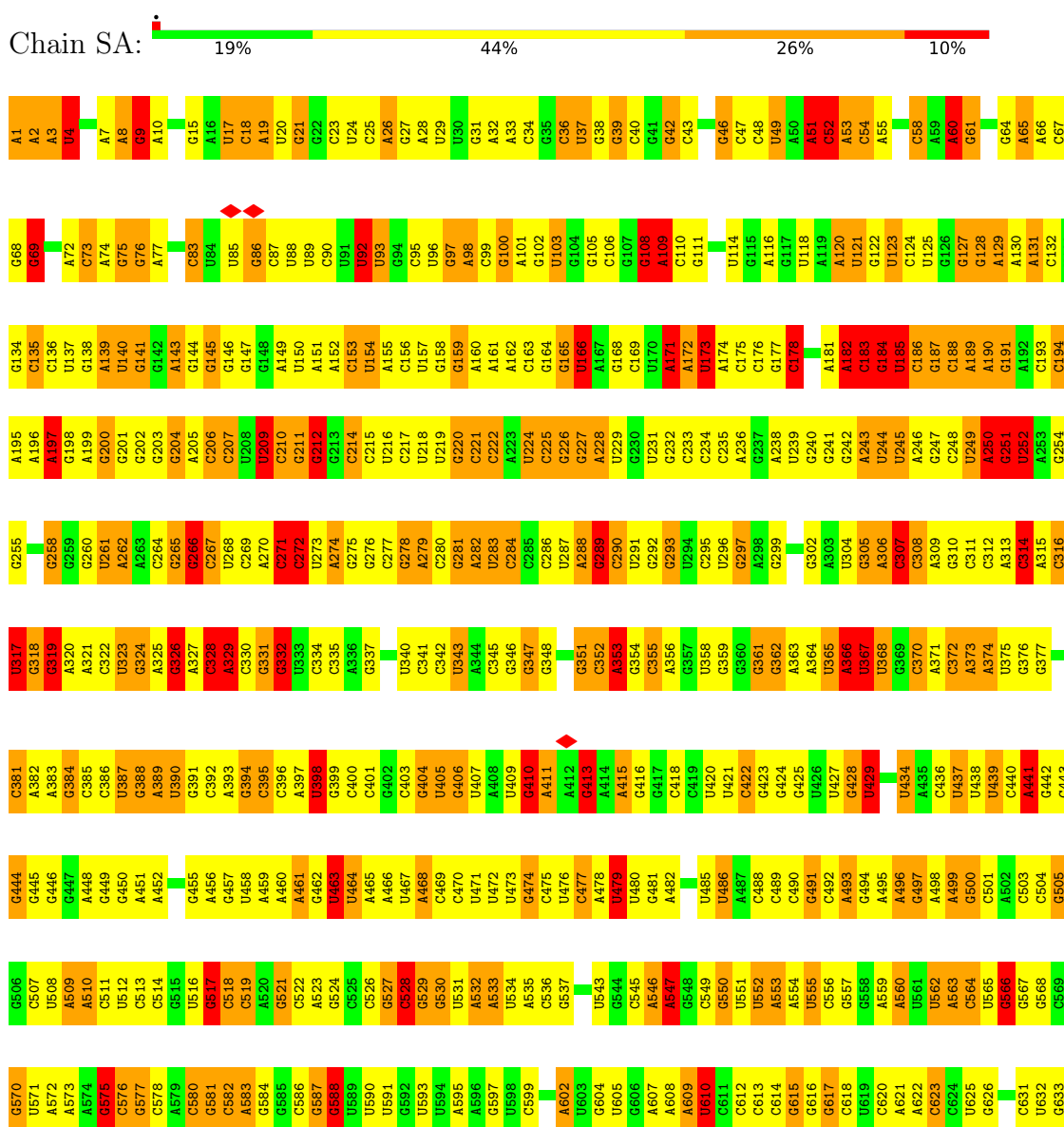


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	S1	1	32	10	5	14	3	0

### 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.

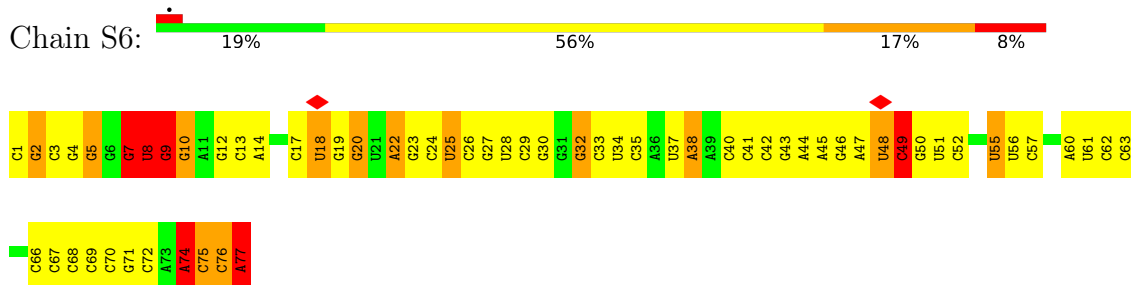
- Molecule 1: 16S ribosomal RNA



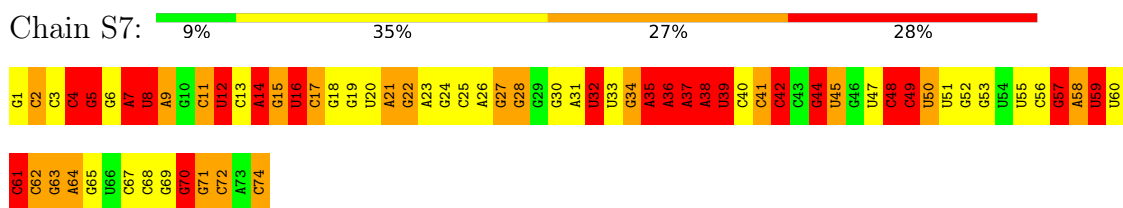




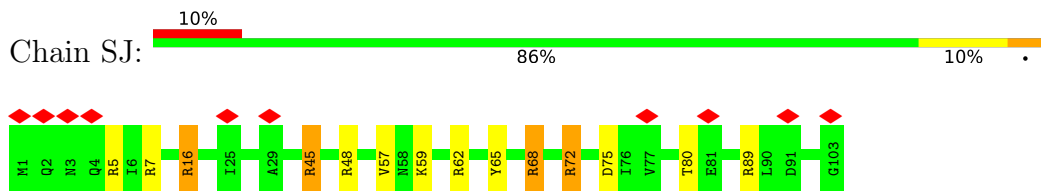
• Molecule 2: P-tRNA



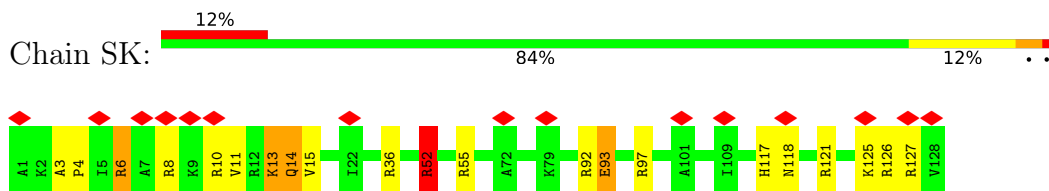
• Molecule 3: E-tRNA



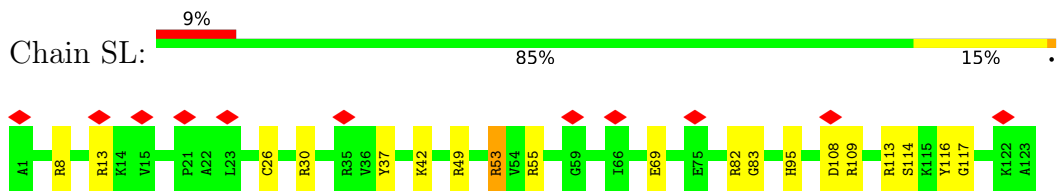
• Molecule 4: 30S ribosomal protein S10



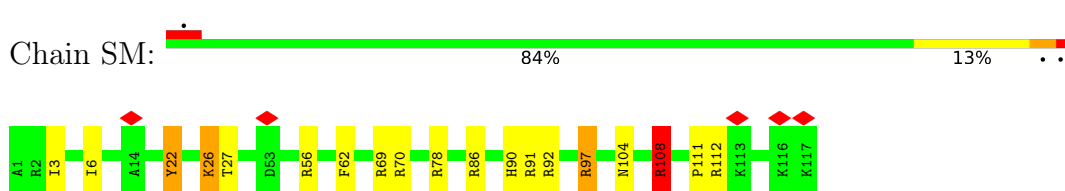
• Molecule 5: 30S ribosomal protein S11




• Molecule 6: 30S ribosomal protein S12



• Molecule 7: 30S ribosomal protein S13




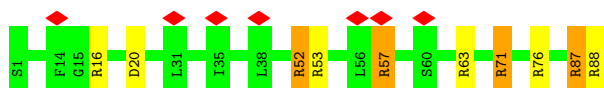
• Molecule 8: 30S ribosomal protein S14

Chain SN:  89% 8%




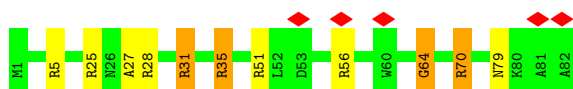
- Molecule 9: 30S ribosomal protein S15

Chain SO:  89% 7% 5%

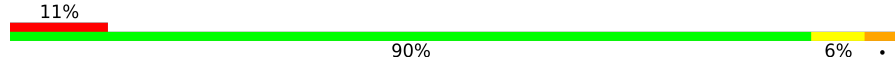


- Molecule 10: 30S ribosomal protein S16

Chain SP:  87% 9% 5%




- Molecule 11: 30S ribosomal protein S17

Chain SQ:  90% 6%




- Molecule 12: 30S ribosomal protein S18

Chain SR:  84% 15%




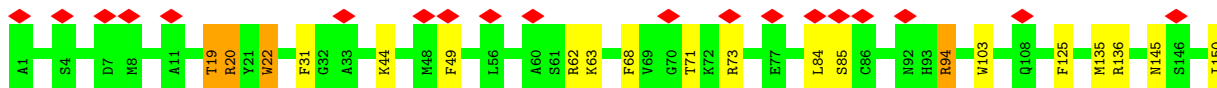
- Molecule 13: 30S ribosomal protein S19

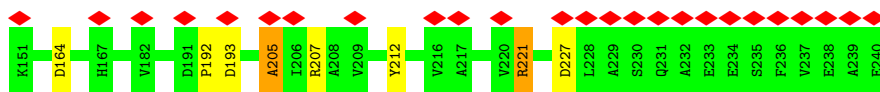
Chain SS:  84% 15%



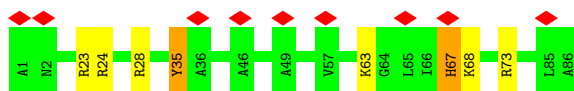
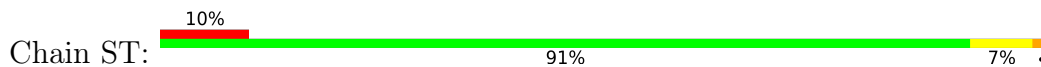
- Molecule 14: 30S ribosomal protein S2

Chain SB:  88% 9%

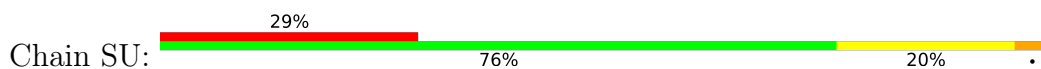




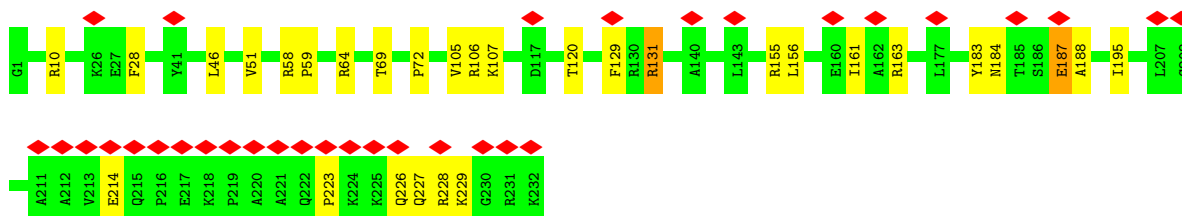
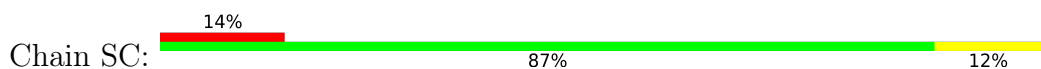
- Molecule 15: 30S ribosomal protein S20



