



## wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 12:21 pm GMT

PDB ID : 7ASO  
EMDB ID : EMD-11902  
Title : Staphylococcus aureus 70S after 30 minutes incubation at 37C  
Authors : Camicata, G.; Bashan, A.; Yonath, A.  
Deposited on : 2020-10-27  
Resolution : 3.11 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>.

---

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

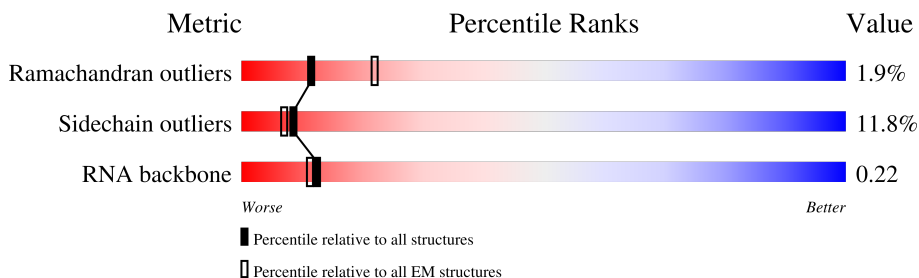
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.11 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	C	114	
2	B	202	
3	I	198	
4	D	156	
5	E	95	
6	G	155	
7	F	130	
8	H	127	

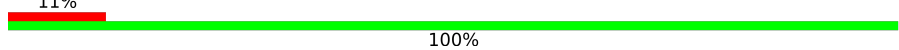

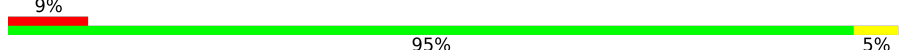

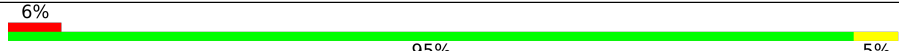
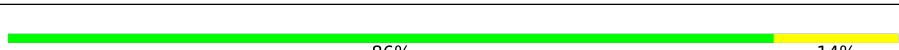



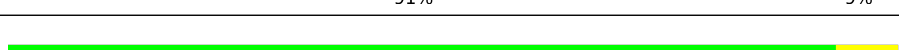
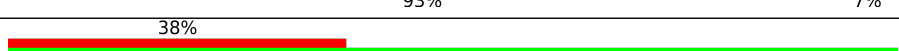
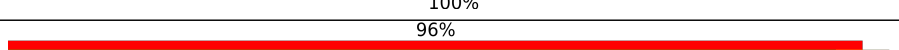
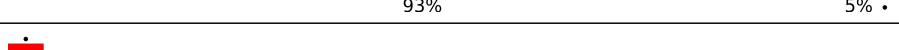
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	1	80	91% 86% 11%
10	2	114	93% 95% 5%
11	3	136	89% 95% 5%
12	4	113	64% 89% 11%
13	5	60	87% 83% 17%
14	6	88	56% 97%
15	7	83	48% 75% 24%
16	8	80	50% 100%
17	9	56	66% 75% 23%
18	I	78	82% 96%
19	A	78	71% 97%
20	X	1415	10% 26% 73%
21	e	215	87% 13%
22	J	205	86% 14%
23	K	165	37% 91% 9%
24	L	174	80% 98%
25	M	145	83% 17%
26	N	122	87% 13%
27	O	145	82% 18%
28	P	136	93% 7%
29	Q	119	85% 14%
30	R	113	96%
31	S	116	86% 14%
32	U	102	78% 22%
33	V	112	84% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	W	89	 81% 18%
35	Z	103	 100% 11%
36	a	93	 100% 65%
37	b	82	 95% 5% 9%
38	c	49	 98% 16%
39	d	62	 95% 5% 6%
40	f	57	 86% 14%
41	g	47	 87% 13%
42	T	47	 77% 21% 55%
43	i	43	 91% 9%
44	j	60	 93% 7%
45	k	37	 100% 38%
46	h	74	 93% 5% 96%
47	Y	2720	 65% 35%

## 2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 125530 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 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C	114	2430	1086	436	794	114	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	202	1551	979	293	278	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	1	198	1058	634	211	213	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	156	1153	727	211	213	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	95	785	496	138	149	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	155	1164	724	220	217	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	130	1007	639	180	184	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	127	975	605	194	175	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	1	80	626	394	116	116	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	2	114	826	507	158	159	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	3	136	976	611	190	173	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	4	113	828	510	168	149	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	5	60	497	314	99	79	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6	88	Total	C	N	O	S	0	0
			713	441	148	123	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	83	Total	C	N	O	S	0	0
			537	335	105	96	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
16	8	80	Total	C	N	O		0	0
			520	327	97	96			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	56	Total	C	N	O	S	0	0
			458	292	88	76	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	78	Total	C	N	O	S	0	0
			541	340	104	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	78	Total	C	N	O	S	0	0
			503	303	100	99	1		

- Molecule 20 is a RNA chain called 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	1415	Total	C	N	O	P	0	0
			30328	13542	5559	9814	1413		

- Molecule 21 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	215	Total	C	N	O	S	0	0
			1570	987	295	283	5		

- Molecule 22 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	205	Total	C	N	O	S	0	0
			1514	953	282	277	2		

- Molecule 23 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	165	Total	C	N	O	S	0	0
			1021	632	184	203	2		

- Molecule 24 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	174	Total	C	N	O	S	0	0
			1062	660	205	195	2		

- Molecule 25 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	145	Total	C	N	O	S	0	0
			1124	703	205	213	3		

- Molecule 26 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 27 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	O	145	Total	C	N	O	0	0
			1020	631	207	182		

- Molecule 28 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	P	136	1043	672	202	165	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Q	119	898	551	176	170	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	R	113	765	474	145	146	0	0

- Molecule 31 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	S	116	942	593	189	156	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	U	102	749	474	140	134	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	V	112	837	526	163	146	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	W	89	694	436	126	128	4	0	0

- Molecule 35 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Z	103	734	462	137	135	0	0

- Molecule 36 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	a	93	648	411	115	122	0	0

- Molecule 37 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	b	82	615	382	122	111	0	0

- Molecule 38 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	c	49	377	233	82	62	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	d	62	493	304	93	96	0	0

- Molecule 40 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	f	57	436	272	83	81	0	0

- Molecule 41 is a protein called 50S ribosomalprotein L32p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g	47	356	218	77	59	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	47	Total	C	N	O	S	0	0
			380	233	75	68	4		

- Molecule 43 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 44 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	60	Total	C	N	O	S	0	0
			446	277	92	75	2		

- Molecule 45 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	37	Total	C	N	O	S	0	0
			272	170	57	40	5		

- Molecule 46 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	h	74	Total	C	N	O	S	0	0
			447	269	86	91	1		

- Molecule 47 is a RNA chain called 23S.

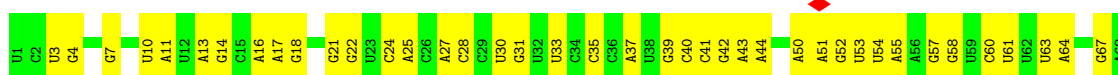
Mol	Chain	Residues	Atoms					AltConf	Trace
47	Y	2720	Total	C	N	O	P	0	0
			58326	26039	10694	18873	2720		

### 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.

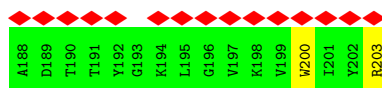
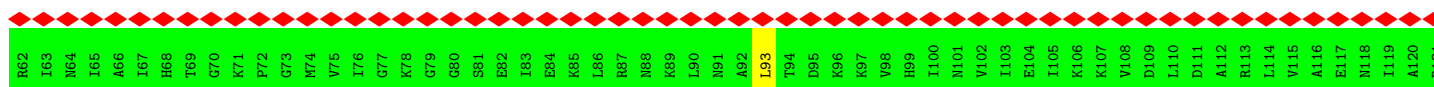
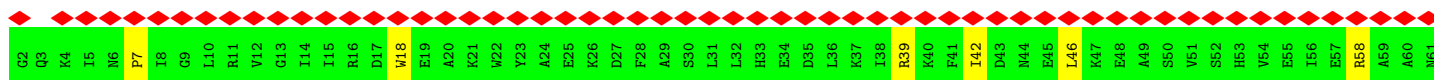
- Molecule 1: 5S

