



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:09 PM EST

PDB ID : 3JCE  
EMDB ID : EMD-6550  
Title : Structure of Escherichia coli EF4 in pretranslocational ribosomes (Pre EF4)  
Authors : Zhang, D.; Yan, K.; Liu, G.; Song, G.; Luo, J.; Shi, Y.; Cheng, E.; Wu, S.;  
Jiang, T.; Low, J.; Gao, N.; Qin, Y.  
Deposited on : 2015-12-01  
Resolution : 3.20 Å(reported)  
Based on initial model : 4V9O

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

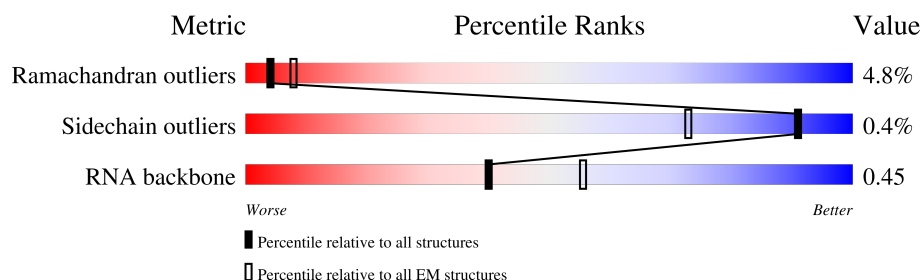
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)
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	a	1533	<div> <div>62%</div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>
2	c	233	<div> <div>73%</div> <div> <div></div> <div>86%</div> <div>12%</div> </div> </div>
3	d	206	<div> <div>82%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
4	e	167	<div> <div>75%</div> <div> <div></div> <div>87%</div> <div>10%</div> </div> </div>
5	f	135	<div> <div>57%</div> <div> <div></div> <div>70%</div> <div>5%</div> <div>24%</div> </div> </div>
6	g	179	<div> <div>70%</div> <div> <div></div> <div>82%</div> <div>.</div> <div>16%</div> </div> </div>
7	h	130	<div> <div>71%</div> <div> <div></div> <div>98%</div> <div>..</div> </div> </div>
8	i	130	<div> <div>75%</div> <div> <div></div> <div>95%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
9	j	103	
10	k	129	
11	l	124	
12	m	118	
13	n	101	
14	o	89	
15	p	82	
16	q	84	
17	r	75	
18	s	92	
19	t	87	
20	u	71	
21	b	241	
22	0	57	
23	1	55	
24	2	46	
25	3	65	
26	4	38	
27	5	234	
28	A	2904	
29	B	120	
30	C	273	
31	D	209	
32	E	201	
33	F	179	

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Mol	Chain	Length	Quality of chain
34	G	177	
35	H	149	
36	I	142	
37	J	142	
38	K	123	
39	L	144	
40	M	136	
41	N	127	
42	O	117	
43	P	115	
44	Q	118	
45	R	103	
46	S	110	
47	T	100	
48	U	104	
49	V	94	
50	W	85	
51	X	78	
52	Y	63	
53	Z	59	
54	6	76	
55	7	15	
56	8	77	
57	x	599	
58	9	76	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 154017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

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

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 21 is a protein called 30S ribosomal protein S2.

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

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a RNA chain called 23 ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	2903	Total	C	N	O	P	0	0
			62320	27801	11467	20149	2903		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	76	Total	C	N	O	P	0	0
			1633	732	291	534	76		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	15	Total	C	N	O	P	0	0
			320	144	59	102	15		

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

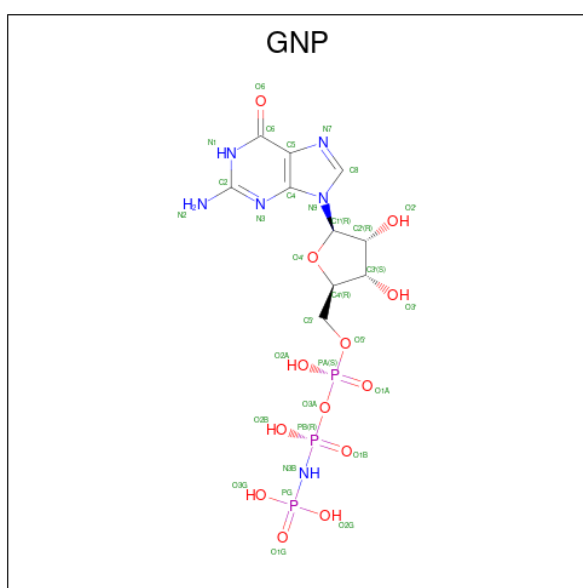
- Molecule 57 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	586	Total	C	N	O	S	0	0
			4573	2885	792	875	21		

- Molecule 58 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	9	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
59	x	1	Total	C	N	O	P	0
			32	10	6	13	3	

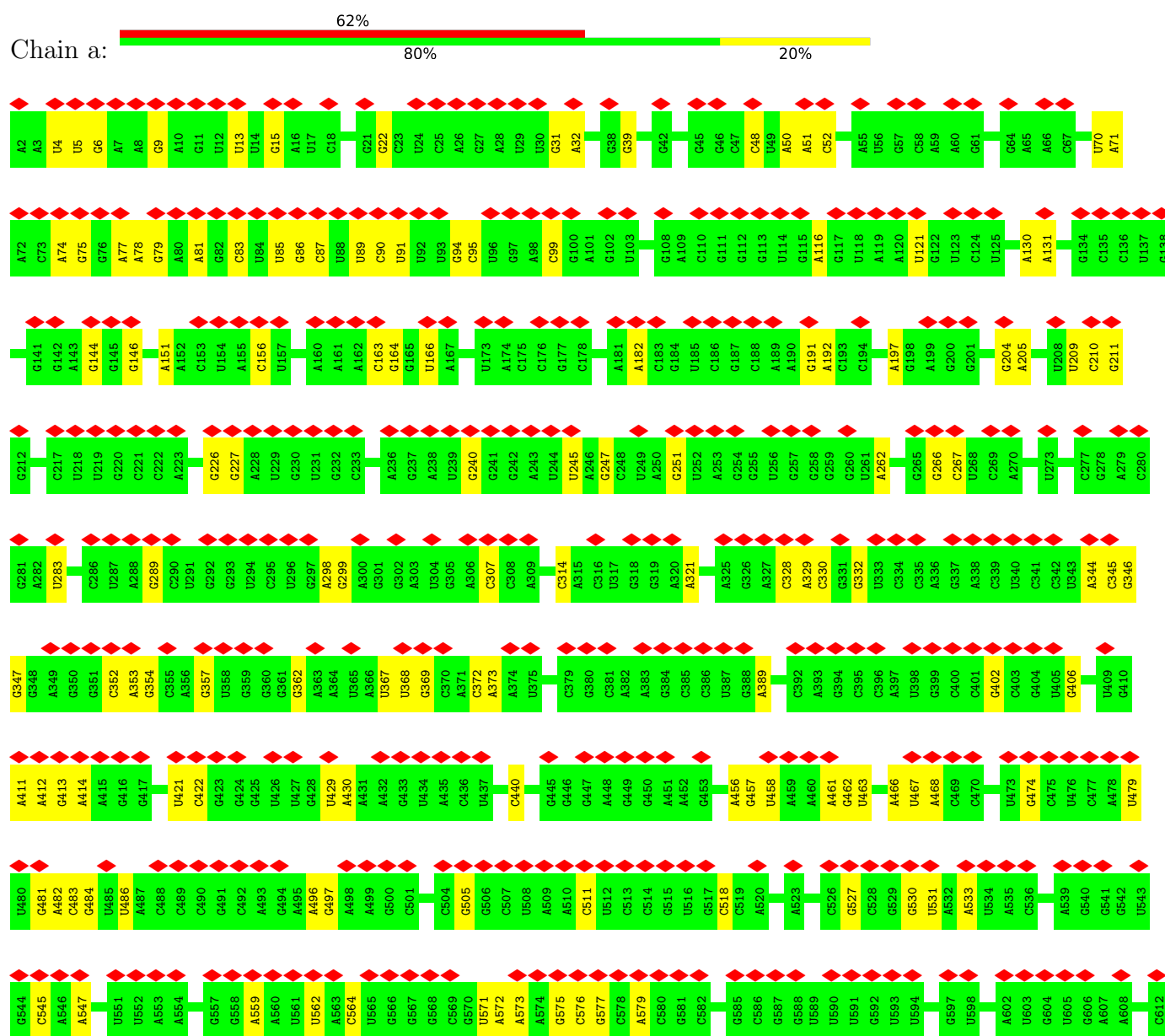
- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

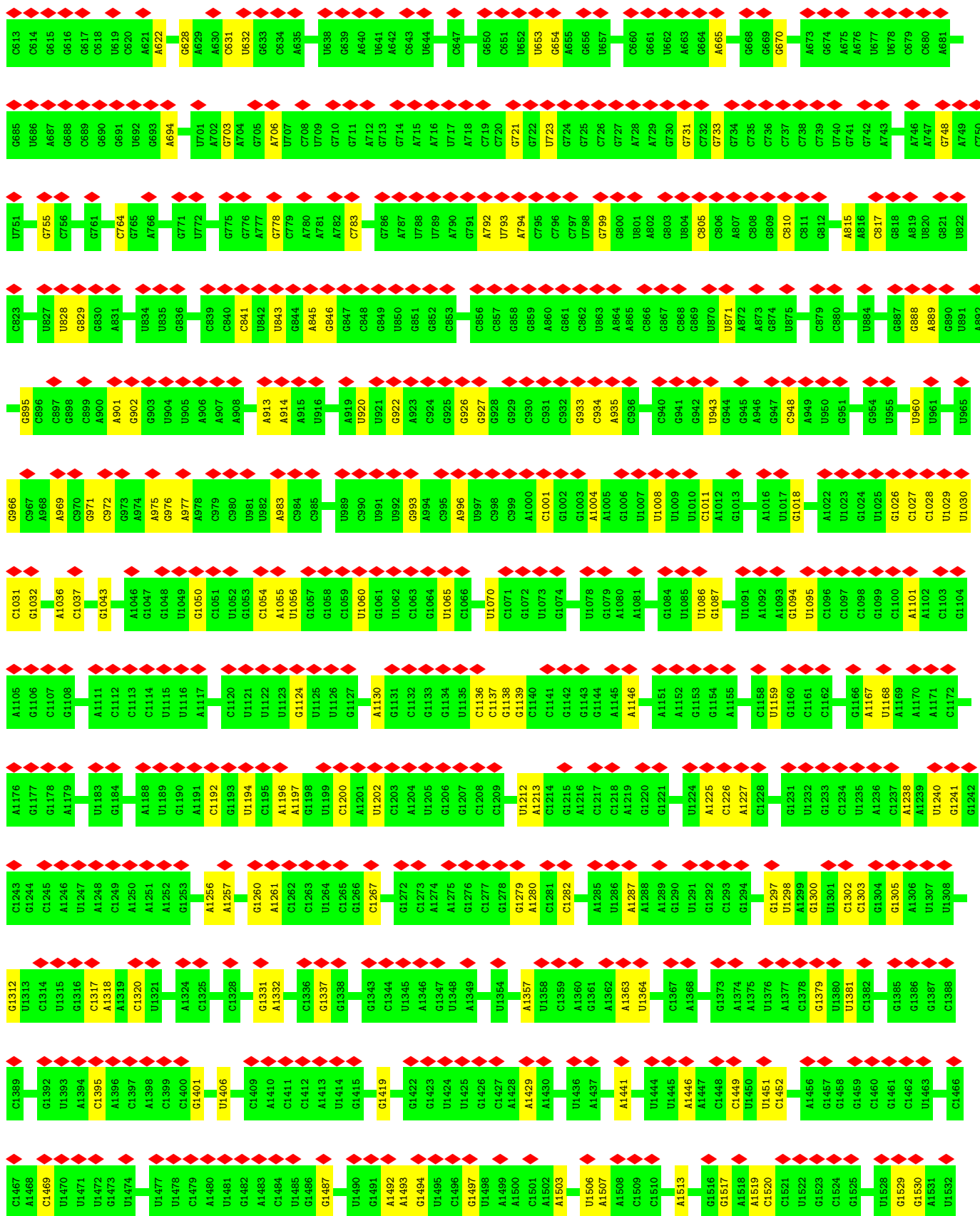
Mol	Chain	Residues	Atoms		AltConf
60	x	1	Total	Mg	0
			1	1	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

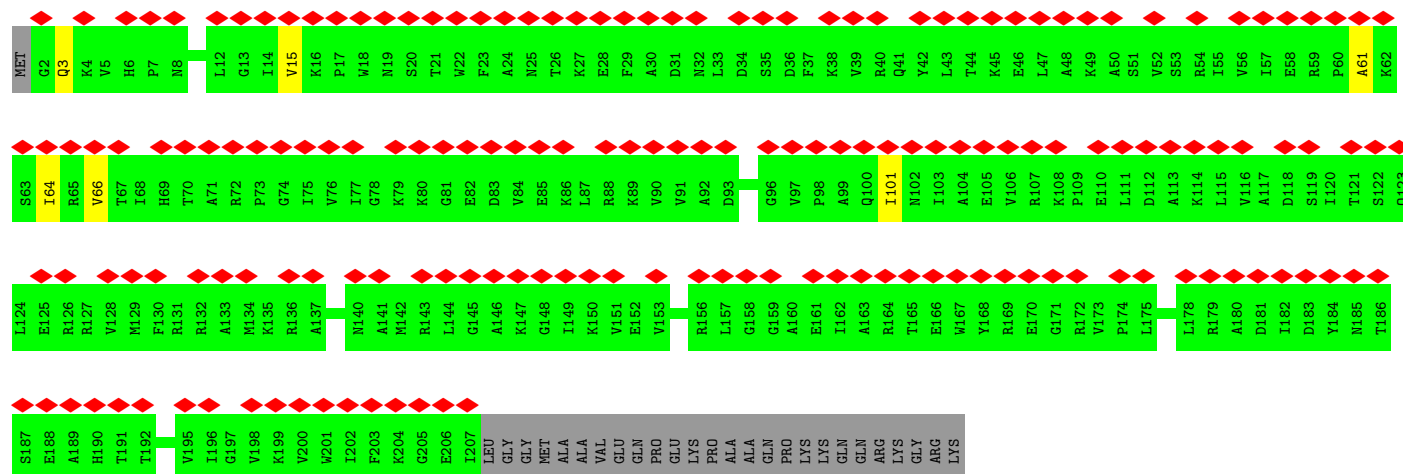
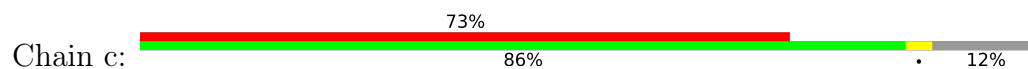
#### • Molecule 1: 16S ribosomal RNA



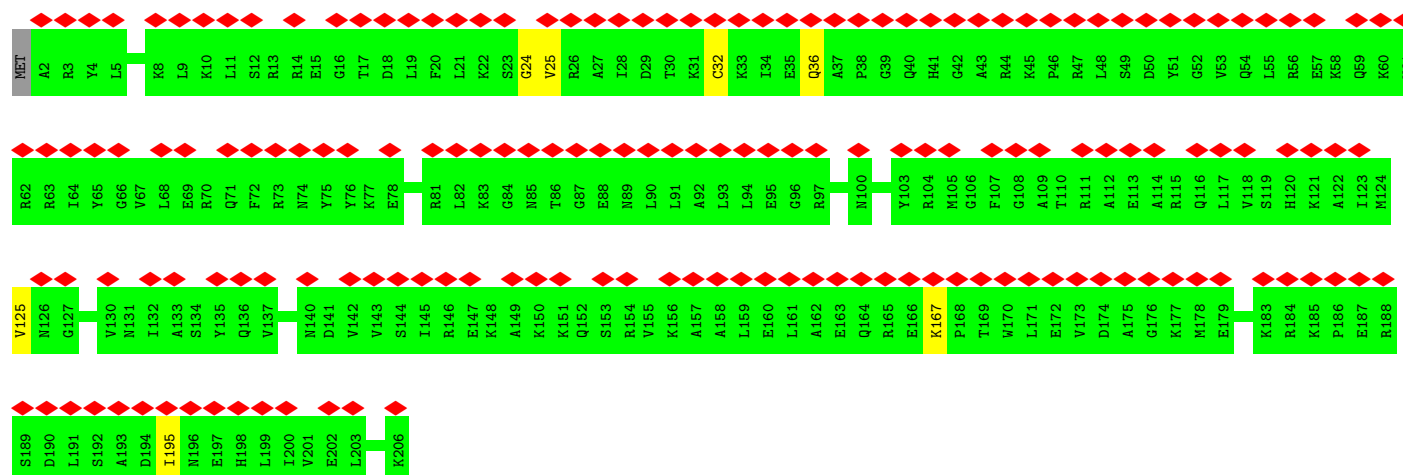
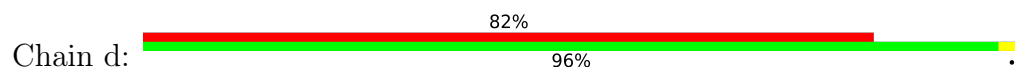




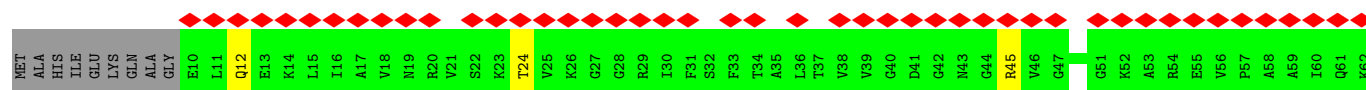
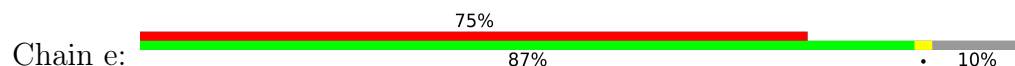
• Molecule 2: 30S ribosomal protein S3



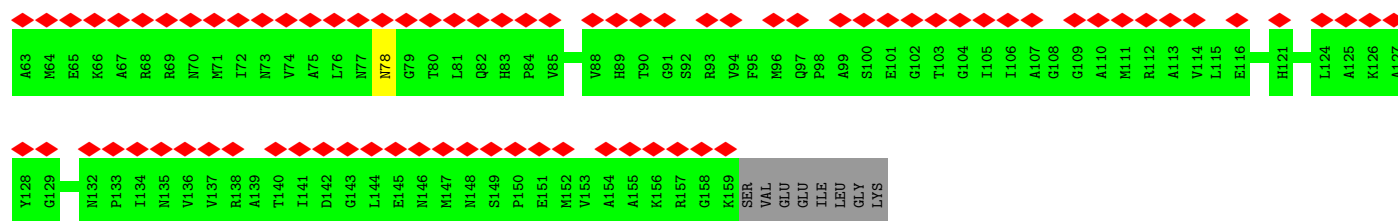
• Molecule 3: 30S ribosomal protein S4



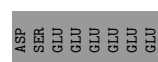
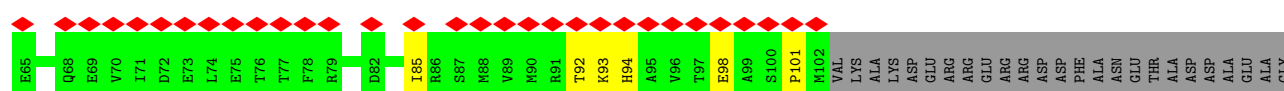
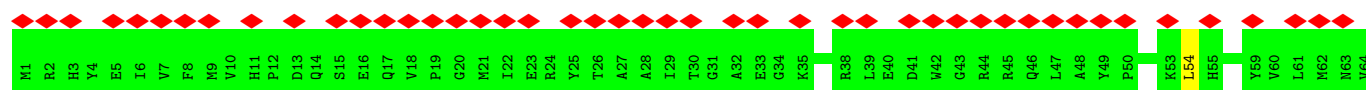
• Molecule 4: 30S ribosomal protein S5



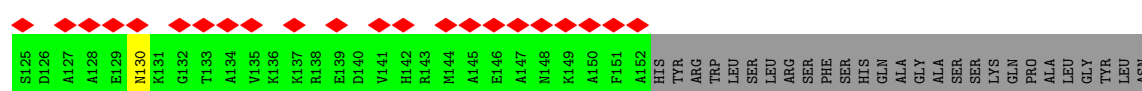
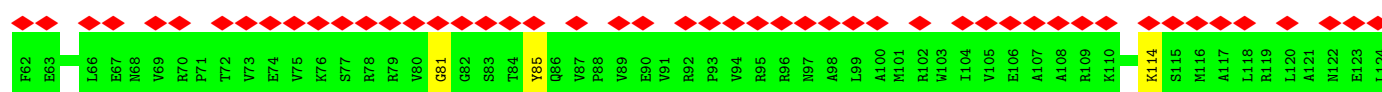
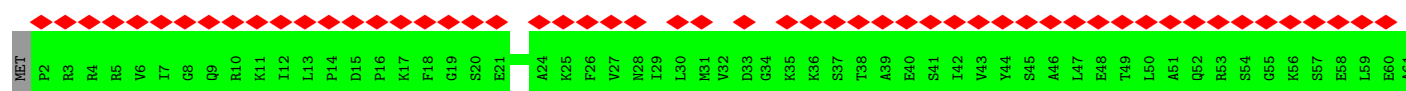
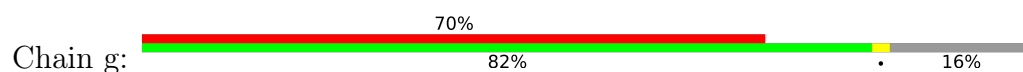