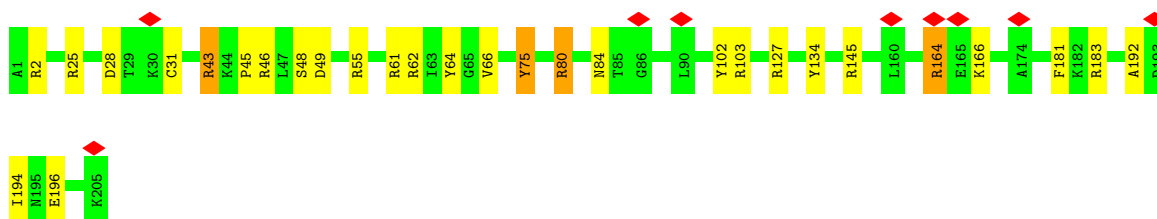
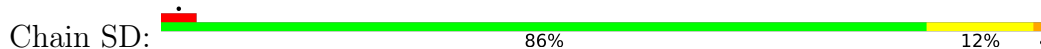
- Molecule 16: 30S ribosomal protein S21



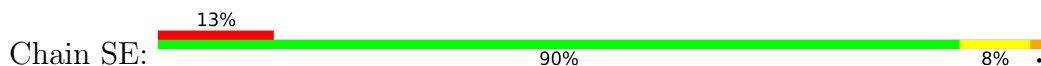
- Molecule 17: 30S ribosomal protein S3



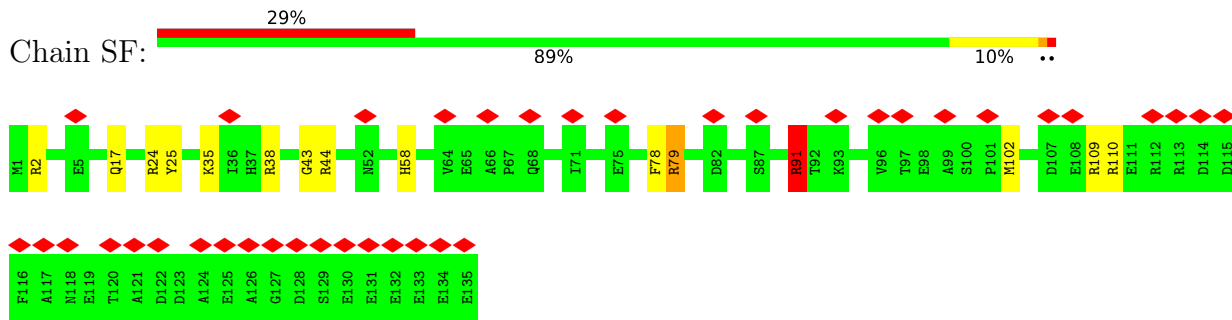
- Molecule 18: 30S ribosomal protein S4



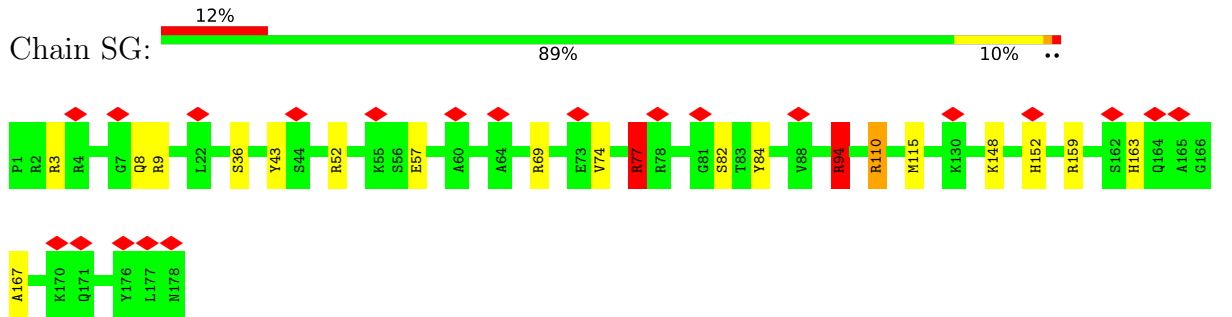
- Molecule 19: 30S ribosomal protein S5



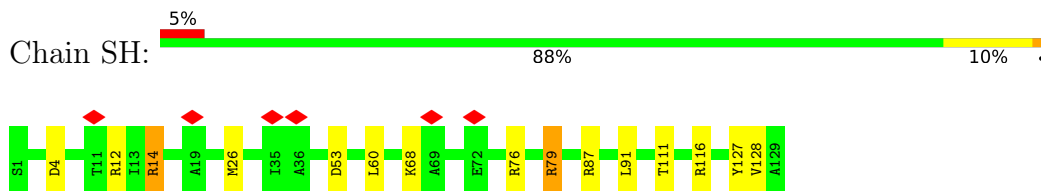
- Molecule 20: 30S ribosomal protein S6



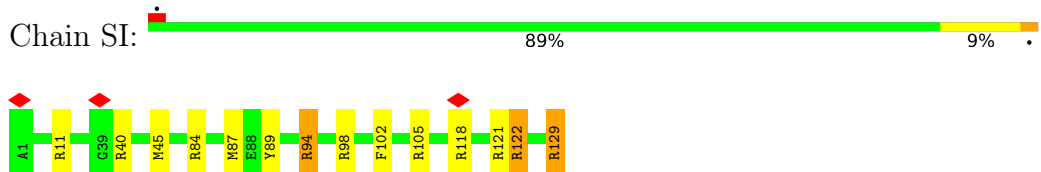
- Molecule 21: 30S ribosomal protein S7



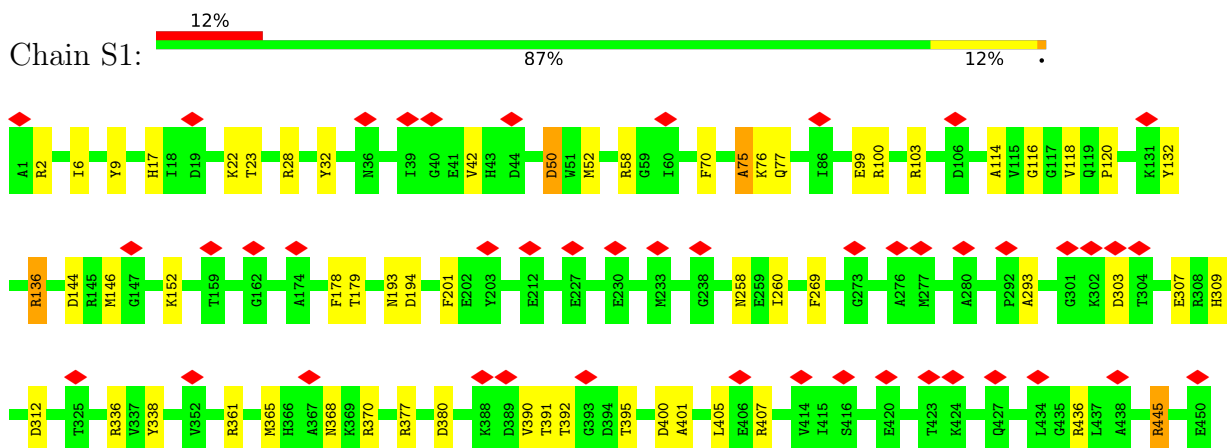
- Molecule 22: 30S ribosomal protein S8

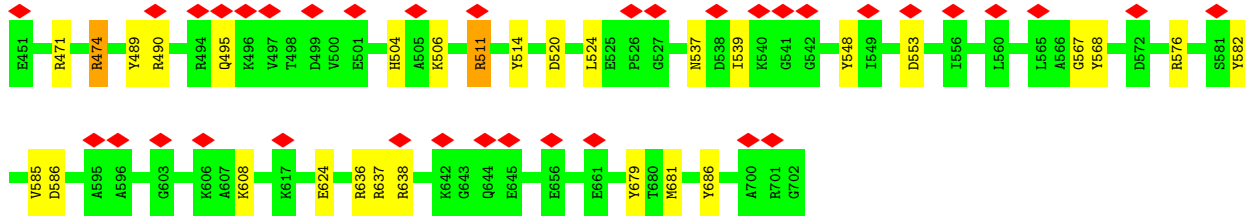


- Molecule 23: 30S ribosomal protein S9

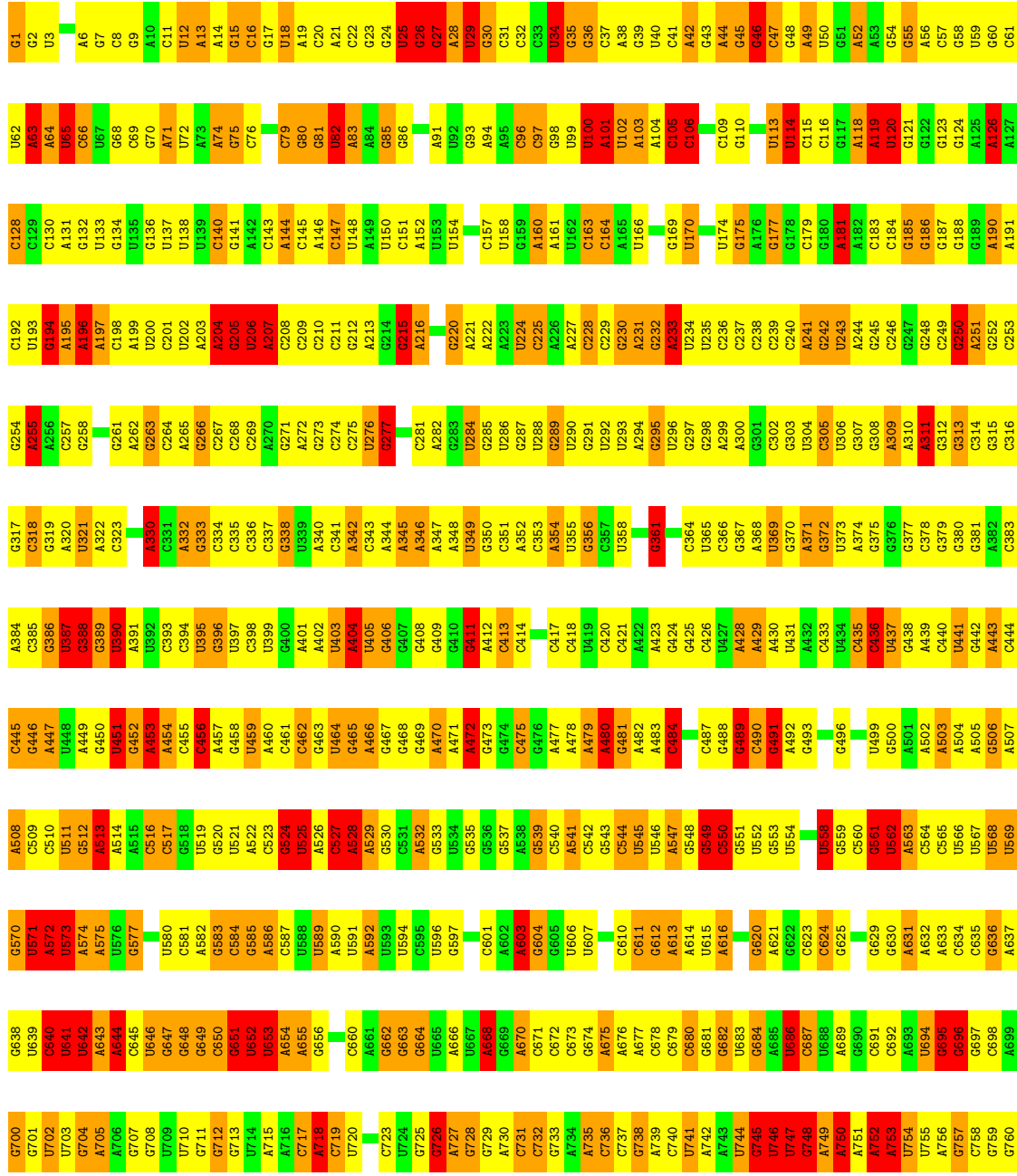
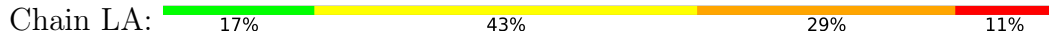