Chain C:  52% 48%



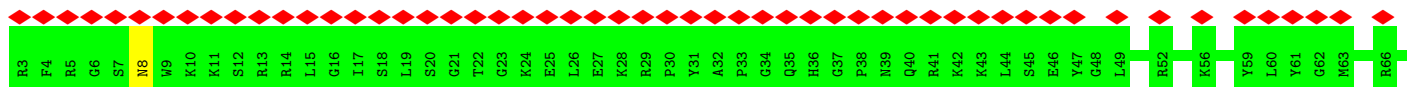
- Molecule 2: 30S ribosomal protein S3

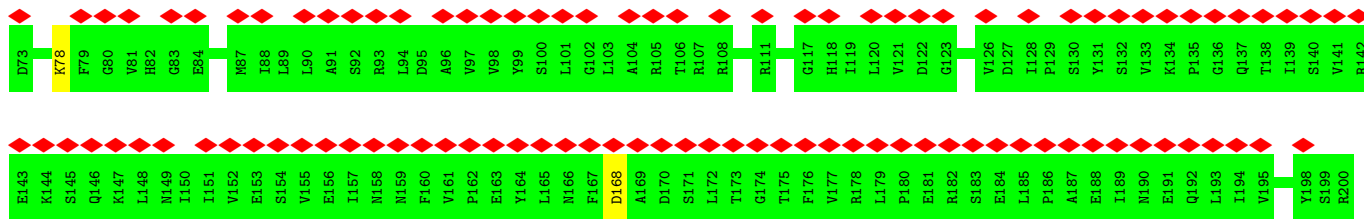
Chain B:  92% 95% 5%



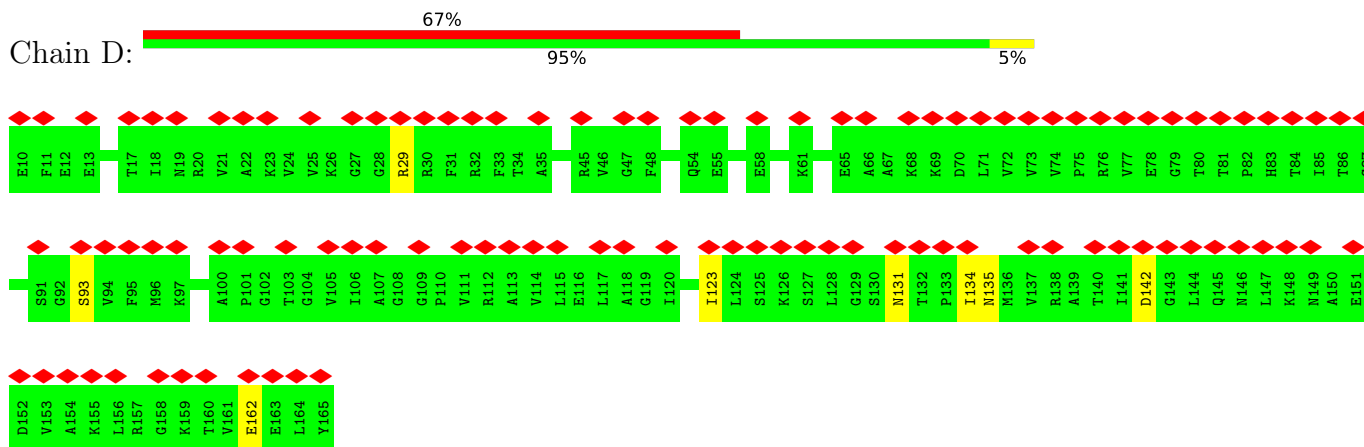
- Molecule 3: 30S ribosomal protein S4

Chain I:  77% 98%

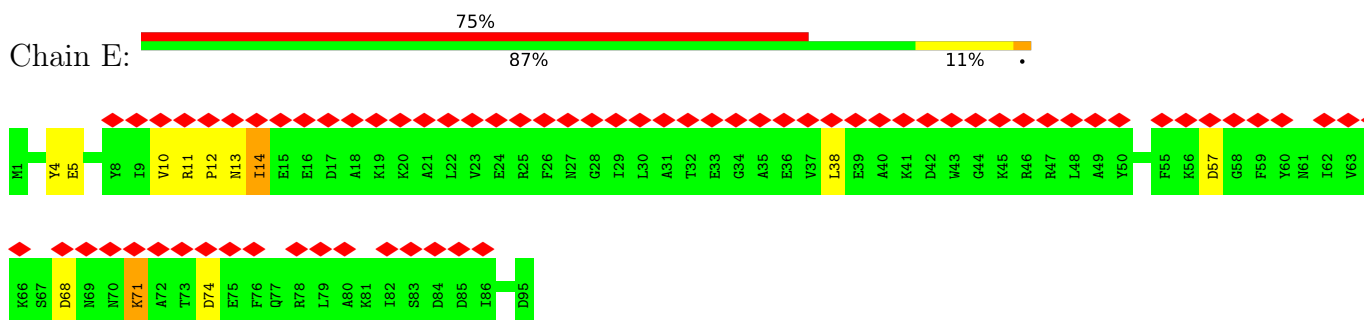




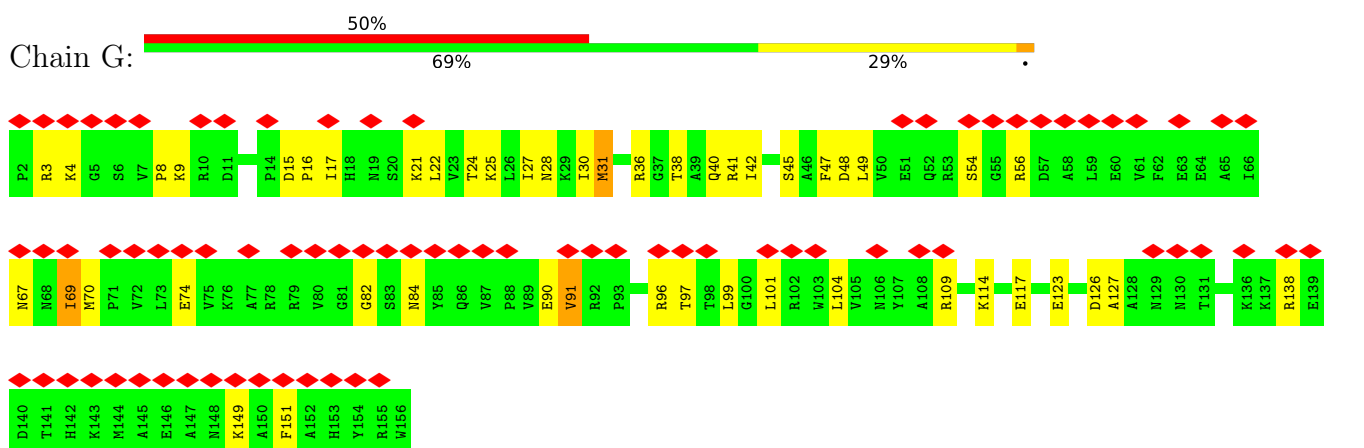
• Molecule 4: 30S ribosomal protein S5



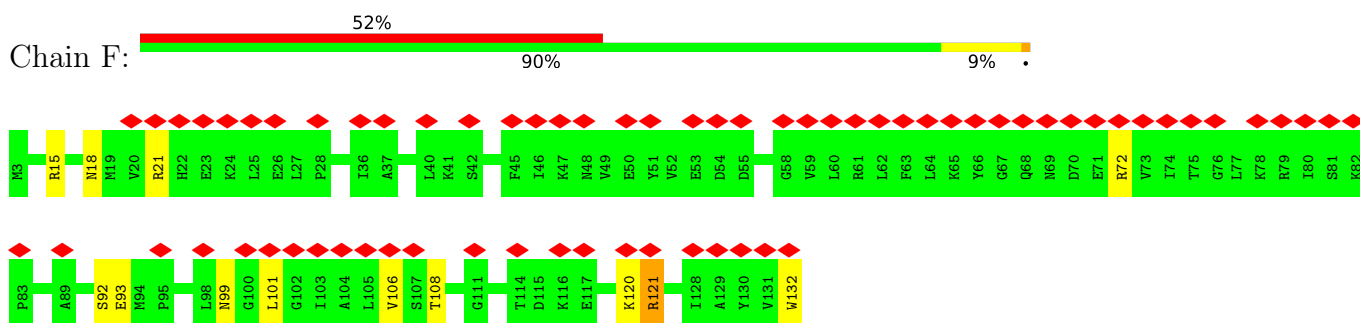
• Molecule 5: 30S ribosomal protein S6



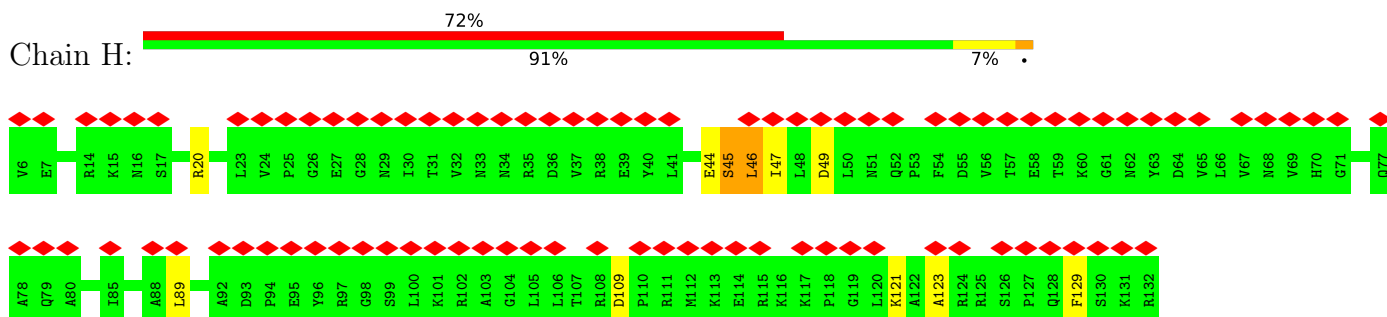
• Molecule 6: 30S ribosomal protein S7



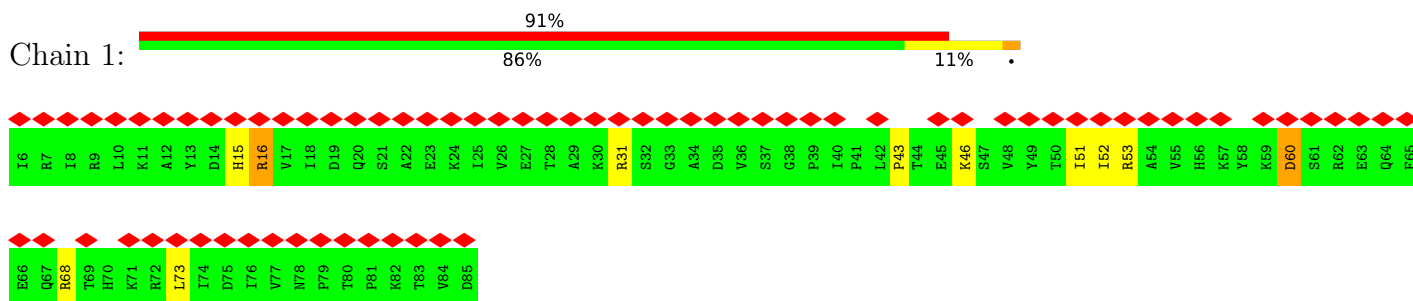
• Molecule 7: 30S ribosomal protein S8



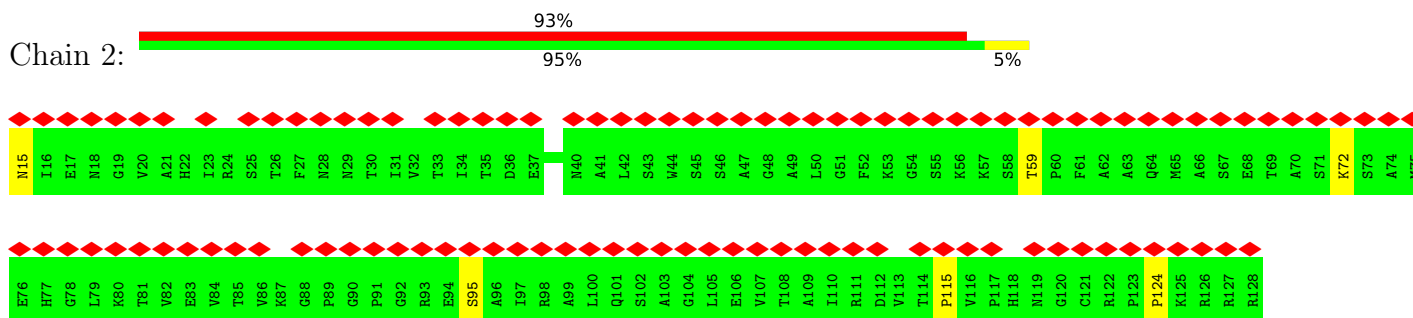
- Molecule 8: 30S ribosomal protein S9



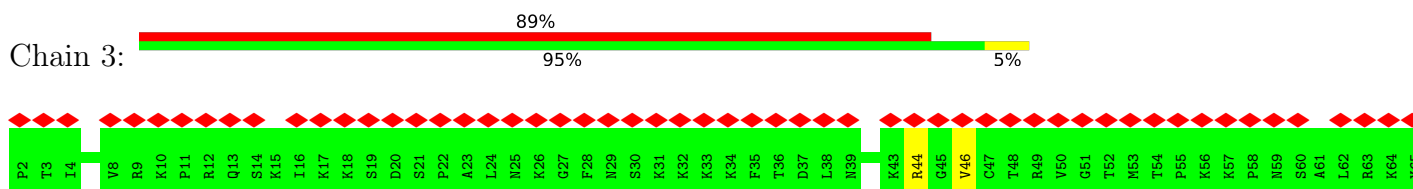
- Molecule 9: 30S ribosomal protein S10

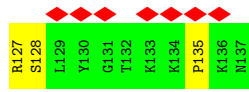
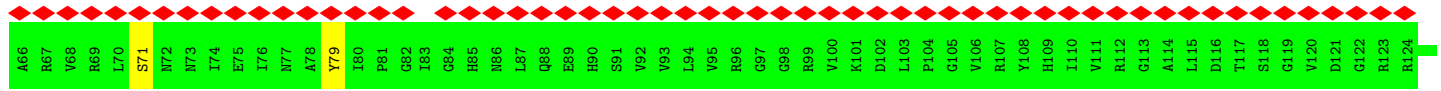


