



## wwPDB EM Validation Summary Report ⓘ

Mar 2, 2024 – 06:29 PM EST

PDB ID : 5UYN  
EMDB ID : EMD-8618  
Title : 70S ribosome bound with near-cognate ternary complex not base-paired to A site codon (Structure I-nc)  
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.  
Deposited on : 2017-02-24  
Resolution : 4.00 Å(reported)

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:

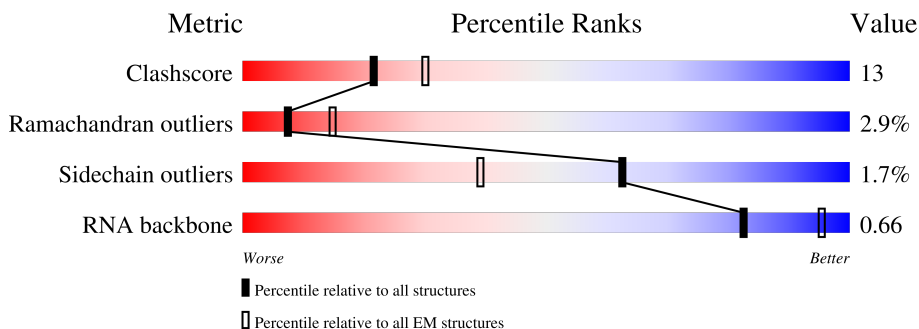
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	04	271	 65% 34%
2	05	209	 59% 40%
3	06	201	 60% 38%
4	07	177	 45% 55%
5	08	176	 62% 37%
6	09	149	 50% 43%
7	10	131	 47% 46% 5%

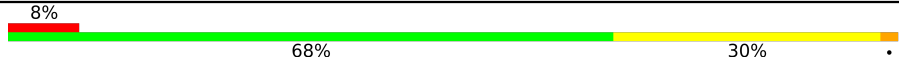

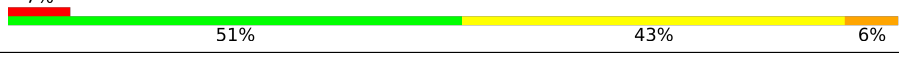
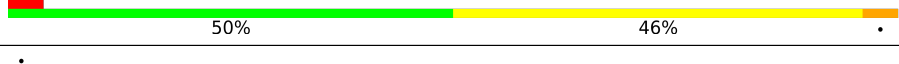



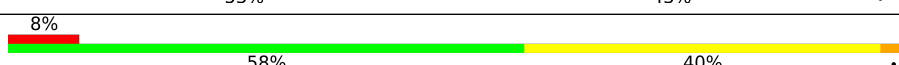



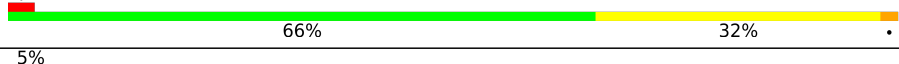
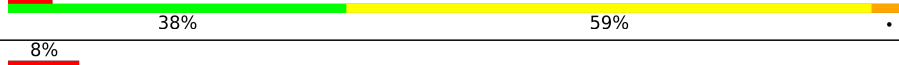




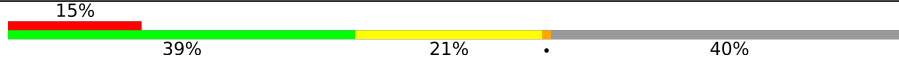







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Mol	Chain	Length	Quality of chain
8	11	141	
9	12	142	
10	13	122	
11	14	143	
12	15	136	
13	16	120	
14	17	116	
15	18	114	
16	19	117	
17	20	103	
18	21	110	
19	22	93	
20	23	102	
21	24	94	
22	25	75	
23	26	77	
24	27	63	
25	28	58	
26	29	66	
27	30	56	
28	31	50	
29	32	46	
30	33	64	
31	34	38	
32	B	218	

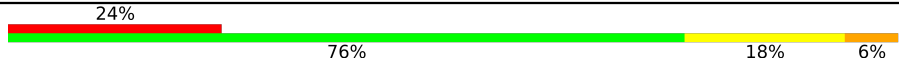


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Mol	Chain	Length	Quality of chain
33	C	206	
34	D	205	
35	E	157	
36	F	100	
37	G	151	
38	H	129	
39	I	127	
40	J	98	
41	K	116	
42	L	123	
43	M	114	
44	N	100	
45	O	88	
46	P	82	
47	Q	80	
48	R	65	
49	S	79	
50	T	85	
51	U	65	
52	03	223	
53	A	1539	
54	01	2903	
55	02	120	
56	W	77	
56	X	77	

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Mol	Chain	Length	Quality of chain
57	V	17	
58	Y	76	
59	Z	392	

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 153717 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	04	271	2083	1288	423	365	7	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	05	209	1565	979	288	294	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	06	201	1552	974	283	290	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	07	177	1411	899	249	257	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	08	176	1323	832	243	246	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	09	149	1111	699	197	214	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	10	131	989	625	175	184	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	11	141	1032	651	179	196	6	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	12	142	1129	714	212	199	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	13	122	939	587	180	166	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	14	143	1045	649	206	189	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	15	136	1074	686	205	177	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	16	120	961	593	196	167	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	E	157	1157	719	218	214	6	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	F	100	818	515	148	149	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	G	151	1182	735	227	216	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	J	98	787	493	150	143	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	K	116	870	535	173	159	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	R	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	S	79	638	408	120	108	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	U	65	545	335	117	92	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	03	134	1027	645	186	194	2	0	0

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	A	1539	33012	14725	6052	10697	1538	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	01	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	02	120	2568	1145	471	833	119	0	0

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	X	77	1640	732	297	535	76	0	0
56	W	77	1640	732	297	535	76	0	0

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	V	17	373	168	79	110	16	0	0

- Molecule 58 is a RNA chain called tRNA<sup>Lys</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
58	Y	76	1618	723	282	536	76	1	0	0

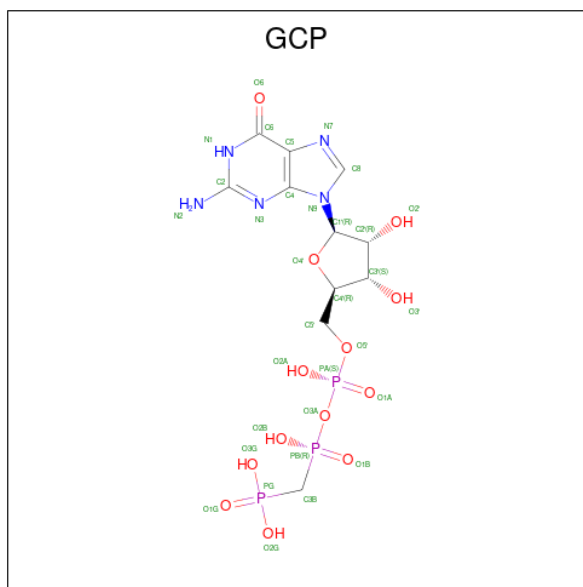
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	34	U8U	-	insertion	GB 558570689

- Molecule 59 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Z	392	3029	1915	521	580	13	0	0