- Molecule 24: Elongation factor G





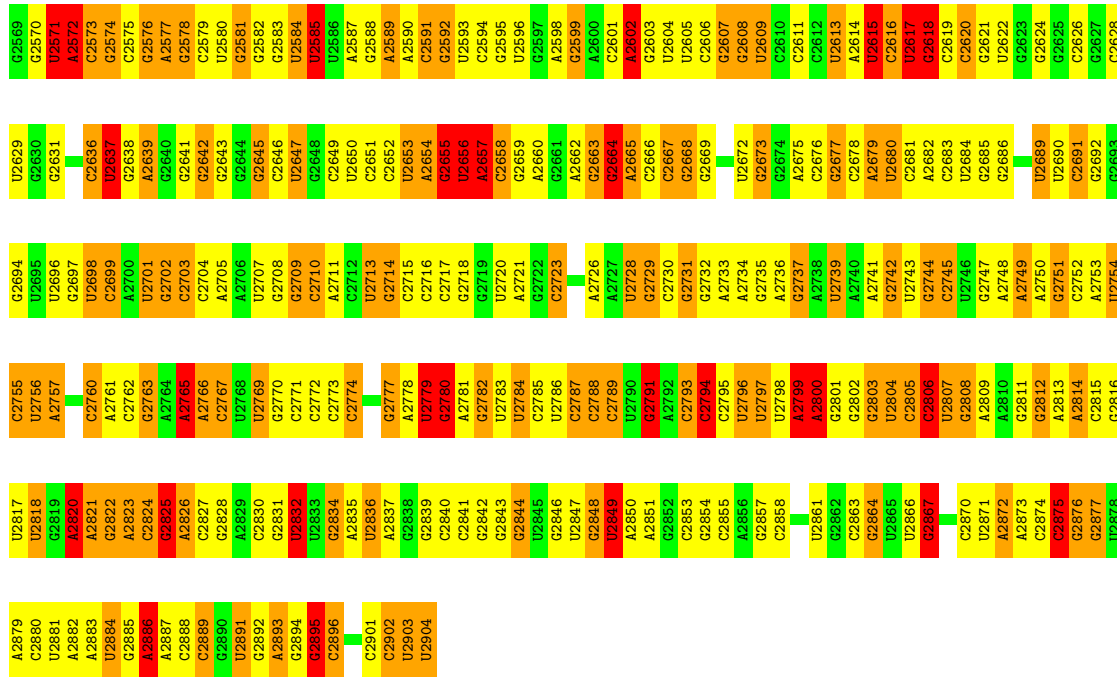
• Molecule 25: 23S ribosomal RNA



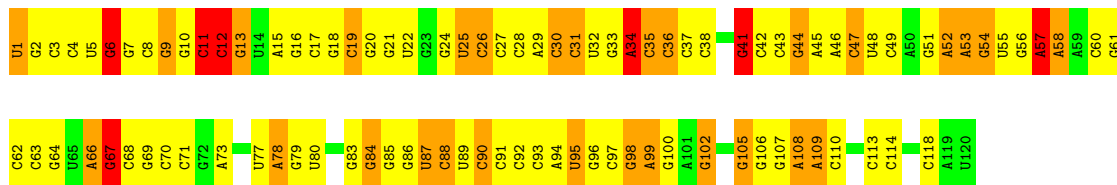
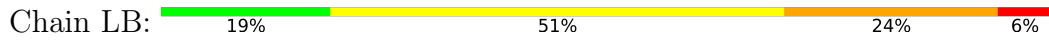
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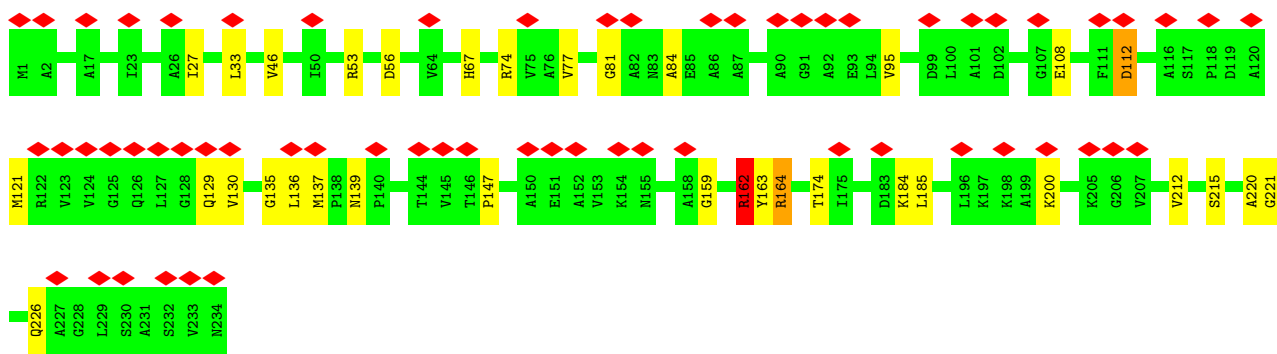
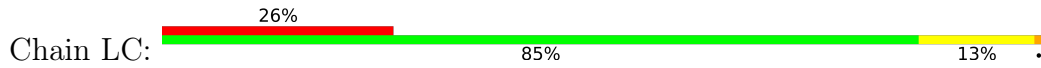




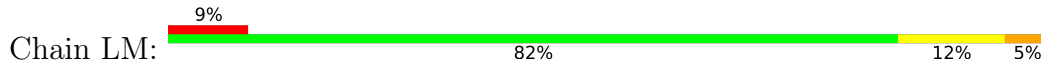
• Molecule 26: 5S ribosomal RNA

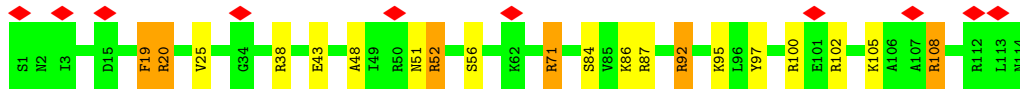


• Molecule 27: 50S ribosomal protein L1

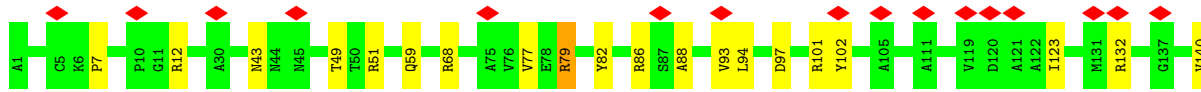
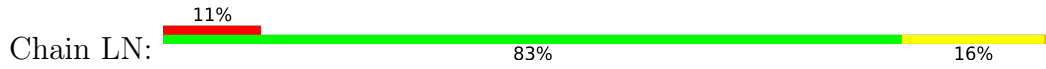


• Molecule 28: 50S ribosomal protein L19

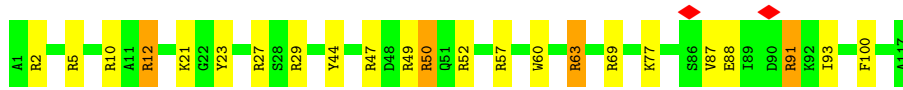
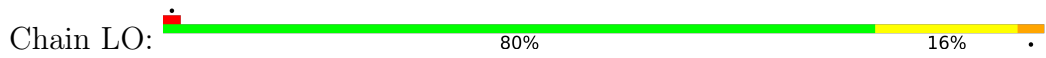




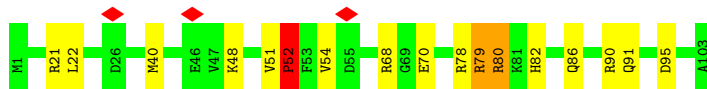
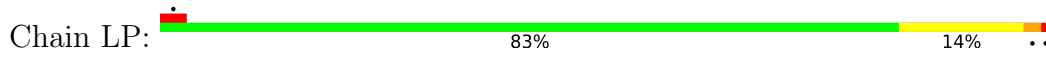
• Molecule 29: 50S ribosomal protein L2



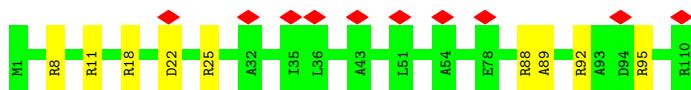
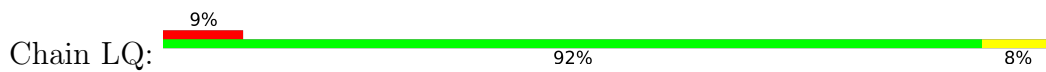
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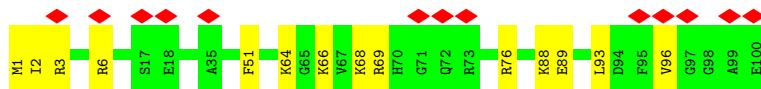
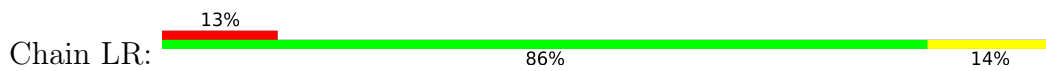
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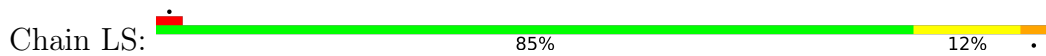
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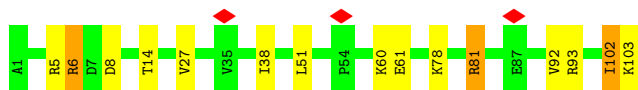


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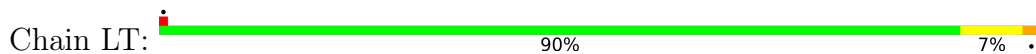


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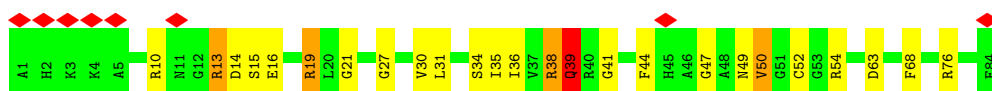




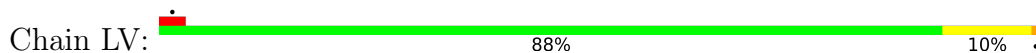
- Molecule 35: 50S ribosomal protein L25



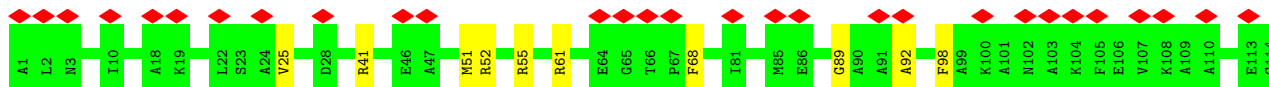
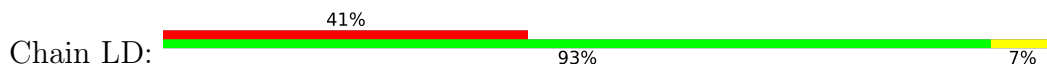
- Molecule 36: 50S ribosomal protein L27



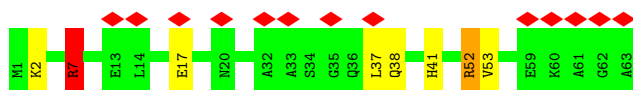
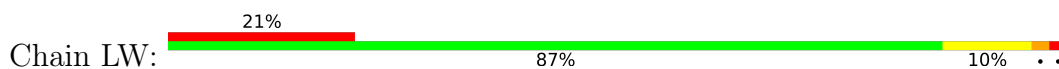
- Molecule 37: 50S ribosomal protein L28



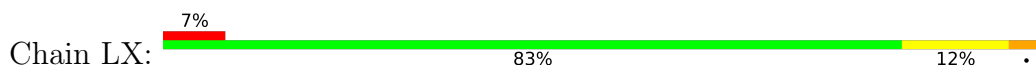
- Molecule 38: 50S ribosomal protein L10

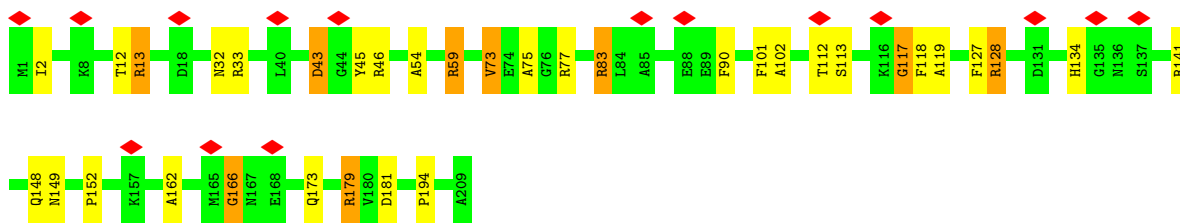


- Molecule 39: 50S ribosomal protein L29



- Molecule 40: 50S ribosomal protein L3

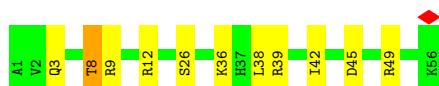
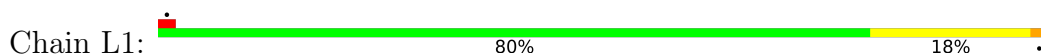