- Molecule 10: 30S ribosomal protein S11

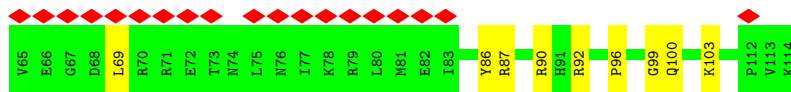
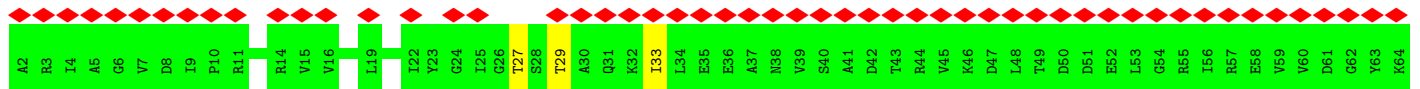
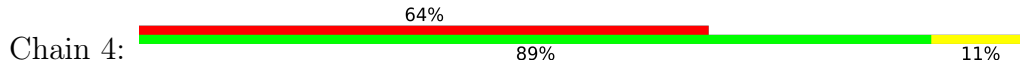


- Molecule 11: 30S ribosomal protein S12

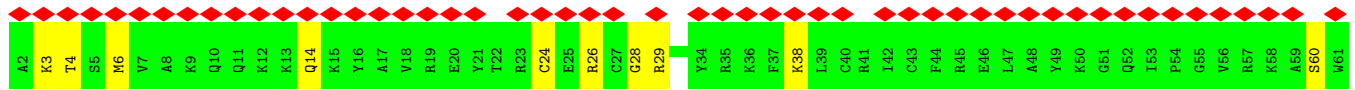
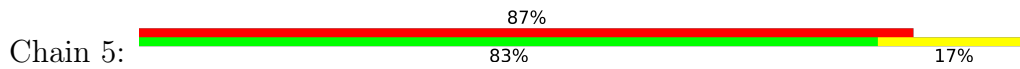




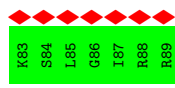
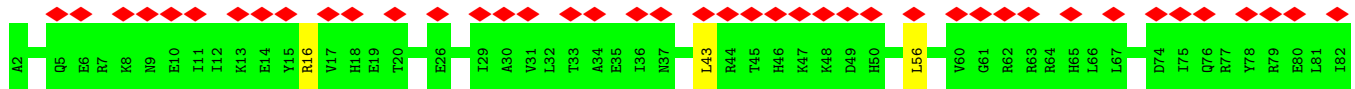
• Molecule 12: 30S ribosomal protein S13



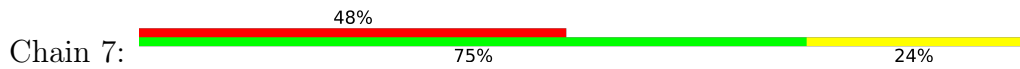
• Molecule 13: 30S ribosomal protein S14 type Z



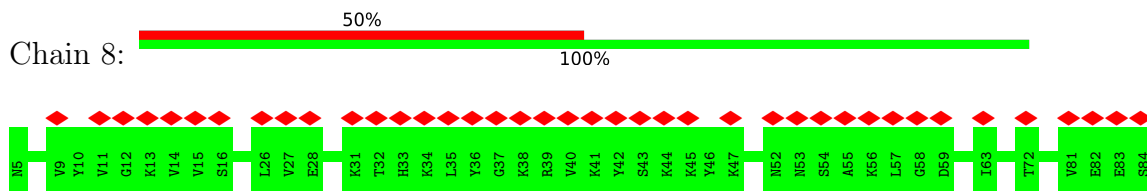
• Molecule 14: 30S ribosomal protein S15



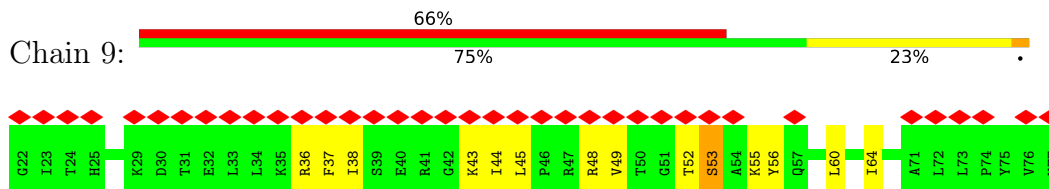
• Molecule 15: 30S ribosomal protein S16



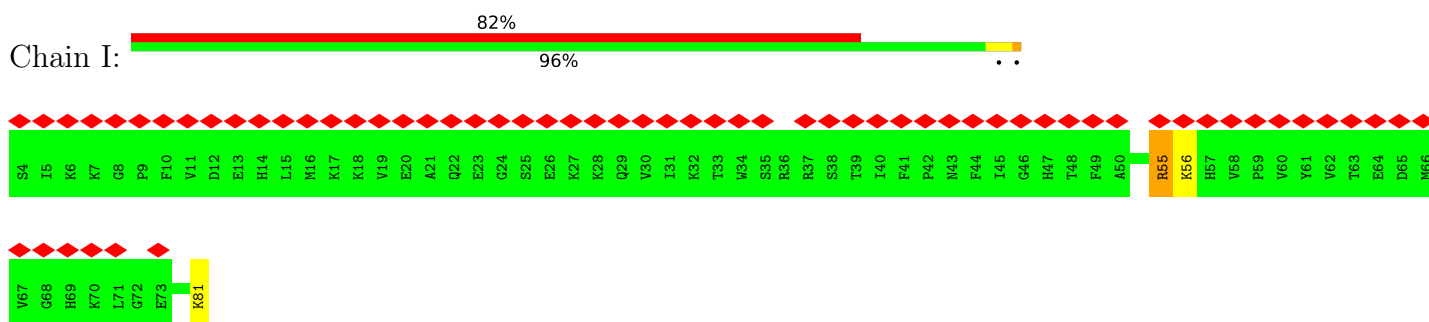
• Molecule 16: 30S ribosomal protein S17



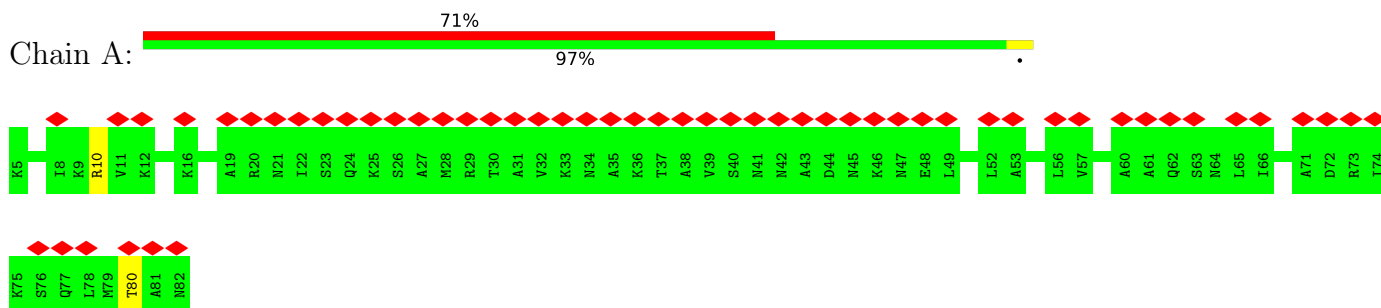
• Molecule 17: 30S ribosomal protein S18