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

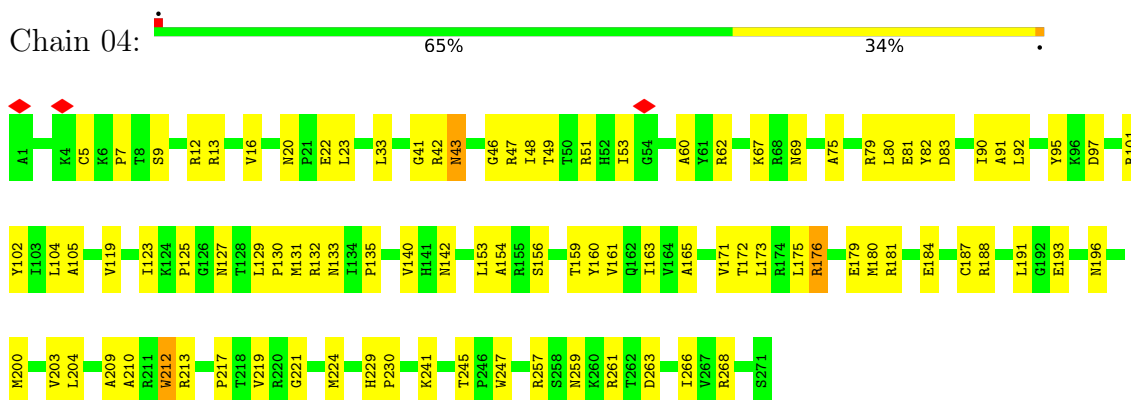


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	Z	1	32	11	5	13	3	0

### 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.

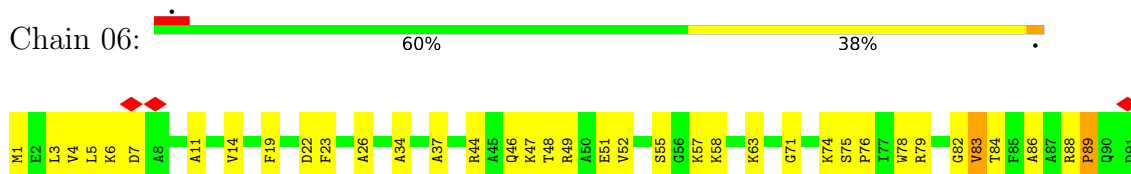
- Molecule 1: 50S ribosomal protein L2



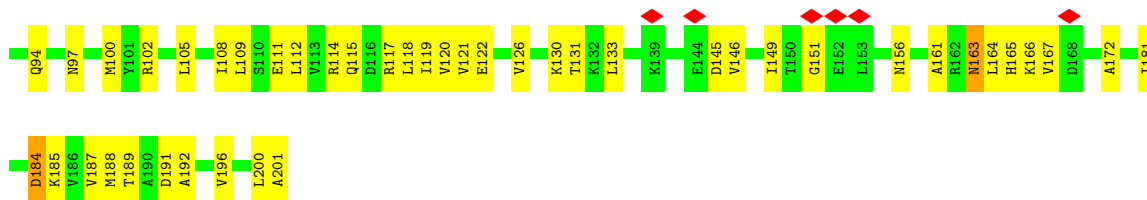
- Molecule 2: 50S ribosomal protein L3



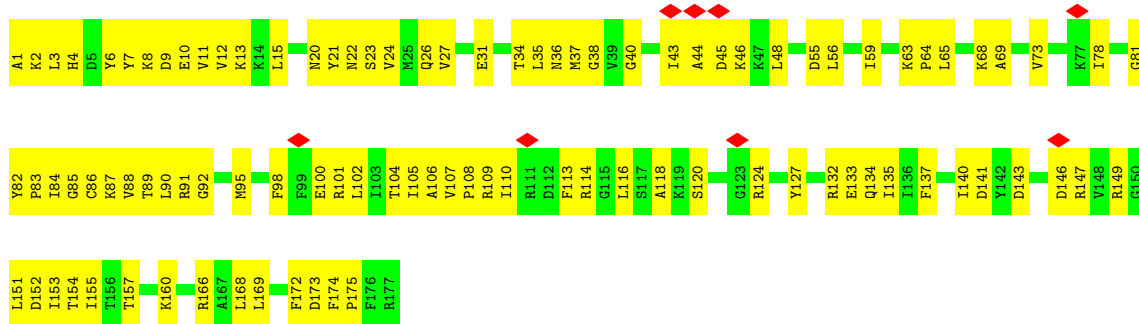
- Molecule 3: 50S ribosomal protein L4



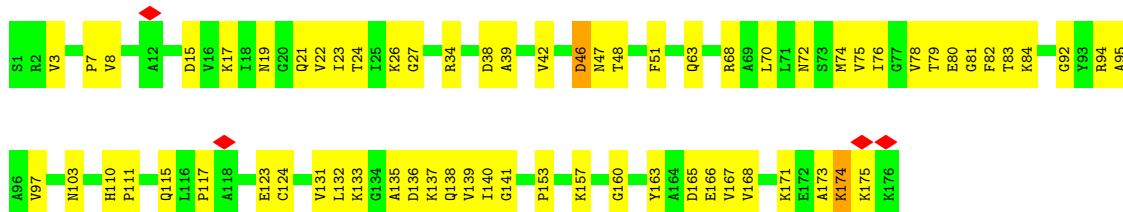




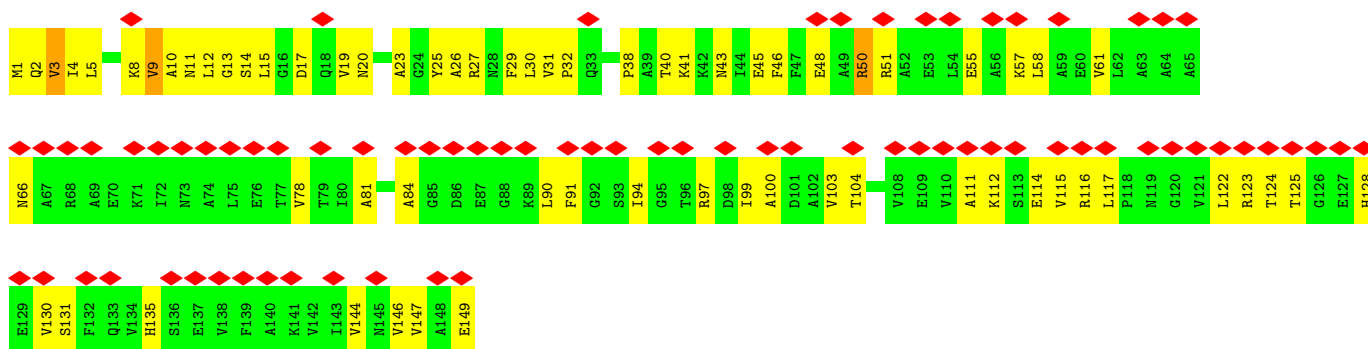
• Molecule 4: 50S ribosomal protein L5



• Molecule 5: 50S ribosomal protein L6

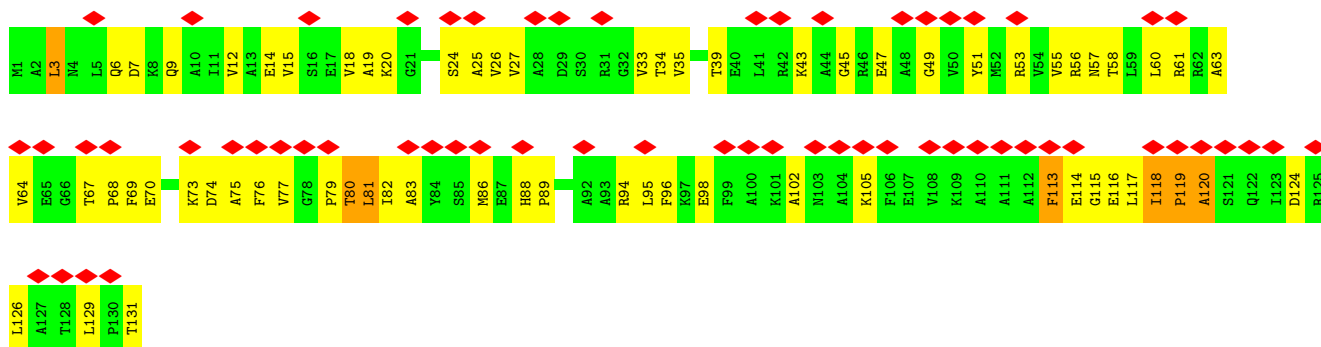


• Molecule 6: 50S ribosomal protein L9

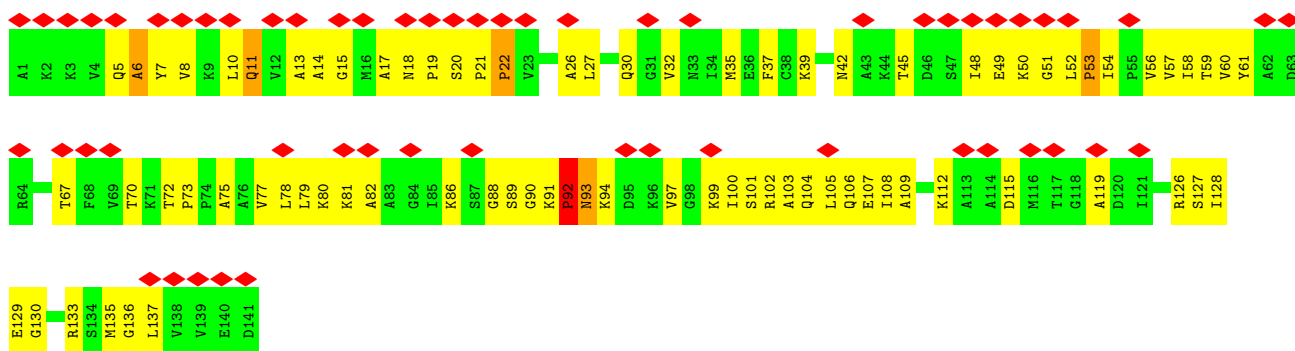
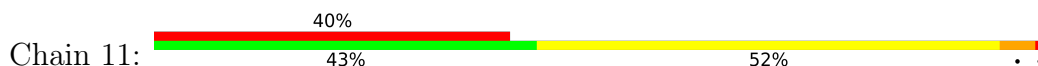


• Molecule 7: 50S ribosomal protein L10

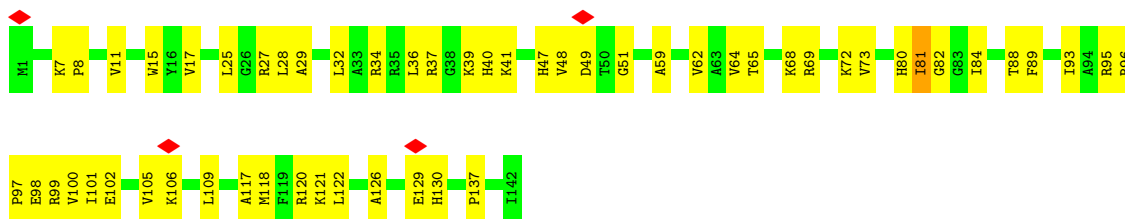




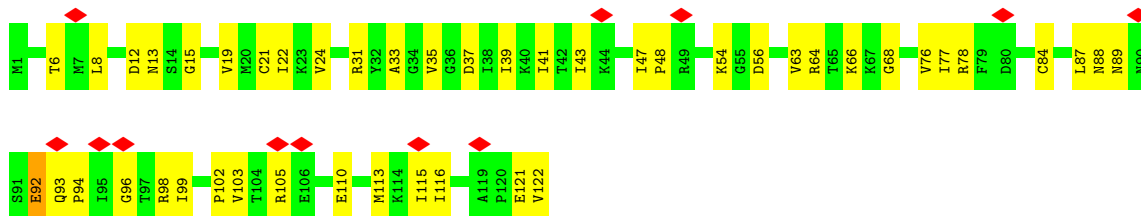
• Molecule 8: 50S ribosomal protein L11



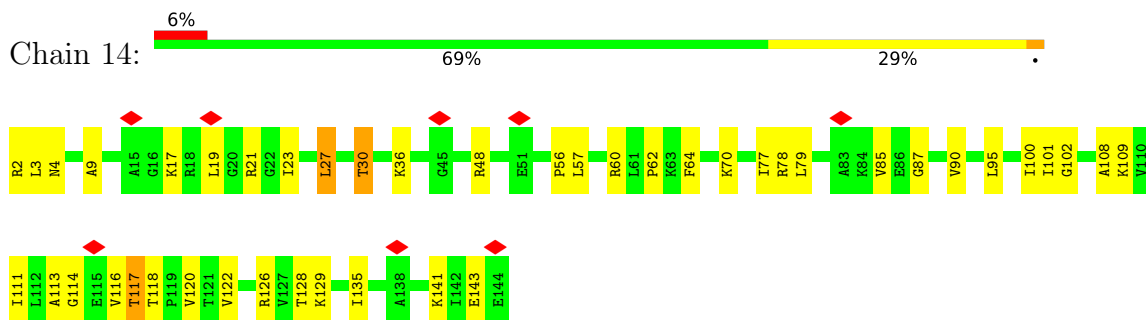
• Molecule 9: 50S ribosomal protein L13



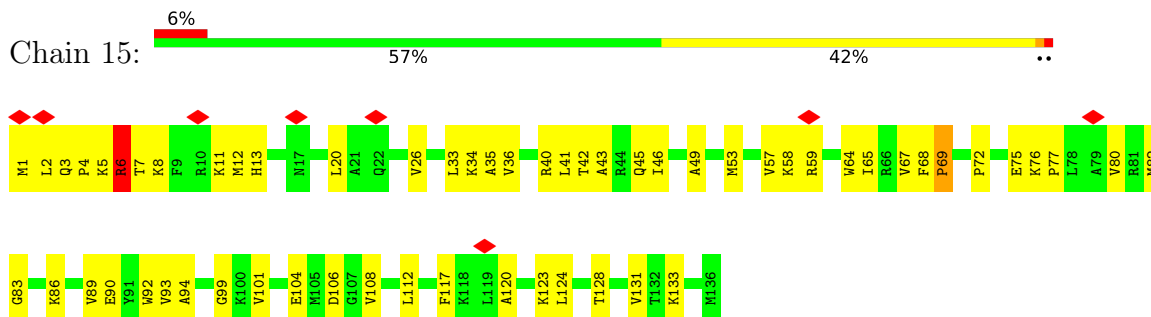
• Molecule 10: 50S ribosomal protein L14



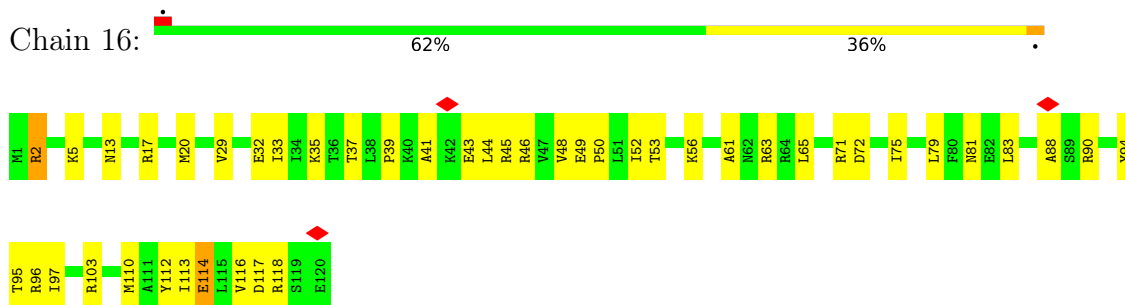
• Molecule 11: 50S ribosomal protein L15



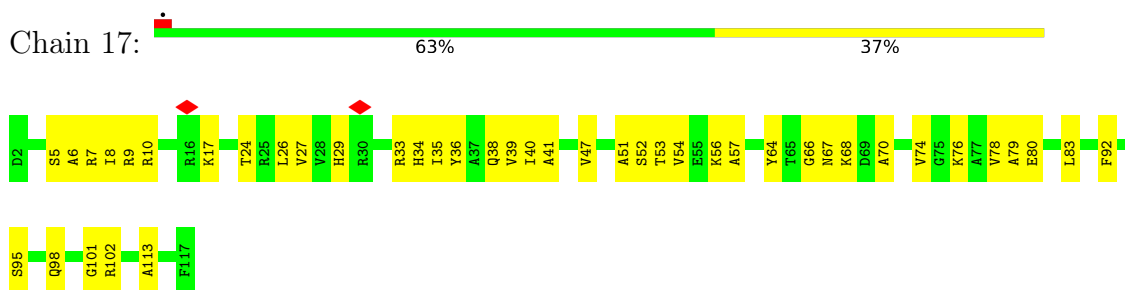
- Molecule 12: 50S ribosomal protein L16



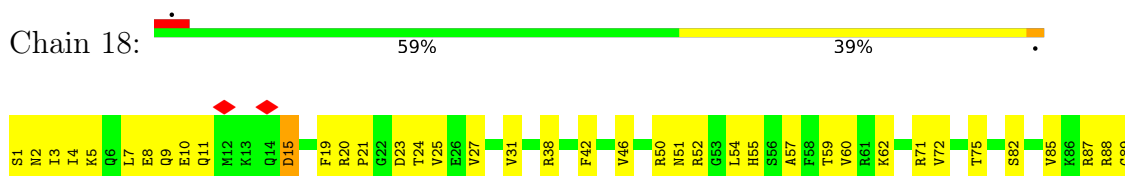
- Molecule 13: 50S ribosomal protein L17

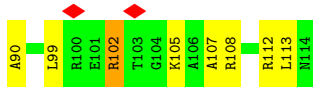


- Molecule 14: 50S ribosomal protein L18

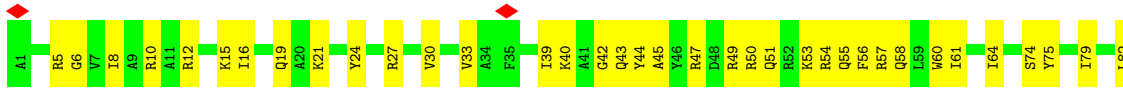


- Molecule 15: 50S ribosomal protein L19





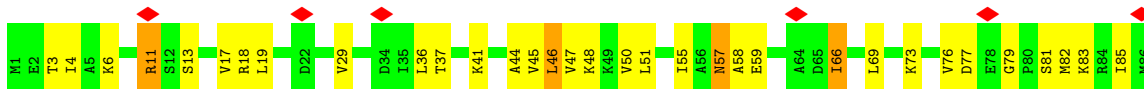
- Molecule 16: 50S ribosomal protein L20



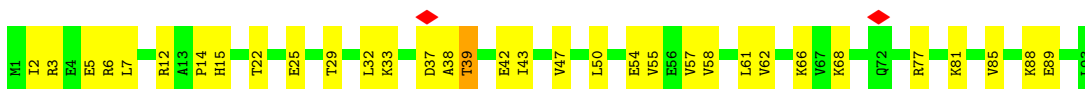
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

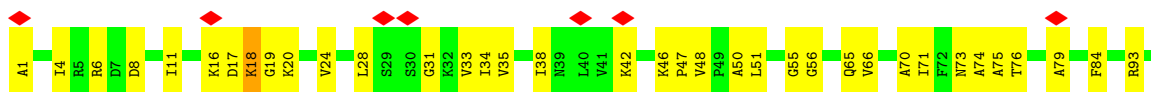


- Molecule 19: 50S ribosomal protein L23

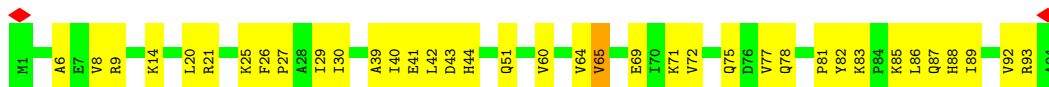


- Molecule 20: 50S ribosomal protein L24

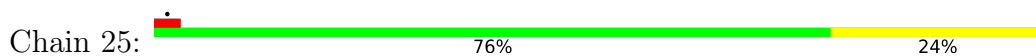




- Molecule 21: 50S ribosomal protein L25



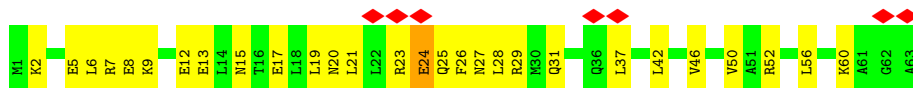
- Molecule 22: 50S ribosomal protein L27



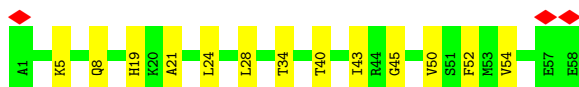
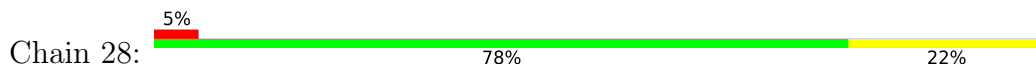
- Molecule 23: 50S ribosomal protein L28



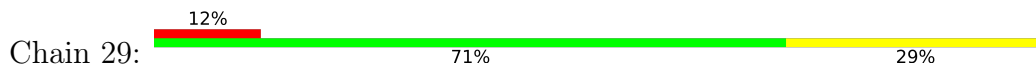
- Molecule 24: 50S ribosomal protein L29

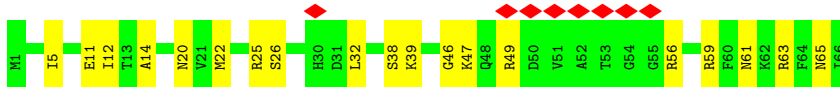


- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31

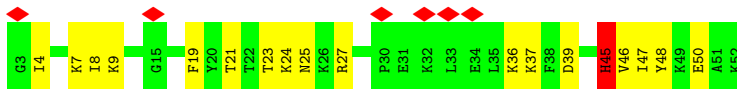




- Molecule 27: 50S ribosomal protein L32



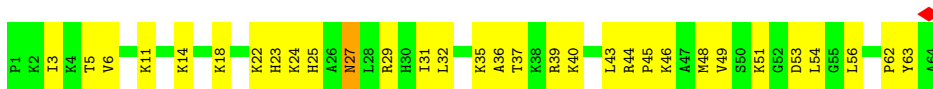
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



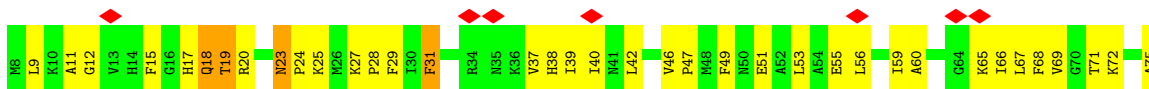
- Molecule 30: 50S ribosomal protein L35