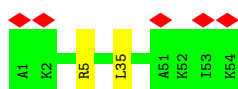
- Molecule 41: 50S ribosomal protein L30



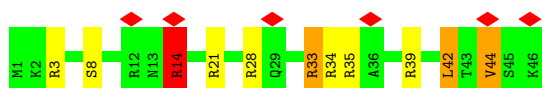
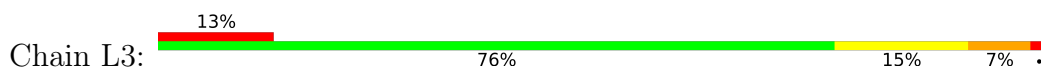
- Molecule 42: 50S ribosomal protein L32



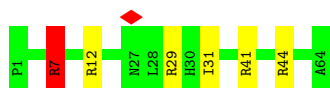
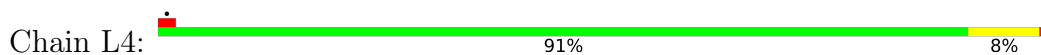
- Molecule 43: 50S ribosomal protein L33



- Molecule 44: 50S ribosomal protein L34



- Molecule 45: 50S ribosomal protein L35

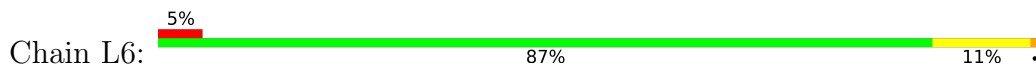


- Molecule 46: 50S ribosomal protein L36

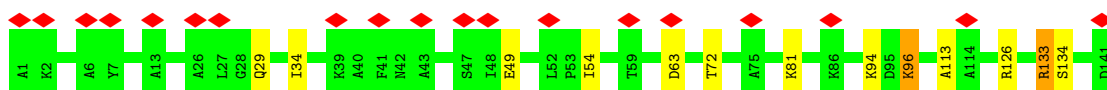
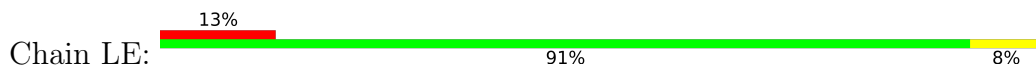




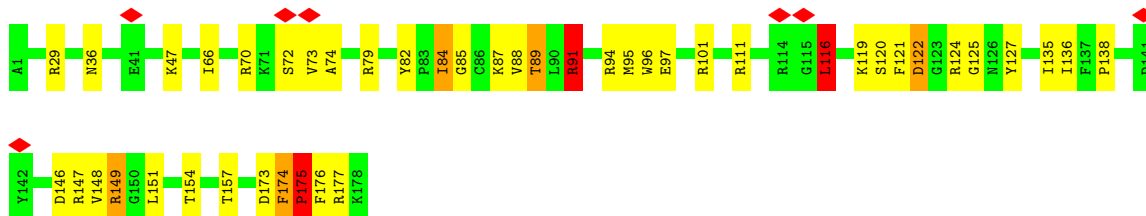
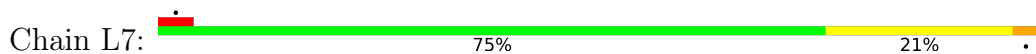
- Molecule 47: 50S ribosomal protein L4



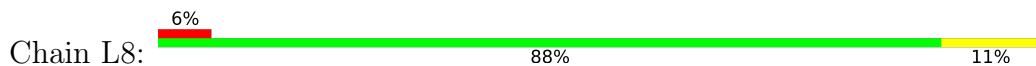
- Molecule 48: 50S ribosomal protein L11



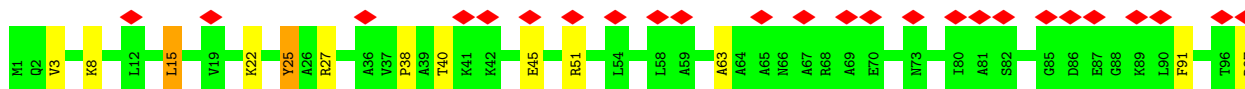
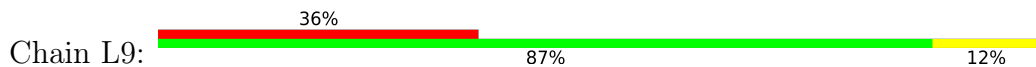
- Molecule 49: 50S ribosomal protein L5



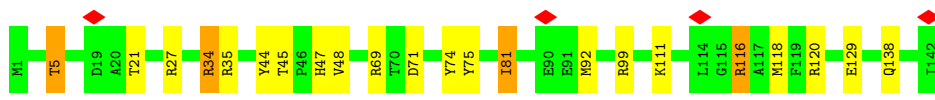
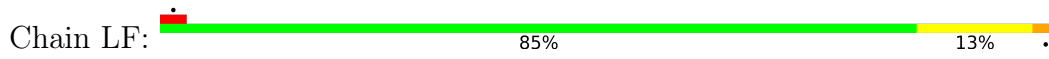
- Molecule 50: 50S ribosomal protein L6



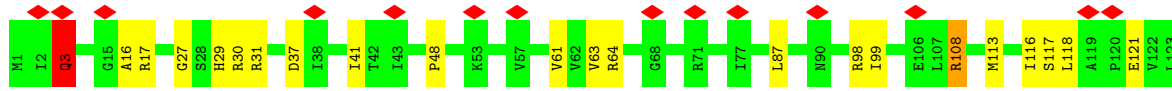
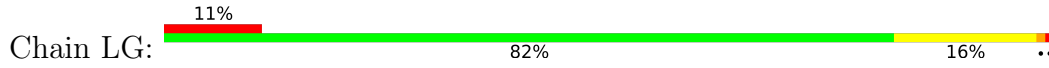
- Molecule 51: 50S ribosomal protein L9



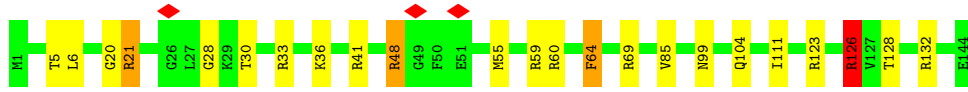
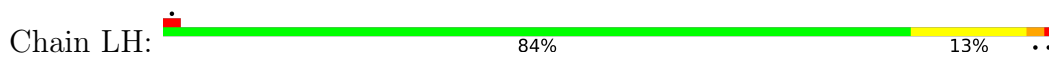
- Molecule 52: 50S ribosomal protein L13



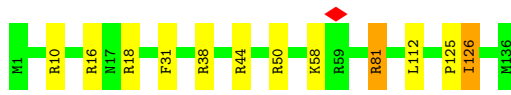
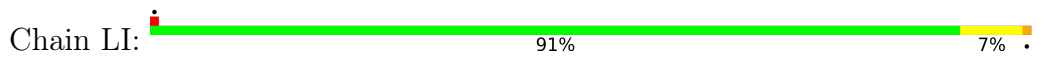
• Molecule 53: 50S ribosomal protein L14



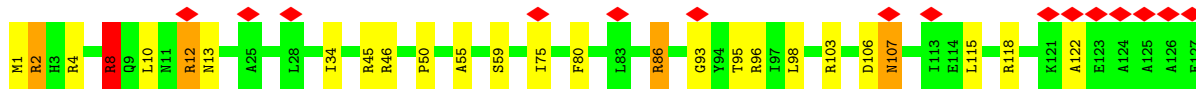
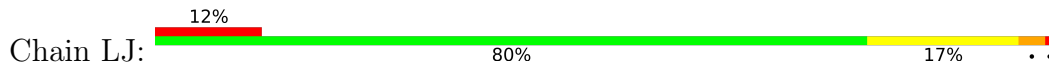
• Molecule 54: 50S ribosomal protein L15



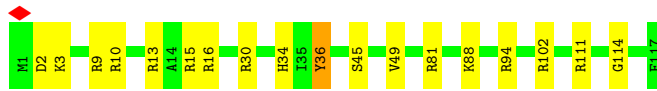
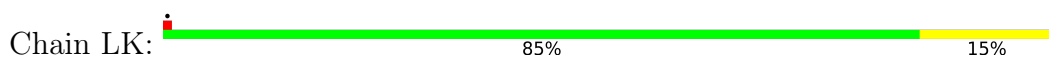
• Molecule 55: 50S ribosomal protein L16



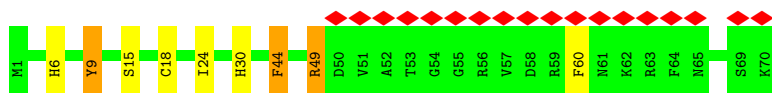
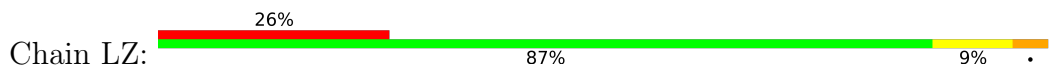
• Molecule 56: 50S ribosomal protein L17



• Molecule 57: 50S ribosomal protein L18



• Molecule 58: 50S ribosomal protein L31



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND3 and CTFIT	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	58000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	SA	1.54	172/37035 (0.5%)	1.91	1570/57774 (2.7%)
2	S6	1.44	5/1831 (0.3%)	1.81	72/2853 (2.5%)
3	S7	1.36	4/1762 (0.2%)	1.97	89/2746 (3.2%)
4	SJ	0.73	0/835	1.28	10/1127 (0.9%)
5	SK	0.75	0/982	1.30	11/1323 (0.8%)
6	SL	0.75	0/969	1.37	9/1300 (0.7%)
7	SM	0.70	0/919	1.33	10/1226 (0.8%)
8	SN	0.73	0/817	1.36	8/1088 (0.7%)
9	SO	0.70	0/724	1.35	12/966 (1.2%)
10	SP	0.73	0/659	1.41	12/884 (1.4%)
11	SQ	0.74	0/681	1.24	5/913 (0.5%)
12	SR	0.76	0/637	1.37	8/851 (0.9%)
13	SS	0.70	0/744	1.28	5/995 (0.5%)
14	SB	0.71	0/1904	1.22	16/2565 (0.6%)
15	ST	0.69	0/676	1.15	3/895 (0.3%)
16	SU	0.84	0/598	1.53	8/792 (1.0%)
17	SC	0.74	0/1852	1.19	7/2490 (0.3%)
18	SD	0.70	0/1665	1.33	16/2227 (0.7%)
19	SE	0.74	0/1239	1.16	2/1664 (0.1%)
20	SF	0.75	0/1121	1.26	6/1509 (0.4%)
21	SG	0.75	0/1422	1.29	12/1908 (0.6%)
22	SH	0.71	0/989	1.22	8/1326 (0.6%)
23	SI	0.75	0/1048	1.35	17/1394 (1.2%)
24	S1	0.70	0/5532	1.21	27/7485 (0.4%)
25	LA	1.66	473/69812 (0.7%)	1.93	2989/108912 (2.7%)
26	LB	1.39	6/2869 (0.2%)	1.84	112/4474 (2.5%)
27	LC	0.70	0/1748	1.21	7/2355 (0.3%)
28	LM	0.77	0/929	1.33	12/1242 (1.0%)
29	LN	0.74	0/2131	1.38	16/2863 (0.6%)
30	LO	0.70	0/960	1.46	18/1278 (1.4%)
31	LP	0.76	0/829	1.21	6/1107 (0.5%)
32	LQ	0.74	0/864	1.28	9/1156 (0.8%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LR	0.73	0/794	1.22	6/1060 (0.6%)
34	LS	0.71	0/797	1.19	6/1062 (0.6%)
35	LT	0.71	0/766	1.18	4/1025 (0.4%)
36	LU	0.78	0/642	1.34	6/848 (0.7%)
37	LV	0.76	0/635	1.32	7/848 (0.8%)
38	LD	0.73	0/1247	1.15	3/1679 (0.2%)
39	LW	0.72	0/510	1.22	4/677 (0.6%)
40	LX	0.77	0/1586	1.35	16/2134 (0.7%)
41	LY	0.68	0/453	1.40	4/605 (0.7%)
42	L1	0.71	0/450	1.28	1/599 (0.2%)
43	L2	0.75	0/448	1.13	1/594 (0.2%)
44	L3	0.77	0/380	1.61	9/498 (1.8%)
45	L4	0.66	0/513	1.28	3/676 (0.4%)
46	L5	0.81	0/303	1.35	3/397 (0.8%)
47	L6	0.71	0/1571	1.27	11/2113 (0.5%)
48	LE	0.68	0/1046	1.19	4/1410 (0.3%)
49	L7	0.73	0/1444	1.35	18/1937 (0.9%)
50	L8	0.70	0/1343	1.20	9/1816 (0.5%)
51	L9	0.71	0/1122	1.16	8/1515 (0.5%)
52	LF	0.77	0/1152	1.30	10/1551 (0.6%)
53	LG	0.78	0/956	1.32	6/1279 (0.5%)
54	LH	0.72	0/1062	1.35	13/1413 (0.9%)
55	LI	0.75	0/1093	1.33	12/1460 (0.8%)
56	LJ	0.75	0/1021	1.36	12/1364 (0.9%)
57	LK	0.73	0/910	1.32	12/1219 (1.0%)
58	LZ	0.71	0/559	1.23	4/745 (0.5%)
All	All	1.38	660/169586 (0.4%)	1.75	5304/252212 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	SA	2	423
2	S6	0	16
3	S7	0	31
4	SJ	0	7
5	SK	0	5
6	SL	0	9
7	SM	0	4
8	SN	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	SO	0	4
10	SP	0	4
11	SQ	0	4
12	SR	0	3
13	SS	0	2
14	SB	0	3
15	ST	0	2
16	SU	0	3
17	SC	0	7
18	SD	0	6
19	SE	0	8
20	SF	0	6
21	SG	0	4
22	SH	0	3
23	SI	0	4
24	S1	0	19
25	LA	1	941
26	LB	0	21
27	LC	0	4
28	LM	0	5
29	LN	0	9
30	LO	0	4
31	LP	0	1
32	LQ	0	2
34	LS	0	3
35	LT	0	2
36	LU	0	5
37	LV	0	3
38	LD	0	3
39	LW	0	4
40	LX	0	10
41	LY	0	1
42	L1	0	2
44	L3	0	5
45	L4	0	3
46	L5	0	1
47	L6	0	6
48	LE	0	1
49	L7	0	8
50	L8	0	3
51	L9	0	2
52	LF	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	LG	0	4
54	LH	0	5
55	LI	0	1
56	LJ	0	6
57	LK	0	3
58	LZ	0	4
All	All	3	1660