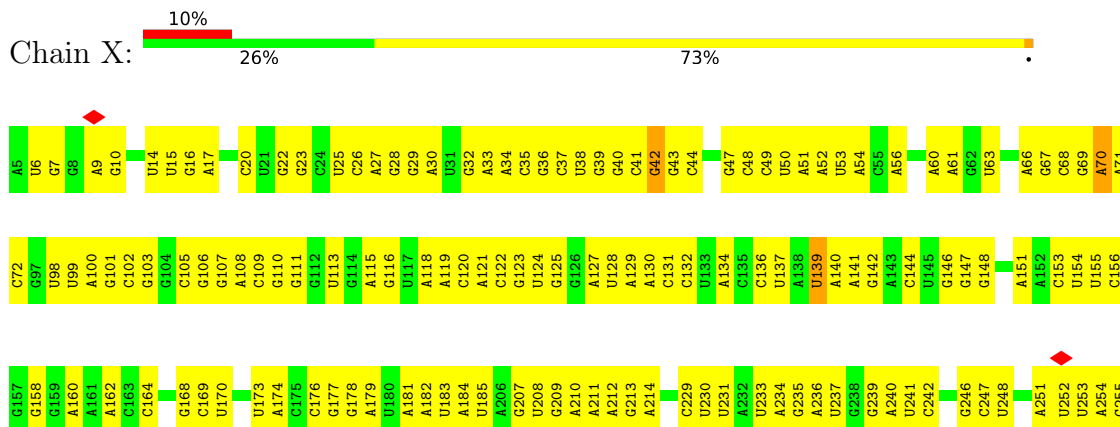
• Molecule 18: 30S ribosomal protein S19



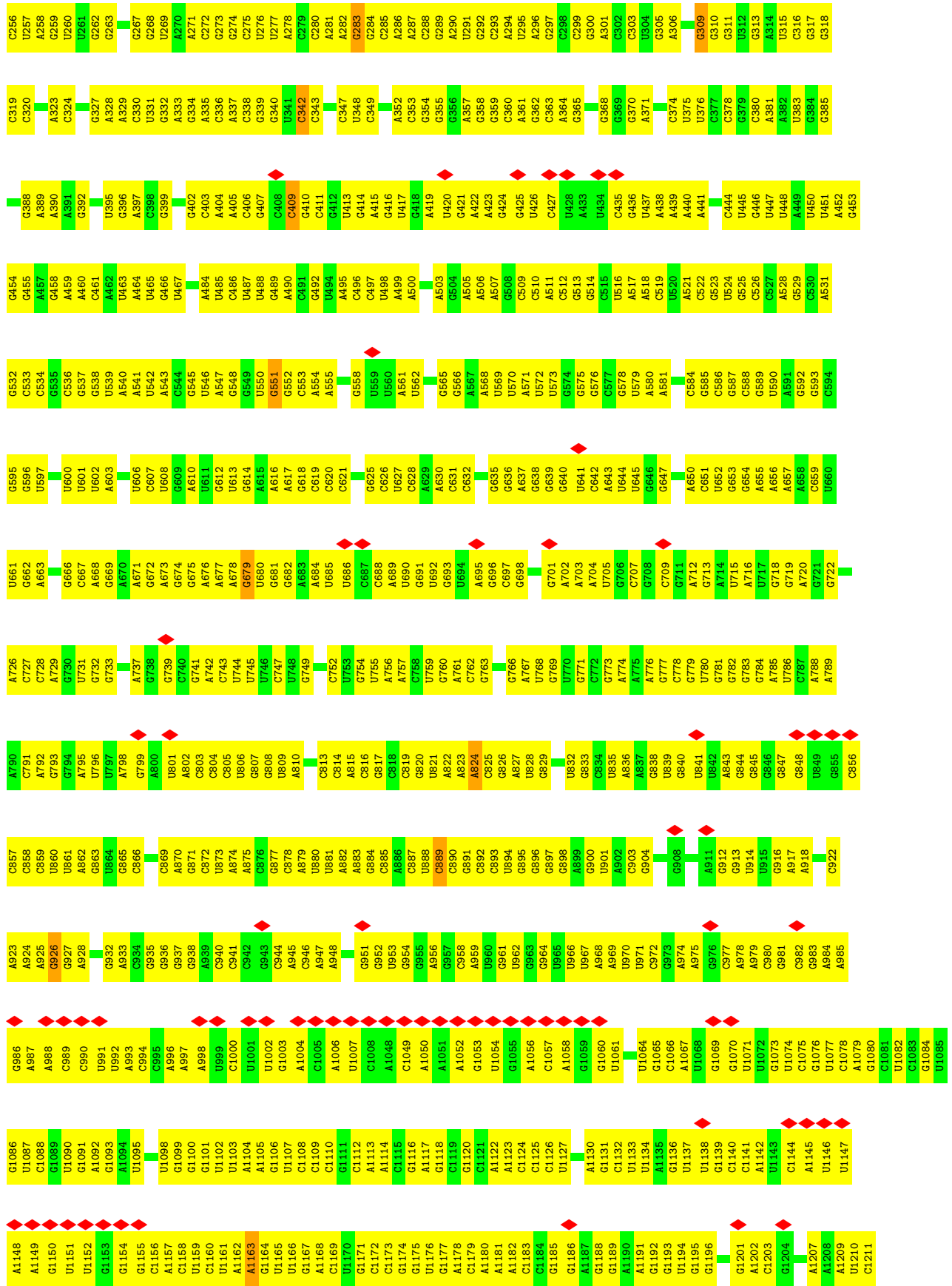
• Molecule 19: 30S ribosomal protein S20

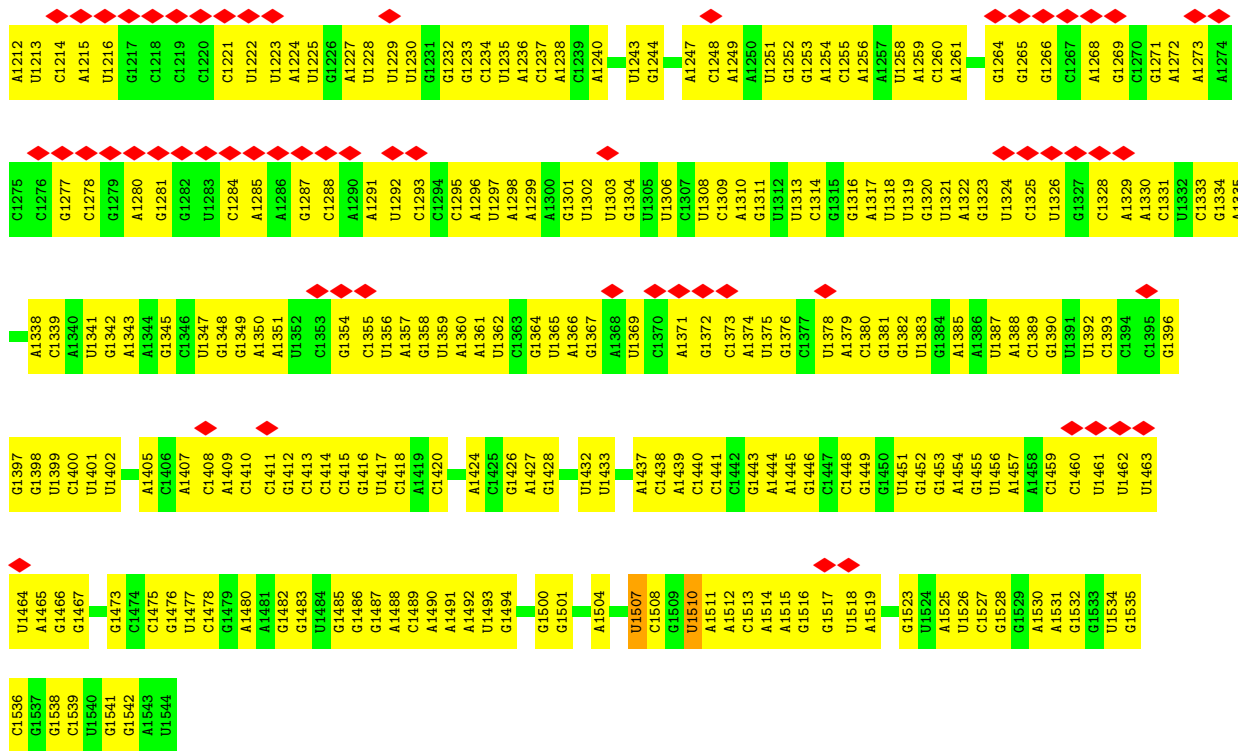


• Molecule 20: 16S

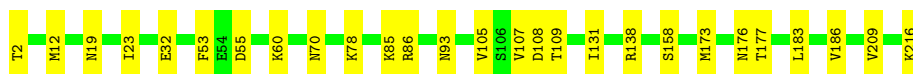
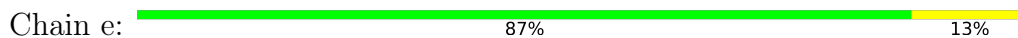




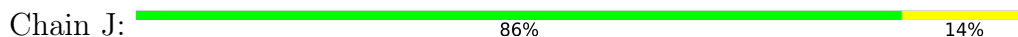




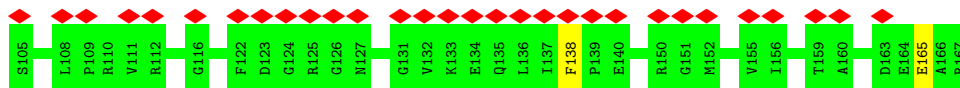
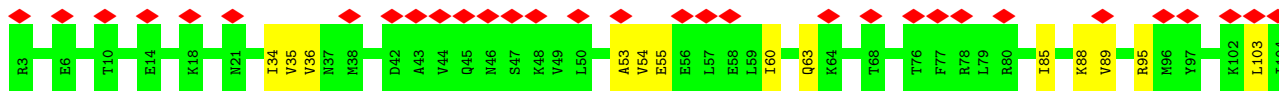
- Molecule 21: 50S ribosomal protein L3