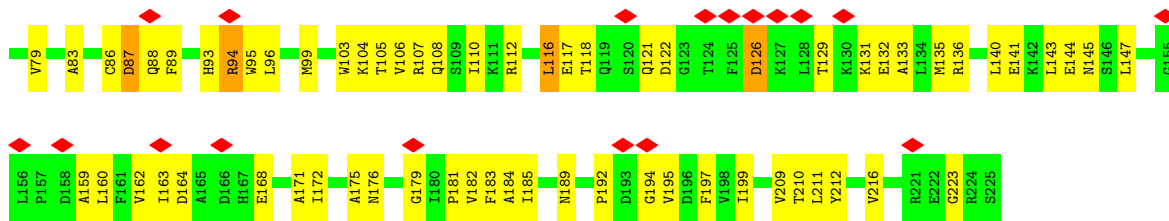


- Molecule 31: 50S ribosomal protein L36

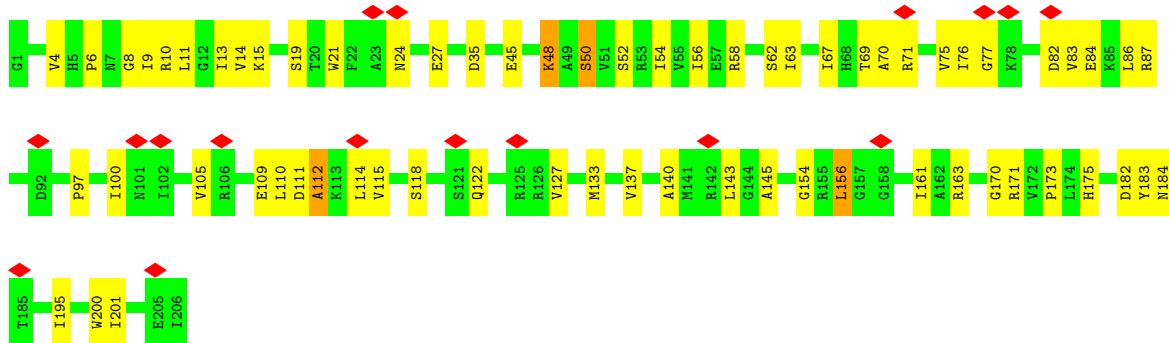


- Molecule 32: 30S ribosomal protein S2

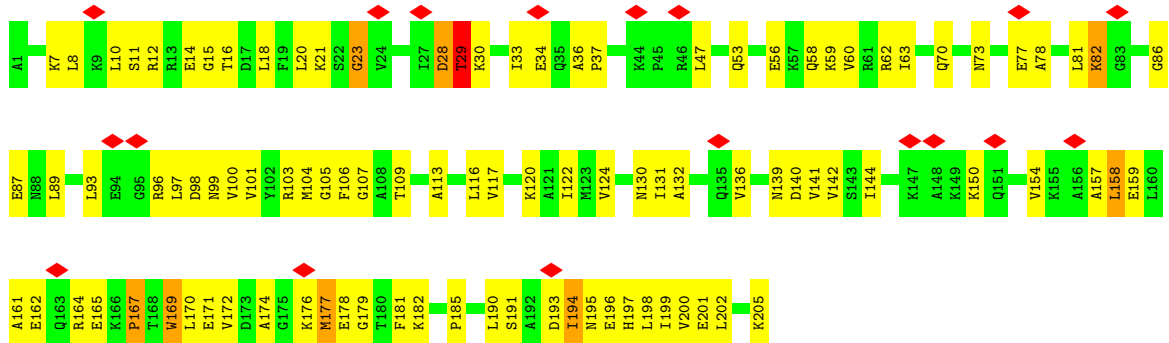




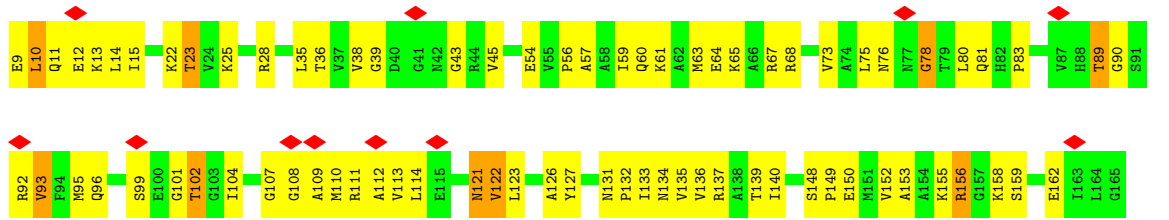
• Molecule 33: 30S ribosomal protein S3



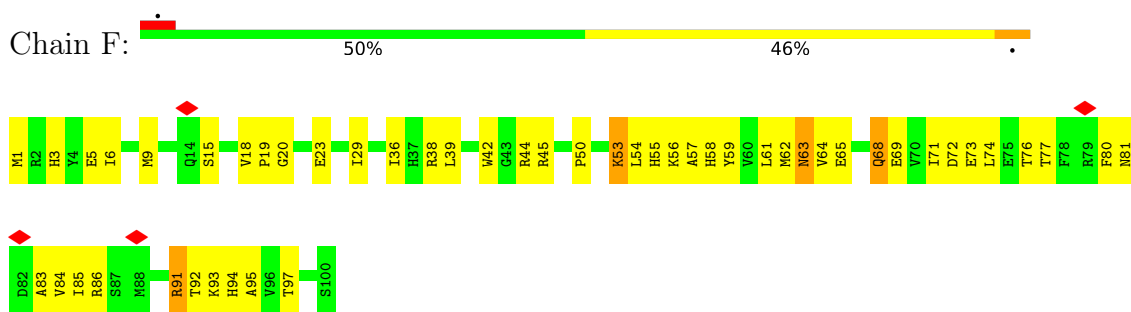
• Molecule 34: 30S ribosomal protein S4



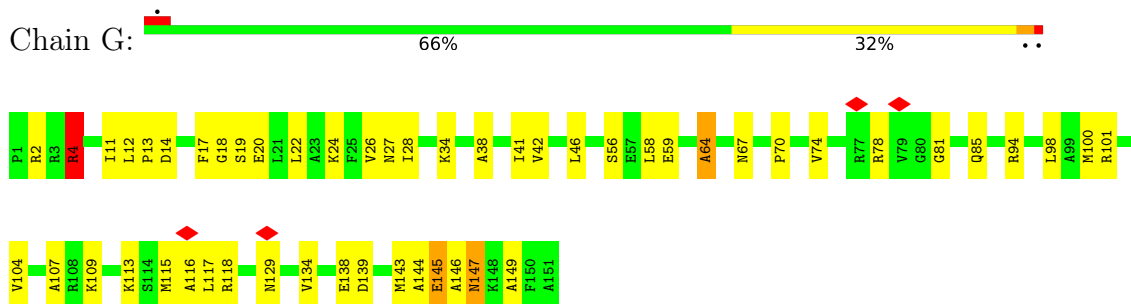
• Molecule 35: 30S ribosomal protein S5



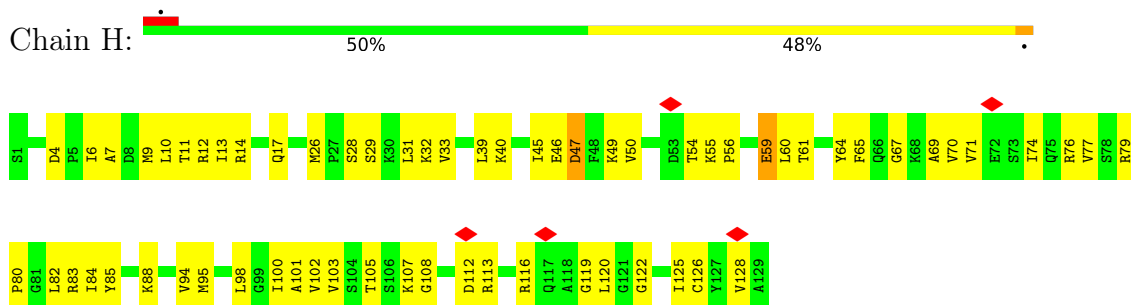
• Molecule 36: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S7



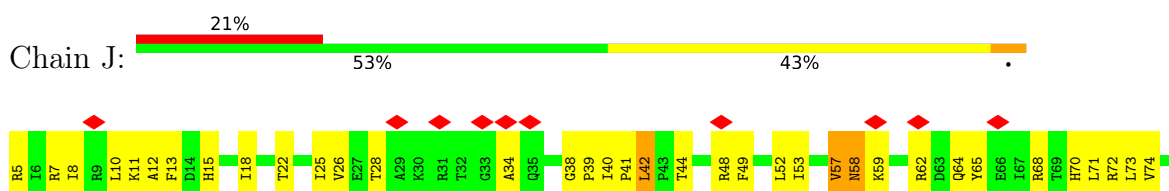
• Molecule 38: 30S ribosomal protein S8



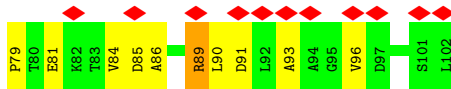
• Molecule 39: 30S ribosomal protein S9



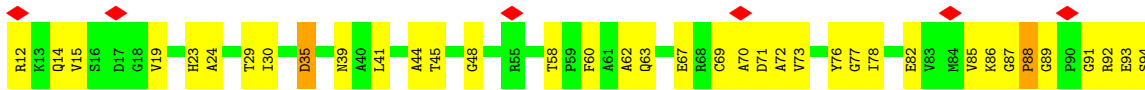
• Molecule 40: 30S ribosomal protein S10



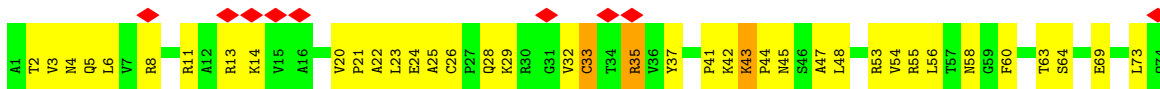




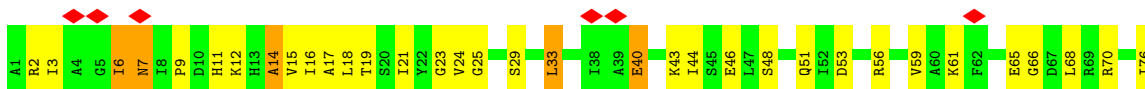
- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12



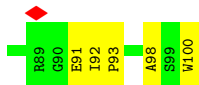
- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14

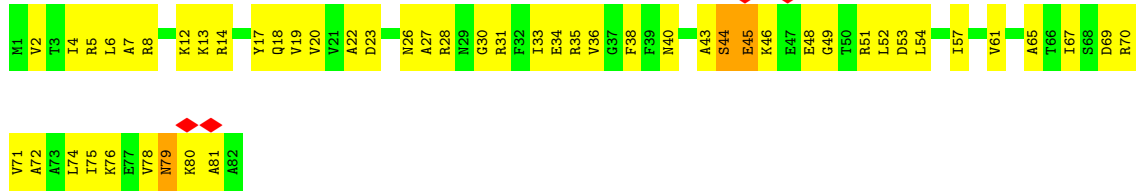


- Molecule 45: 30S ribosomal protein S15

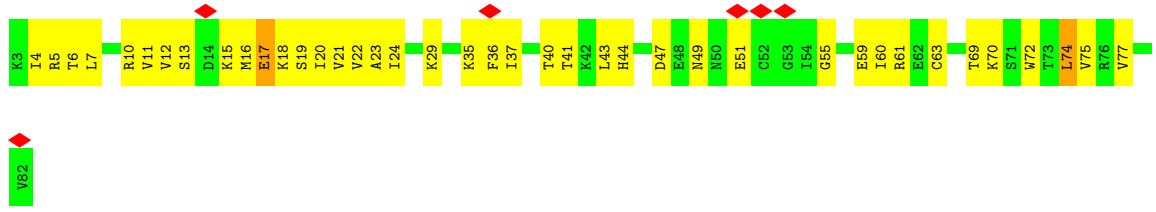




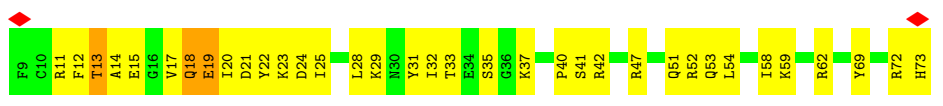
• Molecule 46: 30S ribosomal protein S16



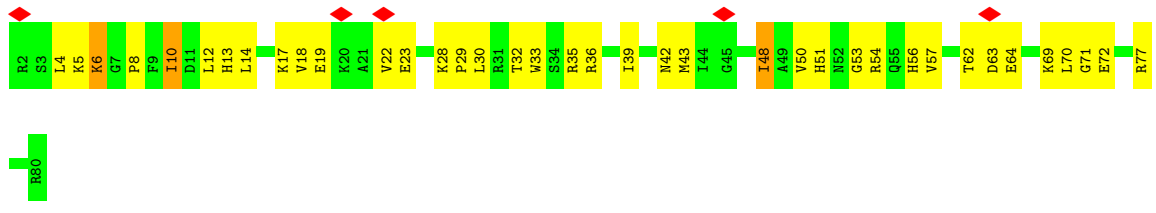
• Molecule 47: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S18

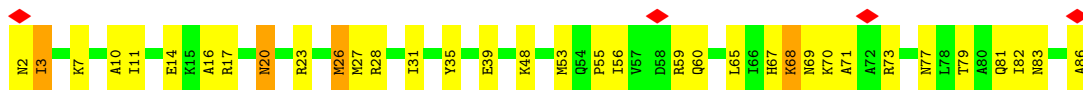


• Molecule 49: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S20

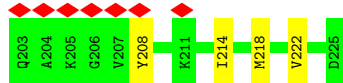
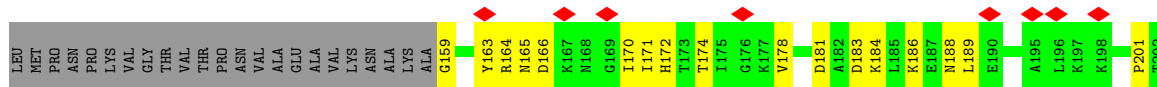
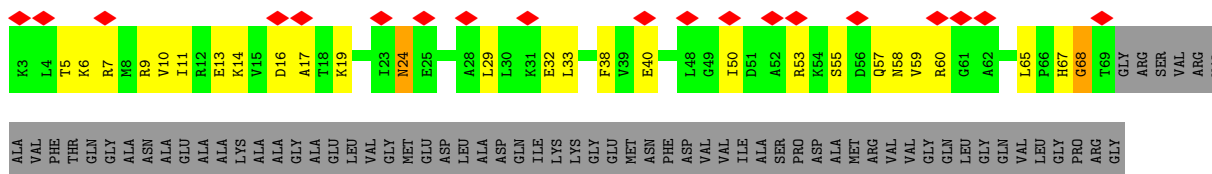