The worst 5 of 660 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	1513	A	N9-C4	-11.15	1.31	1.37
1	SA	781	A	N9-C4	-10.92	1.31	1.37
1	SA	900	A	N9-C4	-10.30	1.31	1.37
25	LA	2571	U	O3'-P	-10.16	1.49	1.61
25	LA	750	A	N9-C4	-10.00	1.31	1.37

The worst 5 of 5304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	LA	2030	C	C6-N1-C2	-27.21	109.42	120.30
25	LA	2251	G	O4'-C1'-N9	26.55	129.44	108.20
25	LA	1900	A	P-O3'-C3'	25.97	150.87	119.70
1	SA	51	A	P-O3'-C3'	25.23	149.97	119.70
25	LA	2656	U	C2-N3-C4	-22.74	113.35	127.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	SA	1498	U	C3',C4'
25	LA	2251	G	C1'

5 of 1660 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	SA	20	U	Sidechain
1	SA	21	G	Sidechain
1	SA	33	A	Sidechain
1	SA	4	U	Sidechain
1	SA	9	G	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SA	33076	0	16648	111	0
2	S6	1639	0	837	1	0
3	S7	1577	0	800	5	0
4	SJ	825	0	865	0	0
5	SK	965	0	997	3	0
6	SL	955	0	1019	1	0
7	SM	910	0	981	2	0
8	SN	805	0	847	1	0
9	SO	716	0	742	0	0
10	SP	649	0	666	0	0
11	SQ	672	0	716	0	0
12	SR	626	0	651	0	0
13	SS	727	0	769	2	0
14	SB	1872	0	1885	1	0
15	ST	670	0	722	3	0
16	SU	590	0	631	0	0
17	SC	1822	0	1913	2	0
18	SD	1643	0	1710	1	0
19	SE	1225	0	1273	1	0
20	SF	1101	0	1050	1	0
21	SG	1400	0	1449	2	0
22	SH	979	0	1034	1	0
23	SI	1036	0	1084	0	0
24	S1	5431	0	5403	16	0
25	LA	62333	0	31349	251	0
26	LB	2566	0	1302	10	0
27	LC	1733	0	1824	6	0
28	LM	917	0	965	1	0
29	LN	2092	0	2170	6	0
30	LO	947	0	1022	1	0
31	LP	816	0	839	2	0
32	LQ	857	0	922	0	0
33	LR	787	0	846	0	0
34	LS	789	0	847	1	0
35	LT	753	0	780	0	0
36	LU	634	0	656	3	0
37	LV	625	0	655	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LD	1233	0	1283	1	0
39	LW	509	0	543	2	0
40	LX	1565	0	1616	1	0
41	LY	449	0	491	1	0
42	L1	444	0	461	5	0
43	L2	441	0	485	0	0
44	L3	377	0	418	0	0
45	L4	504	0	574	0	0
46	L5	302	0	343	0	0
47	L6	1552	0	1619	3	0
48	LE	1032	0	1088	0	0
49	L7	1420	0	1460	4	0
50	L8	1323	0	1374	1	0
51	L9	1111	0	1148	0	0
52	LF	1129	0	1162	6	0
53	LG	947	0	1023	5	0
54	LH	1053	0	1129	2	0
55	LI	1074	0	1157	1	0
56	LJ	1008	0	1045	4	0
57	LK	900	0	935	0	0
58	LZ	549	0	552	1	0
59	S1	32	0	12	15	0
All	All	156714	0	108787	450	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 2.

The worst 5 of 450 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)
24:S1:22:LYS:CE	59:S1:801:GTP:O3G	2.13	0.97
24:S1:23:THR:N	59:S1:801:GTP:O2B	2.08	0.86
24:S1:22:LYS:HE3	59:S1:801:GTP:O3G	1.76	0.85
21:SG:77:ARG:HE	21:SG:152:HIS:CD2	2.05	0.74
24:S1:144:ASP:CG	59:S1:801:GTP:HN1	1.89	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SJ	101/103 (98%)	98 (97%)	0	3 (3%)	4	33
5	SK	126/128 (98%)	104 (82%)	17 (14%)	5 (4%)	3	26
6	SL	121/123 (98%)	109 (90%)	10 (8%)	2 (2%)	9	45
7	SM	115/117 (98%)	101 (88%)	9 (8%)	5 (4%)	2	24
8	SN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	55
9	SO	86/88 (98%)	83 (96%)	1 (1%)	2 (2%)	6	38
10	SP	80/82 (98%)	72 (90%)	4 (5%)	4 (5%)	2	21
11	SQ	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	5	36
12	SR	72/74 (97%)	58 (81%)	11 (15%)	3 (4%)	3	25
13	SS	89/91 (98%)	74 (83%)	10 (11%)	5 (6%)	2	19
14	SB	238/240 (99%)	217 (91%)	13 (6%)	8 (3%)	3	31
15	ST	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	13	51
16	SU	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	13
17	SC	230/232 (99%)	212 (92%)	13 (6%)	5 (2%)	6	39
18	SD	203/205 (99%)	177 (87%)	18 (9%)	8 (4%)	3	27
19	SE	164/166 (99%)	149 (91%)	13 (8%)	2 (1%)	13	51
20	SF	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	19	59
21	SG	176/178 (99%)	158 (90%)	15 (8%)	3 (2%)	9	45
22	SH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	46
23	SI	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
24	S1	700/702 (100%)	632 (90%)	45 (6%)	23 (3%)	4	31
27	LC	232/234 (99%)	206 (89%)	19 (8%)	7 (3%)	4	33
28	LM	112/114 (98%)	99 (88%)	10 (9%)	3 (3%)	5	35
29	LN	270/272 (99%)	244 (90%)	16 (6%)	10 (4%)	3	28
30	LO	115/117 (98%)	108 (94%)	4 (4%)	3 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	LP	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	7	41
32	LQ	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	57
33	LR	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2	20
34	LS	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	3	26
35	LT	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14	53
36	LU	82/84 (98%)	56 (68%)	15 (18%)	11 (13%)	0	4
37	LV	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
38	LD	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
39	LW	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
40	LX	207/209 (99%)	168 (81%)	25 (12%)	14 (7%)	1	15
41	LY	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	8	43
42	L1	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	28
43	L2	52/54 (96%)	44 (85%)	7 (14%)	1 (2%)	8	42
44	L3	44/46 (96%)	39 (89%)	2 (4%)	3 (7%)	1	15
45	L4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	46
46	L5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
47	L6	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	2	23
48	LE	139/141 (99%)	123 (88%)	12 (9%)	4 (3%)	4	33
49	L7	176/178 (99%)	137 (78%)	21 (12%)	18 (10%)	0	7
50	L8	174/176 (99%)	156 (90%)	9 (5%)	9 (5%)	2	20
51	L9	147/149 (99%)	132 (90%)	9 (6%)	6 (4%)	3	26
52	LF	140/142 (99%)	122 (87%)	16 (11%)	2 (1%)	11	48
53	LG	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	9	45
54	LH	142/144 (99%)	129 (91%)	5 (4%)	8 (6%)	2	19
55	LI	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	47
56	LJ	125/127 (98%)	110 (88%)	9 (7%)	6 (5%)	2	22
57	LK	115/117 (98%)	107 (93%)	5 (4%)	3 (3%)	5	35
58	LZ	68/70 (97%)	56 (82%)	10 (15%)	2 (3%)	4	33
All	All	7019/7125 (98%)	6254 (89%)	534 (8%)	231 (3%)	6	31

5 of 231 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SK	125	LYS
7	SM	62	PHE
16	SU	7	GLU
18	SD	48	SER
18	SD	134	TYR

### 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
4	SJ	90/90 (100%)	89 (99%)	1 (1%)	73 88
5	SK	98/98 (100%)	92 (94%)	6 (6%)	18 53
6	SL	103/103 (100%)	101 (98%)	2 (2%)	57 80
7	SM	95/95 (100%)	89 (94%)	6 (6%)	18 53
8	SN	83/83 (100%)	81 (98%)	2 (2%)	49 75
9	SO	76/76 (100%)	75 (99%)	1 (1%)	69 86
10	SP	65/65 (100%)	65 (100%)	0	100 100
11	SQ	77/77 (100%)	75 (97%)	2 (3%)	46 74
12	SR	64/64 (100%)	62 (97%)	2 (3%)	40 71
13	SS	78/78 (100%)	75 (96%)	3 (4%)	33 66
14	SB	198/198 (100%)	189 (96%)	9 (4%)	27 62
15	ST	65/65 (100%)	64 (98%)	1 (2%)	65 84
16	SU	60/60 (100%)	54 (90%)	6 (10%)	7 35
17	SC	189/189 (100%)	178 (94%)	11 (6%)	20 55
18	SD	172/172 (100%)	165 (96%)	7 (4%)	30 64
19	SE	125/125 (100%)	118 (94%)	7 (6%)	21 56
20	SF	116/116 (100%)	112 (97%)	4 (3%)	37 69
21	SG	146/146 (100%)	141 (97%)	5 (3%)	37 69
22	SH	104/104 (100%)	99 (95%)	5 (5%)	25 60
23	SI	106/106 (100%)	104 (98%)	2 (2%)	57 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	S1	575/575 (100%)	549 (96%)	26 (4%)	27	62
27	LC	181/181 (100%)	171 (94%)	10 (6%)	21	57
28	LM	99/99 (100%)	91 (92%)	8 (8%)	11	43
29	LN	217/217 (100%)	207 (95%)	10 (5%)	27	61
30	LO	89/89 (100%)	84 (94%)	5 (6%)	21	56
31	LP	84/84 (100%)	75 (89%)	9 (11%)	6	32
32	LQ	93/93 (100%)	92 (99%)	1 (1%)	73	88
33	LR	84/84 (100%)	79 (94%)	5 (6%)	19	54
34	LS	84/84 (100%)	80 (95%)	4 (5%)	25	60
35	LT	78/78 (100%)	74 (95%)	4 (5%)	24	58
36	LU	62/62 (100%)	57 (92%)	5 (8%)	11	43
37	LV	67/67 (100%)	65 (97%)	2 (3%)	41	71
38	LD	122/122 (100%)	120 (98%)	2 (2%)	62	83
39	LW	55/55 (100%)	53 (96%)	2 (4%)	35	67
40	LX	164/164 (100%)	157 (96%)	7 (4%)	29	63
41	LY	48/48 (100%)	46 (96%)	2 (4%)	30	63
42	L1	47/47 (100%)	44 (94%)	3 (6%)	17	52
43	L2	48/48 (100%)	48 (100%)	0	100	100
44	L3	38/38 (100%)	36 (95%)	2 (5%)	22	58
45	L4	51/51 (100%)	49 (96%)	2 (4%)	32	65
46	L5	34/34 (100%)	33 (97%)	1 (3%)	42	72
47	L6	165/165 (100%)	160 (97%)	5 (3%)	41	71
48	LE	109/109 (100%)	101 (93%)	8 (7%)	14	46
49	L7	149/149 (100%)	138 (93%)	11 (7%)	13	46
50	L8	137/137 (100%)	130 (95%)	7 (5%)	24	58
51	L9	114/114 (100%)	106 (93%)	8 (7%)	15	48
52	LF	116/116 (100%)	112 (97%)	4 (3%)	37	69
53	LG	104/104 (100%)	98 (94%)	6 (6%)	20	55
54	LH	103/103 (100%)	98 (95%)	5 (5%)	25	59
55	LI	109/109 (100%)	106 (97%)	3 (3%)	43	72
56	LJ	103/103 (100%)	98 (95%)	5 (5%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	LK	87/87 (100%)	82 (94%)	5 (6%)	20	55
58	LZ	62/62 (100%)	59 (95%)	3 (5%)	25	60
All	All	5788/5788 (100%)	5526 (96%)	262 (4%)	31	62