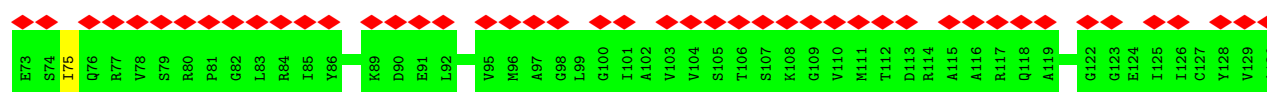
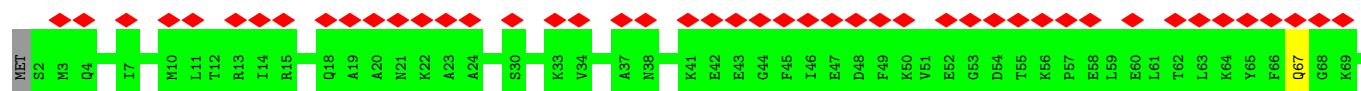
• Molecule 5: 30S ribosomal protein S6



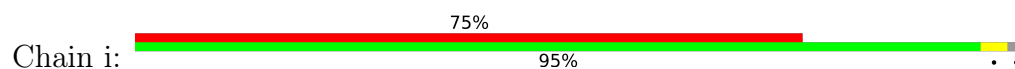
• Molecule 6: 30S ribosomal protein S7

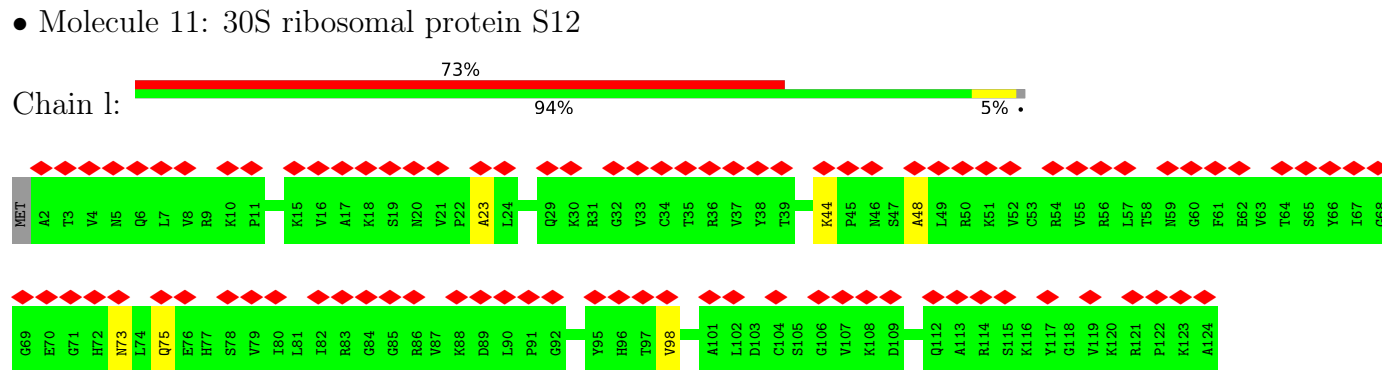
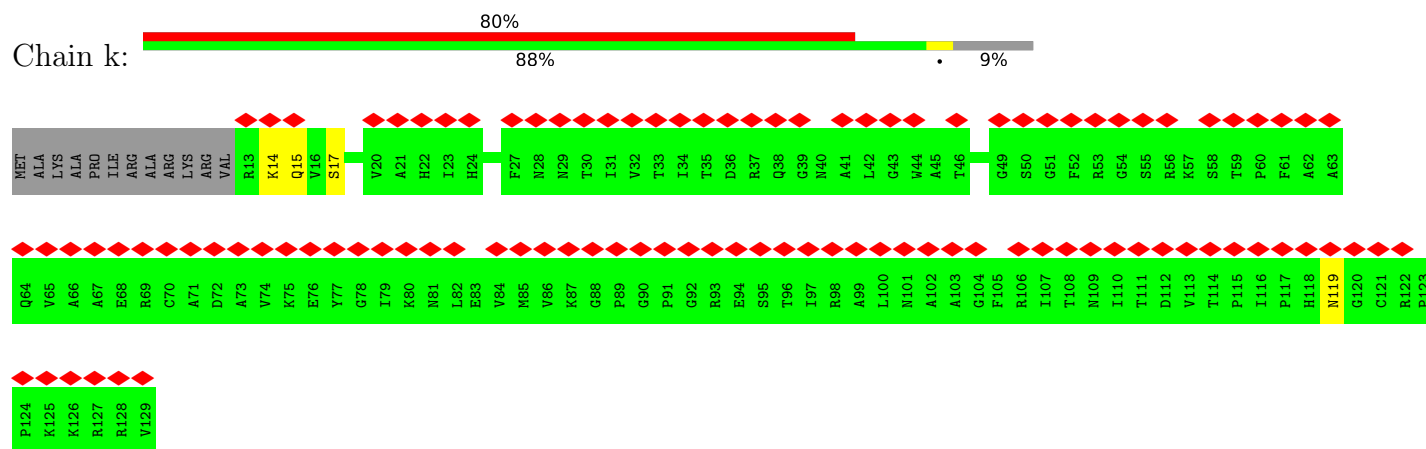
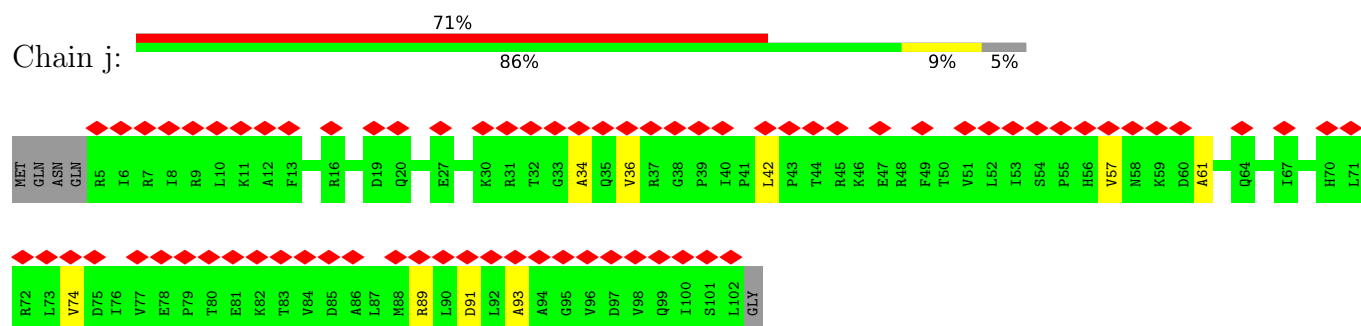
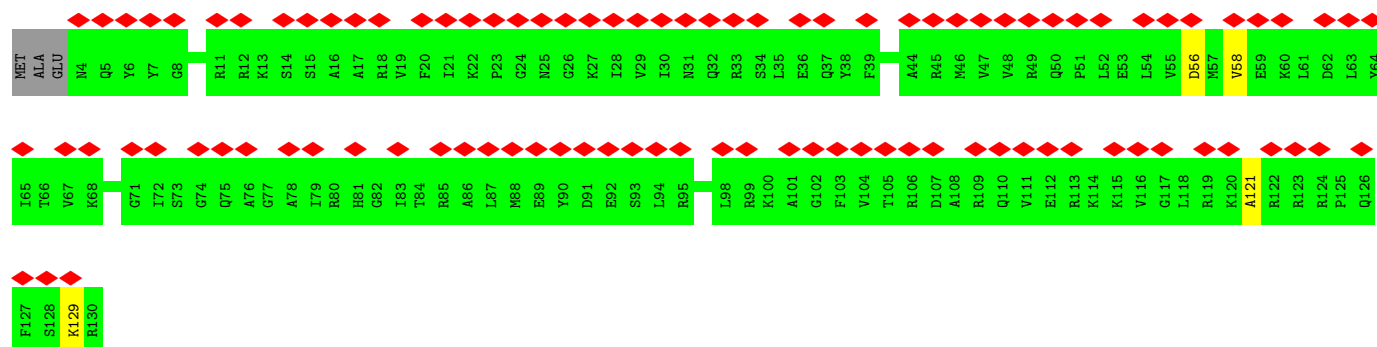


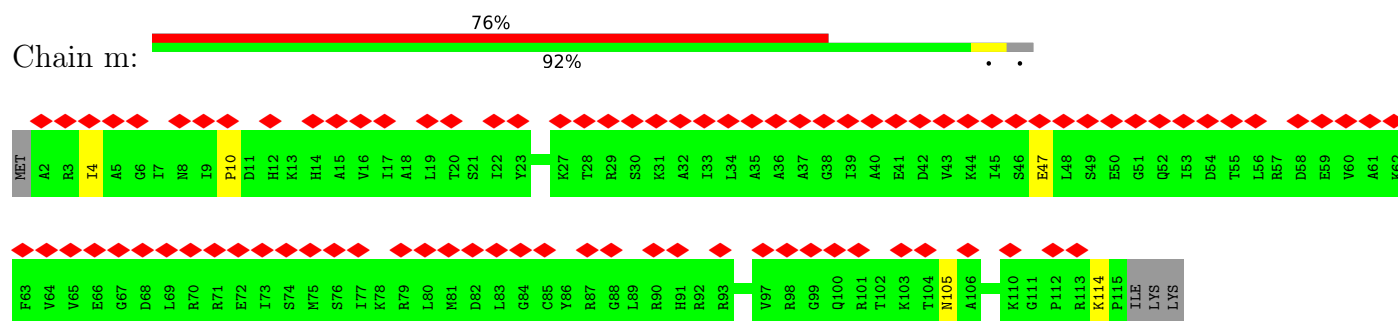
• Molecule 7: 30S ribosomal protein S8



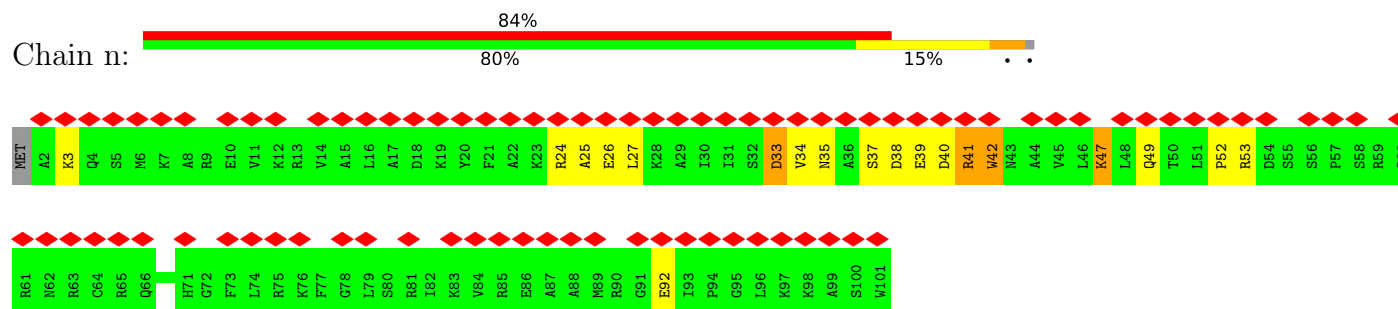
• Molecule 8: 30S ribosomal protein S9



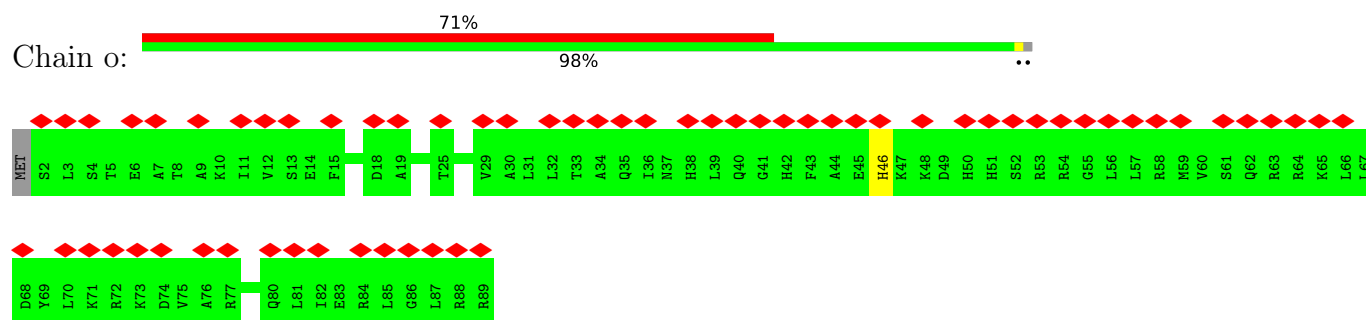




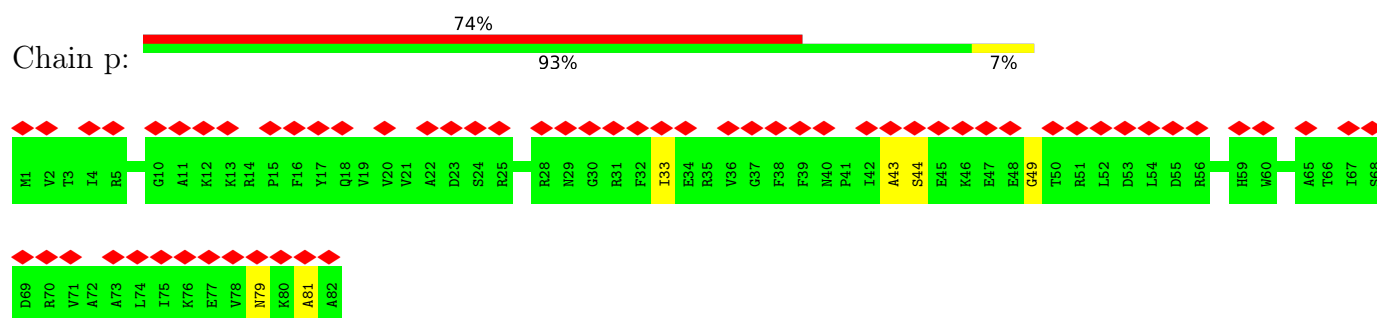
• Molecule 13: 30S ribosomal protein S14



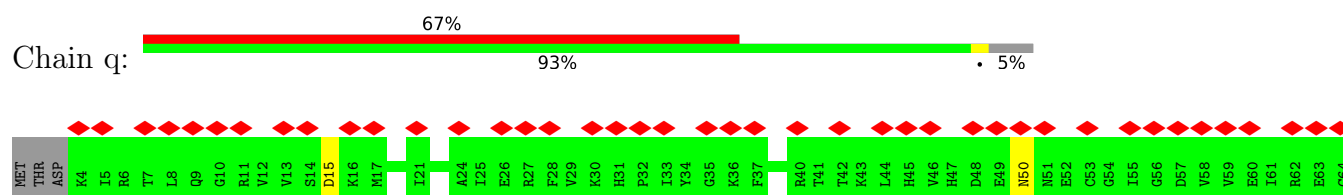
• Molecule 14: 30S ribosomal protein S15

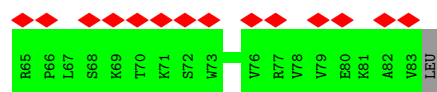


• Molecule 15: 30S ribosomal protein S16

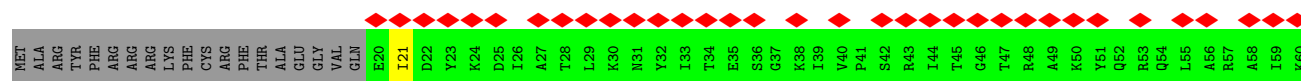


• Molecule 16: 30S ribosomal protein S17

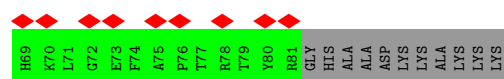
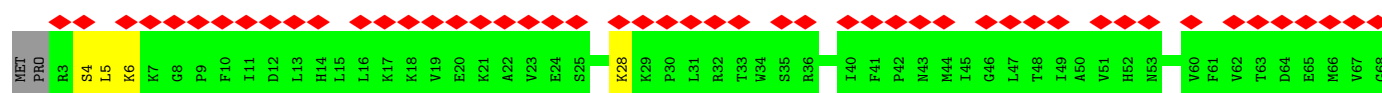
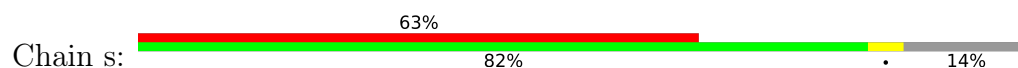




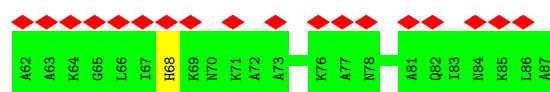
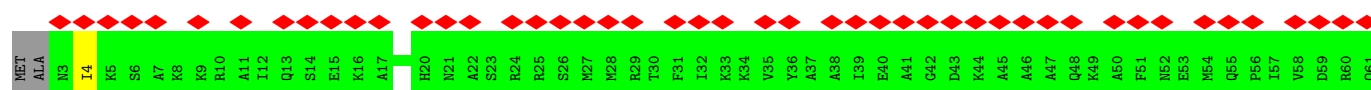
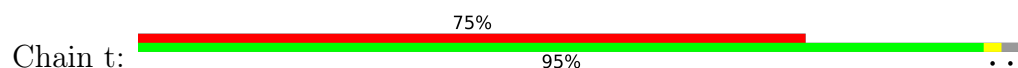
• Molecule 17: 30S ribosomal protein S18



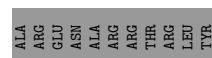
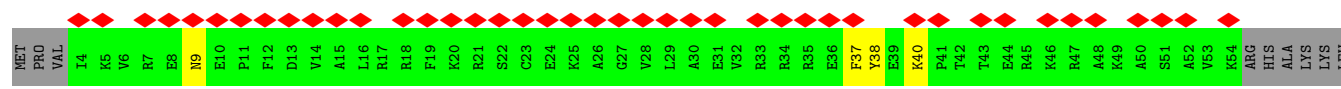
• Molecule 18: 30S ribosomal protein S19



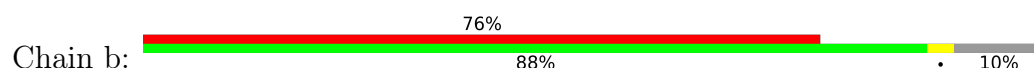
• Molecule 19: 30S ribosomal protein S20

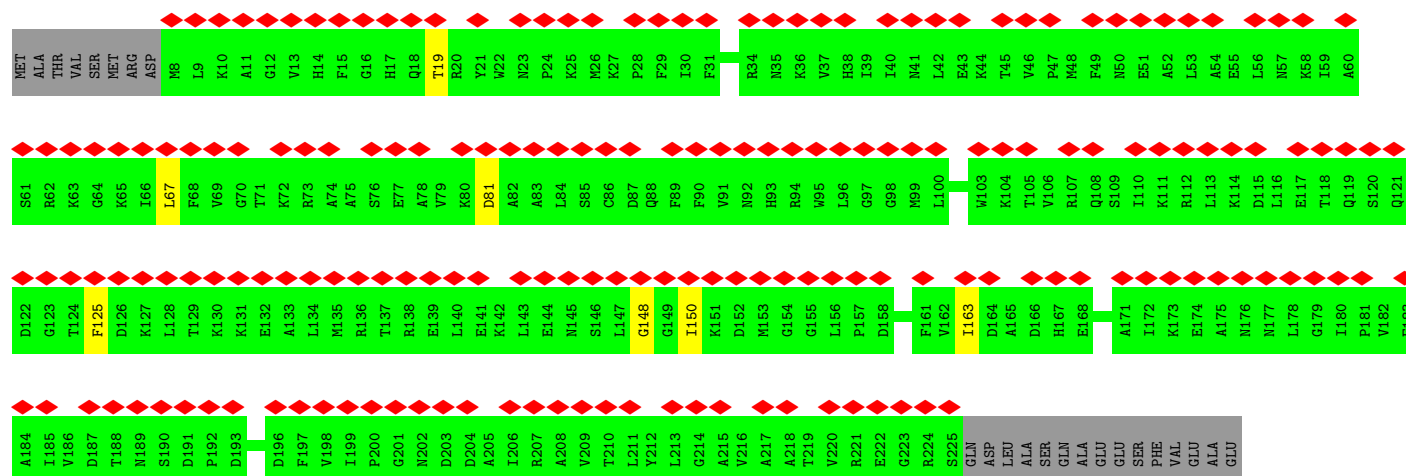


• Molecule 20: 30S ribosomal protein S21

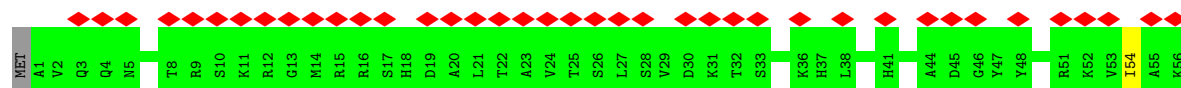


• Molecule 21: 30S ribosomal protein S2

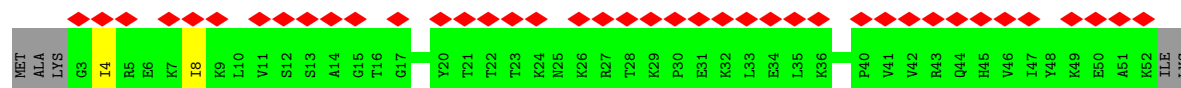
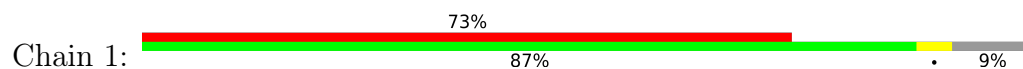




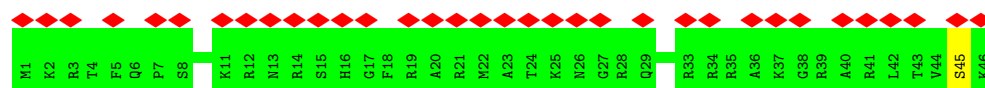
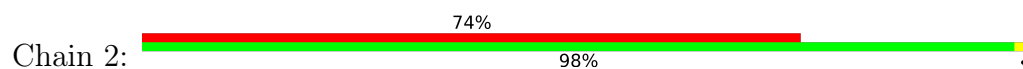
- Molecule 22: 50S ribosomal protein L32