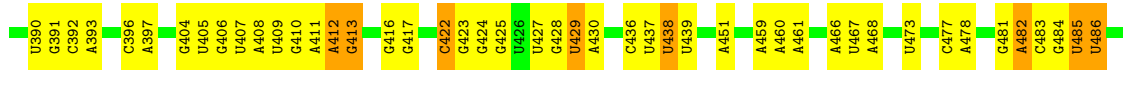
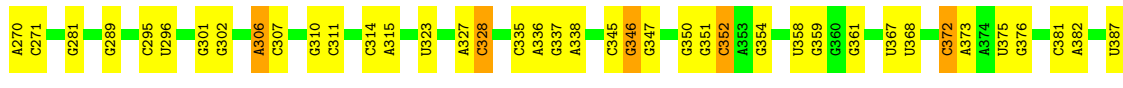
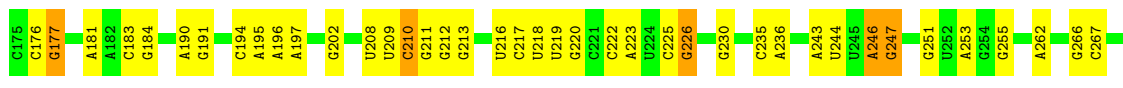
• Molecule 51: 30S ribosomal protein S21

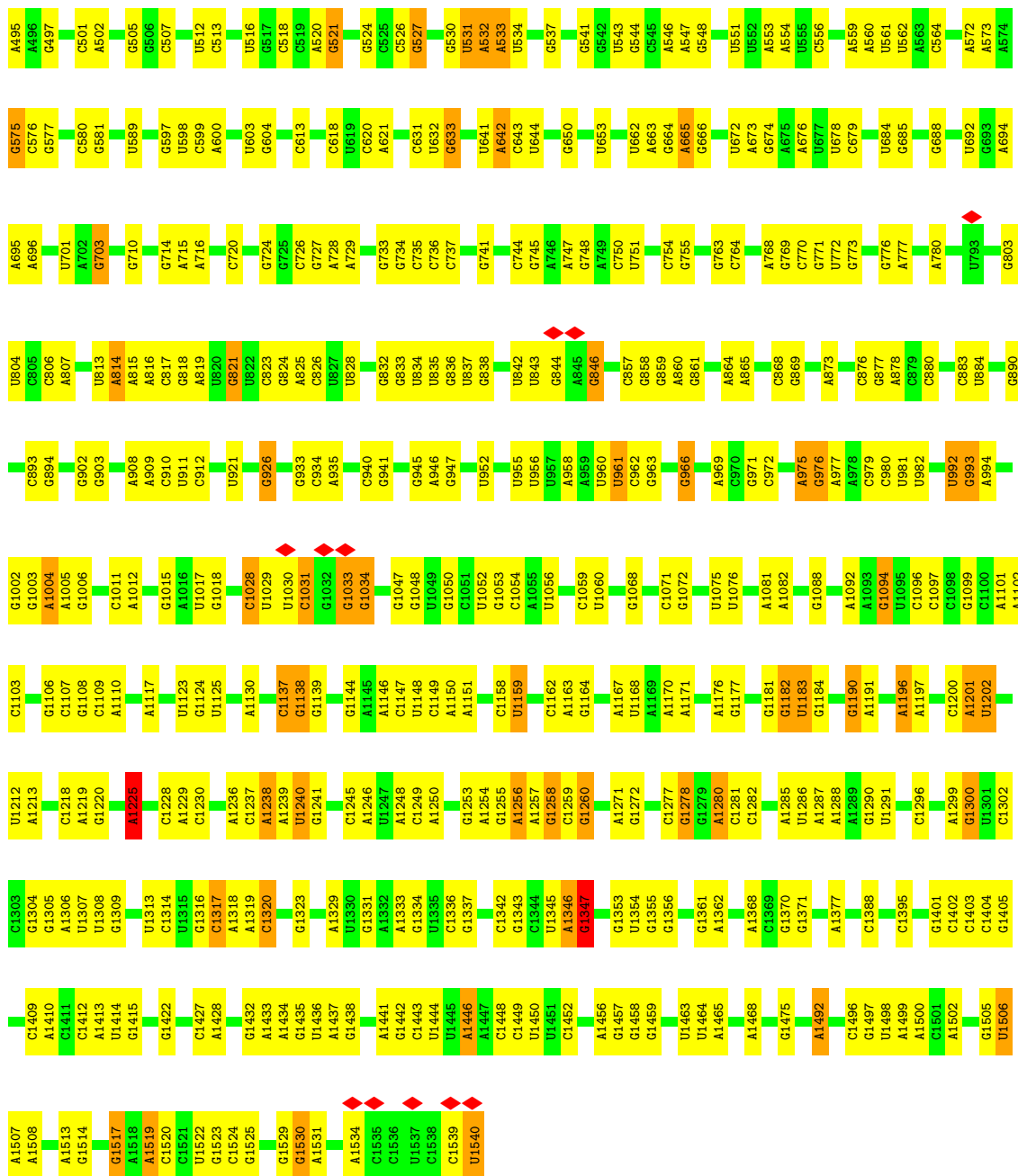


• Molecule 52: 50S ribosomal protein L1

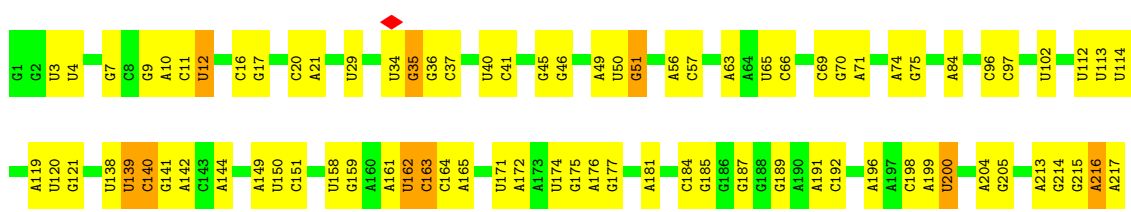


• Molecule 53: 16S ribosomal RNA

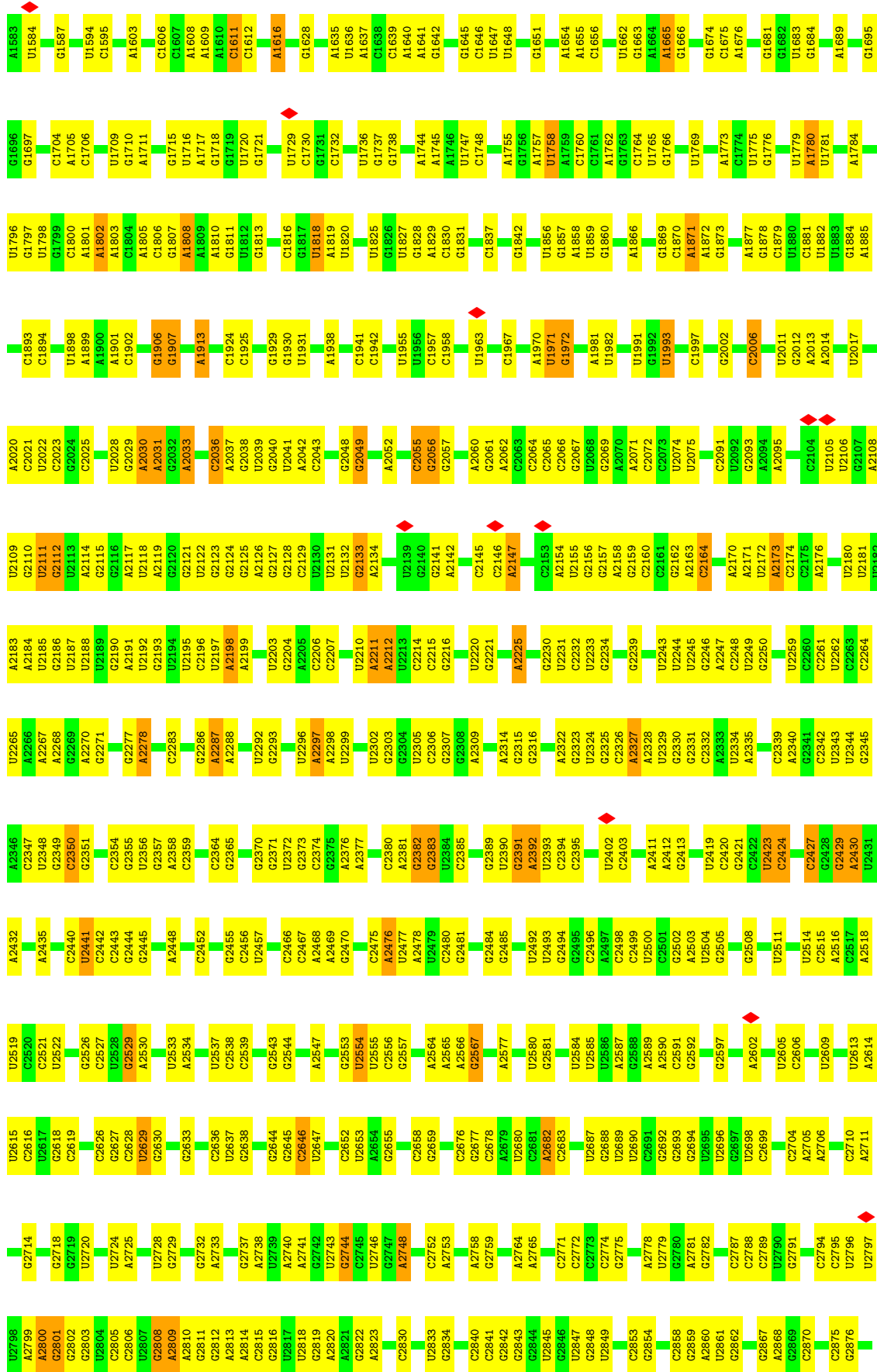


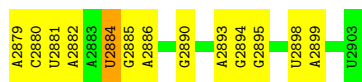


● Molecule 54: 23S ribosomal RNA

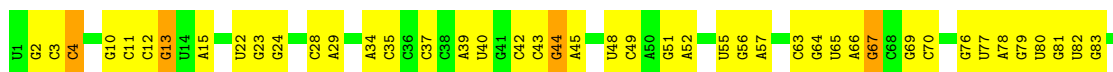




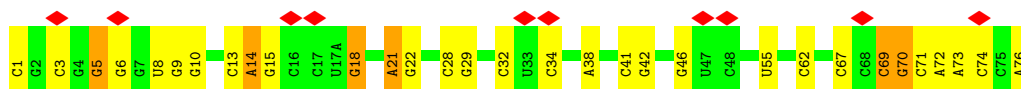




• Molecule 55: 5S ribosomal RNA



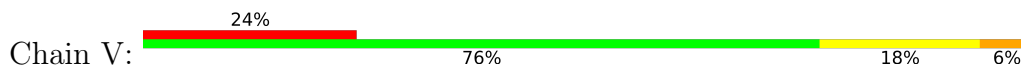
• Molecule 56: tRNAfMet



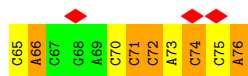
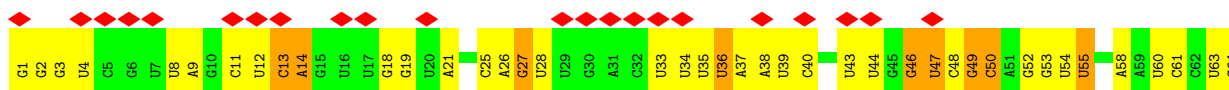
• Molecule 56: tRNAfMet



• Molecule 57: mRNA

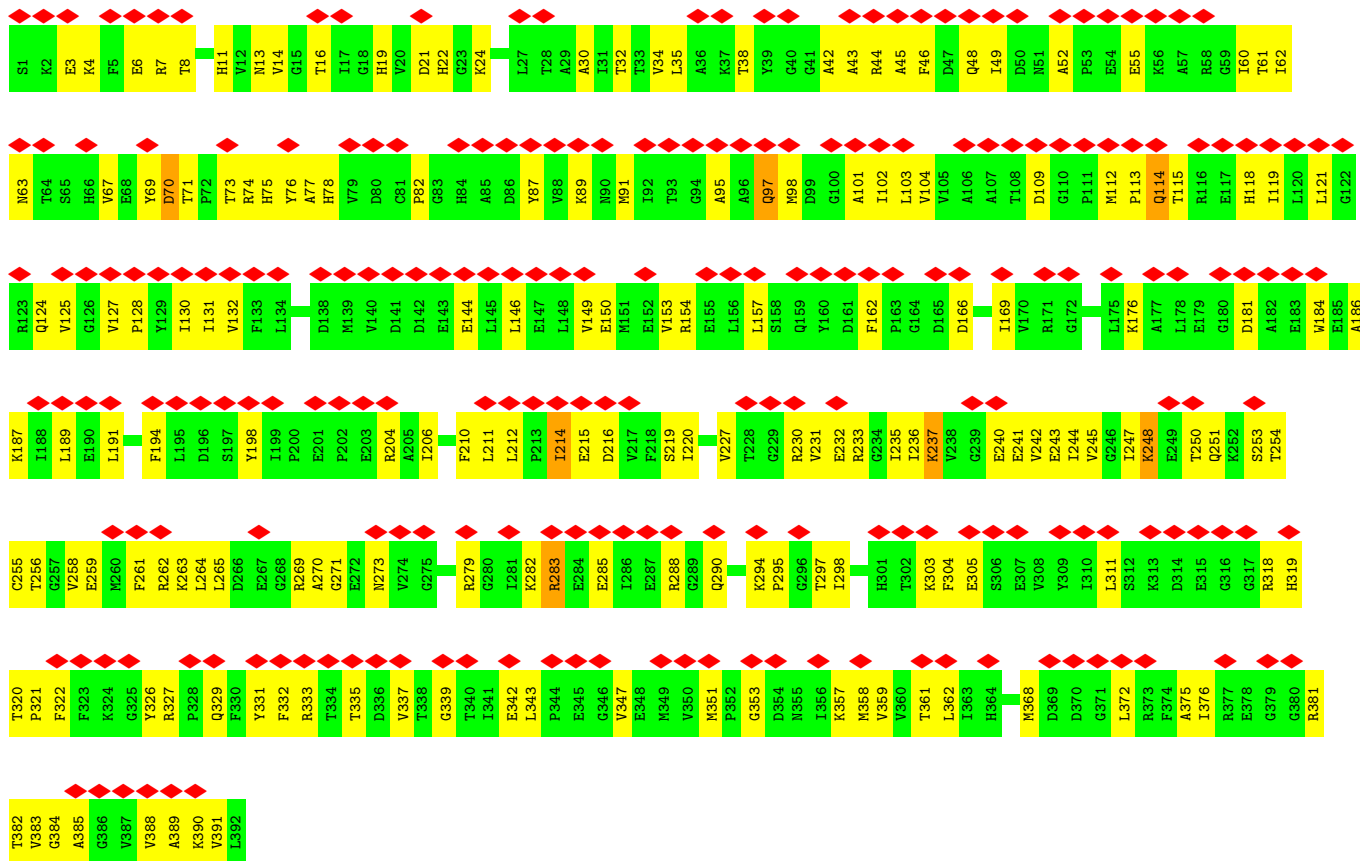


• Molecule 58: tRNA<sup>Lys</sup>



• Molecule 59: Elongation factor Tu 2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.452	Depositor
Minimum map value	-6.336	Depositor
Average map value	-0.325	Depositor
Map value standard deviation	1.041	Depositor
Recommended contour level	2.79	Depositor
Map size ( $\text{\AA}$ )	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	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: GCP, U8U