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	LF	34	ARG
53	LG	41	ILE
58	LZ	44	PHE
24	S1	377	ARG
24	S1	312	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
30	LO	43	GLN
52	LF	47	HIS
36	LU	56	HIS
50	L8	115	GLN
36	LU	45	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	SA	1542/1542 (100%)	308 (19%)	87 (5%)
2	S6	76/77 (98%)	13 (17%)	4 (5%)
25	LA	2903/2904 (99%)	557 (19%)	141 (4%)
26	LB	119/120 (99%)	20 (16%)	11 (9%)
3	S7	73/74 (98%)	29 (39%)	7 (9%)
All	All	4713/4717 (99%)	927 (19%)	250 (5%)

5 of 927 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	SA	2	A
1	SA	3	A
1	SA	4	U
1	SA	7	A

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Mol	Chain	Res	Type
1	SA	8	A

5 of 250 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	LA	428	A
25	LA	2473	U
25	LA	1142	A
25	LA	2452	C
25	LA	2835	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$
59	GTP	S1	801	-	26,34,34	1.81	3 (11%)	32,54,54	2.02	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GTP	S1	801	-	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	S1	801	GTP	C5-C6	-6.84	1.33	1.47
59	S1	801	GTP	C5-C4	-3.59	1.33	1.43
59	S1	801	GTP	O4'-C1'	2.02	1.43	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	S1	801	GTP	PB-O3B-PG	-6.78	109.56	132.83
59	S1	801	GTP	PA-O3A-PB	-3.75	119.94	132.83
59	S1	801	GTP	C2-N1-C6	-3.73	118.24	125.10
59	S1	801	GTP	C5-C6-N1	3.17	119.55	113.95
59	S1	801	GTP	C8-N7-C5	2.69	108.12	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	S1	801	GTP	O4'-C4'-C5'-O5'
59	S1	801	GTP	C3'-C4'-C5'-O5'

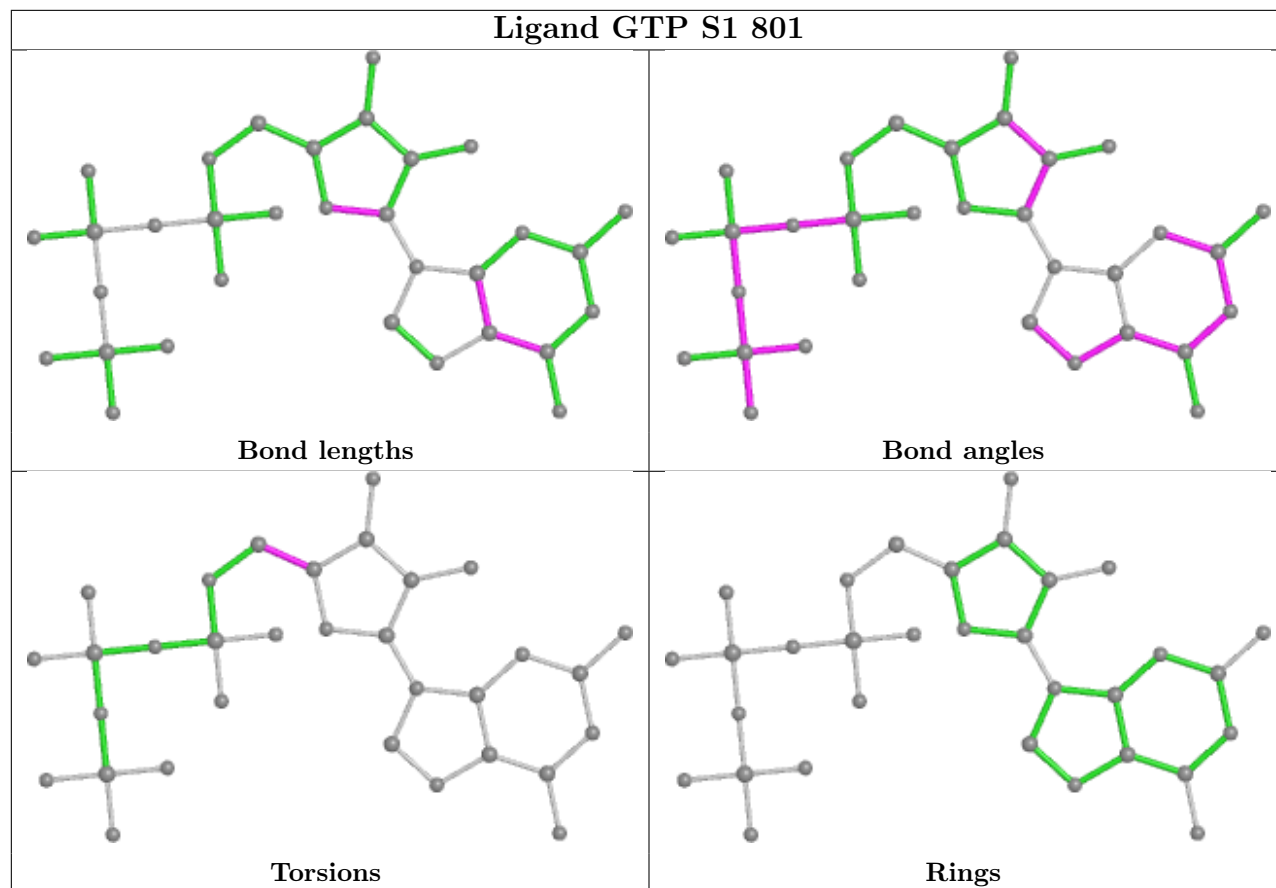
There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	S1	801	GTP	15	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.

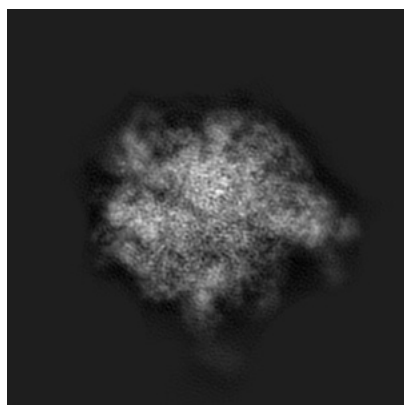
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6315. These allow visual inspection of the internal detail of the map and identification of artifacts.

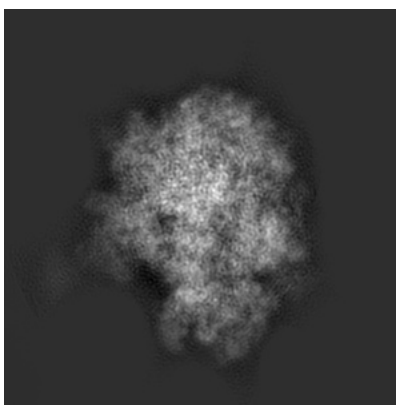
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

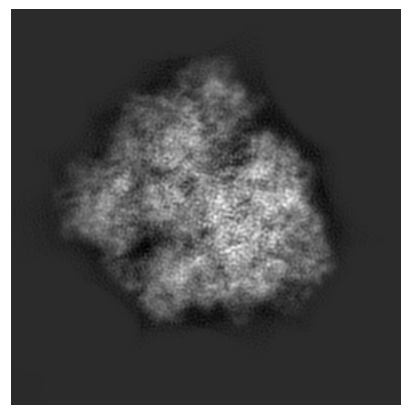
#### 6.1.1 Primary map



X



Y

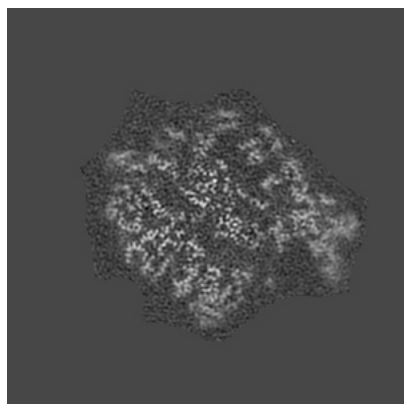


Z

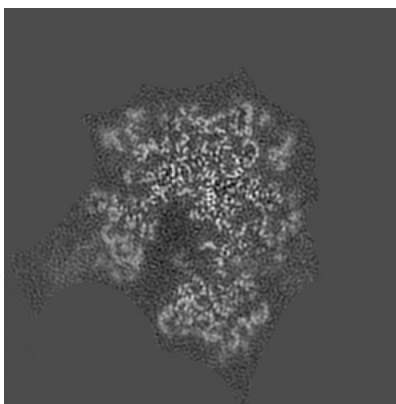
The images above show the map projected in three orthogonal directions.

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

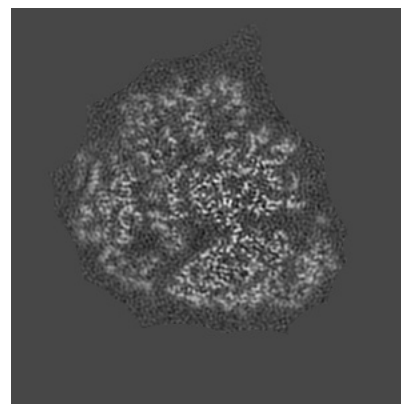
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

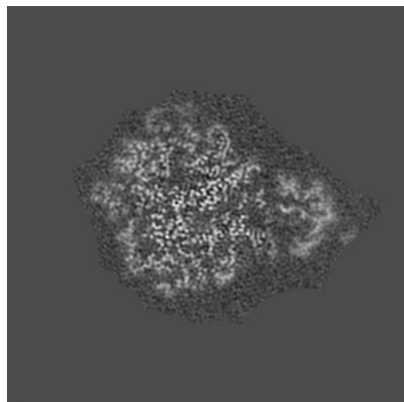


Z Index: 180

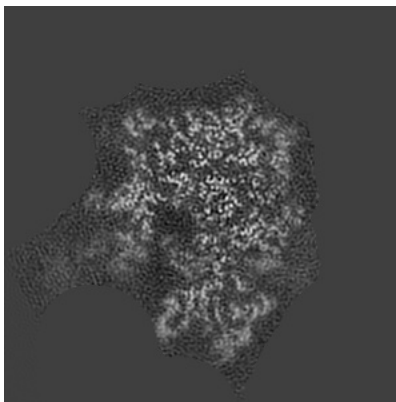
The images above show central slices of the map in three orthogonal directions.

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

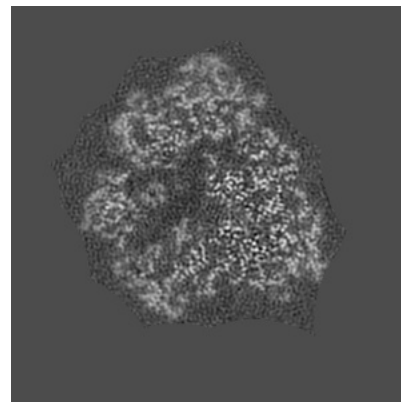
### 6.3.1 Primary map



X Index: 201



Y Index: 187

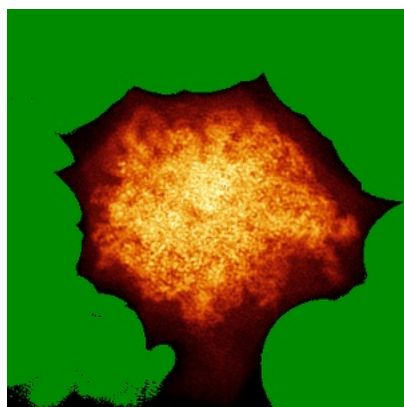


Z Index: 164

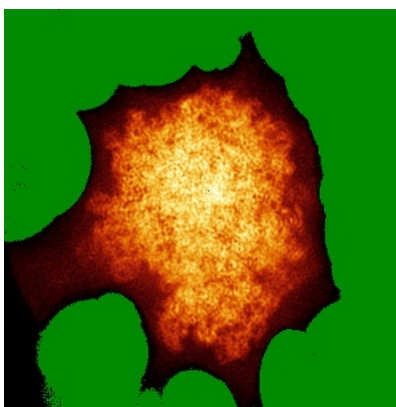
The images above show the largest variance slices of the map in three orthogonal directions.