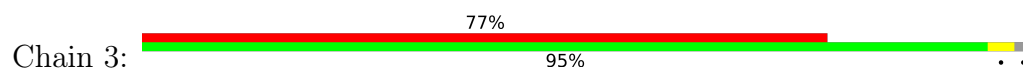
- Molecule 23: 50S ribosomal protein L33



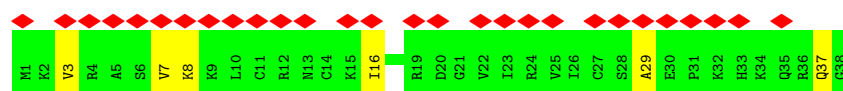
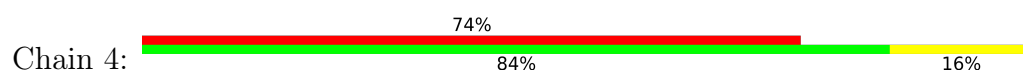
- Molecule 24: 50S ribosomal protein L34



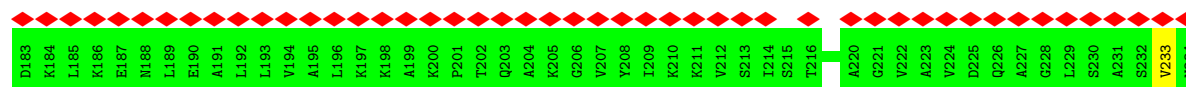
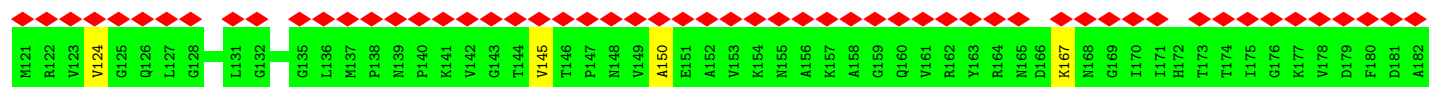
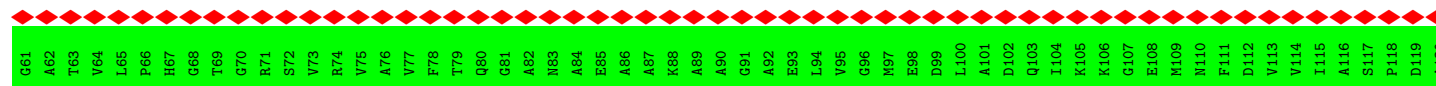
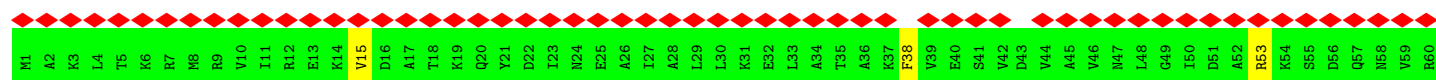
- Molecule 25: 50S ribosomal protein L35



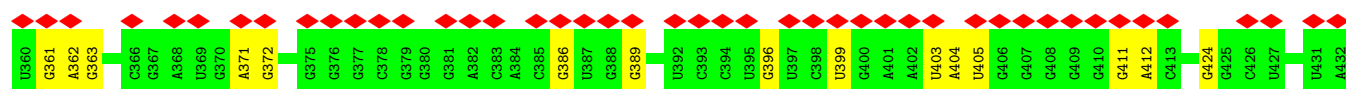
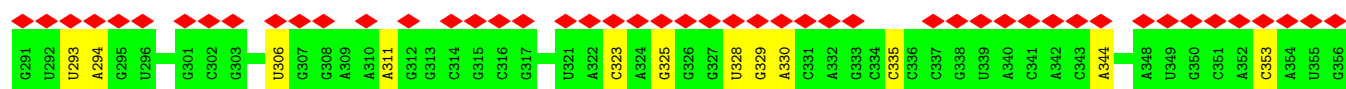
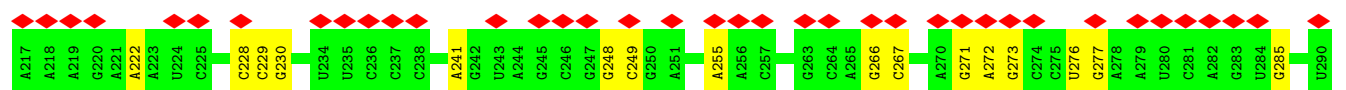
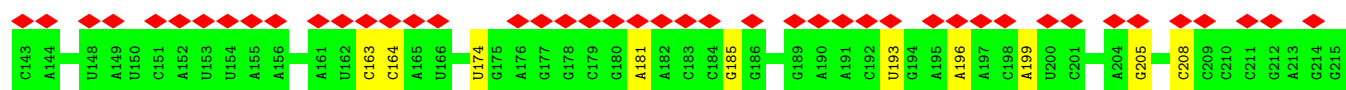
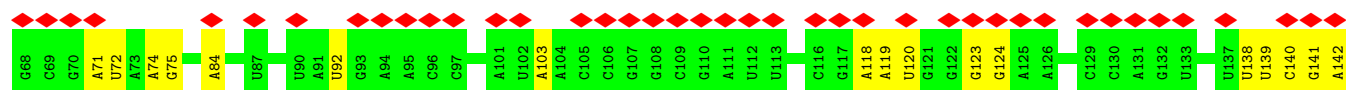
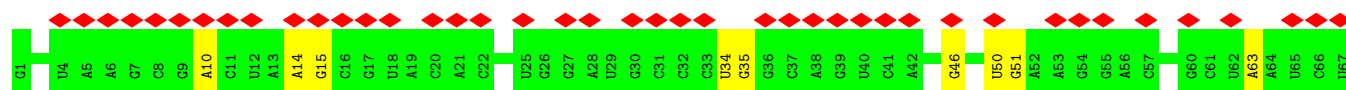
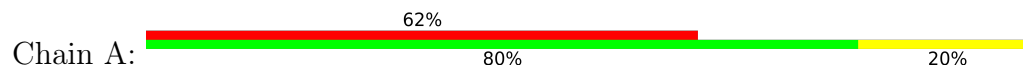
- Molecule 26: 50S ribosomal protein L36

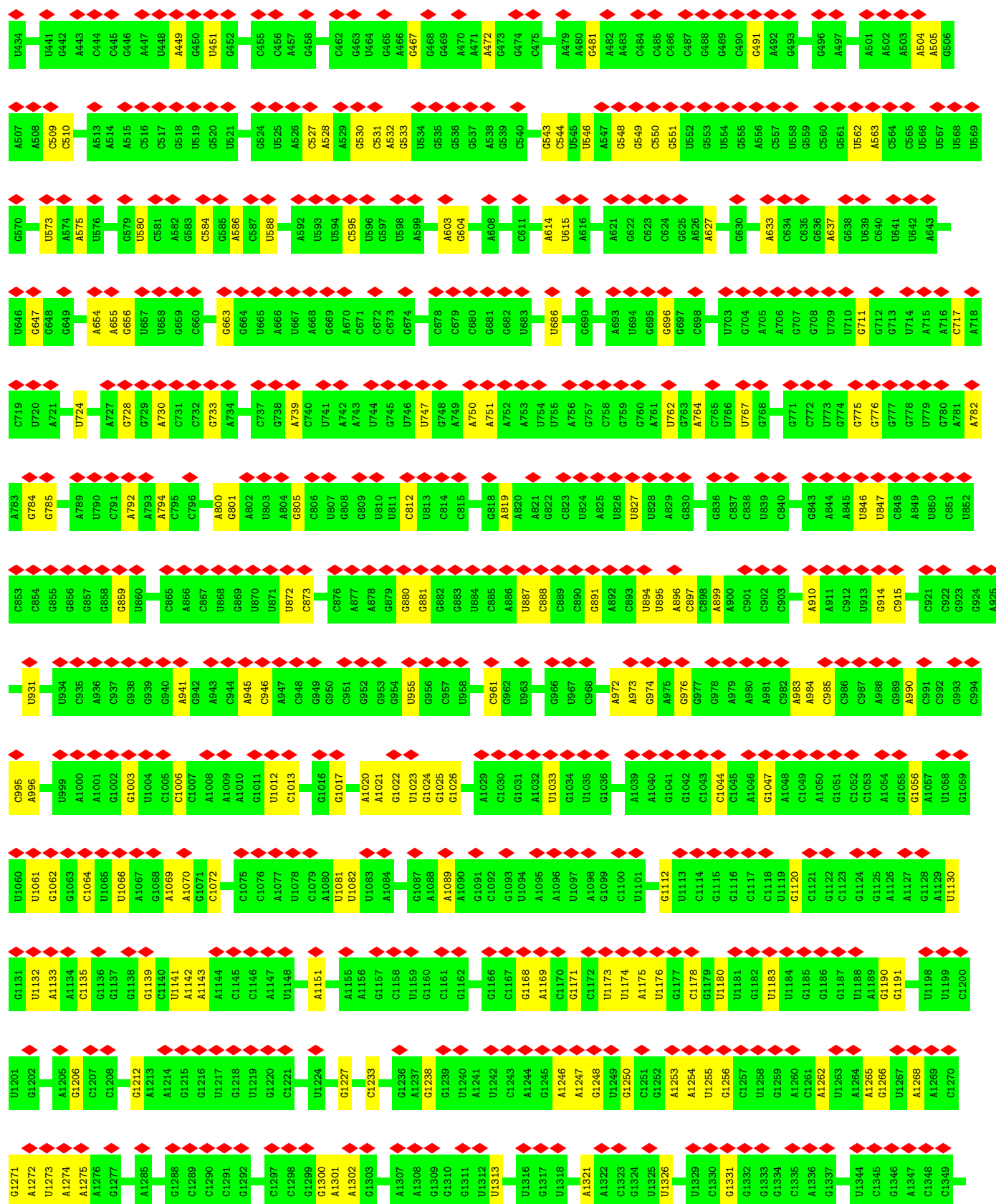


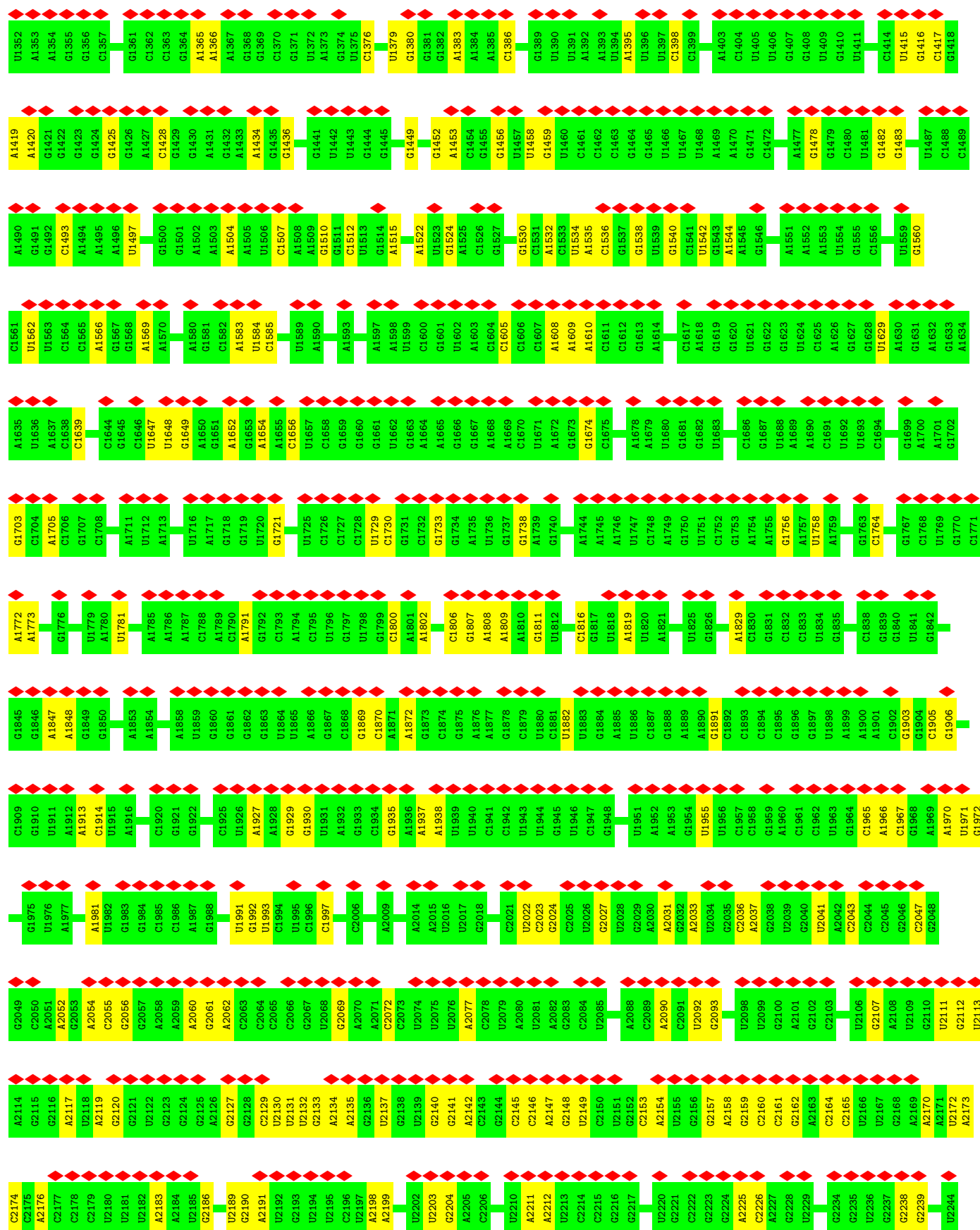
• Molecule 27: 50S ribosomal protein L1



• Molecule 28: 23S ribosomal RNA





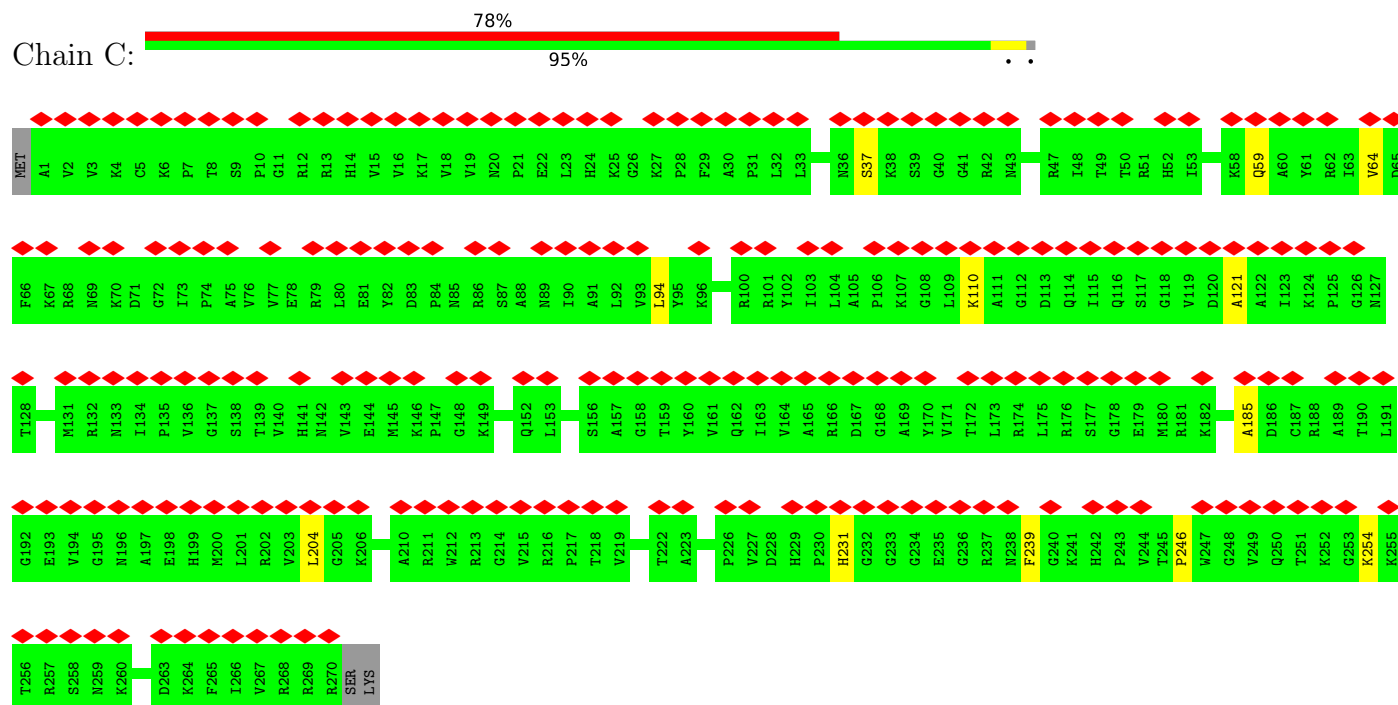






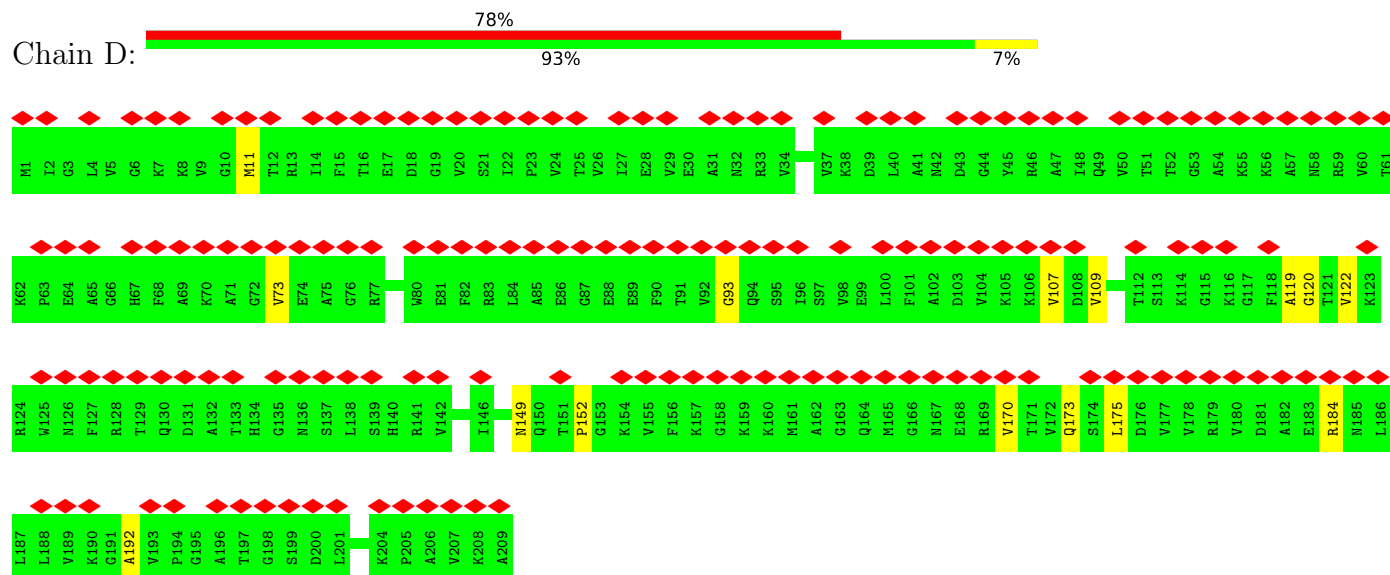
- Molecule 30: 50S ribosomal protein L2

Chain C:



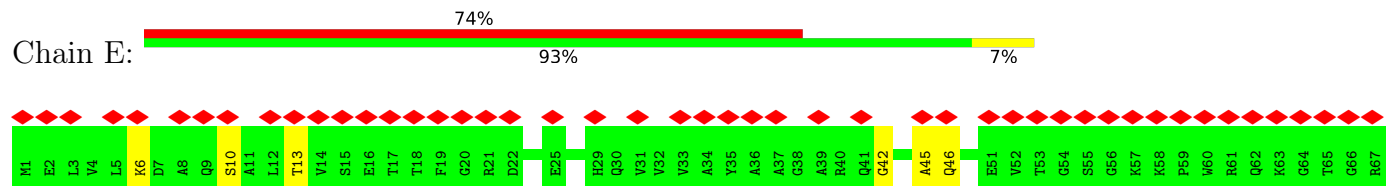
- Molecule 31: 50S ribosomal protein L3

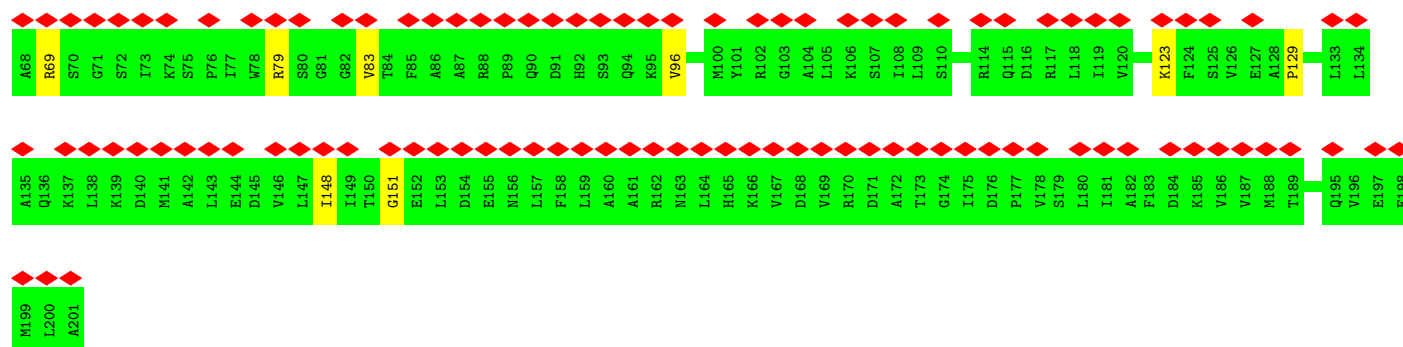
Chain D:



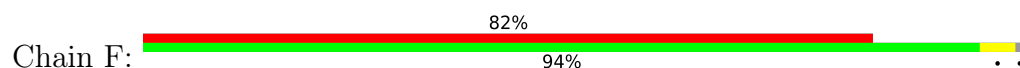
- Molecule 32: 50S ribosomal protein L4

Chain E:

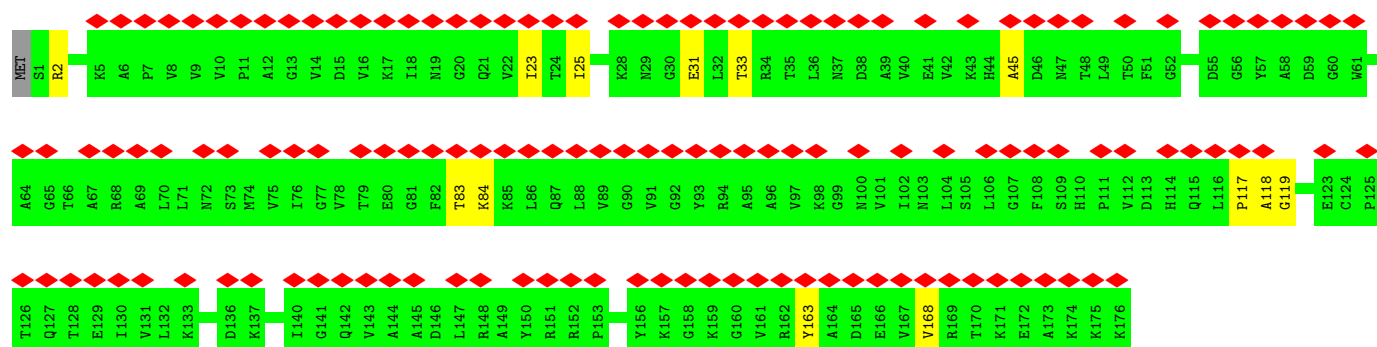
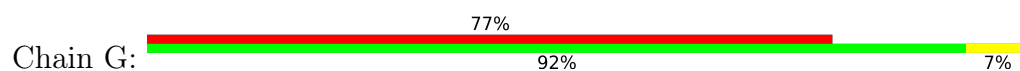




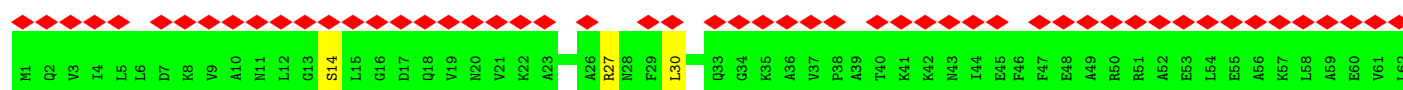
• Molecule 33: 50S ribosomal protein L5

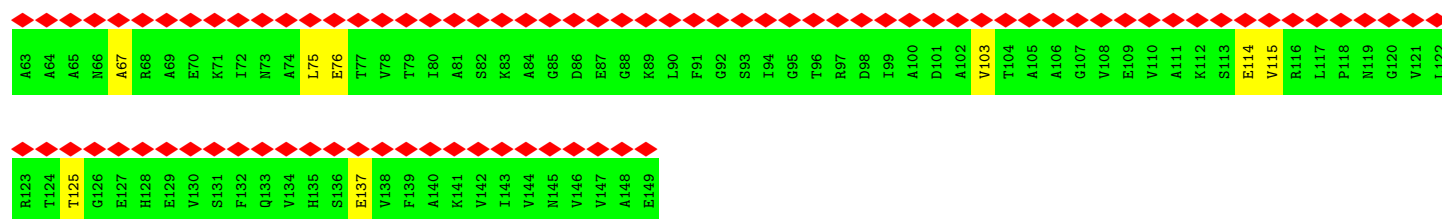


• Molecule 34: 50S ribosomal protein L6



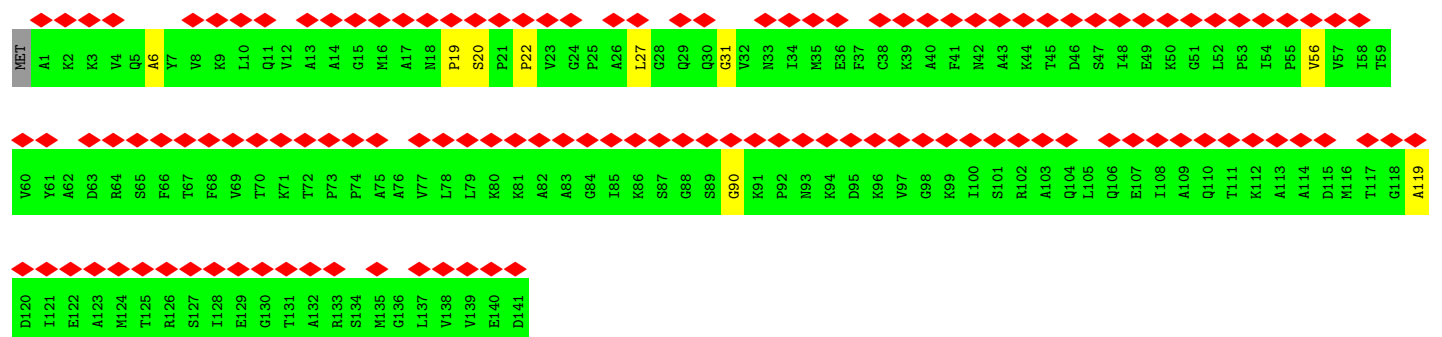
• Molecule 35: 50S ribosomal protein L9





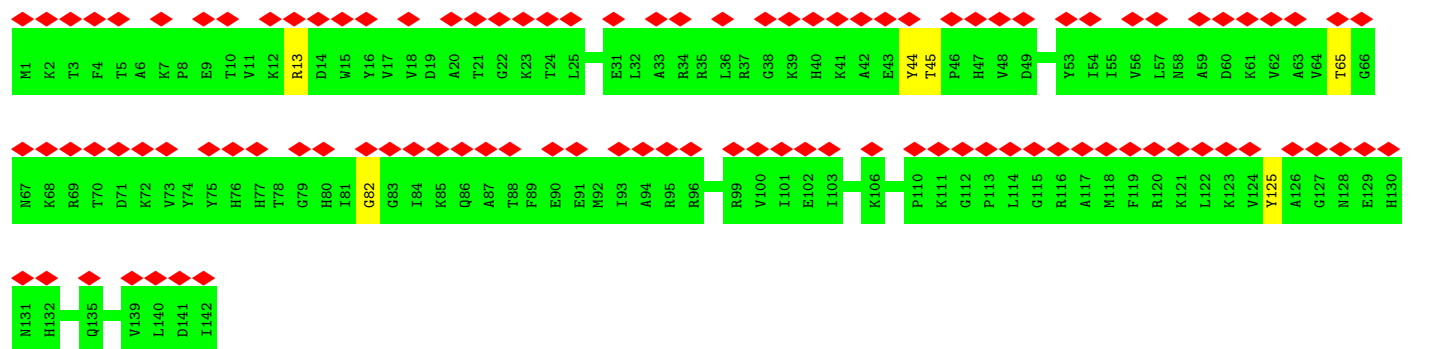
• Molecule 36: 50S ribosomal protein L11

Chain I: 88% 93% 6% .



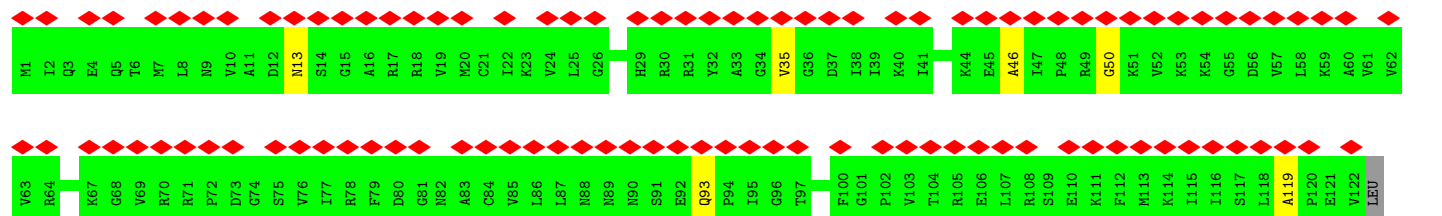
• Molecule 37: 50S ribosomal protein L13

Chain J: 73% 96% .

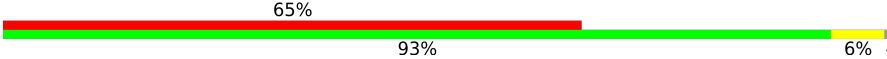


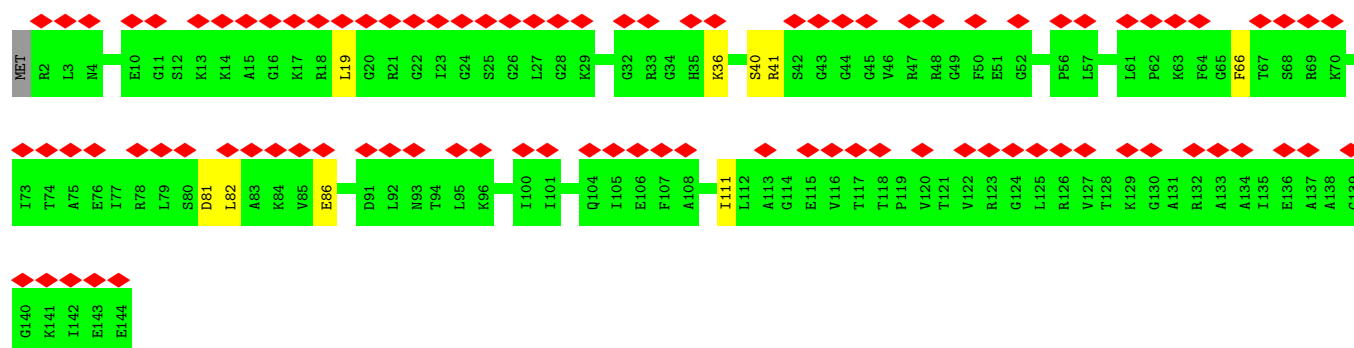
• Molecule 38: 50S ribosomal protein L14

Chain K: 83% 94% 5% .

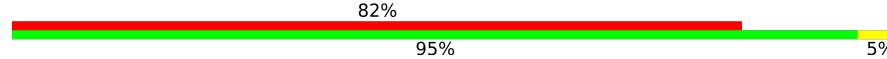


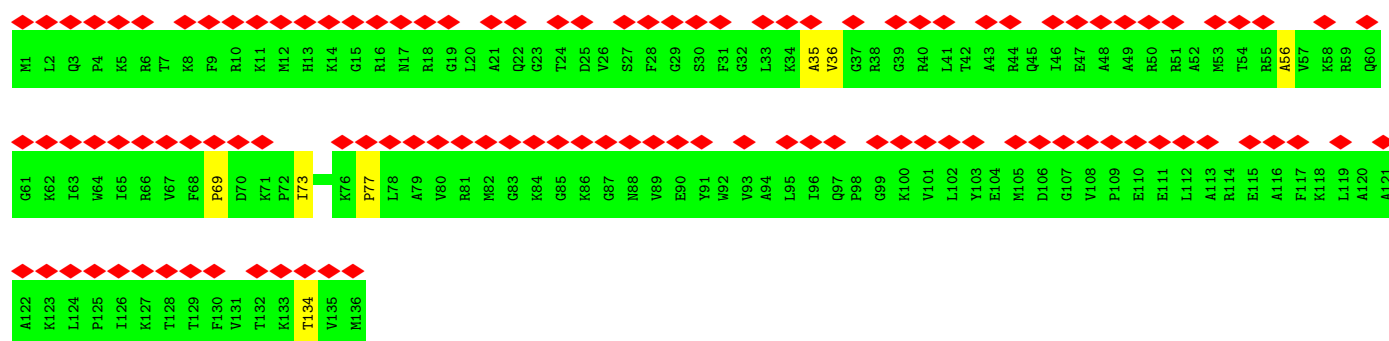
• Molecule 39: 50S ribosomal protein L15

Chain L: 

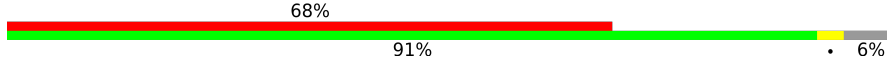


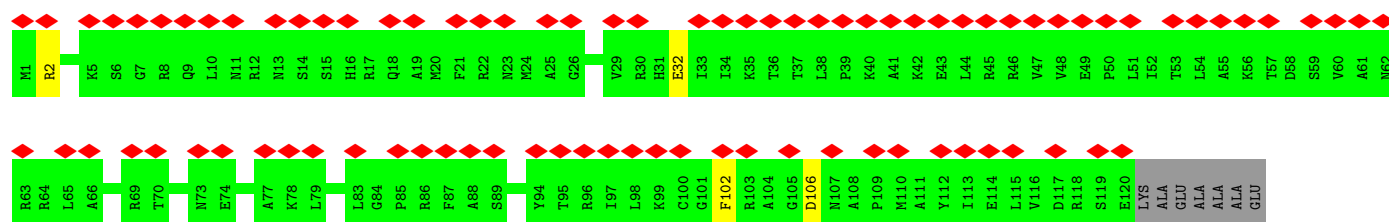
- Molecule 40: 50S ribosomal protein L16

Chain M: 



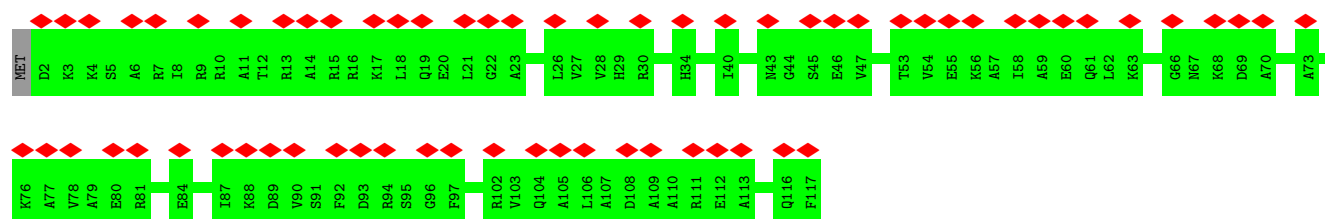
- Molecule 41: 50S ribosomal protein L17

Chain N: 

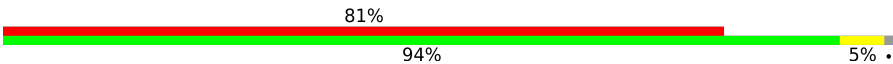


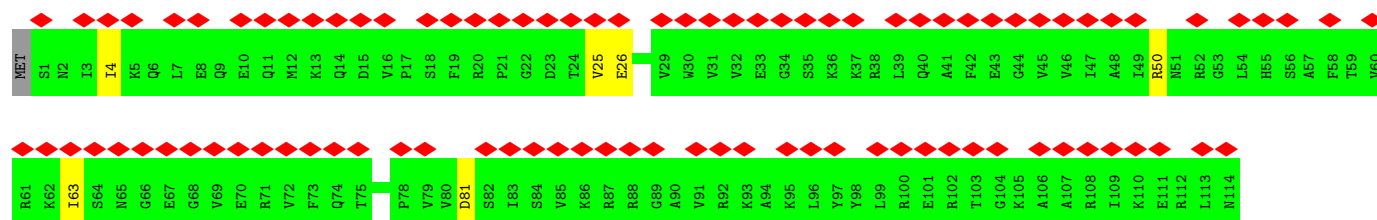
- Molecule 42: 50S ribosomal protein L18

Chain O: 



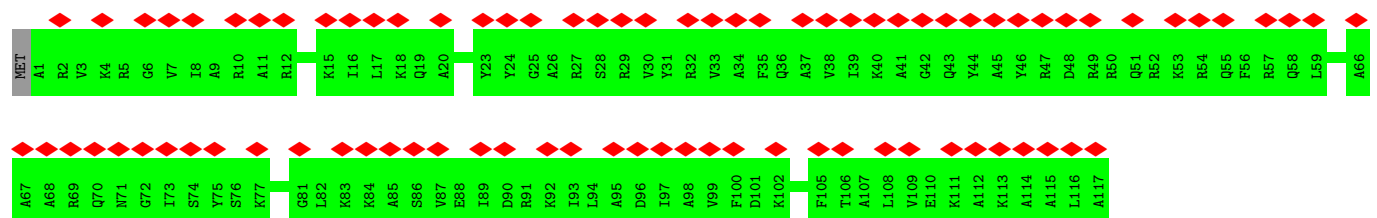
- Molecule 43: 50S ribosomal protein L19

Chain P: 




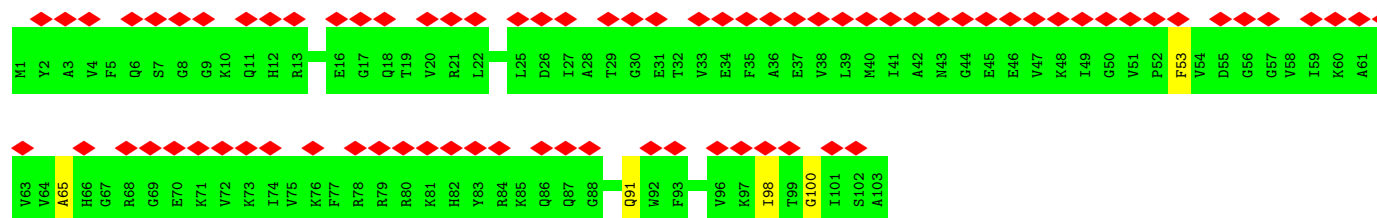
- Molecule 44: 50S ribosomal protein L20

Chain Q: 

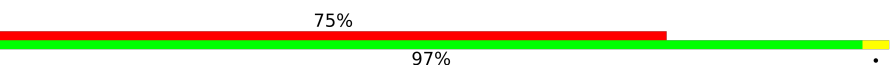


- Molecule 45: 50S ribosomal protein L21

Chain R: 




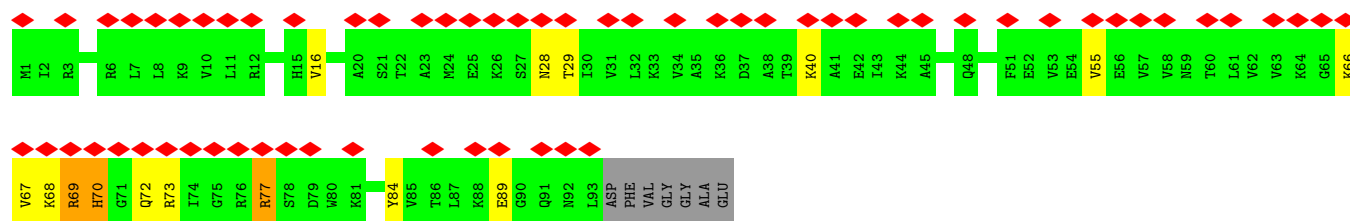
- Molecule 46: 50S ribosomal protein L22

Chain S: 

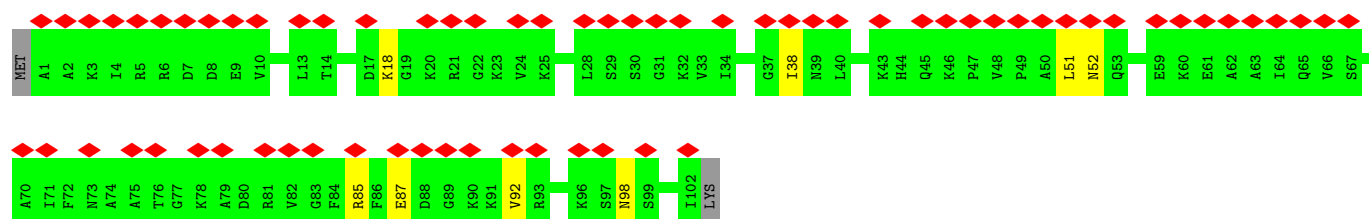
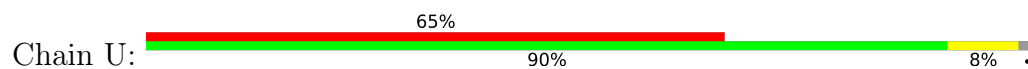


- Molecule 47: 50S ribosomal protein L23

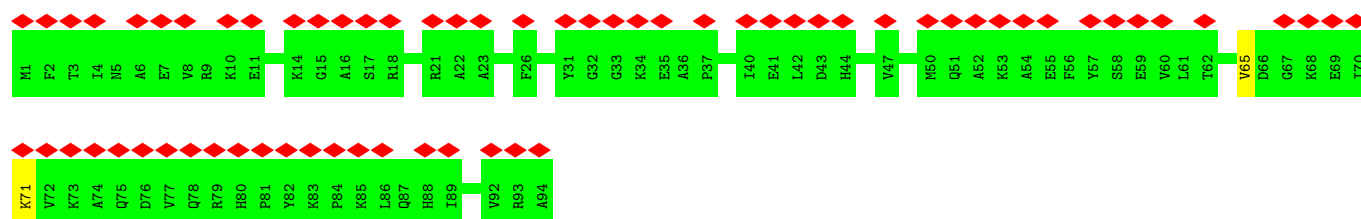
Chain T: 



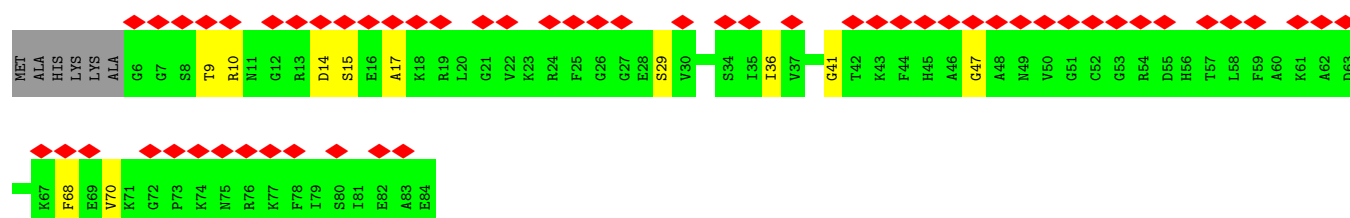
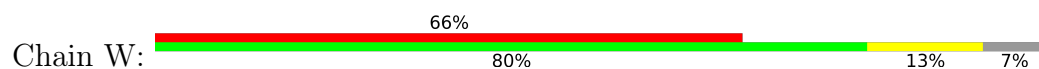
• Molecule 48: 50S ribosomal protein L24