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	04	0.30	0/2122	0.54	0/2852
2	05	0.31	0/1586	0.55	0/2134
3	06	0.31	0/1571	0.56	0/2113
4	07	0.35	0/1435	0.54	0/1926
5	08	0.32	0/1343	0.59	0/1816
6	09	0.36	0/1122	0.61	0/1515
7	10	0.39	0/1002	0.66	0/1350
8	11	0.37	0/1046	0.64	0/1410
9	12	0.33	0/1152	0.55	0/1551
10	13	0.31	0/948	0.55	0/1268
11	14	0.32	0/1054	0.58	0/1403
12	15	0.34	0/1093	0.54	0/1460
13	16	0.33	0/974	0.55	0/1301
14	17	0.31	0/902	0.50	0/1209
15	18	0.32	0/929	0.56	0/1242
16	19	0.34	0/960	0.48	0/1278
17	20	0.34	0/829	0.62	0/1107
18	21	0.30	0/864	0.56	0/1156
19	22	0.32	0/745	0.55	0/994
20	23	0.33	0/788	0.60	1/1051 (0.1%)
21	24	0.33	0/766	0.56	0/1025
22	25	0.33	0/582	0.52	0/769
23	26	0.32	0/635	0.51	0/848
24	27	0.31	0/510	0.56	0/677
25	28	0.31	0/453	0.51	0/605
26	29	0.34	0/532	0.57	0/709
27	30	0.30	0/450	0.52	0/599
28	31	0.37	0/417	0.58	0/554
29	32	0.32	0/380	0.48	0/498
30	33	0.31	0/513	0.54	0/676
31	34	0.29	0/303	0.52	0/397
32	B	0.35	0/1736	0.60	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	C	0.33	0/1652	0.52	0/2225
34	D	0.34	0/1665	0.57	0/2227
35	E	0.33	0/1170	0.57	0/1573
36	F	0.34	0/836	0.56	0/1128
37	G	0.32	0/1196	0.57	0/1602
38	H	0.32	0/989	0.59	0/1326
39	I	0.34	0/1034	0.60	0/1375
40	J	0.32	0/797	0.60	0/1077
41	K	0.33	0/886	0.53	0/1195
42	L	0.32	0/969	0.64	0/1300
43	M	0.31	0/893	0.54	0/1193
44	N	0.33	0/817	0.53	0/1088
45	O	0.31	0/722	0.52	0/964
46	P	0.33	0/659	0.57	0/884
47	Q	0.34	0/658	0.57	0/881
48	R	0.37	0/545	0.59	0/731
49	S	0.35	0/653	0.56	0/877
50	T	0.31	0/671	0.50	0/888
51	U	0.38	0/551	0.62	0/728
52	03	0.35	0/1034	0.62	0/1387
53	A	0.38	0/36963	0.68	5/57662 (0.0%)
54	01	0.38	0/69796	0.68	6/108888 (0.0%)
55	02	0.40	0/2872	0.67	0/4479
56	W	0.42	0/1832	0.67	0/2855
56	X	0.46	0/1832	0.69	0/2855
57	V	0.43	0/421	0.70	0/657
58	Y	0.53	1/1780 (0.1%)	0.70	0/2767
59	Z	0.36	0/3085	0.60	0/4173
All	All	0.37	1/166720 (0.0%)	0.65	12/248816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	1	G	OP3-P	-7.14	1.52	1.61

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	01	1178	C	N1-C1'-C2'	6.88	122.94	114.00
54	01	1130	U	C2'-C3'-O3'	5.71	122.83	113.70
54	01	1818	U	N1-C1'-C2'	5.64	121.33	114.00
53	A	438	U	C2'-C3'-O3'	5.54	122.56	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	23	96	LYS	N-CA-C	-5.41	96.39	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	04	2083	0	2157	83	0
2	05	1565	0	1616	71	0
3	06	1552	0	1619	70	0
4	07	1411	0	1447	81	0
5	08	1323	0	1374	46	0
6	09	1111	0	1148	53	0
7	10	989	0	1025	51	0
8	11	1032	0	1088	71	0
9	12	1129	0	1162	45	0
10	13	939	0	1012	32	0
11	14	1045	0	1117	40	0
12	15	1074	0	1157	50	0
13	16	961	0	1000	39	0
14	17	892	0	923	31	0
15	18	917	0	965	42	0
16	19	947	0	1022	47	0
17	20	816	0	839	44	0
18	21	857	0	922	32	0
19	22	739	0	807	22	0
20	23	780	0	834	29	0
21	24	753	0	780	31	0
22	25	575	0	592	14	0
23	26	625	0	655	25	0
24	27	509	0	543	21	0
25	28	449	0	491	9	0
26	29	523	0	524	15	0
27	30	444	0	461	23	0
28	31	410	0	440	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	32	377	0	418	20	0
30	33	504	0	574	27	0
31	34	302	0	343	25	0
32	B	1705	0	1732	82	0
33	C	1625	0	1699	59	0
34	D	1643	0	1710	74	0
35	E	1157	0	1199	70	0
36	F	818	0	808	41	0
37	G	1182	0	1240	40	0
38	H	979	0	1034	52	0
39	I	1022	0	1070	57	0
40	J	787	0	828	37	0
41	K	870	0	878	43	0
42	L	955	0	1019	60	0
43	M	884	0	944	51	0
44	N	805	0	847	40	0
45	O	714	0	737	25	0
46	P	649	0	666	51	0
47	Q	649	0	691	34	0
48	R	536	0	552	36	0
49	S	638	0	665	37	0
50	T	665	0	714	34	0
51	U	545	0	579	32	0
52	03	1027	0	1092	41	0
53	A	33012	0	16618	461	0
54	01	62317	0	31346	876	0
55	02	2568	0	1303	55	0
56	W	1640	0	837	11	0
56	X	1640	0	837	19	0
57	V	373	0	187	2	0
58	Y	1618	0	821	37	0
59	Z	3029	0	3043	152	0
60	Z	32	0	14	1	0
All	All	153717	0	104765	3363	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 13.

The worst 5 of 3363 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)
54:01:45:G:H5''	54:01:46:G:H5'	1.37	1.06
12:15:45:GLN:HE21	54:01:2485:G:H5''	1.26	1.00
3:06:76:PRO:HA	3:06:82:GLY:HA2	1.45	0.94
54:01:1045:C:H5'	54:01:1046:A:H5'	1.49	0.93
6:09:12:LEU:HD22	6:09:19:VAL:HG11	1.51	0.93

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	04	269/271 (99%)	229 (85%)	37 (14%)	3 (1%)	14	51
2	05	207/209 (99%)	173 (84%)	30 (14%)	4 (2%)	8	40
3	06	199/201 (99%)	177 (89%)	19 (10%)	3 (2%)	10	45
4	07	175/177 (99%)	147 (84%)	26 (15%)	2 (1%)	14	51
5	08	174/176 (99%)	152 (87%)	18 (10%)	4 (2%)	6	37
6	09	147/149 (99%)	117 (80%)	22 (15%)	8 (5%)	2	21
7	10	129/131 (98%)	93 (72%)	26 (20%)	10 (8%)	1	14
8	11	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	1	18
9	12	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	46
10	13	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	3	25
11	14	141/143 (99%)	112 (79%)	23 (16%)	6 (4%)	2	25
12	15	134/136 (98%)	120 (90%)	10 (8%)	4 (3%)	4	32
13	16	118/120 (98%)	100 (85%)	16 (14%)	2 (2%)	9	43
14	17	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	8	41
15	18	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5	34
16	19	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	17	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	20	101/103 (98%)	78 (77%)	21 (21%)	2 (2%)	7	40
18	21	108/110 (98%)	92 (85%)	15 (14%)	1 (1%)	17	55
19	22	91/93 (98%)	72 (79%)	17 (19%)	2 (2%)	6	37
20	23	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	26
21	24	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	14	51
22	25	73/75 (97%)	61 (84%)	12 (16%)	0	100	100
23	26	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
24	27	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	44
25	28	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
26	29	64/66 (97%)	44 (69%)	20 (31%)	0	100	100
27	30	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
28	31	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	39
29	32	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
30	33	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	4	31
31	34	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	20
32	B	216/218 (99%)	174 (81%)	35 (16%)	7 (3%)	4	31
33	C	204/206 (99%)	186 (91%)	15 (7%)	3 (2%)	10	45
34	D	203/205 (99%)	167 (82%)	28 (14%)	8 (4%)	3	26
35	E	155/157 (99%)	123 (79%)	21 (14%)	11 (7%)	1	16
36	F	98/100 (98%)	79 (81%)	11 (11%)	8 (8%)	1	13
37	G	149/151 (99%)	124 (83%)	20 (13%)	5 (3%)	3	30
38	H	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	36
39	I	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	3	26
40	J	96/98 (98%)	67 (70%)	22 (23%)	7 (7%)	1	15
41	K	114/116 (98%)	89 (78%)	20 (18%)	5 (4%)	2	24
42	L	121/123 (98%)	85 (70%)	28 (23%)	8 (7%)	1	17
43	M	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	3	28
44	N	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	7	40
45	O	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	29
46	P	80/82 (98%)	62 (78%)	14 (18%)	4 (5%)	2	22
47	Q	78/80 (98%)	63 (81%)	13 (17%)	2 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R	63/65 (97%)	52 (82%)	8 (13%)	3 (5%)	2	23
49	S	77/79 (98%)	64 (83%)	11 (14%)	2 (3%)	5	34
50	T	83/85 (98%)	75 (90%)	6 (7%)	2 (2%)	6	36
51	U	63/65 (97%)	38 (60%)	21 (33%)	4 (6%)	1	18
52	03	130/223 (58%)	105 (81%)	23 (18%)	2 (2%)	10	45
59	Z	390/392 (100%)	337 (86%)	49 (13%)	4 (1%)	15	53
All	All	6366/6563 (97%)	5298 (83%)	882 (14%)	186 (3%)	7	32

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	06	83	VAL
3	06	184	ASP
5	08	46	ASP
5	08	174	LYS
6	09	9	VAL

### 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	04	216/216 (100%)	210 (97%)	6 (3%)	43	65
2	05	164/164 (100%)	161 (98%)	3 (2%)	59	77
3	06	165/165 (100%)	163 (99%)	2 (1%)	71	84
4	07	148/148 (100%)	146 (99%)	2 (1%)	67	81
5	08	137/137 (100%)	135 (98%)	2 (2%)	65	80
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	100 (100%)	0	100	100
8	11	109/109 (100%)	107 (98%)	2 (2%)	59	77
9	12	116/116 (100%)	116 (100%)	0	100	100
10	13	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	14	102/102 (100%)	100 (98%)	2 (2%)	55	73
12	15	109/109 (100%)	108 (99%)	1 (1%)	78	88
13	16	100/100 (100%)	98 (98%)	2 (2%)	55	73
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	97 (98%)	2 (2%)	55	73
16	19	89/89 (100%)	89 (100%)	0	100	100
17	20	84/84 (100%)	82 (98%)	2 (2%)	49	69
18	21	93/93 (100%)	90 (97%)	3 (3%)	39	62
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	68
20	23	83/83 (100%)	82 (99%)	1 (1%)	71	84
21	24	78/78 (100%)	78 (100%)	0	100	100
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	67 (100%)	0	100	100
24	27	55/55 (100%)	55 (100%)	0	100	100
25	28	48/48 (100%)	48 (100%)	0	100	100
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	46 (98%)	1 (2%)	53	72
28	31	45/45 (100%)	44 (98%)	1 (2%)	52	71
29	32	38/38 (100%)	38 (100%)	0	100	100
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	34 (100%)	0	100	100
32	B	180/180 (100%)	177 (98%)	3 (2%)	60	78
33	C	170/170 (100%)	168 (99%)	2 (1%)	71	84
34	D	172/172 (100%)	165 (96%)	7 (4%)	30	57
35	E	119/119 (100%)	116 (98%)	3 (2%)	47	68
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	122 (98%)	2 (2%)	62	79
38	H	104/104 (100%)	103 (99%)	1 (1%)	76	86
39	I	105/105 (100%)	103 (98%)	2 (2%)	57	75
40	J	86/86 (100%)	85 (99%)	1 (1%)	71	84
41	K	89/89 (100%)	86 (97%)	3 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	L	103/103 (100%)	102 (99%)	1 (1%)	76	86
43	M	92/92 (100%)	89 (97%)	3 (3%)	38	62
44	N	83/83 (100%)	82 (99%)	1 (1%)	71	84
45	O	76/76 (100%)	74 (97%)	2 (3%)	46	67
46	P	65/65 (100%)	64 (98%)	1 (2%)	65	80
47	Q	74/74 (100%)	72 (97%)	2 (3%)	44	66
48	R	56/56 (100%)	55 (98%)	1 (2%)	59	77
49	S	70/70 (100%)	67 (96%)	3 (4%)	29	56
50	T	65/65 (100%)	62 (95%)	3 (5%)	27	54
51	U	55/55 (100%)	53 (96%)	2 (4%)	35	61
52	03	110/174 (63%)	109 (99%)	1 (1%)	78	88
59	Z	324/325 (100%)	313 (97%)	11 (3%)	37	61
All	All	5285/5350 (99%)	5196 (98%)	89 (2%)	62	78

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	K	124	LYS
49	S	42	ASN
43	M	7	ASN
46	P	45	GLU
51	U	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
25	28	8	GLN
50	T	69	ASN
34	D	53	GLN
50	T	51	ASN
59	Z	124	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	150 (9%)	7 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	01	2902/2903 (99%)	348 (11%)	12 (0%)
55	02	119/120 (99%)	11 (9%)	1 (0%)
56	W	76/77 (98%)	8 (10%)	0
56	X	76/77 (98%)	14 (18%)	0
57	V	16/17 (94%)	2 (12%)	0
58	Y	74/76 (97%)	22 (29%)	0
All	All	4801/4809 (99%)	555 (11%)	20 (0%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G
53	A	31	G
53	A	32	A
53	A	39	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	1378	A
54	01	2391	G
55	02	88	C
54	01	2808	G
53	A	1347	G