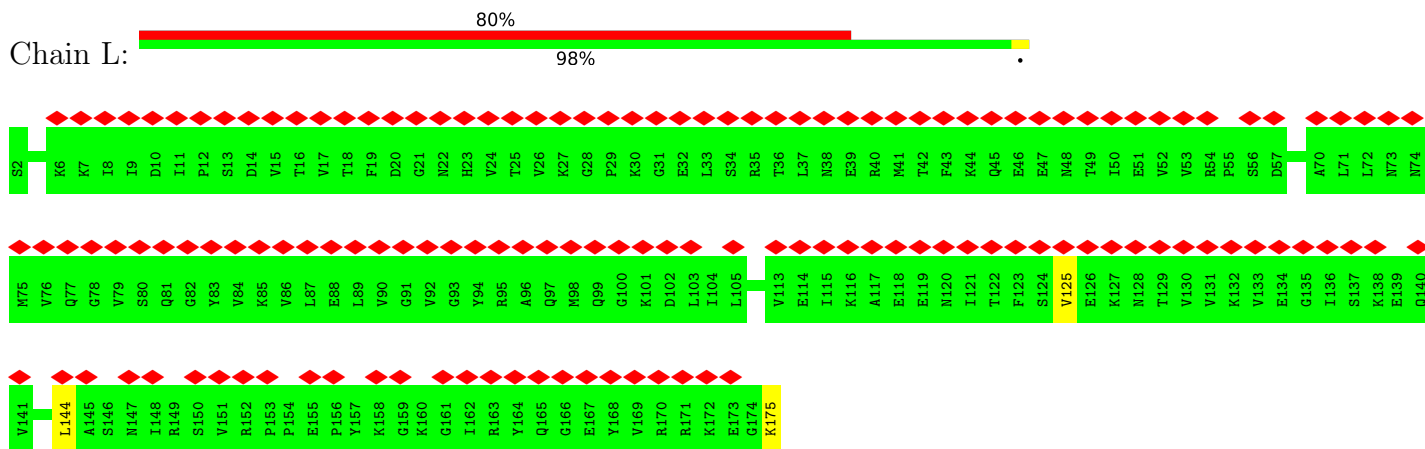
- Molecule 22: 50S ribosomal protein L4



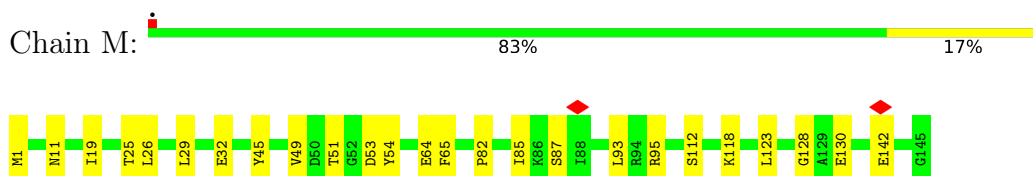
- Molecule 23: 50S ribosomal protein L5



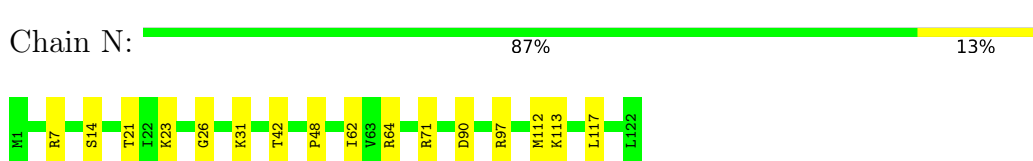
- Molecule 24: 50S ribosomal protein L6



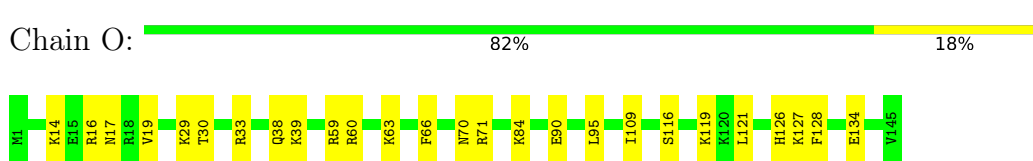
• Molecule 25: 50S ribosomal protein L13



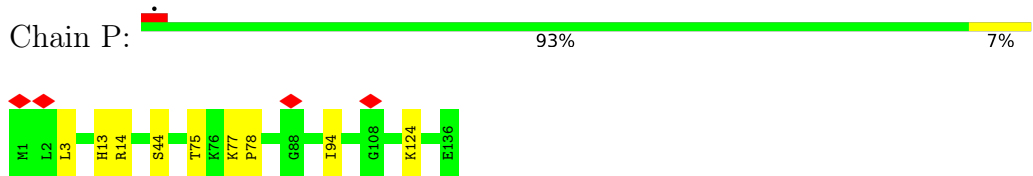
• Molecule 26: 50S ribosomal protein L14



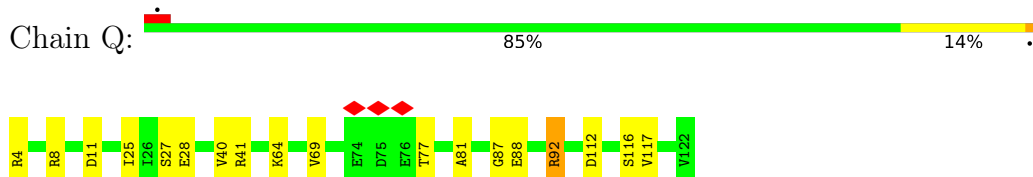
• Molecule 27: 50S ribosomal protein L15



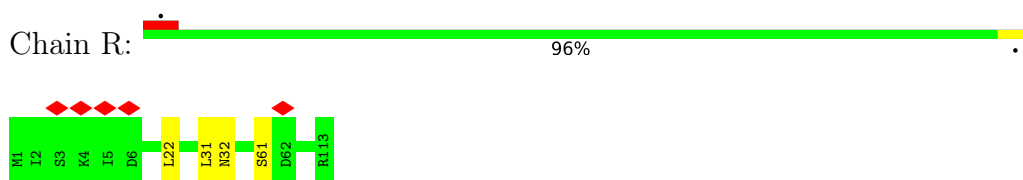
• Molecule 28: 50S ribosomal protein L16



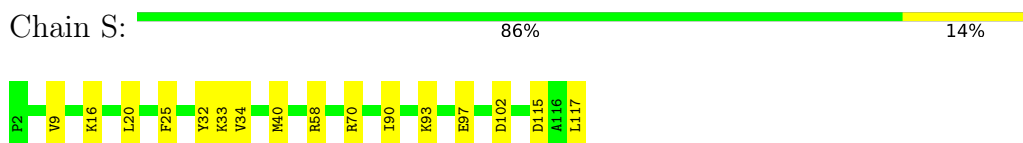
• Molecule 29: 50S ribosomal protein L17



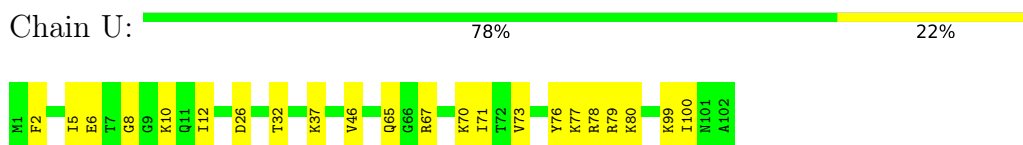
- Molecule 30: 50S ribosomal protein L18



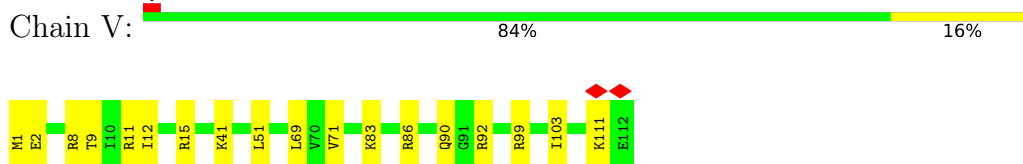
- Molecule 31: 50S ribosomal protein L20



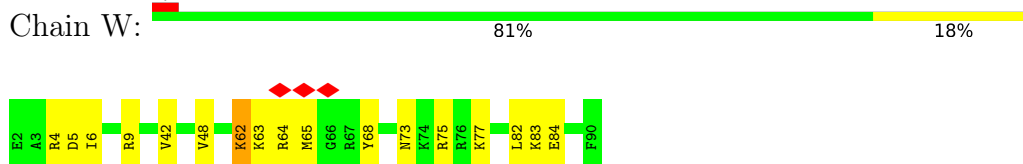
- Molecule 32: 50S ribosomal protein L21



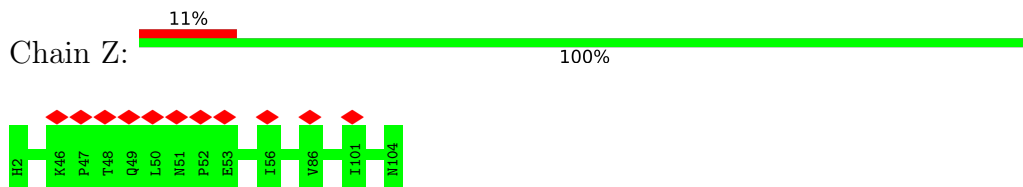
- Molecule 33: 50S ribosomal protein L22



- Molecule 34: 50S ribosomal protein L23



- Molecule 35: 50S ribosomal protein L24

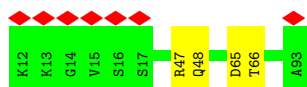


- Molecule 36: 50S ribosomal protein L25

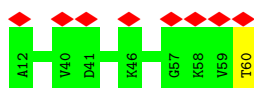




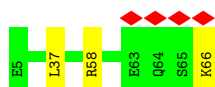
- Molecule 37: 50S ribosomal protein L27