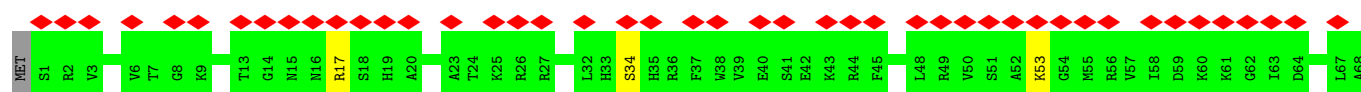
• Molecule 49: 50S ribosomal protein L25

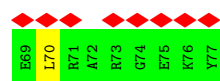


• Molecule 50: 50S ribosomal protein L27

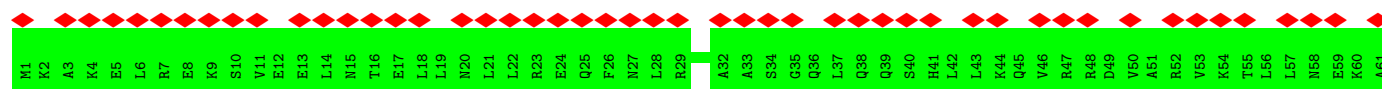
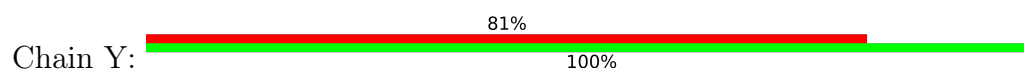


• Molecule 51: 50S ribosomal protein L28

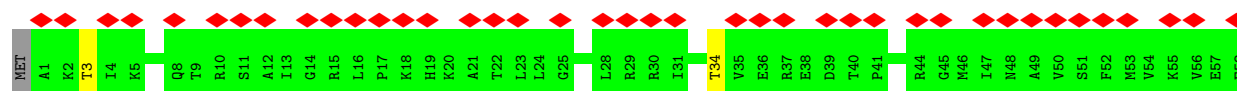




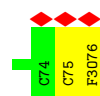
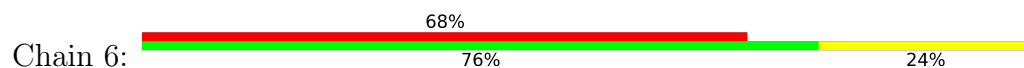
- Molecule 52: 50S ribosomal protein L29



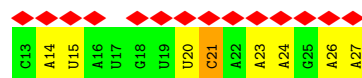
- Molecule 53: 50S ribosomal protein L30



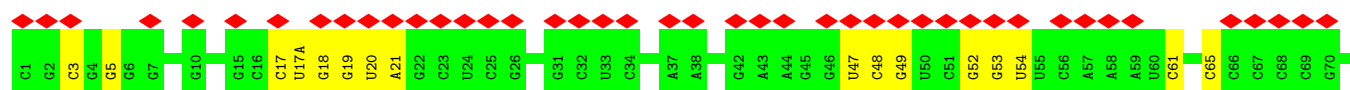
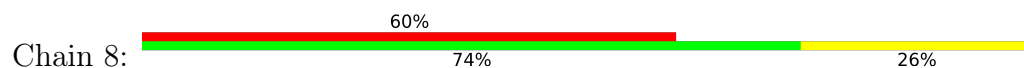
- Molecule 54: tRNA



- Molecule 55: mRNA

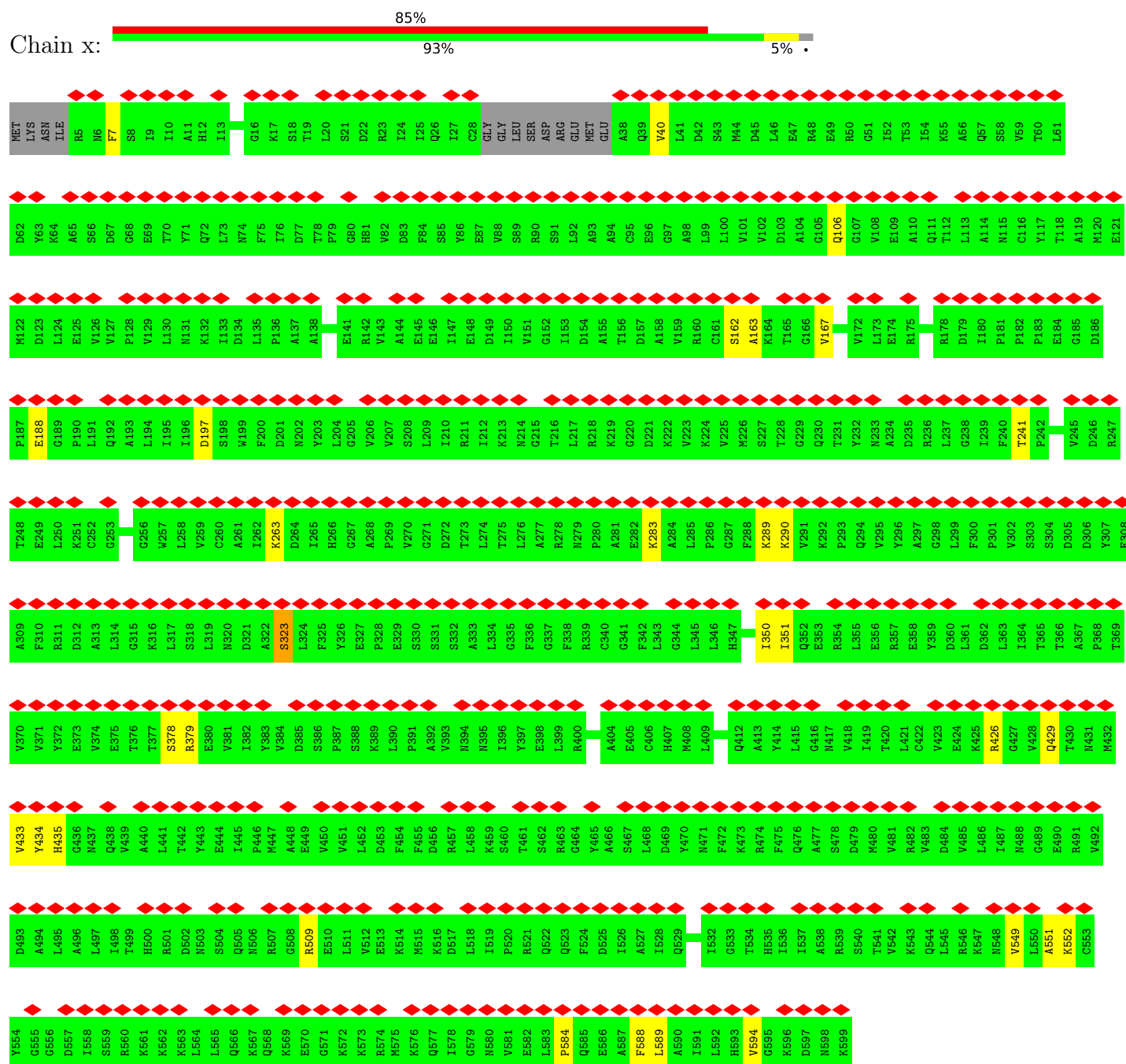


- Molecule 56: tRNA

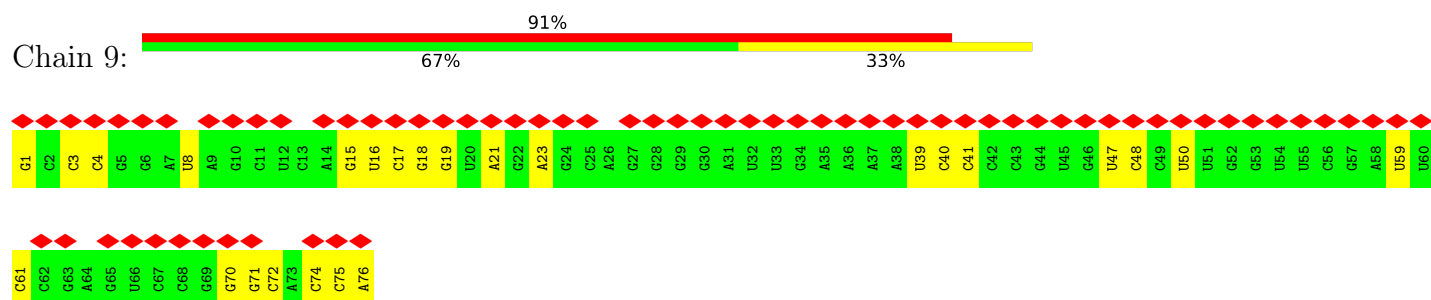




• Molecule 57: Elongation factor 4



• Molecule 58: tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107706	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, F3O, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	a	0.73	0/36834	0.79	0/57462
2	c	0.42	0/1651	0.52	0/2225
3	d	0.38	0/1665	0.50	0/2227
4	e	0.46	0/1118	0.56	0/1504
5	f	0.37	0/851	0.53	0/1150
6	g	0.37	0/1195	0.49	0/1602
7	h	0.43	0/989	0.52	0/1326
8	i	0.39	0/1034	0.56	0/1375
9	j	0.37	0/796	0.51	0/1077
10	k	0.43	0/893	0.54	0/1205
11	l	0.46	0/969	0.55	0/1300
12	m	0.38	0/892	0.55	0/1193
13	n	0.37	0/817	0.52	0/1088
14	o	0.43	0/722	0.50	0/964
15	p	0.36	0/659	0.47	0/884
16	q	0.42	0/657	0.54	0/881
17	r	0.43	0/462	0.49	0/621
18	s	0.36	0/652	0.50	0/877
19	t	0.37	0/671	0.46	0/888
20	u	0.38	0/430	0.53	0/570
21	b	0.35	0/1735	0.51	0/2338
22	0	0.48	0/450	0.54	0/599
23	1	0.44	0/416	0.52	0/554
24	2	0.52	0/380	0.57	0/498
25	3	0.45	0/513	0.58	0/676
26	4	0.45	0/303	0.58	0/397
27	5	0.24	0/1748	0.53	0/2355
28	A	0.84	0/69799	0.81	2/108892 (0.0%)
29	B	0.63	0/2828	0.74	0/4410
30	C	0.52	0/2115	0.58	0/2844
31	D	0.48	0/1586	0.56	0/2134
32	E	0.43	0/1571	0.54	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	F	0.37	0/1434	0.47	0/1926
34	G	0.37	0/1343	0.51	0/1816
35	H	0.30	0/1122	0.57	0/1515
36	I	0.28	0/1046	0.50	0/1410
37	J	0.50	0/1152	0.58	0/1551
38	K	0.49	0/947	0.58	0/1268
39	L	0.45	0/1054	0.57	0/1403
40	M	0.49	0/1093	0.61	0/1460
41	N	0.48	0/973	0.56	0/1301
42	O	0.38	0/902	0.48	0/1209
43	P	0.45	0/929	0.56	0/1242
44	Q	0.57	0/960	0.55	0/1278
45	R	0.48	0/829	0.54	0/1107
46	S	0.48	0/864	0.57	0/1156
47	T	0.40	0/744	0.57	0/994
48	U	0.37	0/787	0.54	0/1051
49	V	0.40	0/766	0.49	0/1025
50	W	0.47	0/603	0.64	0/797
51	X	0.47	0/635	0.56	0/848
52	Y	0.41	0/510	0.51	0/677
53	Z	0.41	0/453	0.58	0/605
54	6	0.63	1/1788 (0.1%)	0.78	0/2784
55	7	0.64	0/358	0.92	2/555 (0.4%)
56	8	0.64	0/1832	0.76	0/2855
57	x	0.39	0/4646	0.52	0/6285
58	9	0.40	1/1813 (0.1%)	0.79	0/2823
All	All	0.70	2/166984 (0.0%)	0.74	4/249170 (0.0%)

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
11	l	0	1
20	u	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	9	1	G	OP3-P	-10.74	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	1	G	OP3-P	-10.67	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	323	C	N1-C2-O2	5.44	122.17	118.90
55	7	21	C	C2-N1-C1'	5.24	124.56	118.80
55	7	21	C	N1-C2-O2	5.22	122.03	118.90
28	A	2689	U	C2-N1-C1'	-5.05	111.64	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	l	23	ALA	Peptide
20	u	37	PHE	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	204/233 (88%)	182 (89%)	16 (8%)	6 (3%)	4	28
3	d	203/206 (98%)	180 (89%)	16 (8%)	7 (3%)	3	24
4	e	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	5	30
5	f	100/135 (74%)	84 (84%)	9 (9%)	7 (7%)	1	8
6	g	149/179 (83%)	134 (90%)	11 (7%)	4 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	127/130 (98%)	114 (90%)	11 (9%)	2 (2%)	9	43
8	i	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	4	26
9	j	96/103 (93%)	76 (79%)	11 (12%)	9 (9%)	0	3
10	k	115/129 (89%)	102 (89%)	9 (8%)	4 (4%)	3	24
11	l	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	21
12	m	112/118 (95%)	101 (90%)	6 (5%)	5 (4%)	2	18
13	n	98/101 (97%)	70 (71%)	15 (15%)	13 (13%)	0	1
14	o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	13	49
15	p	80/82 (98%)	66 (82%)	8 (10%)	6 (8%)	1	7
16	q	78/84 (93%)	62 (80%)	14 (18%)	2 (3%)	5	31
17	r	53/75 (71%)	50 (94%)	2 (4%)	1 (2%)	8	39
18	s	77/92 (84%)	68 (88%)	5 (6%)	4 (5%)	2	15
19	t	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	6	34
20	u	49/71 (69%)	39 (80%)	7 (14%)	3 (6%)	1	12
21	b	216/241 (90%)	189 (88%)	20 (9%)	7 (3%)	4	26
22	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	8	39
23	1	48/55 (87%)	41 (85%)	6 (12%)	1 (2%)	7	37
24	2	44/46 (96%)	43 (98%)	0	1 (2%)	6	34
25	3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	4	26
26	4	36/38 (95%)	25 (69%)	5 (14%)	6 (17%)	0	0
27	5	232/234 (99%)	190 (82%)	34 (15%)	8 (3%)	3	24
30	C	268/273 (98%)	228 (85%)	28 (10%)	12 (4%)	2	18
31	D	207/209 (99%)	169 (82%)	23 (11%)	15 (7%)	1	7
32	E	199/201 (99%)	171 (86%)	14 (7%)	14 (7%)	1	8
33	F	175/179 (98%)	146 (83%)	21 (12%)	8 (5%)	2	18
34	G	174/177 (98%)	140 (80%)	21 (12%)	13 (8%)	1	7
35	H	147/149 (99%)	114 (78%)	22 (15%)	11 (8%)	1	7
36	I	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	1	10
37	J	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	20
38	K	120/123 (98%)	100 (83%)	14 (12%)	6 (5%)	2	16
39	L	141/144 (98%)	115 (82%)	17 (12%)	9 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	M	134/136 (98%)	112 (84%)	15 (11%)	7 (5%)	2	15
41	N	118/127 (93%)	104 (88%)	10 (8%)	4 (3%)	3	24
42	O	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
43	P	112/115 (97%)	93 (83%)	13 (12%)	6 (5%)	2	14
44	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
45	R	101/103 (98%)	81 (80%)	15 (15%)	5 (5%)	2	16
46	S	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	5	29
47	T	91/100 (91%)	61 (67%)	18 (20%)	12 (13%)	0	1
48	U	100/104 (96%)	81 (81%)	11 (11%)	8 (8%)	1	6
49	V	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	6	35
50	W	77/85 (91%)	49 (64%)	17 (22%)	11 (14%)	0	1
51	X	75/78 (96%)	64 (85%)	7 (9%)	4 (5%)	2	15
52	Y	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
53	Z	56/59 (95%)	51 (91%)	3 (5%)	2 (4%)	3	23
57	x	582/599 (97%)	496 (85%)	58 (10%)	28 (5%)	2	17
All	All	6442/6818 (94%)	5465 (85%)	667 (10%)	310 (5%)	4	17

All (310) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	125	VAL
5	f	98	GLU
5	f	101	PRO
9	j	57	VAL
9	j	61	ALA
11	l	44	LYS
12	m	10	PRO
13	n	34	VAL
13	n	35	ASN
13	n	37	SER
13	n	41	ARG
13	n	42	TRP
13	n	49	GLN
13	n	52	PRO
16	q	50	ASN
20	u	9	ASN
20	u	38	TYR

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Mol	Chain	Res	Type
20	u	40	LYS
21	b	150	ILE
21	b	163	ILE
27	5	38	PHE
30	C	59	GLN
30	C	64	VAL
30	C	204	LEU
31	D	11	MET
31	D	73	VAL
31	D	122	VAL
31	D	192	ALA
32	E	69	ARG
32	E	79	ARG
33	F	40	GLY
34	G	2	ARG
34	G	84	LYS
34	G	163	TYR
34	G	168	VAL
35	H	125	THR
36	I	56	VAL
37	J	44	TYR
37	J	45	THR
38	K	13	ASN
39	L	111	ILE
40	M	36	VAL
41	N	106	ASP
43	P	50	ARG
46	S	19	LEU
46	S	96	ILE
47	T	72	GLN
48	U	92	VAL
49	V	65	VAL
50	W	29	SER
50	W	36	ILE
50	W	70	VAL
57	x	40	VAL
57	x	197	ASP
57	x	323	SER
57	x	350	ILE
57	x	351	ILE
57	x	378	SER
57	x	426	ARG

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Mol	Chain	Res	Type
57	x	549	VAL
57	x	584	PRO
57	x	588	PHE
57	x	594	VAL
2	c	15	VAL
2	c	64	ILE
2	c	101	ILE
3	d	24	GLY
3	d	25	VAL
3	d	36	GLN
5	f	85	ILE
5	f	93	LYS
6	g	130	ASN
7	h	67	GLN
7	h	75	ILE
8	i	121	ALA
8	i	129	LYS
9	j	36	VAL
9	j	91	ASP
10	k	119	ASN
11	l	73	ASN
11	l	75	GLN
12	m	4	ILE
12	m	47	GLU
12	m	105	ASN
13	n	25	ALA
13	n	33	ASP
13	n	47	LYS
13	n	53	ARG
13	n	92	GLU
15	p	43	ALA
16	q	15	ASP
18	s	28	LYS
19	t	4	ILE
21	b	19	THR
23	1	4	ILE
25	3	22	LYS
26	4	7	VAL
27	5	124	VAL
27	5	145	VAL
27	5	167	LYS
30	C	185	ALA

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Mol	Chain	Res	Type
30	C	239	PHE
31	D	93	GLY
31	D	170	VAL
31	D	184	ARG
32	E	148	ILE
33	F	176	PHE
34	G	117	PRO
35	H	14	SER
35	H	27	ARG
35	H	75	LEU
35	H	103	VAL
35	H	115	VAL
35	H	137	GLU
36	I	6	ALA
36	I	20	SER
37	J	13	ARG
37	J	82	GLY
37	J	125	TYR
38	K	35	VAL
38	K	50	GLY
39	L	81	ASP
39	L	82	LEU
40	M	73	ILE
41	N	2	ARG
47	T	40	LYS
47	T	69	ARG
47	T	77	ARG
47	T	84	TYR
47	T	89	GLU
48	U	87	GLU
48	U	98	ASN
50	W	17	ALA
50	W	68	PHE
57	x	7	PHE
57	x	163	ALA
57	x	263	LYS
57	x	289	LYS
57	x	379	ARG
57	x	552	LYS
3	d	32	CYS
4	e	12	GLN
4	e	24	THR

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Mol	Chain	Res	Type
4	e	45	ARG
4	e	78	ASN
5	f	54	LEU
5	f	92	THR
5	f	94	HIS
10	k	17	SER
12	m	114	LYS
15	p	49	GLY
18	s	4	SER
18	s	5	LEU
21	b	81	ASP
21	b	125	PHE
25	3	27	ASN
27	5	53	ARG
31	D	119	ALA
32	E	6	LYS
32	E	13	THR
32	E	123	LYS
34	G	31	GLU
34	G	33	THR
34	G	45	ALA
34	G	118	ALA
35	H	30	LEU
35	H	67	ALA
35	H	76	GLU
35	H	114	GLU
39	L	41	ARG
40	M	56	ALA
40	M	69	PRO
40	M	77	PRO
47	T	29	THR
47	T	55	VAL
47	T	70	HIS
48	U	18	LYS
50	W	14	ASP
50	W	41	GLY
50	W	47	GLY
51	X	53	LYS
57	x	429	GLN
57	x	433	VAL
57	x	434	TYR
57	x	435	HIS

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Mol	Chain	Res	Type
6	g	114	LYS
8	i	56	ASP
8	i	58	VAL
9	j	34	ALA
10	k	14	LYS
10	k	15	GLN
11	l	98	VAL
13	n	3	LYS
14	o	46	HIS
15	p	44	SER
15	p	79	ASN
15	p	81	ALA
18	s	6	LYS
21	b	148	GLY
26	4	29	ALA
26	4	37	GLN
27	5	15	VAL
30	C	37	SER
30	C	110	LYS
32	E	10	SER
32	E	42	GLY
32	E	45	ALA
34	G	83	THR
36	I	19	PRO
36	I	27	LEU
38	K	93	GLN
39	L	19	LEU
39	L	40	SER
43	P	81	ASP
45	R	100	GLY
47	T	28	ASN
48	U	52	ASN
49	V	71	LYS
50	W	9	THR
53	Z	3	THR
57	x	188	GLU
57	x	283	LYS
2	c	61	ALA
2	c	66	VAL
3	d	167	LYS
6	g	85	TYR
9	j	89	ARG