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

1 non-standard protein/DNA/RNA residue 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
58	U8U	Y	34	58	19,24,25	1.33	2 (10%)	23,34,37	1.04	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	U8U	Y	34	58	-	2/9/28/29	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	34	U8U	C6-N1	3.80	1.44	1.38
58	Y	34	U8U	C4-C5	3.02	1.51	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Y	34	U8U	C2'-C1'-N1	2.52	120.36	113.22
58	Y	34	U8U	O4-C4-C5	-2.29	121.56	124.96
58	Y	34	U8U	C5-C6-N1	2.04	125.64	122.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Y	34	U8U	N-C-C5-C4
58	Y	34	U8U	N-C-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 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
60	GCP	Z	401	-	27,34,34	1.89	7 (25%)	34,54,54	3.96	18 (52%)

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
60	GCP	Z	401	-	-	9/15/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Z	401	GCP	PB-O3A	-4.11	1.53	1.58
60	Z	401	GCP	C5-C6	3.93	1.48	1.41
60	Z	401	GCP	O4'-C1'	3.79	1.46	1.41
60	Z	401	GCP	C6-N1	3.48	1.39	1.33
60	Z	401	GCP	C2'-C1'	2.58	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z	401	GCP	C1'-N9-C4	13.76	150.81	126.64
60	Z	401	GCP	C5-C6-N1	-8.56	111.72	123.43
60	Z	401	GCP	O1G-PG-C3B	-7.40	95.29	111.24
60	Z	401	GCP	C2-N1-C6	6.56	126.35	115.93
60	Z	401	GCP	O4'-C1'-C2'	-5.67	98.65	106.93

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	Z	401	GCP	PB-C3B-PG-O1G
60	Z	401	GCP	PB-C3B-PG-O2G
60	Z	401	GCP	PG-C3B-PB-O1B
60	Z	401	GCP	C5'-O5'-PA-O3A

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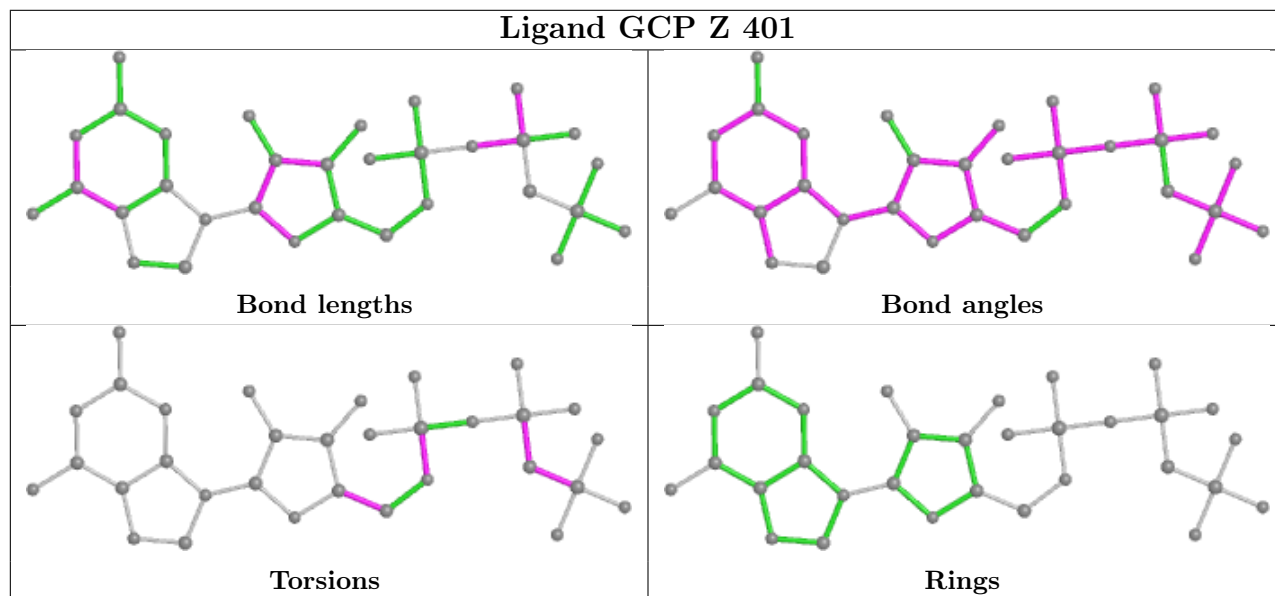
Mol	Chain	Res	Type	Atoms
60	Z	401	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	Z	401	GCP	1	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

There are no chain breaks in this entry.

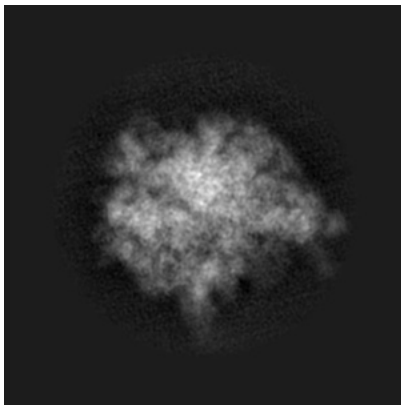
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8618. These allow visual inspection of the internal detail of the map and identification of artifacts.

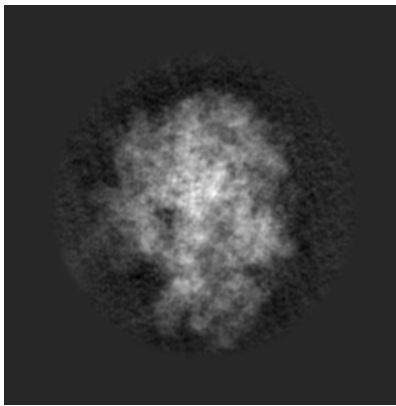
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

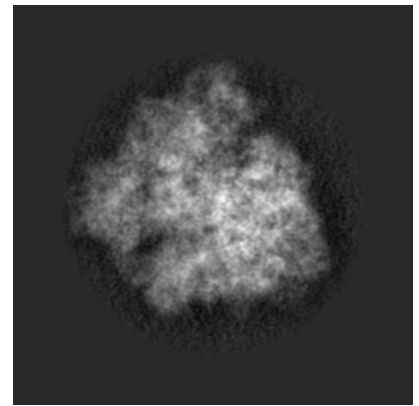
#### 6.1.1 Primary map



X

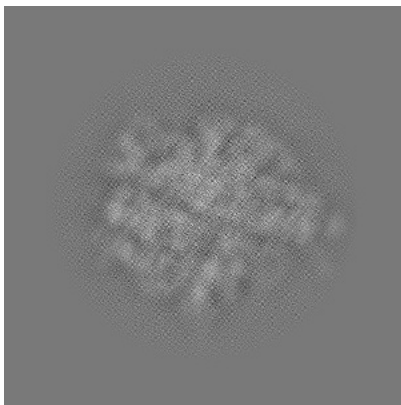


Y

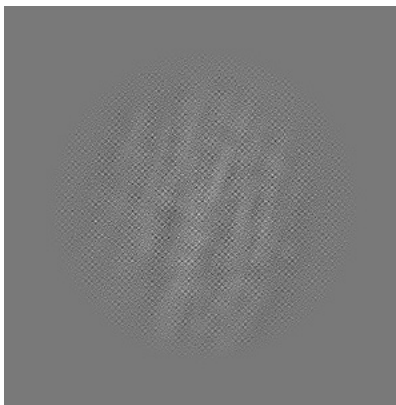


Z

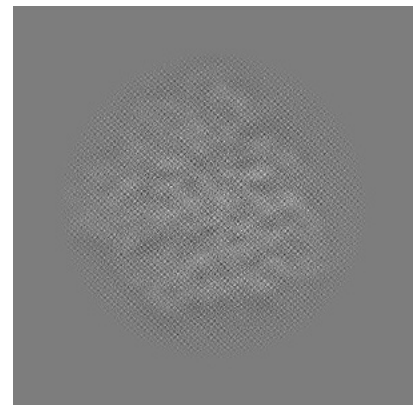
#### 6.1.2 Raw map



X



Y



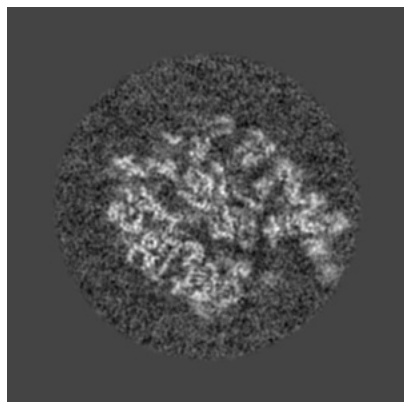
Z

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

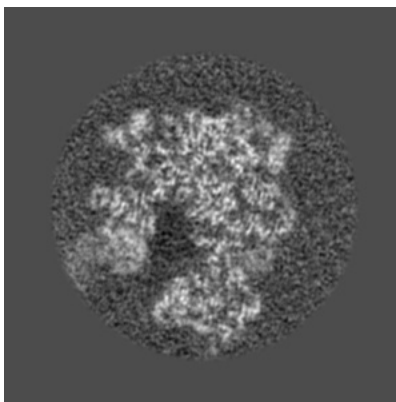


## 6.2 Central slices [i](#)

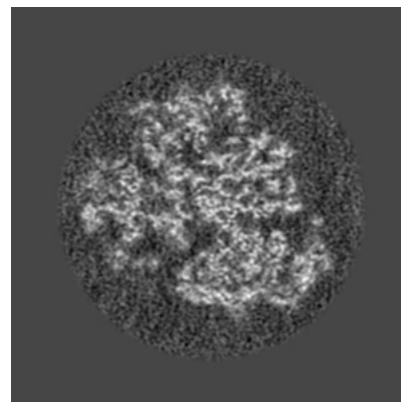
### 6.2.1 Primary map



X Index: 240

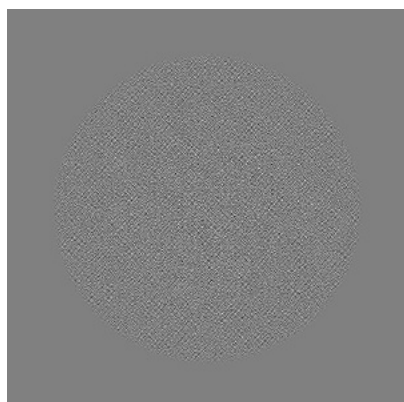


Y Index: 240

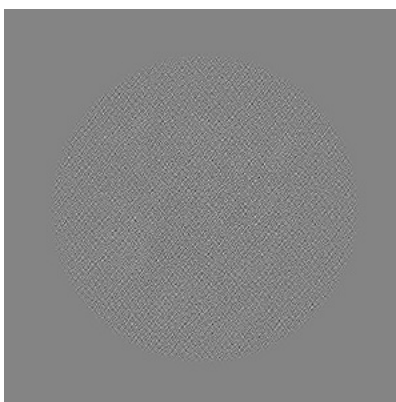


Z Index: 240

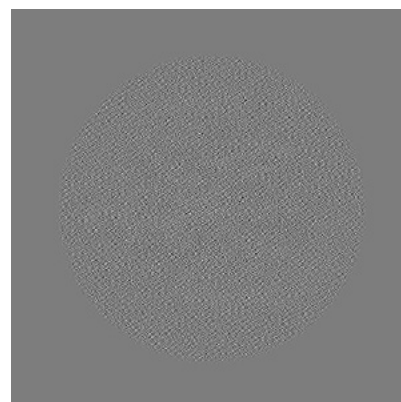
### 6.2.2 Raw map



X Index: 240



Y Index: 240

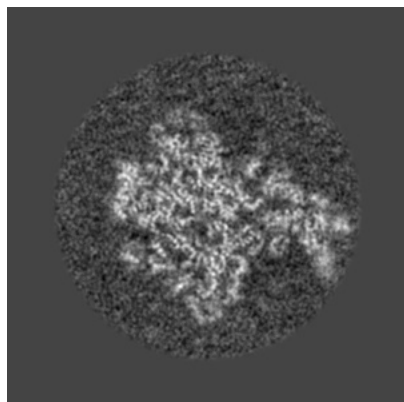


Z Index: 240

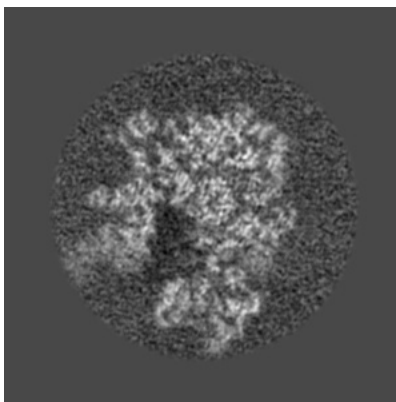
The images above show central slices of the map in three orthogonal directions.

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

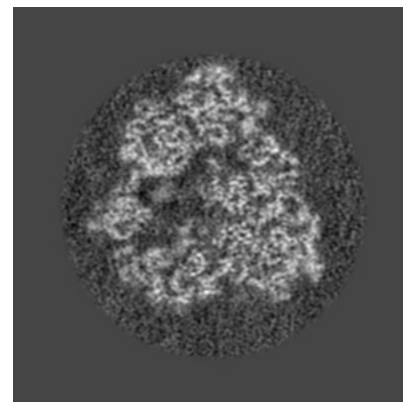
### 6.3.1 Primary map



X Index: 251

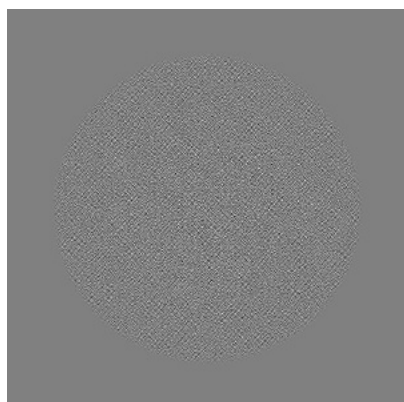


Y Index: 244

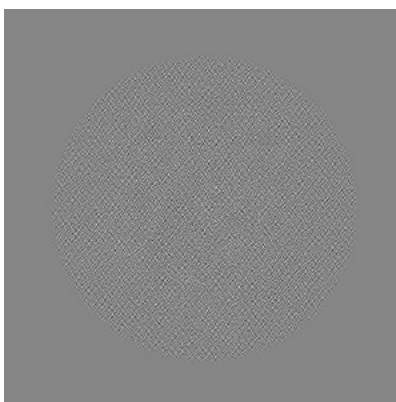


Z Index: 219

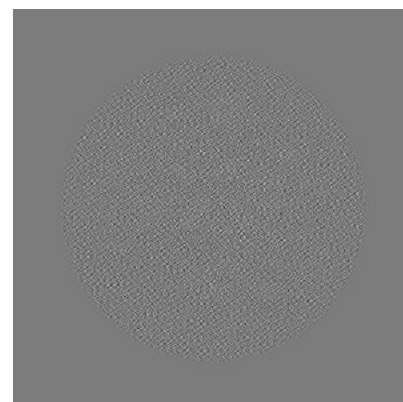
### 6.3.2 Raw map



X Index: 240



Y Index: 234

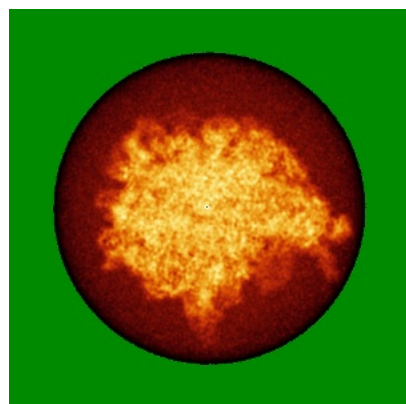


Z Index: 252

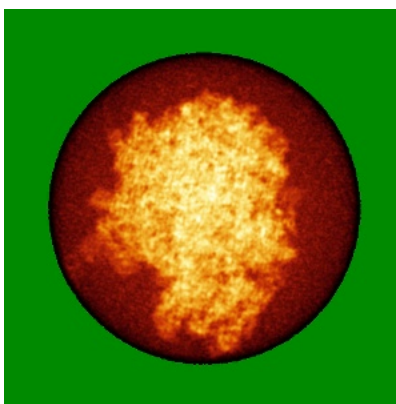
The images above show the largest variance slices of the map in three orthogonal directions.