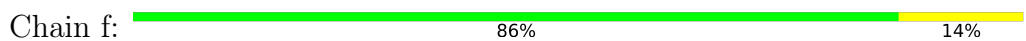
- Molecule 38: 50S ribosomal protein L28



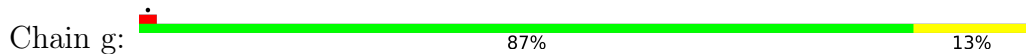
- Molecule 39: 50S ribosomal protein L29



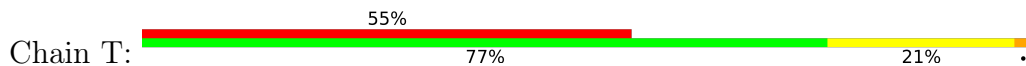
- Molecule 40: 50S ribosomal protein L30



- Molecule 41: 50S ribosomal protein L32p

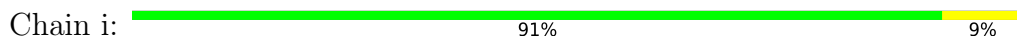


- Molecule 42: 50S ribosomal protein L33





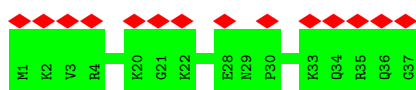
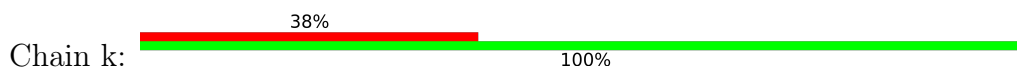
• Molecule 43: 50S ribosomal protein L34



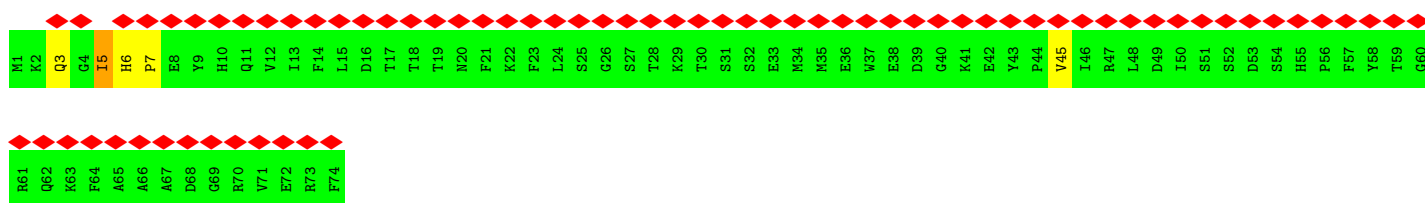
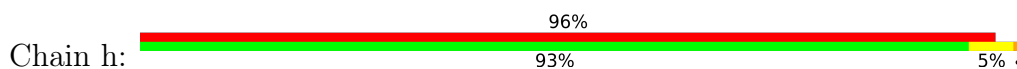
• Molecule 44: 50S ribosomal protein L35



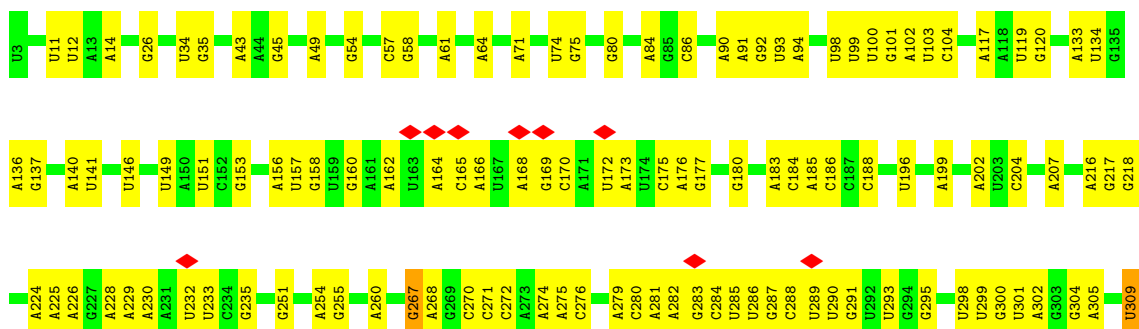
• Molecule 45: 50S ribosomal protein L36

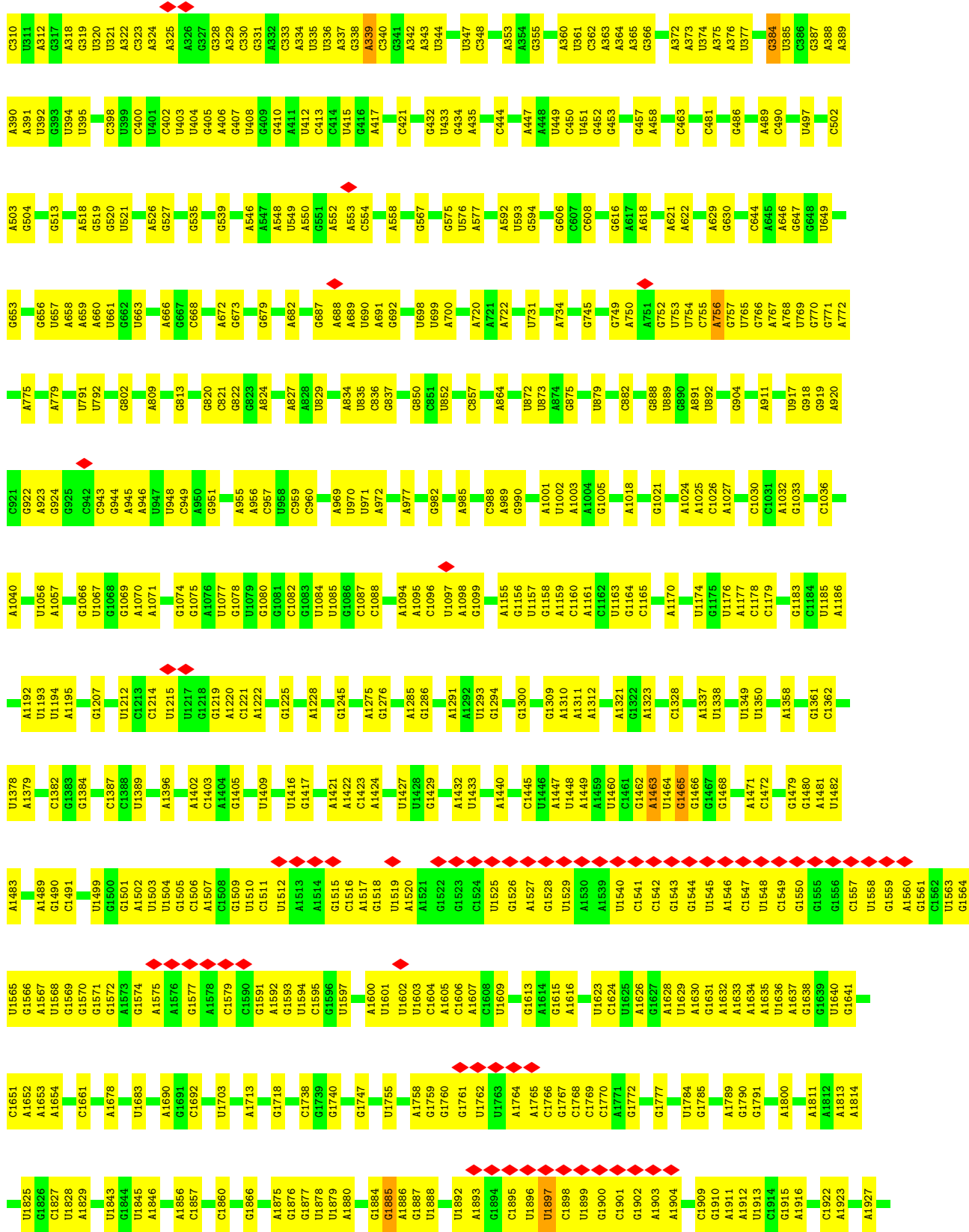


• Molecule 46: 50S ribosomal protein L31 type B



• Molecule 47: 23S









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	Depositor
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	0.039	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0052	Depositor
Map size ( $\text{\AA}$ )	361.2, 361.2, 361.2	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	C	0.20	0/2717	0.63	0/4232
2	B	0.42	0/1573	0.71	1/2121 (0.0%)
3	I	0.32	0/1062	0.62	0/1465
4	D	0.47	0/1167	0.75	0/1576
5	E	0.50	0/796	0.78	1/1069 (0.1%)
6	G	0.66	0/1180	0.60	0/1595
7	F	0.49	0/1019	0.80	0/1371
8	H	0.46	0/990	0.72	1/1332 (0.1%)
9	1	0.48	0/637	0.61	0/865
10	2	0.42	0/840	0.70	0/1137
11	3	0.47	0/991	0.77	0/1337
12	4	0.45	0/835	0.71	1/1123 (0.1%)
13	5	0.54	0/507	0.77	0/674
14	6	0.38	0/721	0.73	2/964 (0.2%)
15	7	0.72	0/541	0.70	0/733
16	8	0.36	0/527	0.70	0/721
17	9	0.54	0/465	0.66	0/620
18	I	0.43	0/551	0.72	0/747
19	A	0.44	0/502	0.60	0/679
20	X	0.21	0/33951	0.65	15/52921 (0.0%)
21	e	0.67	0/1593	0.59	0/2143
22	J	0.66	0/1536	0.57	0/2078
23	K	0.49	0/1028	0.68	1/1405 (0.1%)
24	L	0.33	0/1074	0.68	1/1467 (0.1%)
25	M	0.65	0/1146	0.56	0/1546
26	N	0.66	0/925	0.59	0/1242
27	O	0.68	0/1034	0.60	0/1388
28	P	0.60	1/1067 (0.1%)	0.68	0/1436
29	Q	0.66	0/900	0.57	0/1205
30	R	0.42	0/770	0.65	0/1044
31	S	0.63	0/954	0.55	0/1264
32	U	0.67	0/758	0.57	0/1014
33	V	0.66	0/845	0.59	0/1140
34	W	0.65	0/701	0.57	0/939