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Mol	Chain	Res	Type
9	j	93	ALA
11	l	48	ALA
19	t	68	HIS
24	2	45	SER
26	4	8	LYS
26	4	16	ILE
27	5	150	ALA
30	C	94	LEU
30	C	121	ALA
30	C	231	HIS
30	C	254	LYS
31	D	149	ASN
31	D	152	PRO
31	D	173	GLN
32	E	46	GLN
32	E	83	VAL
32	E	96	VAL
33	F	11	VAL
33	F	128	SER
33	F	133	GLU
33	F	160	LYS
34	G	119	GLY
36	I	90	GLY
36	I	119	ALA
38	K	46	ALA
39	L	36	LYS
39	L	86	GLU
40	M	35	ALA
43	P	63	ILE
45	R	65	ALA
45	R	91	GLN
45	R	98	ILE
46	S	65	ASP
47	T	67	VAL
48	U	85	ARG
50	W	10	ARG
50	W	15	SER
51	X	34	SER
51	X	70	LEU
53	Z	34	THR
57	x	162	SER
57	x	290	LYS

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Mol	Chain	Res	Type
2	c	3	GLN
3	d	195	ILE
9	j	42	LEU
21	b	67	LEU
22	o	54	ILE
31	D	109	VAL
31	D	120	GLY
31	D	175	LEU
32	E	151	GLY
33	F	132	ARG
36	I	22	PRO
37	J	65	THR
38	K	119	ALA
39	L	66	PHE
40	M	134	THR
41	N	32	GLU
41	N	102	PHE
43	P	4	ILE
43	P	25	VAL
43	P	26	GLU
45	R	53	PHE
47	T	16	VAL
48	U	51	LEU
51	X	17	ARG
57	x	551	ALA
30	C	246	PRO
33	F	59	ILE
36	I	31	GLY
15	p	33	ILE
26	4	3	VAL
31	D	107	VAL
34	G	25	ILE
48	U	38	ILE
57	x	167	VAL
6	g	81	GLY
17	r	21	ILE
27	5	233	VAL
34	G	23	ILE
57	x	241	THR
9	j	74	VAL
32	E	129	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	170/190 (90%)	170 (100%)	0	100	100
3	d	172/173 (99%)	172 (100%)	0	100	100
4	e	113/126 (90%)	113 (100%)	0	100	100
5	f	89/116 (77%)	89 (100%)	0	100	100
6	g	124/147 (84%)	124 (100%)	0	100	100
7	h	104/105 (99%)	104 (100%)	0	100	100
8	i	105/107 (98%)	105 (100%)	0	100	100
9	j	86/90 (96%)	86 (100%)	0	100	100
10	k	90/99 (91%)	90 (100%)	0	100	100
11	l	103/104 (99%)	103 (100%)	0	100	100
12	m	92/96 (96%)	92 (100%)	0	100	100
13	n	83/84 (99%)	73 (88%)	10 (12%)	5	22
14	o	76/77 (99%)	76 (100%)	0	100	100
15	p	65/65 (100%)	65 (100%)	0	100	100
16	q	74/78 (95%)	74 (100%)	0	100	100
17	r	48/65 (74%)	48 (100%)	0	100	100
18	s	70/79 (89%)	70 (100%)	0	100	100
19	t	65/66 (98%)	65 (100%)	0	100	100
20	u	44/61 (72%)	44 (100%)	0	100	100
21	b	180/199 (90%)	180 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	44 (98%)	1 (2%)	52	79
24	2	38/38 (100%)	38 (100%)	0	100	100
25	3	51/52 (98%)	51 (100%)	0	100	100
26	4	34/34 (100%)	34 (100%)	0	100	100
27	5	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	C	215/218 (99%)	215 (100%)	0	100	100
31	D	164/164 (100%)	164 (100%)	0	100	100
32	E	165/165 (100%)	165 (100%)	0	100	100
33	F	148/150 (99%)	148 (100%)	0	100	100
34	G	137/138 (99%)	137 (100%)	0	100	100
35	H	114/114 (100%)	114 (100%)	0	100	100
36	I	109/110 (99%)	109 (100%)	0	100	100
37	J	116/116 (100%)	116 (100%)	0	100	100
38	K	103/104 (99%)	103 (100%)	0	100	100
39	L	102/103 (99%)	102 (100%)	0	100	100
40	M	109/109 (100%)	109 (100%)	0	100	100
41	N	100/103 (97%)	100 (100%)	0	100	100
42	O	86/87 (99%)	86 (100%)	0	100	100
43	P	99/100 (99%)	99 (100%)	0	100	100
44	Q	89/90 (99%)	89 (100%)	0	100	100
45	R	84/84 (100%)	84 (100%)	0	100	100
46	S	93/93 (100%)	93 (100%)	0	100	100
47	T	80/84 (95%)	74 (92%)	6 (8%)	13	45
48	U	83/85 (98%)	83 (100%)	0	100	100
49	V	78/78 (100%)	78 (100%)	0	100	100
50	W	59/63 (94%)	59 (100%)	0	100	100
51	X	67/68 (98%)	67 (100%)	0	100	100
52	Y	55/55 (100%)	55 (100%)	0	100	100
53	Z	48/49 (98%)	48 (100%)	0	100	100
57	x	500/511 (98%)	496 (99%)	4 (1%)	81	93
All	All	5352/5570 (96%)	5331 (100%)	21 (0%)	91	95

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	n	24	ARG
13	n	26	GLU
13	n	27	LEU

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Mol	Chain	Res	Type
13	n	33	ASP
13	n	38	ASP
13	n	39	GLU
13	n	40	ASP
13	n	41	ARG
13	n	42	TRP
13	n	47	LYS
23	1	8	ILE
47	T	66	LYS
47	T	68	LYS
47	T	69	ARG
47	T	70	HIS
47	T	73	ARG
47	T	77	ARG
57	x	106	GLN
57	x	323	SER
57	x	509	ARG
57	x	589	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	d	120	HIS
5	f	46	GLN
5	f	55	HIS
5	f	63	ASN
6	g	86	GLN
7	h	67	GLN
8	i	75	GLN
9	j	35	GLN
10	k	22	HIS
11	l	5	ASN
12	m	14	HIS
13	n	35	ASN
13	n	43	ASN
13	n	60	GLN
14	o	35	GLN
16	q	51	ASN
18	s	69	HIS
19	t	48	GLN
19	t	82	GLN
21	b	119	GLN

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Mol	Chain	Res	Type
22	0	4	GLN
22	0	5	ASN
22	0	18	HIS
27	5	58	ASN
27	5	83	ASN
27	5	110	ASN
30	C	52	HIS
30	C	57	HIS
30	C	114	GLN
30	C	259	ASN
31	D	49	GLN
31	D	130	GLN
32	E	62	GLN
32	E	165	HIS
34	G	21	GLN
34	G	72	ASN
34	G	103	ASN
34	G	110	HIS
35	H	2	GLN
35	H	18	GLN
35	H	28	ASN
37	J	40	HIS
37	J	135	GLN
39	L	54	GLN
40	M	22	GLN
41	N	9	GLN
43	P	9	GLN
43	P	11	GLN
44	Q	43	GLN
45	R	66	HIS
47	T	15	HIS
47	T	70	HIS
47	T	91	GLN
48	U	65	GLN
49	V	44	HIS
49	V	51	GLN
49	V	80	HIS
50	W	39	GLN
51	X	16	ASN
52	Y	20	ASN
52	Y	27	ASN
52	Y	41	HIS

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Mol	Chain	Res	Type
53	Z	19	HIS
57	x	81	HIS
57	x	192	GLN
57	x	214	ASN
57	x	266	HIS
57	x	294	GLN
57	x	407	HIS
57	x	429	GLN
57	x	476	GLN
57	x	548	ASN
57	x	568	GLN
57	x	593	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1532/1533 (99%)	302 (19%)	0
28	A	2902/2904 (99%)	566 (19%)	24 (0%)
29	B	117/120 (97%)	18 (15%)	0
54	6	74/76 (97%)	15 (20%)	3 (4%)
55	7	14/15 (93%)	7 (50%)	1 (7%)
56	8	76/77 (98%)	20 (26%)	0
58	9	75/76 (98%)	24 (32%)	2 (2%)
All	All	4790/4801 (99%)	952 (19%)	30 (0%)

All (952) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	13	U
1	a	15	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	39	G
1	a	48	C
1	a	50	A
1	a	51	A

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Mol	Chain	Res	Type
1	a	52	C
1	a	70	U
1	a	71	A
1	a	74	A
1	a	75	G
1	a	77	A
1	a	78	A
1	a	79	G
1	a	81	A
1	a	83	C
1	a	85	U
1	a	86	G
1	a	87	C
1	a	89	U
1	a	90	C
1	a	91	U
1	a	94	G
1	a	95	C
1	a	99	C
1	a	116	A
1	a	121	U
1	a	130	A
1	a	131	A
1	a	144	G
1	a	146	G
1	a	151	A
1	a	156	C
1	a	163	C
1	a	164	G
1	a	166	U
1	a	182	A
1	a	191	G
1	a	192	A
1	a	197	A
1	a	204	G
1	a	205	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	226	G
1	a	227	G
1	a	240	G

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Mol	Chain	Res	Type
1	a	245	U
1	a	247	G
1	a	251	G
1	a	262	A
1	a	266	G
1	a	267	C
1	a	283	U
1	a	289	G
1	a	298	A
1	a	299	G
1	a	307	C
1	a	314	C
1	a	321	A
1	a	328	C
1	a	329	A
1	a	330	C
1	a	332	G
1	a	344	A
1	a	345	C
1	a	346	G
1	a	347	G
1	a	352	C
1	a	353	A
1	a	354	G
1	a	357	G
1	a	362	G
1	a	367	U
1	a	368	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	389	A
1	a	402	G
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	429	U
1	a	430	A

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Mol	Chain	Res	Type
1	a	440	C
1	a	456	A
1	a	457	G
1	a	458	U
1	a	461	A
1	a	462	G
1	a	463	U
1	a	466	A
1	a	467	U
1	a	468	A
1	a	474	G
1	a	479	U
1	a	481	G
1	a	482	A
1	a	483	C
1	a	484	G
1	a	486	U
1	a	496	A
1	a	497	G
1	a	505	G
1	a	511	C
1	a	518	C
1	a	527	G
1	a	530	G
1	a	531	U
1	a	533	A
1	a	545	C
1	a	547	A
1	a	559	A
1	a	562	U
1	a	564	C
1	a	571	U
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	622	A
1	a	628	G
1	a	631	C
1	a	632	U

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Mol	Chain	Res	Type
1	a	653	U
1	a	654	G
1	a	665	A
1	a	670	G
1	a	694	A
1	a	703	G
1	a	706	A
1	a	721	G
1	a	723	U
1	a	731	G
1	a	733	G
1	a	748	G
1	a	755	G
1	a	764	C
1	a	778	G
1	a	783	C
1	a	792	A
1	a	793	U
1	a	794	A
1	a	799	G
1	a	805	C
1	a	810	C
1	a	815	A
1	a	817	C
1	a	828	U
1	a	829	G
1	a	841	C
1	a	843	U
1	a	845	A
1	a	846	G
1	a	871	U
1	a	888	G
1	a	889	A
1	a	895	G
1	a	901	A
1	a	902	G
1	a	913	A
1	a	914	A
1	a	920	U
1	a	922	G
1	a	926	G
1	a	927	G

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Mol	Chain	Res	Type
1	a	933	G
1	a	934	C
1	a	935	A
1	a	943	U
1	a	948	C
1	a	960	U
1	a	966	G
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	983	A
1	a	993	G
1	a	996	A
1	a	1001	C
1	a	1004	A
1	a	1008	U
1	a	1011	C
1	a	1018	G
1	a	1026	G
1	a	1027	C
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1036	A
1	a	1037	C
1	a	1043	G
1	a	1050	G
1	a	1054	C
1	a	1055	A
1	a	1056	U
1	a	1060	U
1	a	1065	U
1	a	1070	U
1	a	1086	U
1	a	1087	G
1	a	1094	G
1	a	1095	U

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Mol	Chain	Res	Type
1	a	1101	A
1	a	1124	G
1	a	1130	A
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1146	A
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1192	C
1	a	1194	U
1	a	1196	A
1	a	1197	A
1	a	1200	C
1	a	1202	U
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1257	A
1	a	1260	G
1	a	1261	A
1	a	1267	C
1	a	1279	G
1	a	1280	A
1	a	1282	C
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1303	C
1	a	1305	G
1	a	1312	G
1	a	1317	C

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Mol	Chain	Res	Type
1	a	1318	A
1	a	1320	C
1	a	1331	G
1	a	1332	A
1	a	1337	G
1	a	1357	A
1	a	1363	A
1	a	1364	U
1	a	1379	G
1	a	1381	U
1	a	1395	C
1	a	1401	G
1	a	1406	U
1	a	1419	G
1	a	1429	A
1	a	1441	A
1	a	1446	A
1	a	1449	C
1	a	1451	U
1	a	1452	C
1	a	1469	C
1	a	1487	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1497	G
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1513	A
1	a	1517	G
1	a	1519	A
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
28	A	10	A
28	A	14	A
28	A	15	G
28	A	34	U
28	A	35	G

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Mol	Chain	Res	Type
28	A	46	G
28	A	50	U
28	A	51	G
28	A	63	A
28	A	71	A
28	A	72	U
28	A	74	A
28	A	75	G
28	A	84	A
28	A	92	U
28	A	103	A
28	A	118	A
28	A	120	U
28	A	123	G
28	A	124	G
28	A	138	U
28	A	139	U
28	A	140	C
28	A	141	G
28	A	142	A
28	A	163	C
28	A	164	C
28	A	174	U
28	A	181	A
28	A	185	G
28	A	193	U
28	A	196	A
28	A	199	A
28	A	205	G
28	A	208	C
28	A	216	A
28	A	222	A
28	A	228	C
28	A	230	G
28	A	241	A
28	A	248	G
28	A	249	C
28	A	255	A
28	A	266	G
28	A	267	C
28	A	272	A
28	A	273	G

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Mol	Chain	Res	Type
28	A	276	U
28	A	277	G
28	A	285	G
28	A	293	U
28	A	294	A
28	A	306	U
28	A	311	A
28	A	325	G
28	A	329	G
28	A	330	A
28	A	335	C
28	A	353	C
28	A	361	G
28	A	362	A
28	A	363	G
28	A	371	A
28	A	372	G
28	A	386	G
28	A	389	G
28	A	396	G
28	A	399	U
28	A	404	A
28	A	405	U
28	A	411	G
28	A	412	A
28	A	424	G
28	A	449	A
28	A	451	U
28	A	467	G
28	A	472	A
28	A	481	G
28	A	491	G
28	A	504	A
28	A	505	A
28	A	509	C
28	A	510	C
28	A	528	A
28	A	531	C
28	A	532	A
28	A	533	G
28	A	543	G
28	A	544	C

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Mol	Chain	Res	Type
28	A	546	U
28	A	548	G
28	A	549	G
28	A	550	C
28	A	551	G
28	A	562	U
28	A	563	A
28	A	573	U
28	A	575	A
28	A	580	U
28	A	584	C
28	A	586	A
28	A	588	U
28	A	595	C
28	A	603	A
28	A	604	G
28	A	614	A
28	A	615	U
28	A	627	A
28	A	633	A
28	A	637	A
28	A	647	G
28	A	654	A
28	A	655	A
28	A	656	G
28	A	663	G
28	A	686	U
28	A	696	G
28	A	711	G
28	A	717	C
28	A	724	U
28	A	728	G
28	A	730	A
28	A	733	G
28	A	739	A
28	A	747	U
28	A	750	A
28	A	751	A
28	A	762	U
28	A	764	A
28	A	767	U
28	A	775	G

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Mol	Chain	Res	Type
28	A	776	G
28	A	782	A
28	A	784	G
28	A	785	G
28	A	792	A
28	A	794	A
28	A	801	G
28	A	805	G
28	A	812	C
28	A	819	A
28	A	827	U
28	A	846	U
28	A	847	U
28	A	859	G
28	A	872	U
28	A	873	C
28	A	880	G
28	A	881	G
28	A	887	U
28	A	888	C
28	A	891	G
28	A	895	U
28	A	896	A
28	A	897	C
28	A	899	A
28	A	910	A
28	A	914	G
28	A	915	C
28	A	931	U
28	A	941	A
28	A	945	A
28	A	946	C
28	A	955	U
28	A	961	C
28	A	972	A
28	A	973	A
28	A	974	G
28	A	976	G
28	A	983	A
28	A	984	A
28	A	985	C
28	A	990	A

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Mol	Chain	Res	Type
28	A	995	C
28	A	996	A
28	A	1003	G
28	A	1006	C
28	A	1012	U
28	A	1013	C
28	A	1017	G
28	A	1021	A
28	A	1022	G
28	A	1023	U
28	A	1024	G
28	A	1025	G
28	A	1026	G
28	A	1033	U
28	A	1044	C
28	A	1047	G
28	A	1056	G
28	A	1061	U
28	A	1062	G
28	A	1064	C
28	A	1066	U
28	A	1069	A
28	A	1070	A
28	A	1072	C
28	A	1081	U
28	A	1082	U
28	A	1089	A
28	A	1112	G
28	A	1120	G
28	A	1130	U
28	A	1132	U
28	A	1133	A
28	A	1135	C
28	A	1139	G
28	A	1141	U
28	A	1142	A
28	A	1143	A
28	A	1151	A
28	A	1168	G
28	A	1169	A
28	A	1171	G
28	A	1173	U

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Mol	Chain	Res	Type
28	A	1174	U
28	A	1175	A
28	A	1176	U
28	A	1178	C
28	A	1180	U
28	A	1183	U
28	A	1190	G
28	A	1191	G
28	A	1206	G
28	A	1212	G
28	A	1227	G
28	A	1233	C
28	A	1238	G
28	A	1246	A
28	A	1247	A
28	A	1248	G
28	A	1250	G
28	A	1253	A
28	A	1254	A
28	A	1255	U
28	A	1256	G
28	A	1262	A
28	A	1265	A
28	A	1266	G
28	A	1268	A
28	A	1271	G
28	A	1272	A
28	A	1273	U
28	A	1274	A
28	A	1275	A
28	A	1300	G
28	A	1301	A
28	A	1302	A
28	A	1313	U
28	A	1321	A
28	A	1326	U
28	A	1365	A
28	A	1366	A
28	A	1376	C
28	A	1379	U
28	A	1380	G
28	A	1383	A

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Mol	Chain	Res	Type
28	A	1386	C
28	A	1395	A
28	A	1398	C
28	A	1415	U
28	A	1416	G
28	A	1417	C
28	A	1419	A
28	A	1420	A
28	A	1425	G
28	A	1428	C
28	A	1434	A
28	A	1436	G
28	A	1449	G
28	A	1452	G
28	A	1453	A
28	A	1456	G
28	A	1458	U
28	A	1459	G
28	A	1478	G
28	A	1482	G
28	A	1483	G
28	A	1493	C
28	A	1497	U
28	A	1504	A
28	A	1507	C
28	A	1510	G
28	A	1512	C
28	A	1515	A
28	A	1522	A
28	A	1524	G
28	A	1530	G
28	A	1532	A
28	A	1534	U
28	A	1535	A
28	A	1536	C
28	A	1538	G
28	A	1540	G
28	A	1542	U
28	A	1544	A
28	A	1560	G
28	A	1562	U
28	A	1566	A

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Mol	Chain	Res	Type
28	A	1569	A
28	A	1583	A
28	A	1585	C
28	A	1605	C
28	A	1608	A
28	A	1609	A
28	A	1610	A
28	A	1629	U
28	A	1639	C
28	A	1647	U
28	A	1648	U
28	A	1649	G
28	A	1652	A
28	A	1654	A
28	A	1656	C
28	A	1674	G
28	A	1703	G
28	A	1705	A
28	A	1721	G
28	A	1729	U
28	A	1730	C
28	A	1733	G
28	A	1738	G
28	A	1756	G
28	A	1758	U
28	A	1764	C
28	A	1772	A
28	A	1773	A
28	A	1781	U
28	A	1791	A
28	A	1800	C
28	A	1802	A
28	A	1806	C
28	A	1807	G
28	A	1808	A
28	A	1809	A
28	A	1811	G
28	A	1816	C
28	A	1819	A
28	A	1829	A
28	A	1847	A
28	A	1848	A

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Mol	Chain	Res	Type
28	A	1869	G
28	A	1870	C
28	A	1872	A
28	A	1882	U
28	A	1891	G
28	A	1903	G
28	A	1906	G
28	A	1913	A
28	A	1914	C
28	A	1927	A
28	A	1929	G
28	A	1930	G
28	A	1935	G
28	A	1937	A
28	A	1938	A
28	A	1955	U
28	A	1965	C
28	A	1966	A
28	A	1967	C
28	A	1970	A
28	A	1971	U
28	A	1972	G
28	A	1981	A
28	A	1991	U
28	A	1992	G
28	A	1993	U
28	A	1997	C
28	A	2022	U
28	A	2023	C
28	A	2024	G
28	A	2027	G
28	A	2031	A
28	A	2033	A
28	A	2036	C
28	A	2037	A
28	A	2041	U
28	A	2043	C
28	A	2047	C
28	A	2052	A
28	A	2054	A
28	A	2055	C
28	A	2056	G

*Continued on next page...*

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Mol	Chain	Res	Type
28	A	2060	A
28	A	2061	G
28	A	2062	A
28	A	2069	G
28	A	2072	C
28	A	2077	A
28	A	2090	A
28	A	2092	U
28	A	2093	G
28	A	2107	G
28	A	2111	U
28	A	2112	G
28	A	2113	U
28	A	2117	A
28	A	2119	A
28	A	2120	G
28	A	2127	G
28	A	2129	C
28	A	2130	U
28	A	2131	U
28	A	2132	U
28	A	2133	G
28	A	2134	A
28	A	2135	A
28	A	2137	U
28	A	2140	G
28	A	2141	G
28	A	2142	A
28	A	2145	C
28	A	2146	C
28	A	2147	A
28	A	2148	G
28	A	2149	U
28	A	2153	C
28	A	2154	A
28	A	2157	G
28	A	2158	A
28	A	2159	G
28	A	2160	C
28	A	2161	C
28	A	2162	G
28	A	2164	C