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

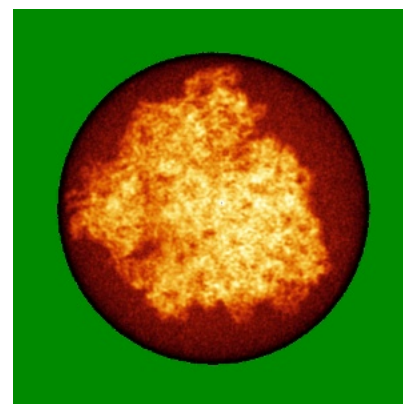
### 6.4.1 Primary map



X

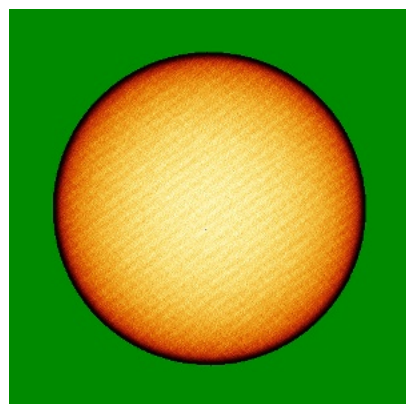


Y

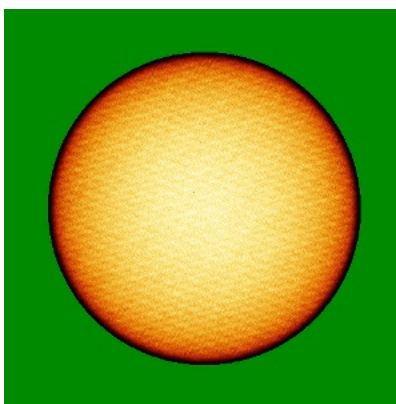


Z

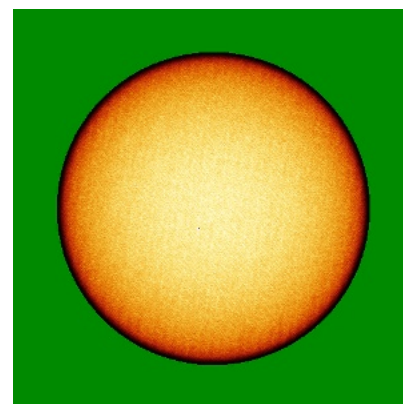
### 6.4.2 Raw map



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.

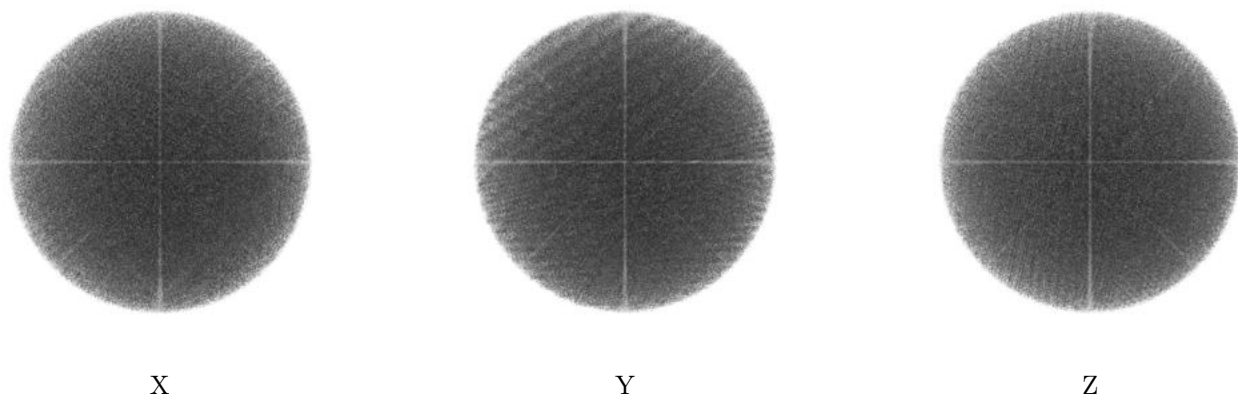
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.79. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

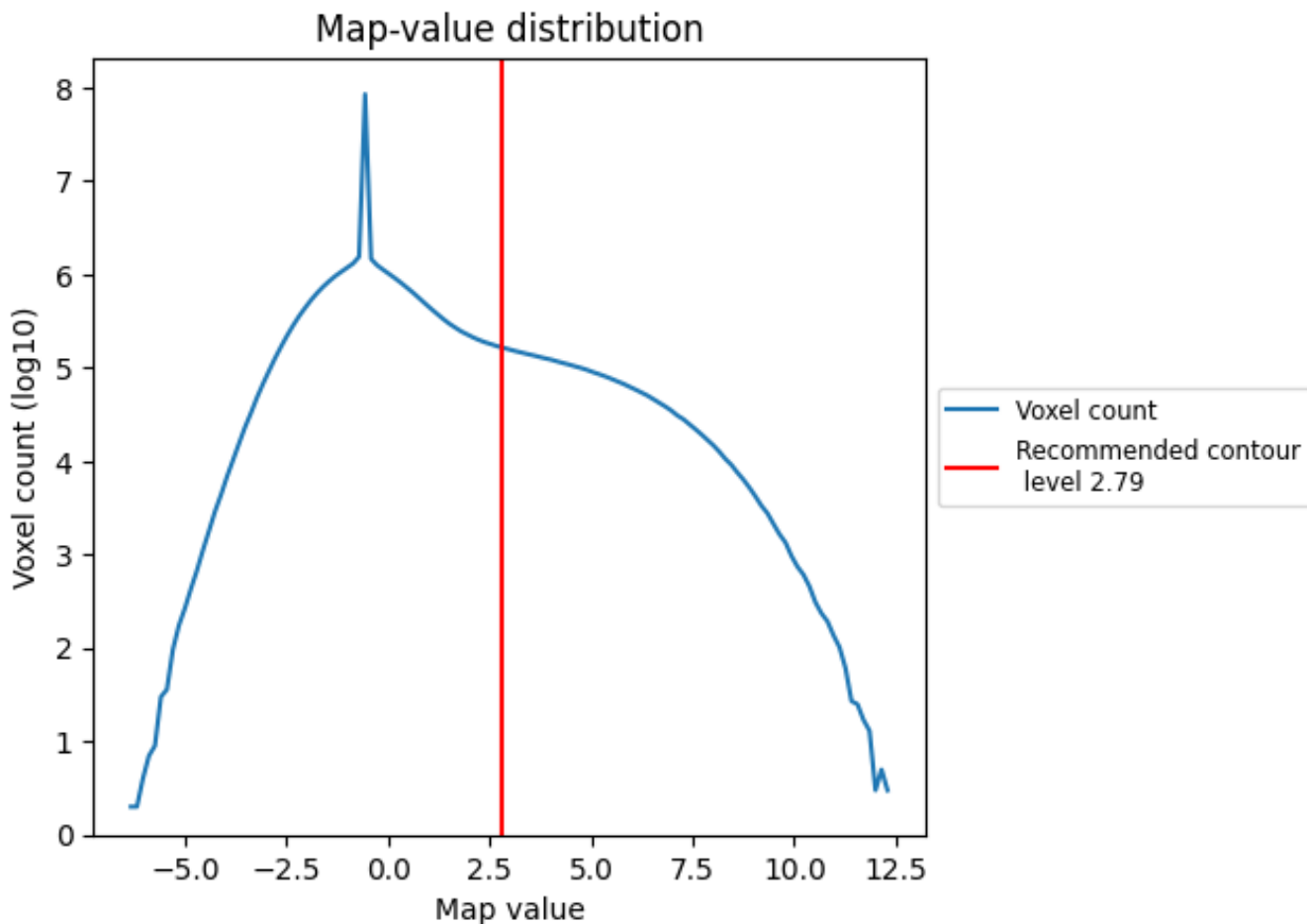
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

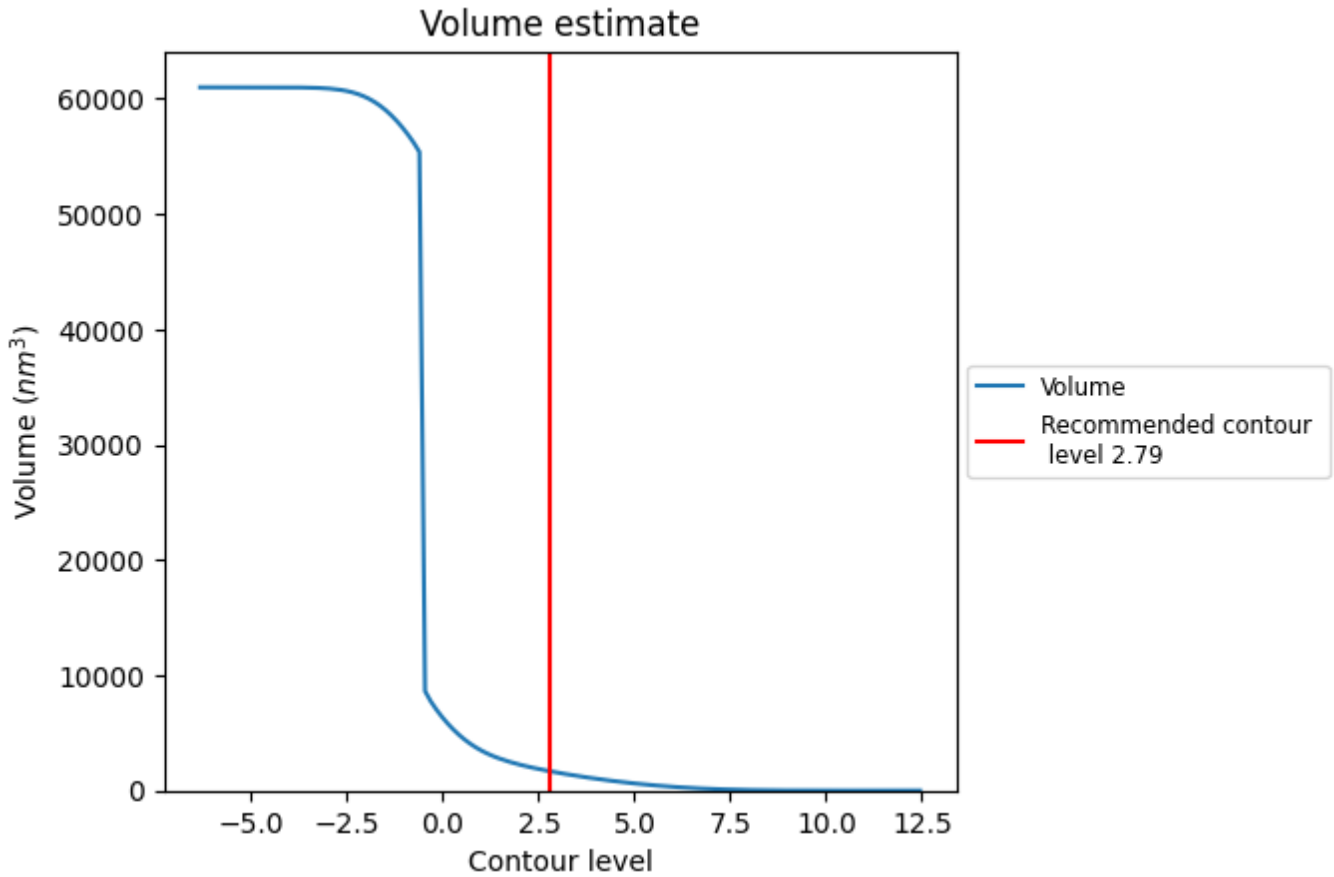
This section contains the results of statistical analysis of the map.

### 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.

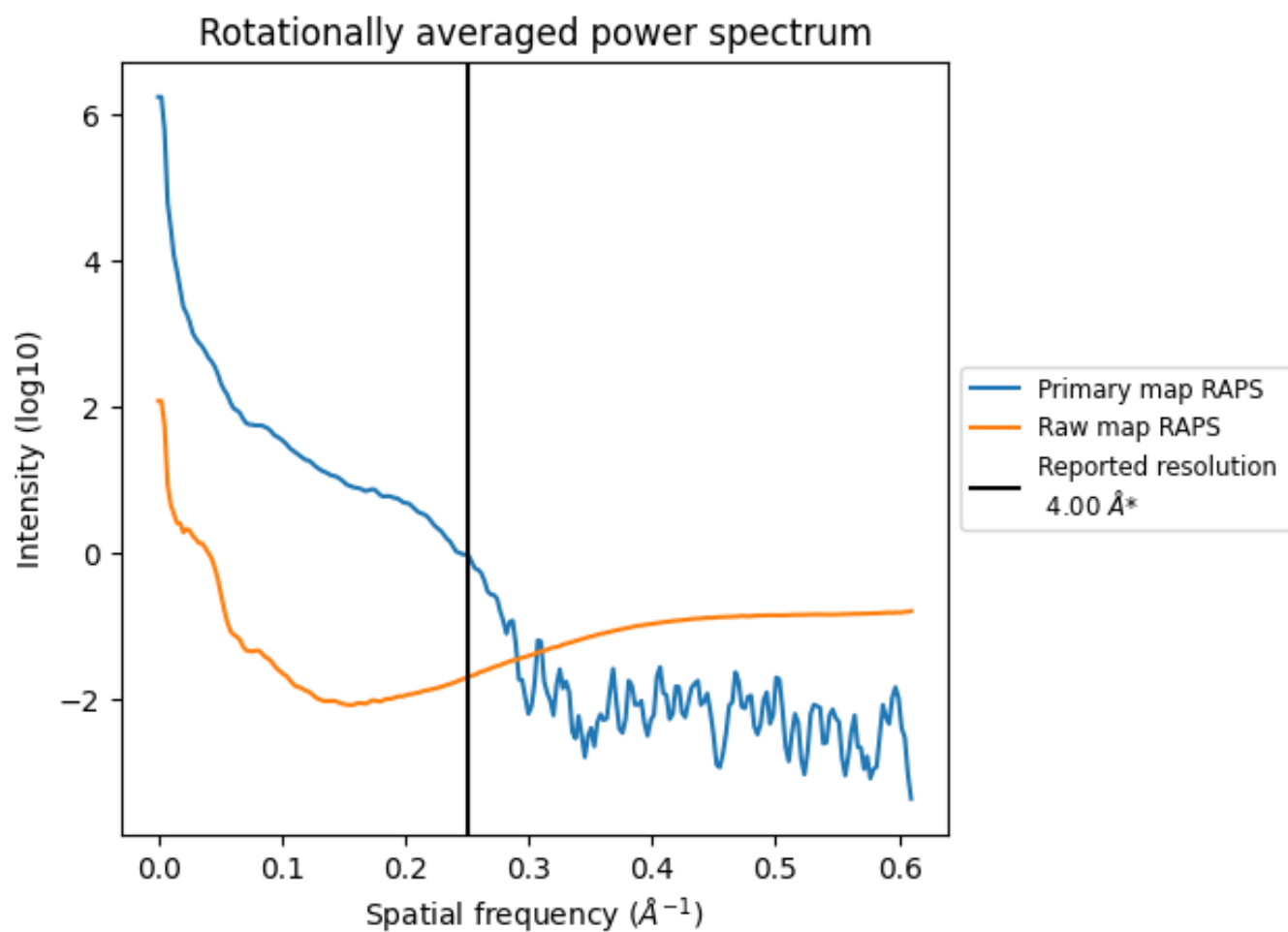
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1679 nm<sup>3</sup>; this corresponds to an approximate mass of 1517 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