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	Z	0.46	0/742	0.66	0/1001
36	a	0.41	0/655	0.77	0/888
37	b	0.72	0/621	0.71	0/824
38	c	0.57	0/382	0.65	0/512
39	d	0.47	0/494	0.69	0/660
40	f	0.66	0/438	0.58	0/591
41	g	0.65	0/361	0.58	0/481
42	T	0.63	0/385	0.57	0/518
43	i	0.62	0/371	0.57	0/484
44	j	0.70	0/450	0.83	1/597 (0.2%)
45	k	0.38	0/275	0.69	0/366
46	h	0.39	0/454	0.62	0/624
47	Y	0.21	1/65313 (0.0%)	0.63	9/101832 (0.0%)
All	All	0.33	2/136844 (0.0%)	0.64	33/205971 (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
2	B	0	2
3	l	0	3
4	D	0	1
7	F	0	1
8	H	0	1
10	2	0	2
11	3	0	3
12	4	0	2
13	5	0	1
19	A	0	1
23	K	0	1
24	L	0	1
30	R	0	3
39	d	0	1
44	j	0	2
46	h	0	1
All	All	0	26

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y	765	U	O3'-P	7.60	1.70	1.61
28	P	124	LYS	C-N	-5.85	1.20	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Y	1463	A	C2'-C3'-O3'	7.93	126.95	109.50
47	Y	756	A	C2'-C3'-O3'	7.61	126.24	109.50
47	Y	267	G	C2'-C3'-O3'	7.36	125.69	109.50
20	X	409	C	C2'-C3'-O3'	7.05	125.00	109.50
20	X	139	U	C2'-C3'-O3'	7.01	124.92	109.50

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	58	ARG	Peptide
2	B	7	PRO	Peptide
3	1	168	ASP	Peptide
3	1	78	LYS	Peptide
3	1	8	ASN	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	B	200/202 (99%)	155 (78%)	43 (22%)	2 (1%)	15	48
3	1	196/198 (99%)	128 (65%)	68 (35%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	154/156 (99%)	118 (77%)	35 (23%)	1 (1%)	25	59
5	E	93/95 (98%)	66 (71%)	23 (25%)	4 (4%)	2	15
6	G	153/155 (99%)	105 (69%)	39 (26%)	9 (6%)	1	9
7	F	128/130 (98%)	89 (70%)	36 (28%)	3 (2%)	6	28
8	H	125/127 (98%)	88 (70%)	33 (26%)	4 (3%)	4	21
9	1	78/80 (98%)	63 (81%)	12 (15%)	3 (4%)	3	18
10	2	112/114 (98%)	78 (70%)	33 (30%)	1 (1%)	17	51
11	3	134/136 (98%)	92 (69%)	40 (30%)	2 (2%)	10	38
12	4	111/113 (98%)	79 (71%)	29 (26%)	3 (3%)	5	24
13	5	58/60 (97%)	39 (67%)	18 (31%)	1 (2%)	9	35
14	6	86/88 (98%)	64 (74%)	22 (26%)	0	100	100
15	7	81/83 (98%)	55 (68%)	18 (22%)	8 (10%)	0	3
16	8	78/80 (98%)	51 (65%)	27 (35%)	0	100	100
17	9	54/56 (96%)	41 (76%)	12 (22%)	1 (2%)	8	32
18	I	76/78 (97%)	47 (62%)	27 (36%)	2 (3%)	5	25
19	A	76/78 (97%)	64 (84%)	12 (16%)	0	100	100
21	e	213/215 (99%)	173 (81%)	37 (17%)	3 (1%)	11	39
22	J	203/205 (99%)	175 (86%)	26 (13%)	2 (1%)	15	48
23	K	163/165 (99%)	112 (69%)	46 (28%)	5 (3%)	4	22
24	L	172/174 (99%)	115 (67%)	57 (33%)	0	100	100
25	M	143/145 (99%)	123 (86%)	15 (10%)	5 (4%)	3	19
26	N	120/122 (98%)	99 (82%)	18 (15%)	3 (2%)	5	26
27	O	143/145 (99%)	111 (78%)	30 (21%)	2 (1%)	11	39
28	P	134/136 (98%)	115 (86%)	17 (13%)	2 (2%)	10	38
29	Q	117/119 (98%)	97 (83%)	14 (12%)	6 (5%)	2	12
30	R	111/113 (98%)	80 (72%)	31 (28%)	0	100	100
31	S	114/116 (98%)	108 (95%)	4 (4%)	2 (2%)	8	33
32	U	100/102 (98%)	73 (73%)	24 (24%)	3 (3%)	4	23
33	V	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
34	W	87/89 (98%)	70 (80%)	13 (15%)	4 (5%)	2	14
35	Z	101/103 (98%)	74 (73%)	27 (27%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	a	91/93 (98%)	69 (76%)	22 (24%)	0	100	100
37	b	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	5	26
38	c	47/49 (96%)	38 (81%)	9 (19%)	0	100	100
39	d	60/62 (97%)	49 (82%)	11 (18%)	0	100	100
40	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
41	g	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	6	28
42	T	45/47 (96%)	41 (91%)	3 (7%)	1 (2%)	6	28
43	i	41/43 (95%)	36 (88%)	5 (12%)	0	100	100
44	j	58/60 (97%)	43 (74%)	15 (26%)	0	100	100
45	k	35/37 (95%)	24 (69%)	11 (31%)	0	100	100
46	h	72/74 (97%)	40 (56%)	30 (42%)	2 (3%)	5	24
All	All	4653/4741 (98%)	3540 (76%)	1026 (22%)	87 (2%)	11	32

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	12	PRO
15	7	13	LYS
21	e	19	ASN
23	K	95	ARG
28	P	78	PRO

### 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	
2	B	151/164 (92%)	145 (96%)	6 (4%)	31	64
3	l	23/174 (13%)	23 (100%)	0	100	100
4	D	120/122 (98%)	114 (95%)	6 (5%)	24	56
5	E	82/83 (99%)	73 (89%)	9 (11%)	6	24
6	G	115/131 (88%)	73 (64%)	42 (36%)	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	107/111 (96%)	97 (91%)	10 (9%)	9	32
8	H	96/105 (91%)	89 (93%)	7 (7%)	14	42
9	1	67/73 (92%)	57 (85%)	10 (15%)	3	13
10	2	85/90 (94%)	82 (96%)	3 (4%)	36	67
11	3	95/118 (80%)	93 (98%)	2 (2%)	53	78
12	4	75/97 (77%)	69 (92%)	6 (8%)	12	39
13	5	51/52 (98%)	43 (84%)	8 (16%)	2	11
14	6	74/80 (92%)	73 (99%)	1 (1%)	67	85
15	7	36/70 (51%)	22 (61%)	14 (39%)	0	0
16	8	35/75 (47%)	35 (100%)	0	100	100
17	9	49/50 (98%)	35 (71%)	14 (29%)	0	1
18	I	45/69 (65%)	43 (96%)	2 (4%)	28	60
19	A	37/65 (57%)	36 (97%)	1 (3%)	44	73
21	e	158/173 (91%)	134 (85%)	24 (15%)	3	12
22	J	154/168 (92%)	127 (82%)	27 (18%)	2	9
23	K	67/146 (46%)	59 (88%)	8 (12%)	5	20
24	L	61/152 (40%)	60 (98%)	1 (2%)	62	84
25	M	117/123 (95%)	97 (83%)	20 (17%)	2	9
26	N	100/100 (100%)	87 (87%)	13 (13%)	4	18
27	O	91/111 (82%)	67 (74%)	24 (26%)	0	1
28	P	101/113 (89%)	95 (94%)	6 (6%)	19	50
29	Q	90/100 (90%)	77 (86%)	13 (14%)	3	14
30	R	63/90 (70%)	62 (98%)	1 (2%)	62	84
31	S	96/96 (100%)	82 (85%)	14 (15%)	3	13
32	U	68/86 (79%)	49 (72%)	19 (28%)	0	1
33	V	84/91 (92%)	66 (79%)	18 (21%)	1	4
34	W	72/80 (90%)	58 (81%)	14 (19%)	1	6
35	Z	71/88 (81%)	71 (100%)	0	100	100
36	a	58/82 (71%)	58 (100%)	0	100	100
37	b	61/64 (95%)	59 (97%)	2 (3%)	38	68
38	c	38/41 (93%)	37 (97%)	1 (3%)	46	74

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	d	52/57 (91%)	50 (96%)	2 (4%)	33	65
40	f	50/51 (98%)	42 (84%)	8 (16%)	2	11
41	g	35/43 (81%)	30 (86%)	5 (14%)	3	14
42	T	42/45 (93%)	31 (74%)	11 (26%)	0	1
43	i	39/39 (100%)	35 (90%)	4 (10%)	7	26
44	j	44/52 (85%)	43 (98%)	1 (2%)	50	76
45	k	29/35 (83%)	29 (100%)	0	100	100
46	h	23/66 (35%)	20 (87%)	3 (13%)	4	18
All	All	3207/4021 (80%)	2827 (88%)	380 (12%)	8	21

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	N	112	MET
31	S	70	ARG
27	O	30	THR
28	P	14	ARG
32	U	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
25	M	137	GLN
31	S	29	HIS
42	T	26	ASN
26	N	4	GLN
27	O	143	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	113/114 (99%)	55 (48%)	2 (1%)
20	X	1401/1415 (99%)	1035 (73%)	80 (5%)
47	Y	2703/2720 (99%)	954 (35%)	36 (1%)
All	All	4217/4249 (99%)	2044 (48%)	118 (2%)

5 of 2044 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	C	3	U
1	C	4	G
1	C	7	G
1	C	10	U
1	C	11	A

5 of 118 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	X	936	G
47	Y	1885	G
20	X	1298	A
47	Y	1845	U
47	Y	1463	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	Y	16
20	X	11

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	1492:G	O3'	1498:U	P	29.74
1	Y	2135:U	O3'	2208:A	P	19.22
1	Y	1530:A	O3'	1539:A	P	17.34
1	Y	1550:G	O3'	1555:G	P	16.75
1	X	215:C	O3'	228:A	P	16.72