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

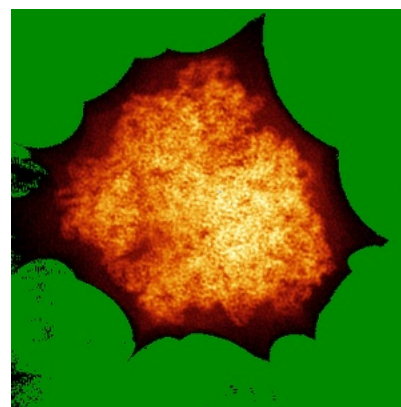
### 6.4.1 Primary map



X



Y

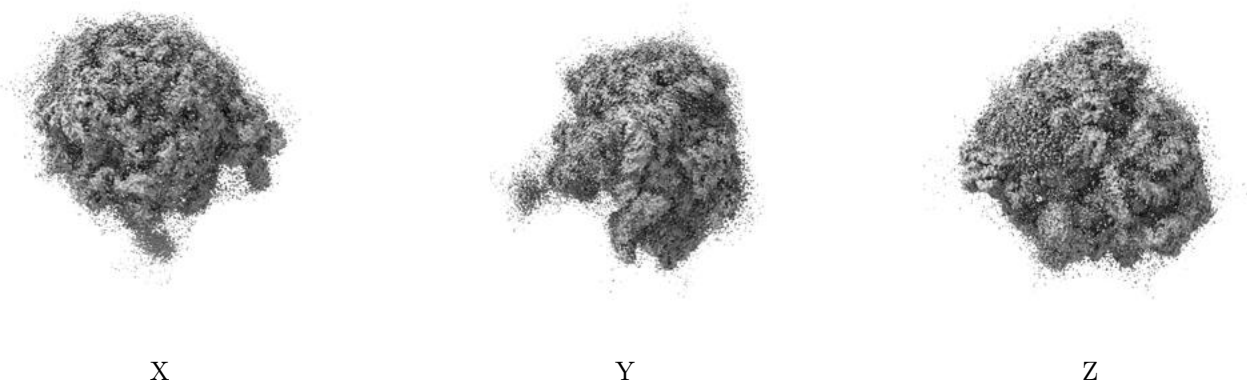


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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](#)

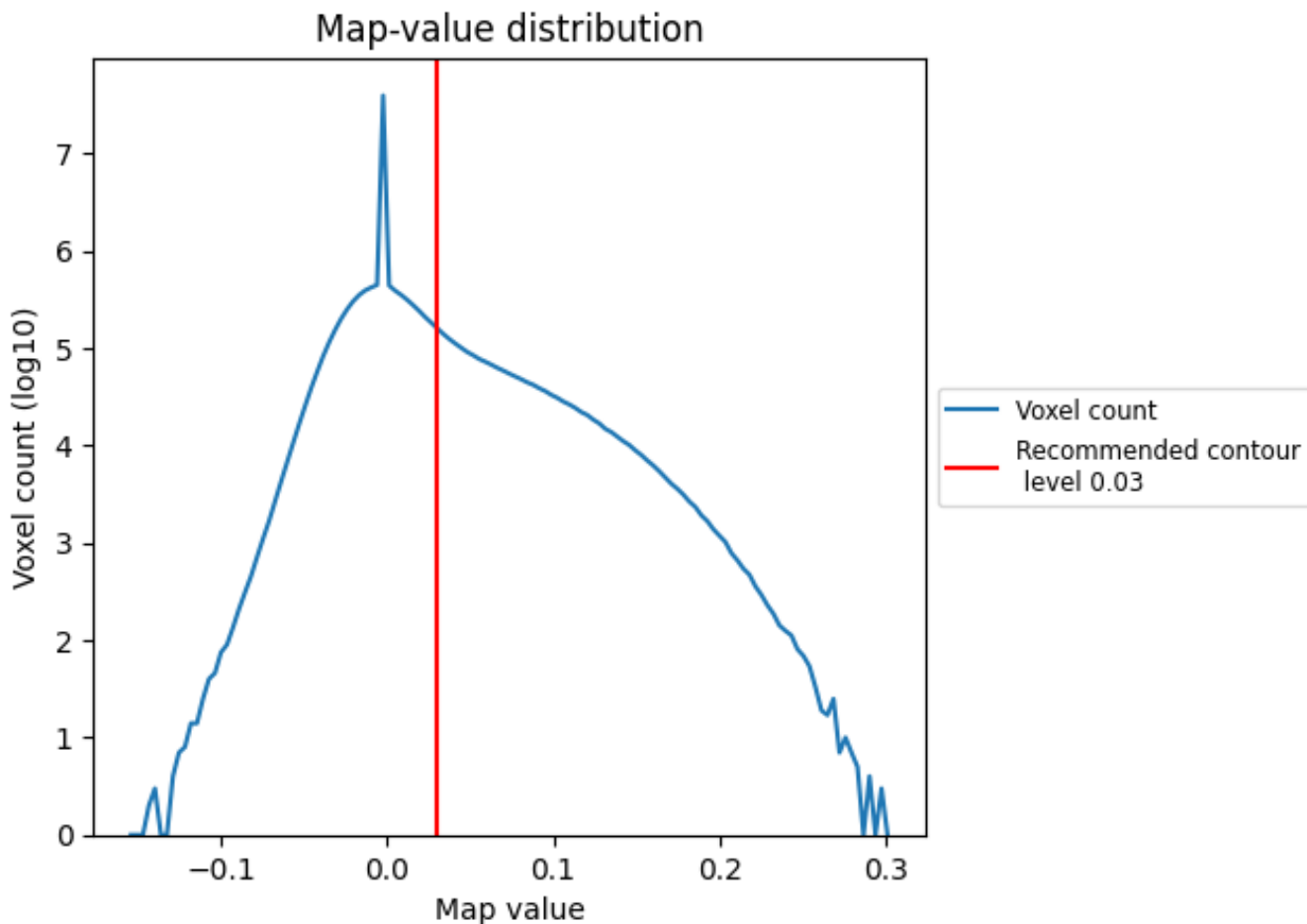
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

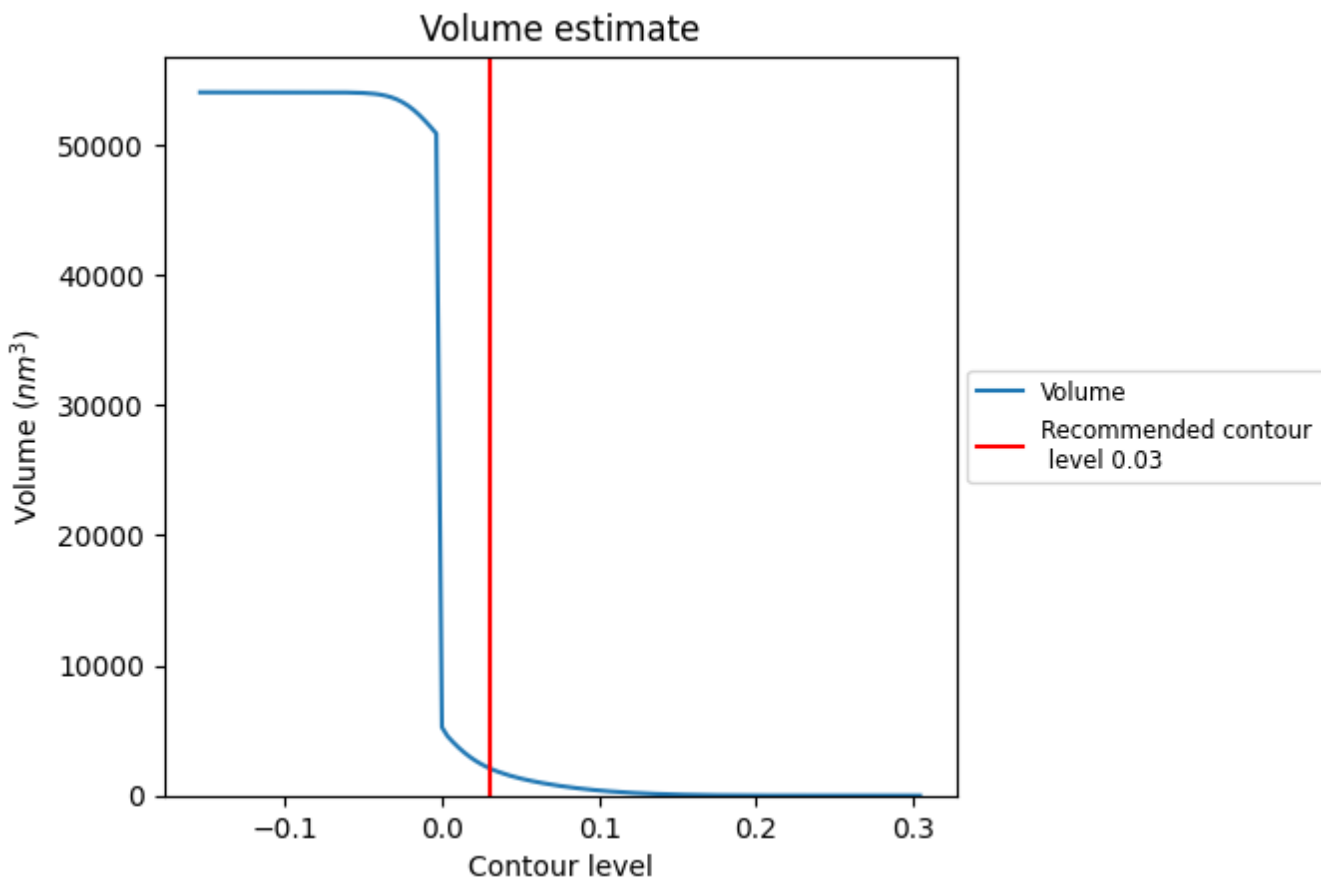
This section contains the results of statistical analysis of the map.

### 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.

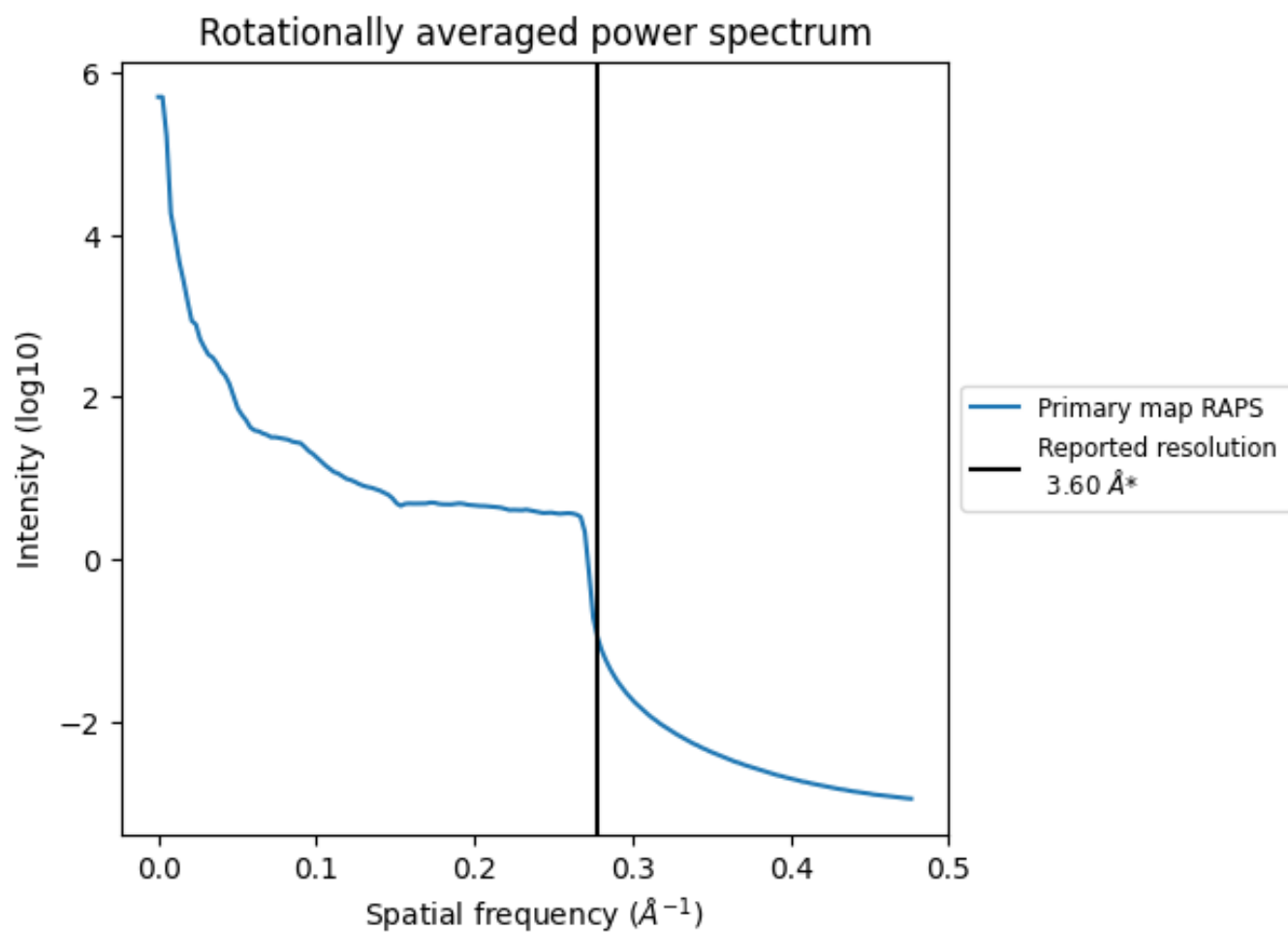
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2119 nm<sup>3</sup>; this corresponds to an approximate mass of 1915 kDa.