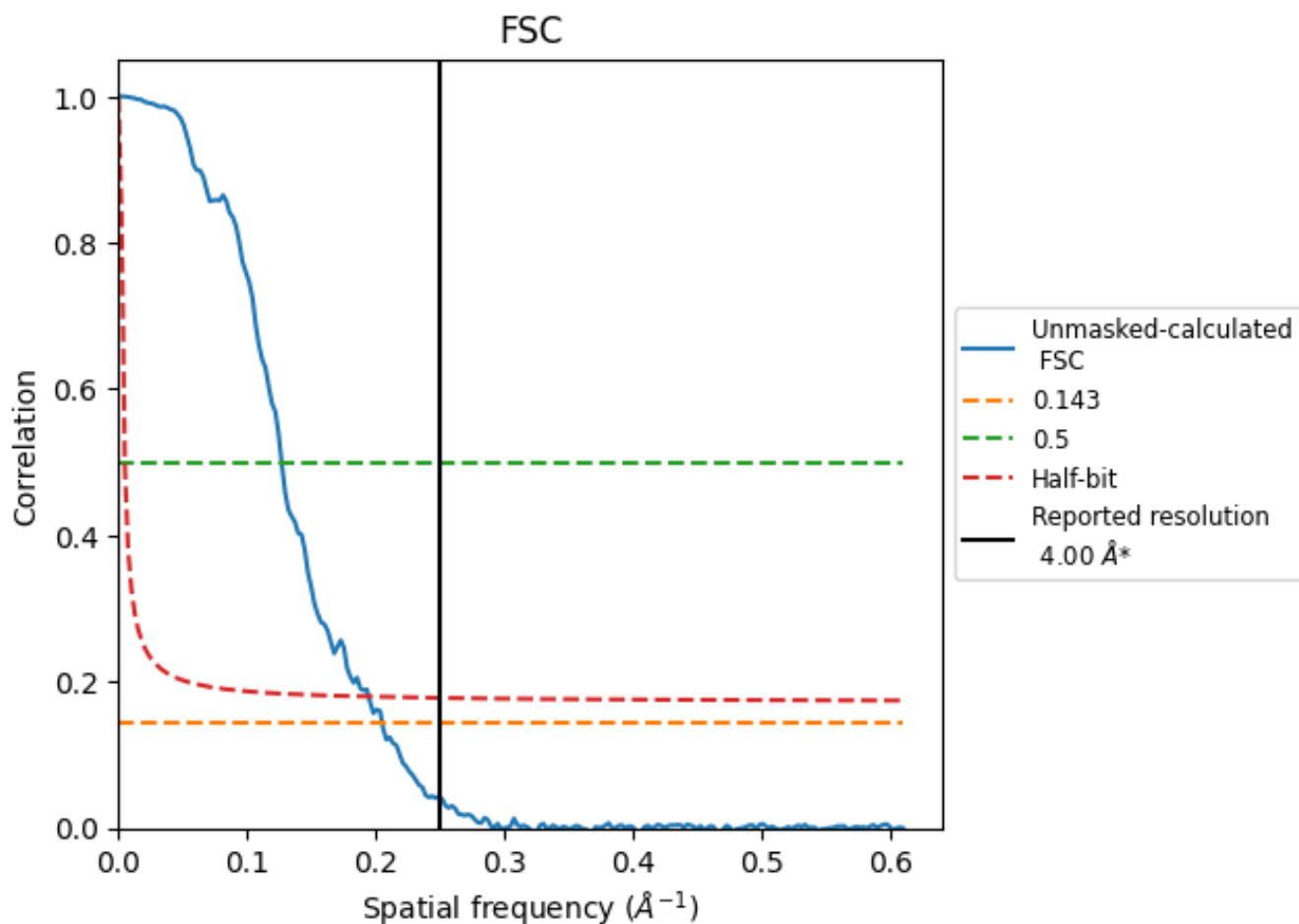
\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

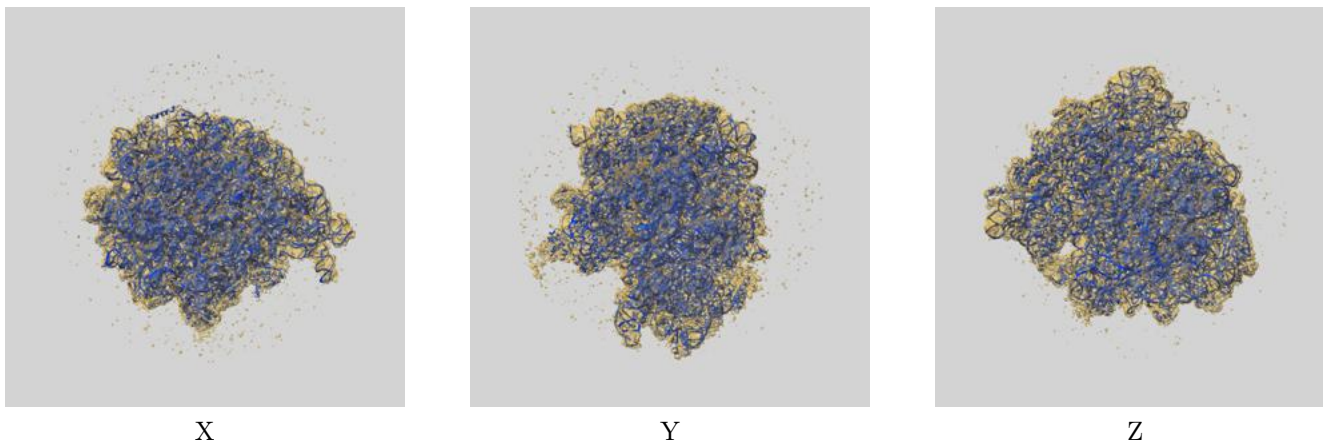
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.88	7.88	5.14

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.88 differs from the reported value 4.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-8618 and PDB model 5UYN. Per-residue inclusion information can be found in section 3 on page 16.

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



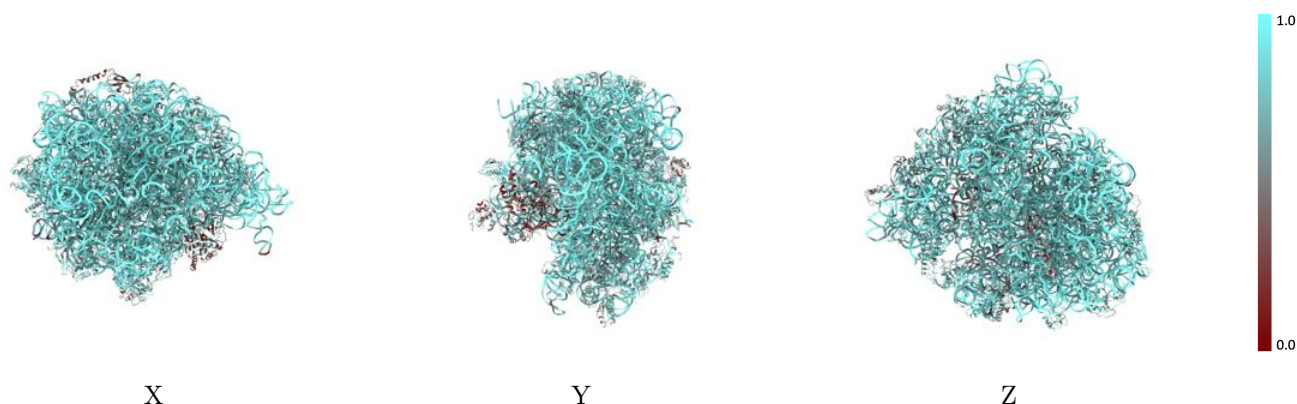
The images above show the 3D surface view of the map at the recommended contour level 2.79 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



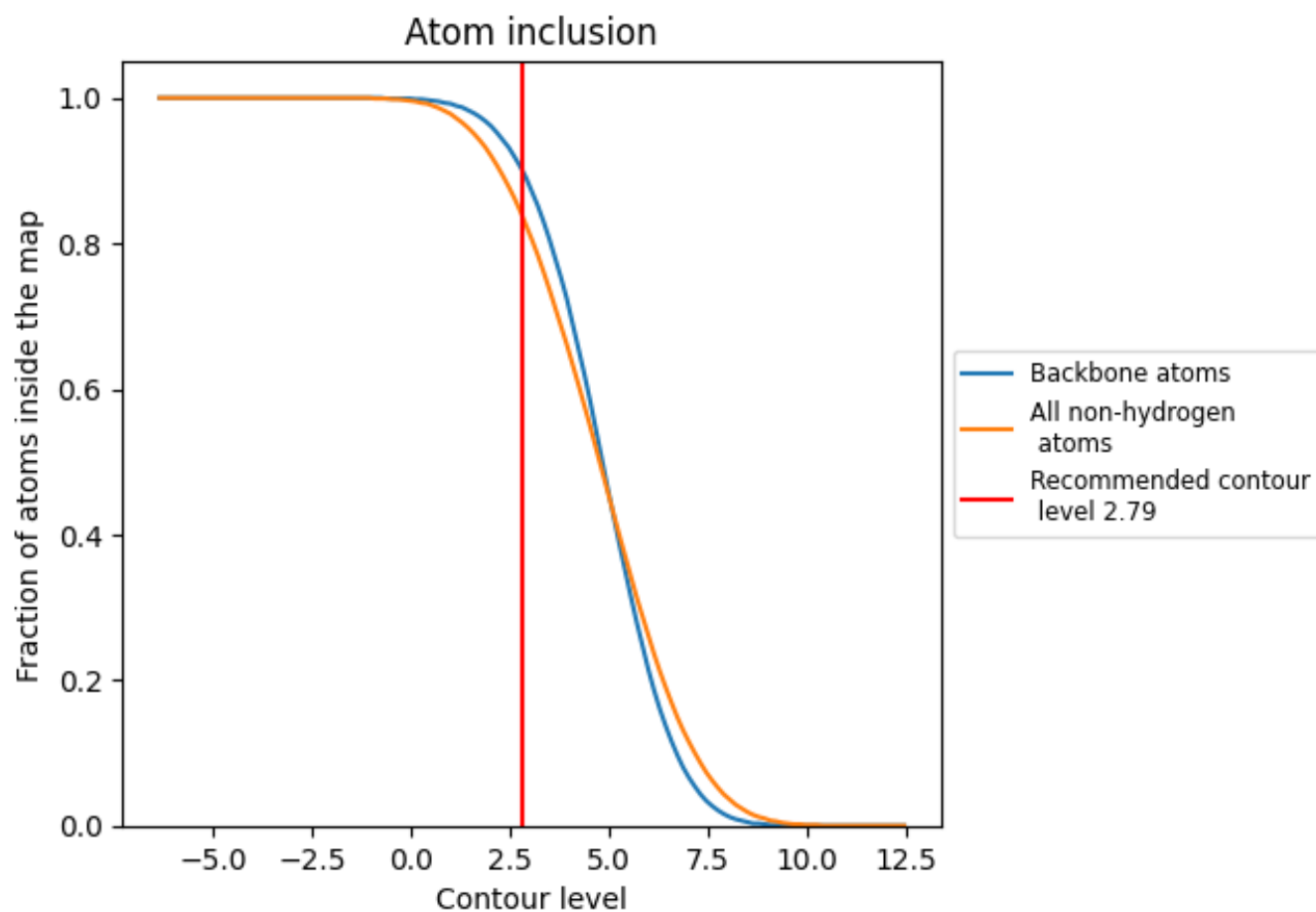
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.79).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (2.79) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.3160
01	 0.9270	 0.3300
02	 0.9360	 0.3190
03	 0.5890	 0.2000
04	 0.7880	 0.3640
05	 0.7680	 0.3660
06	 0.7440	 0.3180
07	 0.7550	 0.3010
08	 0.7980	 0.3200
09	 0.4200	 0.2620
10	 0.4410	 0.1700
11	 0.5460	 0.2060
12	 0.7500	 0.3500
13	 0.6630	 0.3550
14	 0.7580	 0.3250
15	 0.6810	 0.3550
16	 0.7980	 0.3280
17	 0.7990	 0.3150
18	 0.7190	 0.3290
19	 0.7660	 0.3220
20	 0.7140	 0.3100
21	 0.7050	 0.3190
22	 0.7650	 0.3240
23	 0.7550	 0.2910
24	 0.7910	 0.3420
25	 0.7660	 0.3600
26	 0.7470	 0.3400
27	 0.7240	 0.2610
28	 0.7300	 0.3210
29	 0.7270	 0.2810
30	 0.7710	 0.3410
31	 0.6770	 0.2940
32	 0.8080	 0.3360
33	 0.7960	 0.3450
34	 0.7940	 0.3580



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Chain	Atom inclusion	Q-score
A	 0.9160	 0.3230
B	 0.6690	 0.2810
C	 0.6830	 0.3300
D	 0.7080	 0.2920
E	 0.7010	 0.3320
F	 0.7590	 0.3060
G	 0.7320	 0.2930
H	 0.7530	 0.3280
I	 0.7600	 0.2830
J	 0.5910	 0.2730
K	 0.7330	 0.3170
L	 0.7420	 0.3390
M	 0.7200	 0.2950
N	 0.7020	 0.3020
O	 0.7940	 0.3270
P	 0.8170	 0.3300
Q	 0.7160	 0.3060
R	 0.7510	 0.2930
S	 0.7600	 0.2950
T	 0.7550	 0.2940
U	 0.6330	 0.2610
V	 0.6170	 0.2090
W	 0.8310	 0.2930
X	 0.6590	 0.1740
Y	 0.5180	 0.1620
Z	 0.3720	 0.2160