*Continued on next page...*

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Mol	Chain	Res	Type
28	A	2165	C
28	A	2170	A
28	A	2172	U
28	A	2173	A
28	A	2174	C
28	A	2176	A
28	A	2183	A
28	A	2186	G
28	A	2189	U
28	A	2190	G
28	A	2191	A
28	A	2198	A
28	A	2199	A
28	A	2203	U
28	A	2204	G
28	A	2211	A
28	A	2212	A
28	A	2225	A
28	A	2226	C
28	A	2238	G
28	A	2239	G
28	A	2250	G
28	A	2257	U
28	A	2279	G
28	A	2283	C
28	A	2286	G
28	A	2287	A
28	A	2288	A
28	A	2292	U
28	A	2305	U
28	A	2308	G
28	A	2309	A
28	A	2311	A
28	A	2322	A
28	A	2325	G
28	A	2327	A
28	A	2334	U
28	A	2345	G
28	A	2347	C
28	A	2355	G
28	A	2361	G
28	A	2371	G

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Mol	Chain	Res	Type
28	A	2383	G
28	A	2385	C
28	A	2396	G
28	A	2402	U
28	A	2403	C
28	A	2406	A
28	A	2423	U
28	A	2424	C
28	A	2425	A
28	A	2429	G
28	A	2430	A
28	A	2431	U
28	A	2434	A
28	A	2439	A
28	A	2440	C
28	A	2441	U
28	A	2448	A
28	A	2464	G
28	A	2475	C
28	A	2476	A
28	A	2478	A
28	A	2479	U
28	A	2480	C
28	A	2482	A
28	A	2491	U
28	A	2492	U
28	A	2501	C
28	A	2502	G
28	A	2503	A
28	A	2504	U
28	A	2505	G
28	A	2506	U
28	A	2507	C
28	A	2513	A
28	A	2518	A
28	A	2520	C
28	A	2529	G
28	A	2530	A
28	A	2542	A
28	A	2546	U
28	A	2553	G
28	A	2554	U

*Continued on next page...*

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Mol	Chain	Res	Type
28	A	2566	A
28	A	2567	G
28	A	2573	C
28	A	2585	U
28	A	2586	U
28	A	2587	A
28	A	2589	A
28	A	2590	A
28	A	2601	C
28	A	2602	A
28	A	2604	U
28	A	2609	U
28	A	2613	U
28	A	2615	U
28	A	2629	U
28	A	2630	G
28	A	2638	G
28	A	2682	A
28	A	2689	U
28	A	2690	U
28	A	2714	G
28	A	2716	C
28	A	2727	A
28	A	2728	U
28	A	2729	G
28	A	2733	A
28	A	2744	G
28	A	2748	A
28	A	2758	A
28	A	2778	A
28	A	2791	G
28	A	2793	C
28	A	2795	C
28	A	2797	U
28	A	2798	U
28	A	2800	A
28	A	2811	G
28	A	2820	A
28	A	2821	A
28	A	2824	C
28	A	2832	U
28	A	2833	U

*Continued on next page...*

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Mol	Chain	Res	Type
28	A	2834	G
28	A	2835	A
28	A	2837	A
28	A	2851	A
28	A	2861	U
28	A	2867	G
28	A	2872	A
28	A	2873	A
28	A	2879	A
28	A	2880	C
28	A	2883	A
28	A	2884	U
28	A	2885	G
28	A	2887	A
28	A	2901	C
29	B	15	A
29	B	16	G
29	B	35	C
29	B	37	C
29	B	44	G
29	B	52	A
29	B	56	G
29	B	66	A
29	B	87	U
29	B	88	C
29	B	89	U
29	B	90	C
29	B	97	C
29	B	99	A
29	B	107	G
29	B	109	A
29	B	116	G
29	B	119	A
54	6	6	G
54	6	9	A
54	6	17	C
54	6	18	G
54	6	19	G
54	6	20	U
54	6	21	A
54	6	22	G
54	6	36	A

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Mol	Chain	Res	Type
54	6	37	A
54	6	44	G
54	6	46	G
54	6	59	U
54	6	65	G
54	6	75	C
55	7	14	A
55	7	15	U
55	7	21	C
55	7	23	A
55	7	24	A
55	7	26	A
55	7	27	A
56	8	3	C
56	8	5	G
56	8	17	C
56	8	17(A)	U
56	8	18	G
56	8	19	G
56	8	20	U
56	8	21	A
56	8	47	U
56	8	48	C
56	8	49	G
56	8	52	G
56	8	53	G
56	8	54	U
56	8	61	C
56	8	65	C
56	8	73	A
56	8	74	C
56	8	75	C
56	8	76	A
58	9	3	C
58	9	4	C
58	9	8	U
58	9	15	G
58	9	16	U
58	9	17	C
58	9	18	G
58	9	19	G
58	9	21	A

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Mol	Chain	Res	Type
58	9	23	A
58	9	39	U
58	9	40	C
58	9	41	C
58	9	47	U
58	9	48	C
58	9	50	U
58	9	59	U
58	9	61	C
58	9	70	G
58	9	71	G
58	9	72	C
58	9	74	C
58	9	75	C
58	9	76	A

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	119	A
28	A	229	C
28	A	271	G
28	A	328	U
28	A	344	A
28	A	403	U
28	A	404	A
28	A	527	C
28	A	530	G
28	A	784	G
28	A	800	A
28	A	894	U
28	A	976	G
28	A	1020	A
28	A	1331	G
28	A	1584	U
28	A	1847	A
28	A	1905	C
28	A	2119	A
28	A	2130	U
28	A	2326	C
28	A	2423	U
28	A	2481	G

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Mol	Chain	Res	Type
28	A	2820	A
54	6	17	C
54	6	35	A
54	6	36	A
55	7	20	U
58	9	15	G
58	9	74	C

## 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	$\# Z  > 2$
54	F3O	6	76	54	30,35,37	1.14	1 (3%)	33,49,54	1.49	5 (15%)

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
54	F3O	6	76	54	-	9/15/36/38	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	76	F3O	O3'-C	4.87	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	6	76	F3O	N3-C2-N1	-4.71	121.31	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	6	76	F3O	O3'-C-CA	3.69	120.15	111.35
54	6	76	F3O	C3'-O3'-C	-3.05	112.54	117.78
54	6	76	F3O	C3'-C2'-C1'	2.68	105.82	99.89
54	6	76	F3O	O3'-C-O	-2.58	119.12	123.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	6	76	F3O	CA-C-O3'-C3'
54	6	76	F3O	C-CA-CB-CG
54	6	76	F3O	O-C-O3'-C3'
54	6	76	F3O	N-CA-CB-CG
54	6	76	F3O	CA-CB-CG-CD2
54	6	76	F3O	CA-CB-CG-CD1
54	6	76	F3O	C4'-C5'-O5'-P
54	6	76	F3O	O-C-CA-N
54	6	76	F3O	O3'-C-CA-N

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GNP	x	701	60	29,34,34	1.86	8 (27%)	33,54,54	2.51	10 (30%)

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	GNP	x	701	60	-	6/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	701	GNP	PB-O3A	-5.75	1.51	1.59
59	x	701	GNP	C6-N1	3.63	1.39	1.33
59	x	701	GNP	PB-O2B	-3.22	1.48	1.56
59	x	701	GNP	PG-O1G	3.15	1.51	1.46
59	x	701	GNP	C8-N7	-2.30	1.30	1.34
59	x	701	GNP	PG-O2G	-2.25	1.50	1.56
59	x	701	GNP	PG-O3G	-2.23	1.50	1.56
59	x	701	GNP	PB-N3B	-2.06	1.58	1.63

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	701	GNP	C5-C6-N1	-8.47	111.85	123.43
59	x	701	GNP	C2-N1-C6	5.63	124.88	115.93
59	x	701	GNP	O2B-PB-O1B	4.20	118.72	109.92
59	x	701	GNP	O1B-PB-N3B	-4.02	105.85	111.77
59	x	701	GNP	PB-O3A-PA	-3.71	119.55	132.62
59	x	701	GNP	O1G-PG-N3B	-3.55	106.54	111.77
59	x	701	GNP	C2-N3-C4	-3.14	111.77	115.36
59	x	701	GNP	O3G-PG-O1G	-3.08	105.70	113.45
59	x	701	GNP	O2G-PG-O3G	2.62	114.62	107.64
59	x	701	GNP	N3-C2-N1	-2.51	123.88	127.22

There are no chirality outliers.

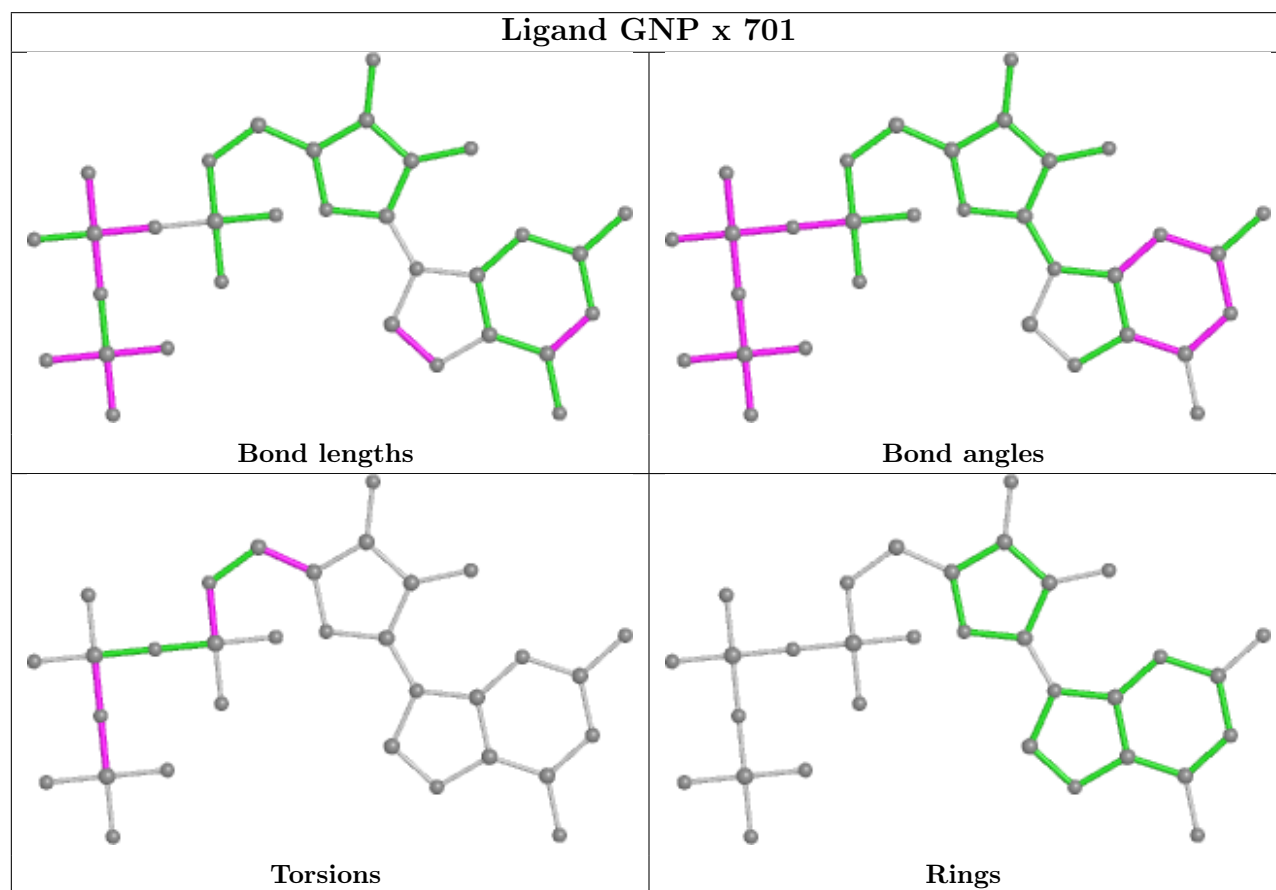
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	x	701	GNP	PB-N3B-PG-O1G
59	x	701	GNP	PG-N3B-PB-O1B
59	x	701	GNP	PG-N3B-PB-O3A
59	x	701	GNP	O4'-C4'-C5'-O5'
59	x	701	GNP	C3'-C4'-C5'-O5'
59	x	701	GNP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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.

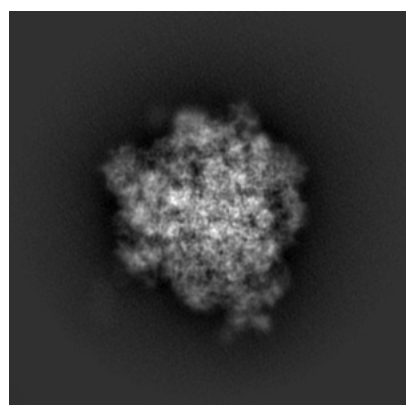
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6550. These allow visual inspection of the internal detail of the map and identification of artifacts.

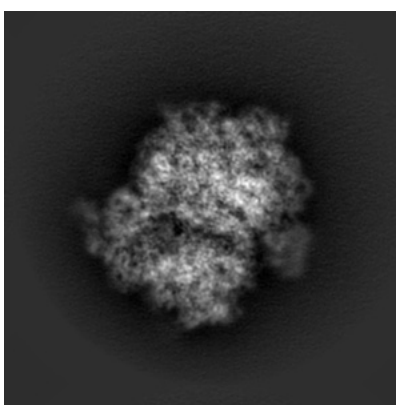
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

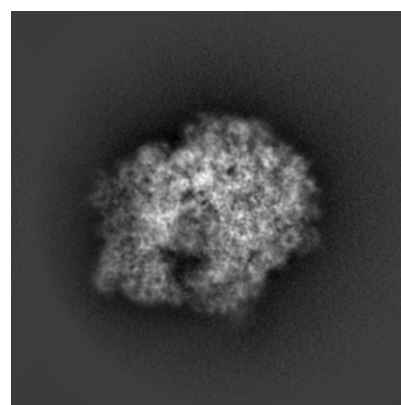
#### 6.1.1 Primary map



X



Y

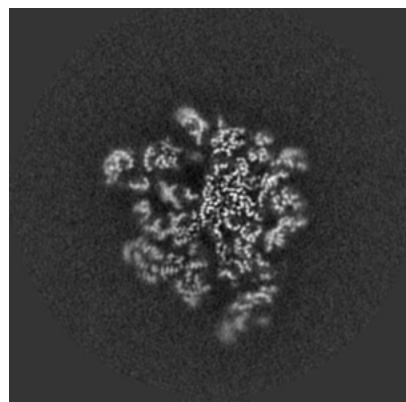


Z

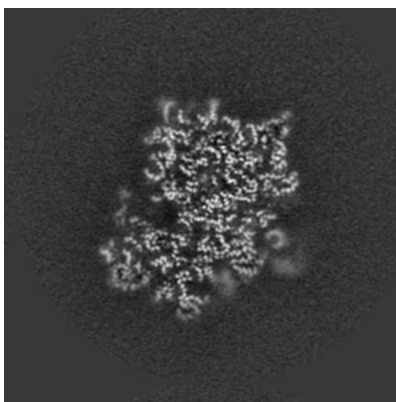
The images above show the map projected in three orthogonal directions.

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

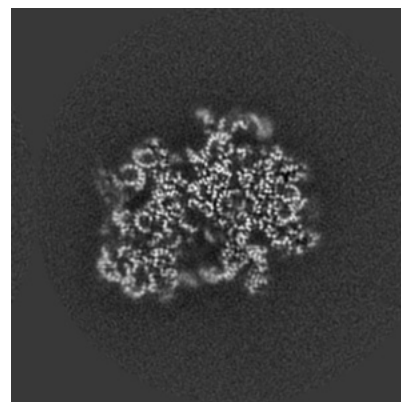
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



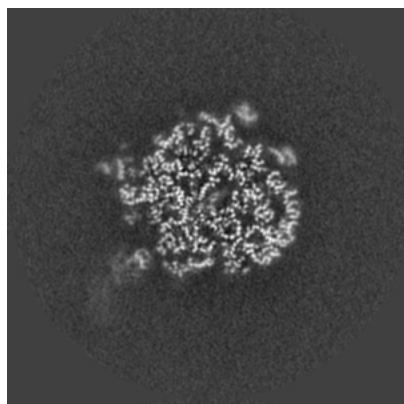
Z Index: 160



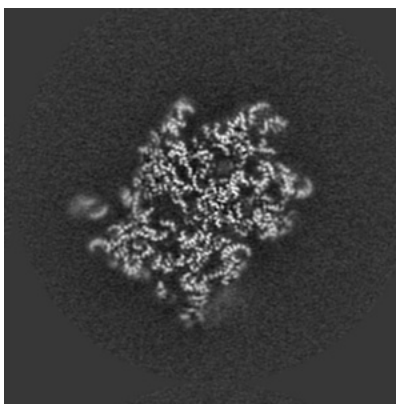
The images above show central slices of the map in three orthogonal directions.

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

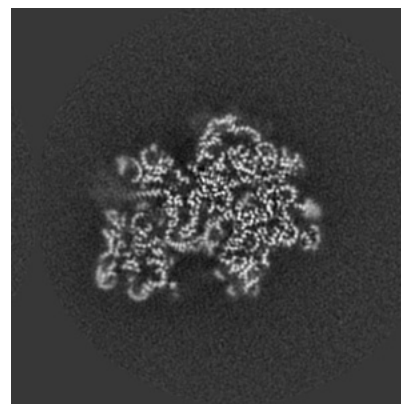
### 6.3.1 Primary map



X Index: 186



Y Index: 178



Z Index: 167

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

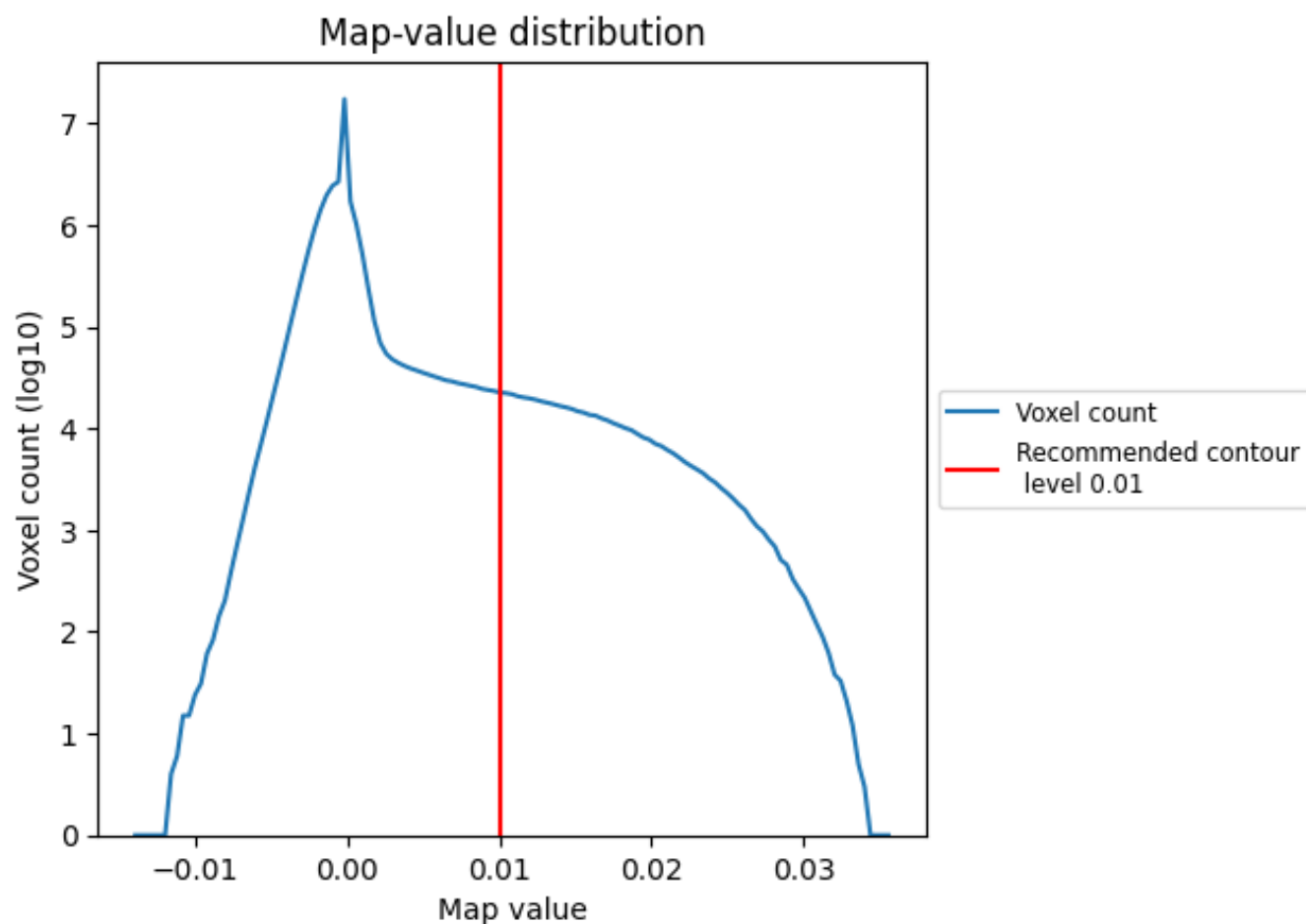
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

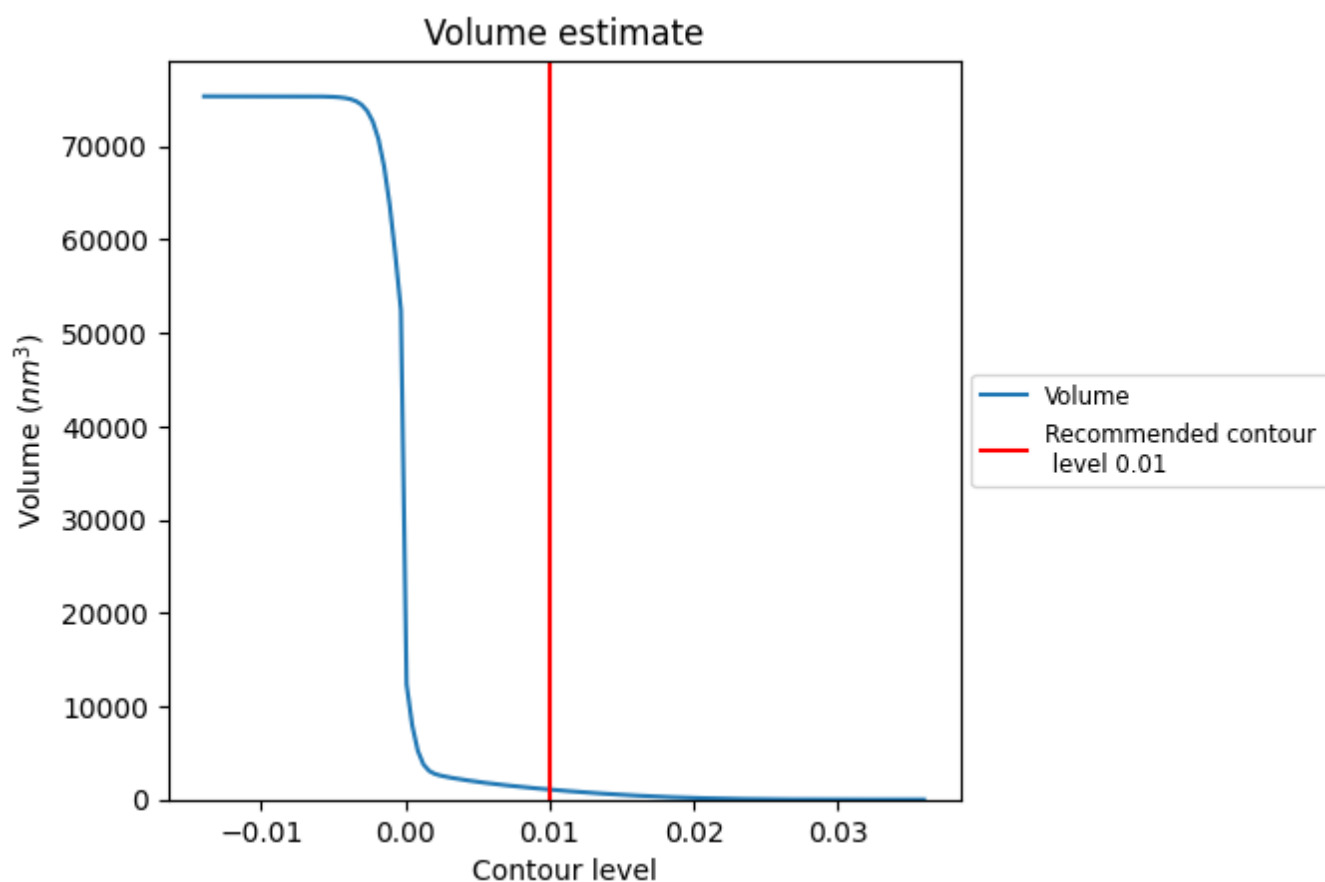
This section contains the results of statistical analysis of the map.