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

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



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

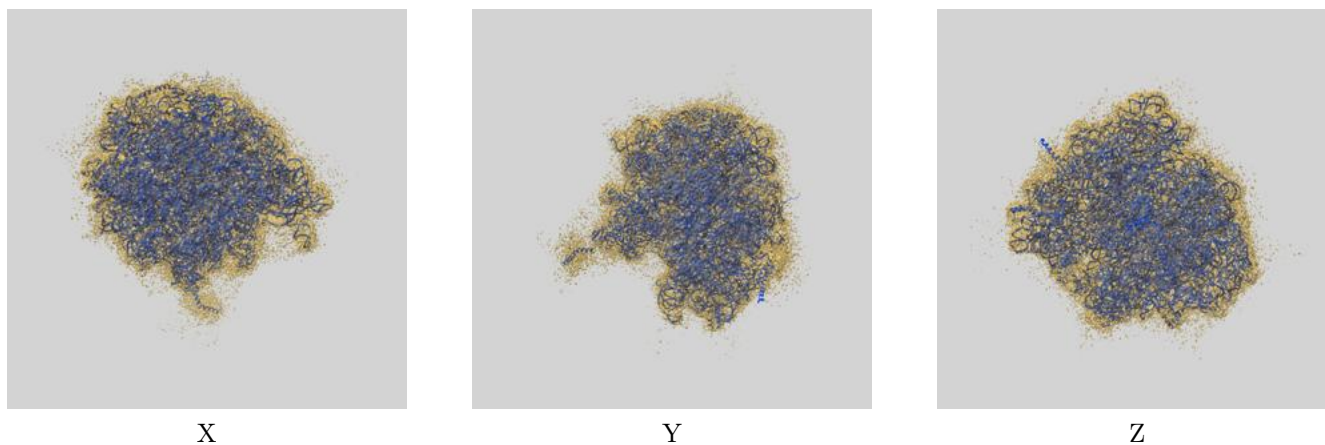
## 8 Fourier-Shell correlation

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

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

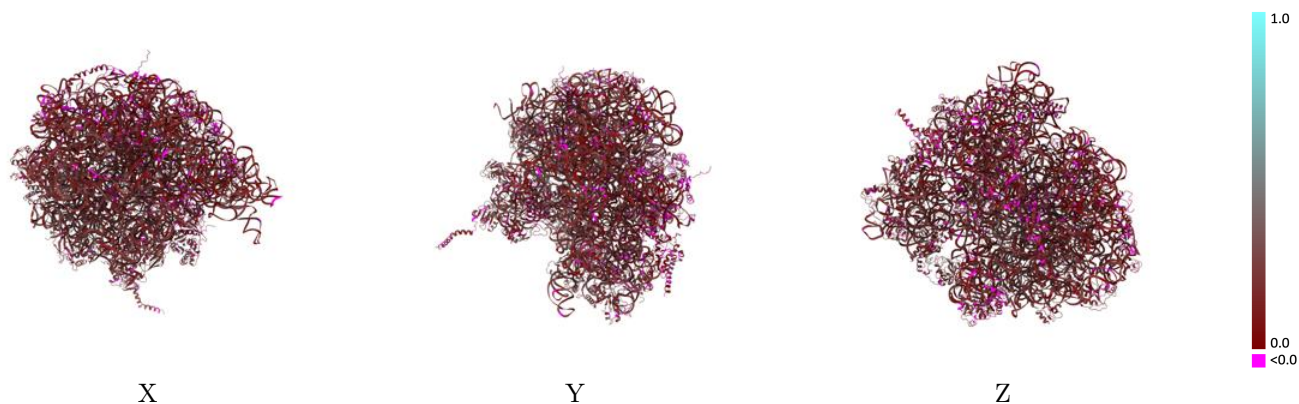
This section contains information regarding the fit between EMDB map EMD-6315 and PDB model 3J9Z. Per-residue inclusion information can be found in section 3 on page 16.

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



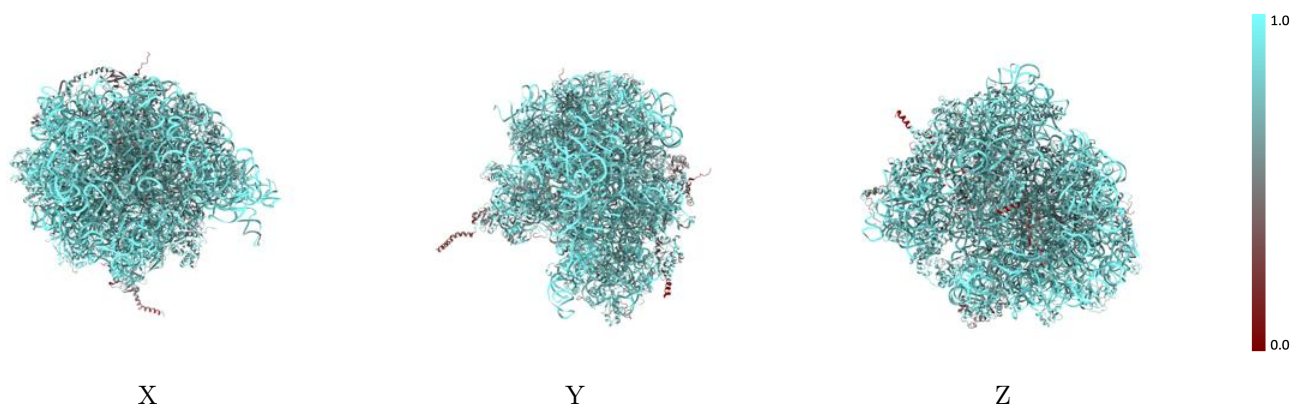
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



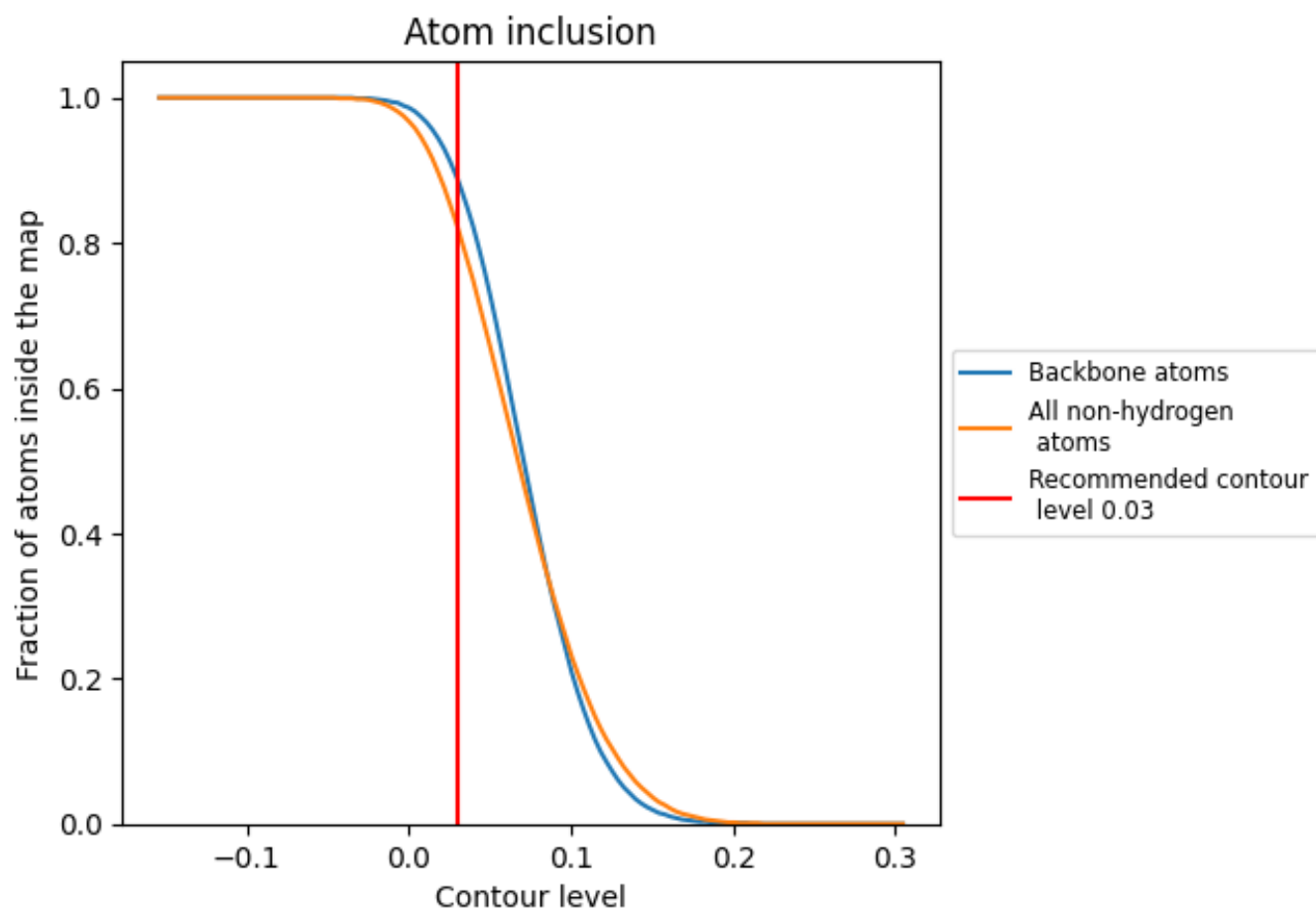
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.03) and Q-score for the entire model and for each chain.

















































Chain	Atom inclusion	Q-score
All	 0.8210	 0.1940
L1	 0.7380	 0.1660
L2	 0.7570	 0.2300
L3	 0.6760	 0.1490
L4	 0.7720	 0.2340
L5	 0.7880	 0.2560
L6	 0.7570	 0.1840
L7	 0.8160	 0.2540
L8	 0.8020	 0.2460
L9	 0.5100	 0.1070
LA	 0.8750	 0.2050
LB	 0.9630	 0.2750
LC	 0.6100	 0.1060
LD	 0.4940	 0.1870
LE	 0.7120	 0.1980
LF	 0.7910	 0.2260
LG	 0.6440	 0.1730
LH	 0.7810	 0.2110
LI	 0.8080	 0.2900
LJ	 0.6830	 0.1270
LK	 0.8530	 0.2540
LM	 0.6860	 0.1430
LN	 0.6740	 0.1470
LO	 0.7950	 0.2170
LP	 0.7880	 0.2220
LQ	 0.7140	 0.1760
LR	 0.6780	 0.1130
LS	 0.7900	 0.1340
LT	 0.8500	 0.3110
LU	 0.7280	 0.2380
LV	 0.7350	 0.1800
LW	 0.6800	 0.0770
LX	 0.7220	 0.1850
LY	 0.7990	 0.2660
LZ	 0.6410	 0.1850



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Chain	Atom inclusion	Q-score
S1	 0.7010	 0.1850
S6	 0.8650	 0.2260
S7	 0.8100	 0.1550
SA	 0.8840	 0.1920
SB	 0.6410	 0.1240
SC	 0.6850	 0.1890
SD	 0.7720	 0.1700
SE	 0.6680	 0.1570
SF	 0.5730	 0.0870
SG	 0.7070	 0.1740
SH	 0.7160	 0.1140
SI	 0.7600	 0.1720
SJ	 0.7000	 0.1970
SK	 0.6910	 0.1670
SL	 0.7130	 0.1850
SM	 0.7940	 0.2500
SN	 0.8000	 0.2190
SO	 0.6800	 0.0970
SP	 0.7580	 0.1140
SQ	 0.6980	 0.1110
SR	 0.6760	 0.1380
SS	 0.7610	 0.2490
ST	 0.7270	 0.1220
SU	 0.5980	 0.1600