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



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

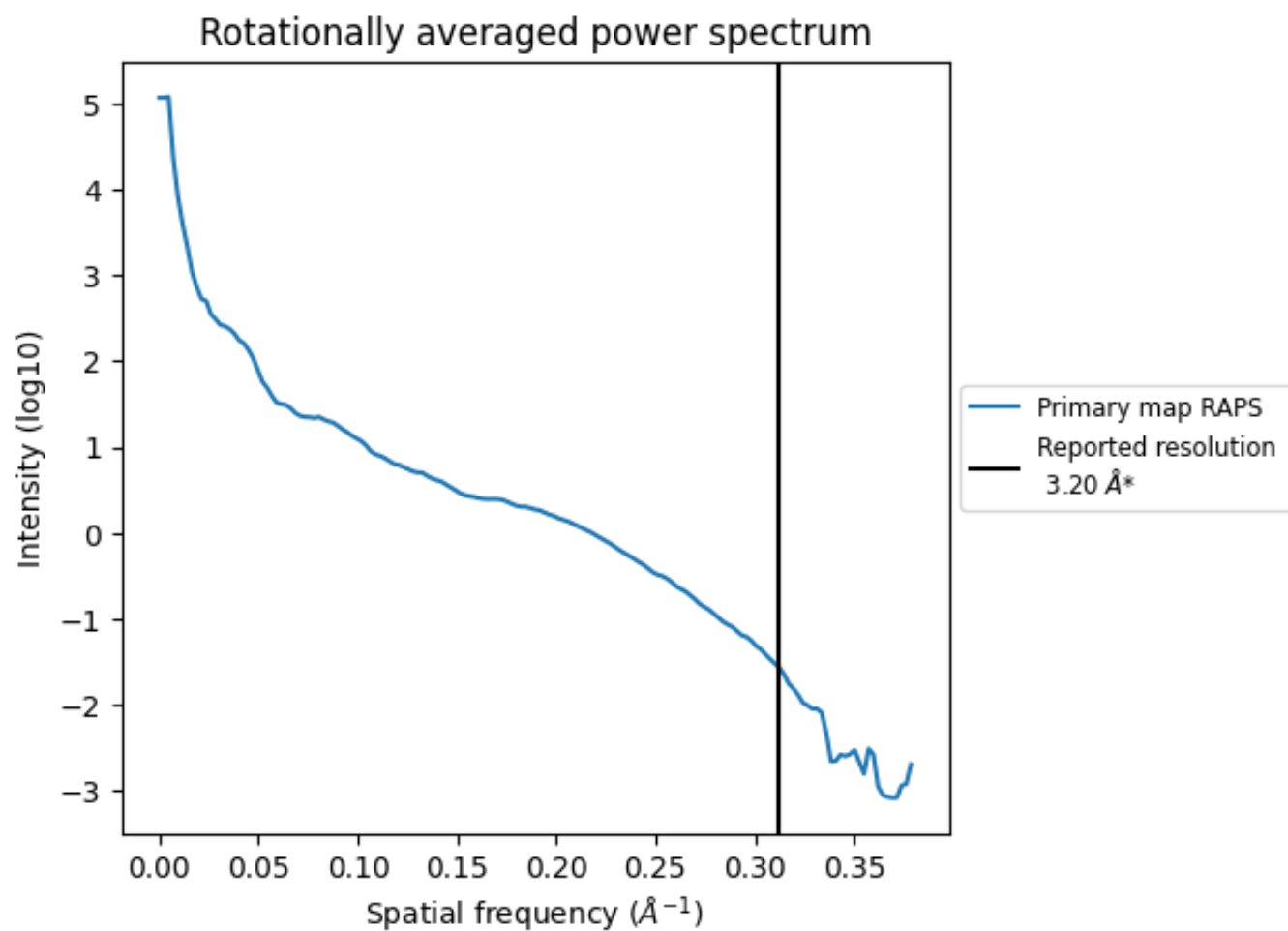
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1075 nm<sup>3</sup>; this corresponds to an approximate mass of 971 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

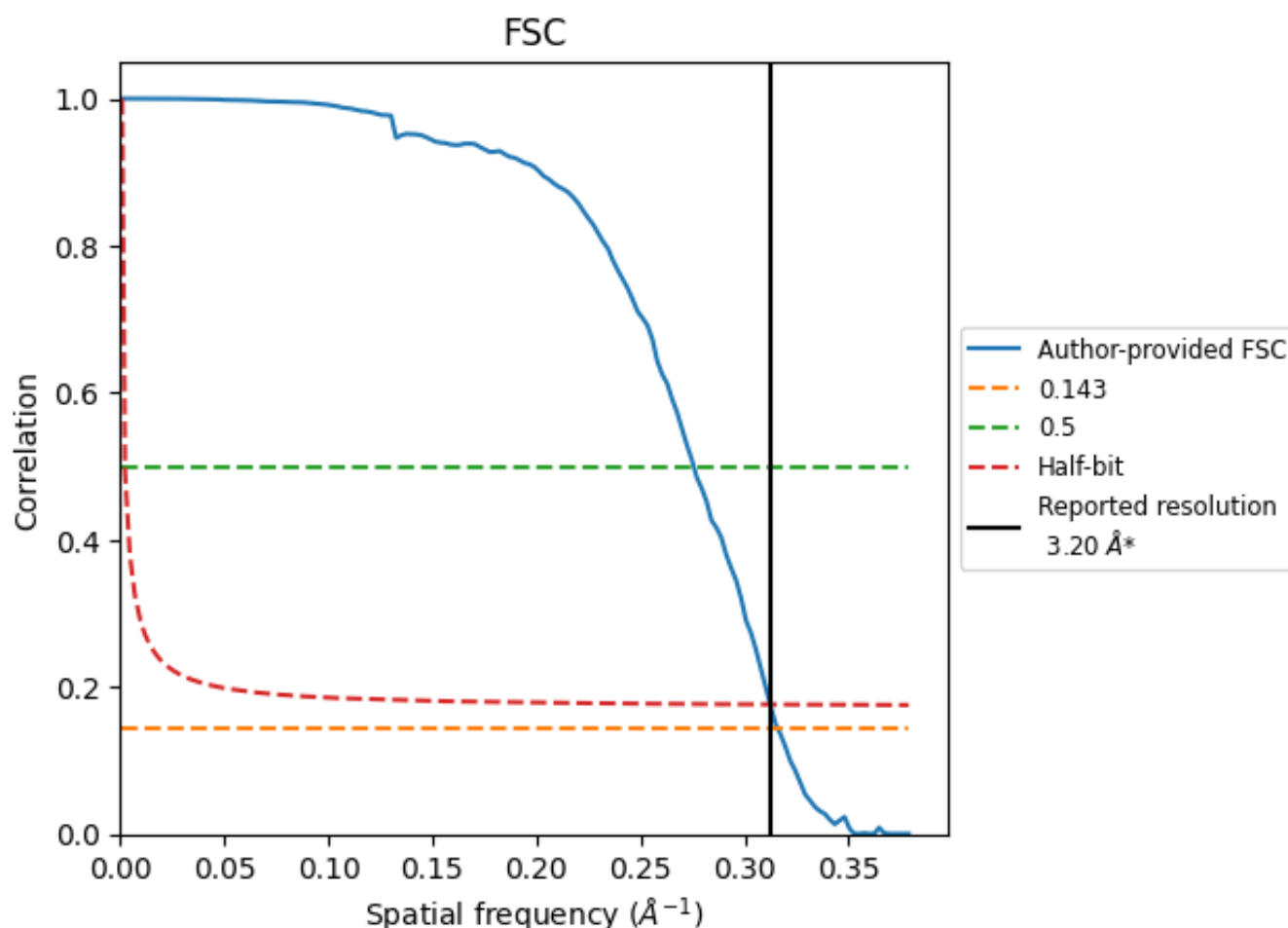


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

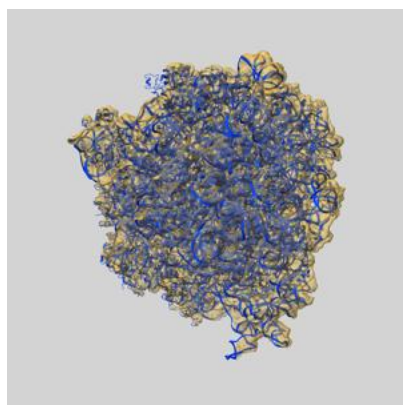
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.17	3.63	3.20
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

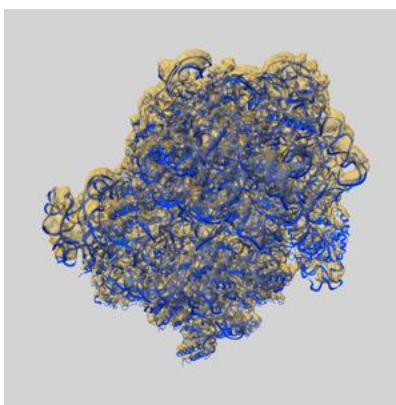
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6550 and PDB model 3JCE. Per-residue inclusion information can be found in section [3](#) on page [14](#).

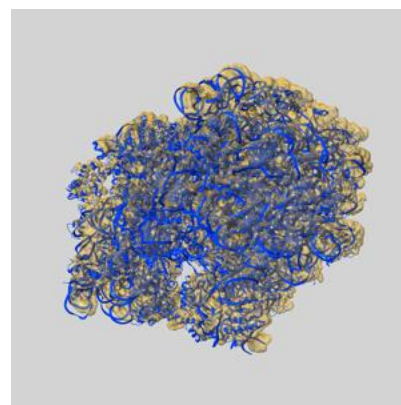
### 9.1 Map-model overlay [i](#)



X



Y

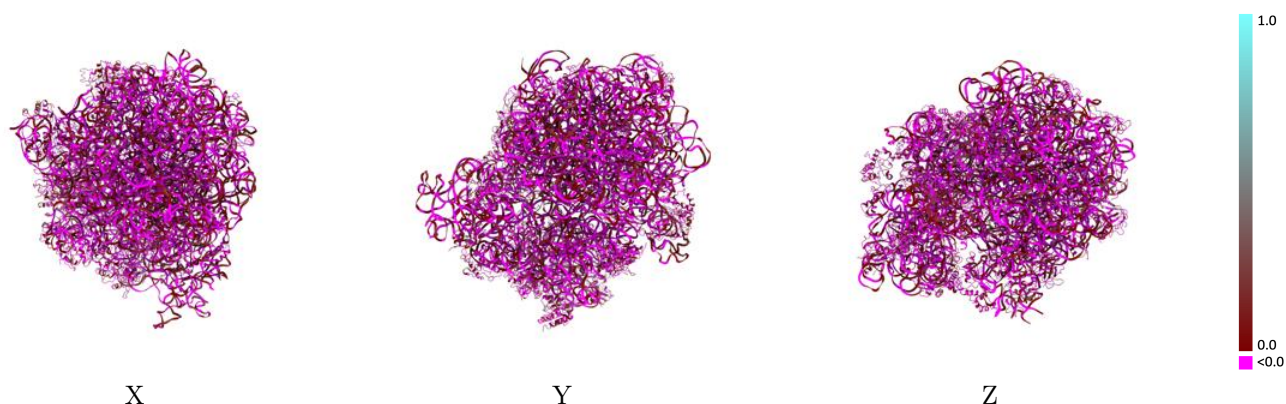


Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

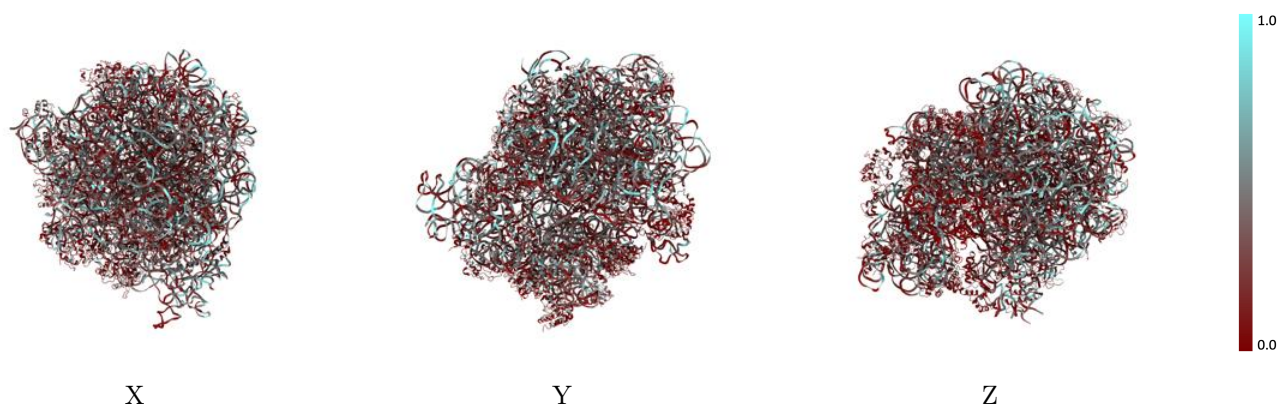


## 9.2 Q-score mapped to coordinate model [i](#)



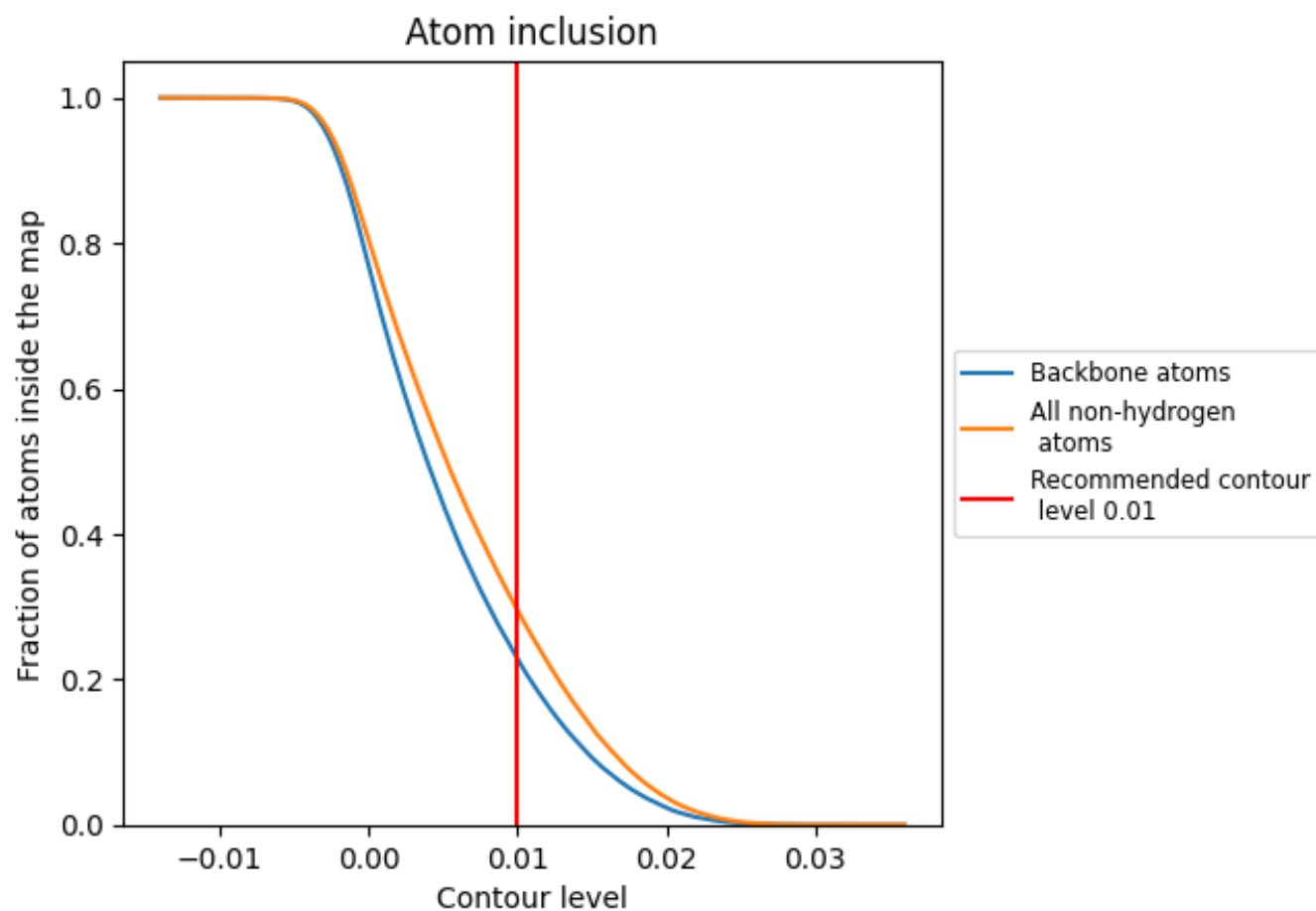
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 23% of all backbone atoms, 30% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2951	-0.0160
0	0.2500	-0.0710
1	0.1845	-0.0080
2	0.2197	-0.0580
3	0.2383	-0.0330
4	0.2329	-0.0340
5	0.0468	0.0240
6	0.2774	0.0080
7	0.1375	-0.0660
8	0.3165	0.0250
9	0.1152	0.0280
A	0.3462	-0.0170
B	0.3772	-0.0130
C	0.1915	-0.0390
D	0.2224	-0.0230
E	0.2336	-0.0220
F	0.1529	-0.0490
G	0.1981	-0.0270
H	0.0575	0.0200
I	0.1047	-0.0080
J	0.2373	-0.0310
K	0.1993	-0.0050
L	0.2884	-0.0050
M	0.1756	-0.0140
N	0.2549	-0.0380
O	0.3465	0.0420
P	0.1971	-0.0010
Q	0.2665	-0.0250
R	0.2522	-0.0370
S	0.2428	-0.0400
T	0.2784	-0.0040
U	0.2881	-0.0080
V	0.2764	0.0170
W	0.2793	-0.0120
X	0.2562	-0.0360



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Chain	Atom inclusion	Q-score
Y	 0.2032	 -0.0360
Z	 0.2654	 -0.0170
a	 0.3491	 -0.0200
b	 0.1427	 -0.0020
c	 0.1857	 -0.0380
d	 0.1761	 -0.0060
e	 0.1588	 -0.0490
f	 0.2158	 -0.0120
g	 0.1836	 -0.0270
h	 0.2333	 0.0260
i	 0.1992	 -0.0310
j	 0.2313	 0.0510
k	 0.1547	 -0.0580
l	 0.2432	 -0.0190
m	 0.1974	 -0.0140
n	 0.1770	 -0.0250
o	 0.2594	 -0.0290
p	 0.2297	 0.0270
q	 0.2484	 -0.0090
r	 0.1881	 -0.0310
s	 0.2158	 -0.0360
t	 0.2338	 -0.0390
u	 0.1552	 0.0270
x	 0.1386	 -0.0120