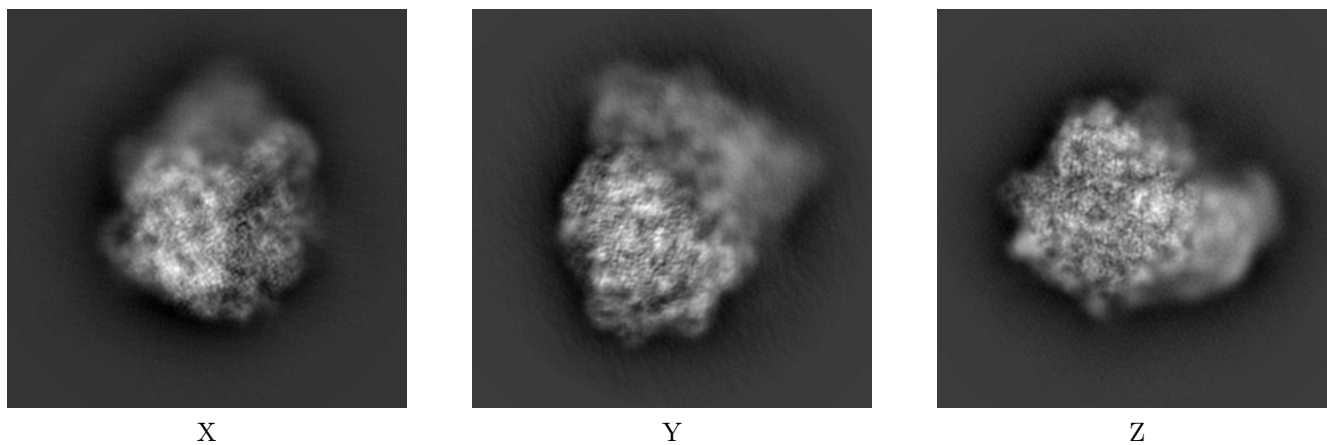
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11902. 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](#)

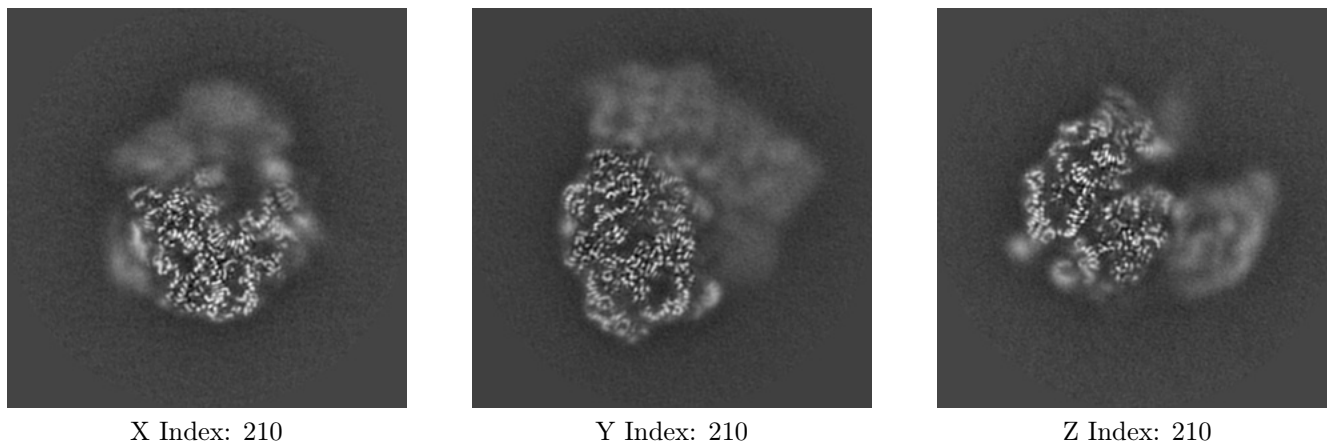
#### 6.1.1 Primary map



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

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

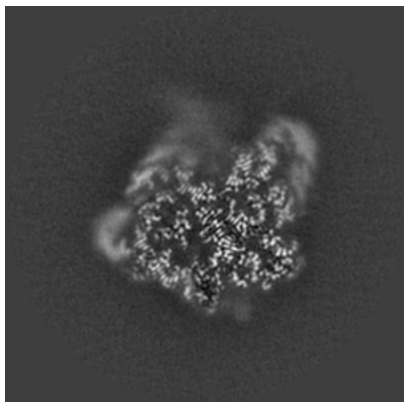
#### 6.2.1 Primary map



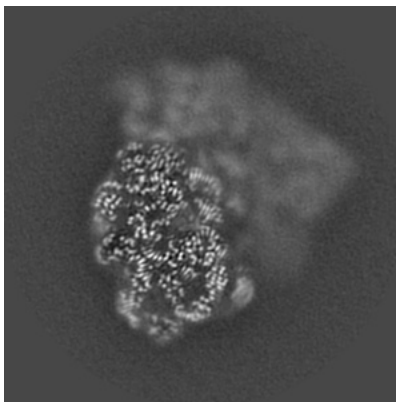
The images above show central slices of the map in three orthogonal directions.

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

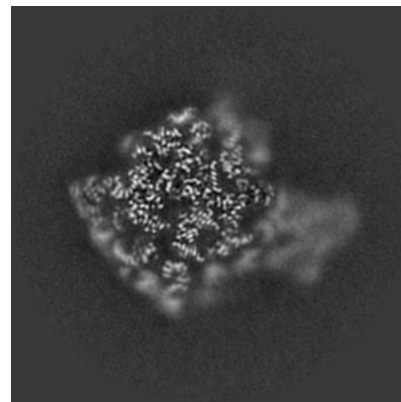
### 6.3.1 Primary map



X Index: 167



Y Index: 214



Z Index: 167

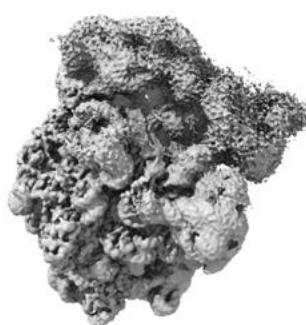
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.0052. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

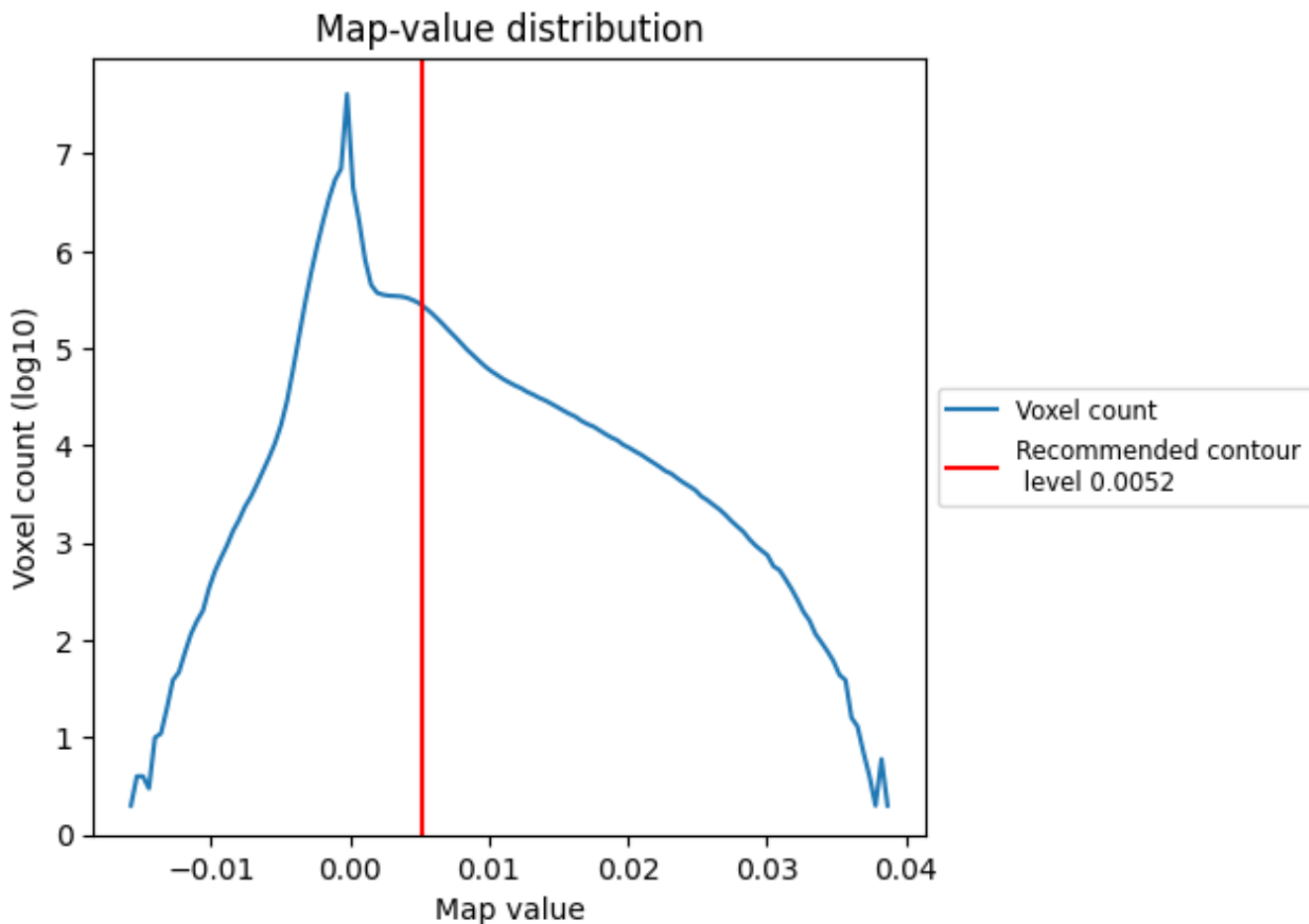
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

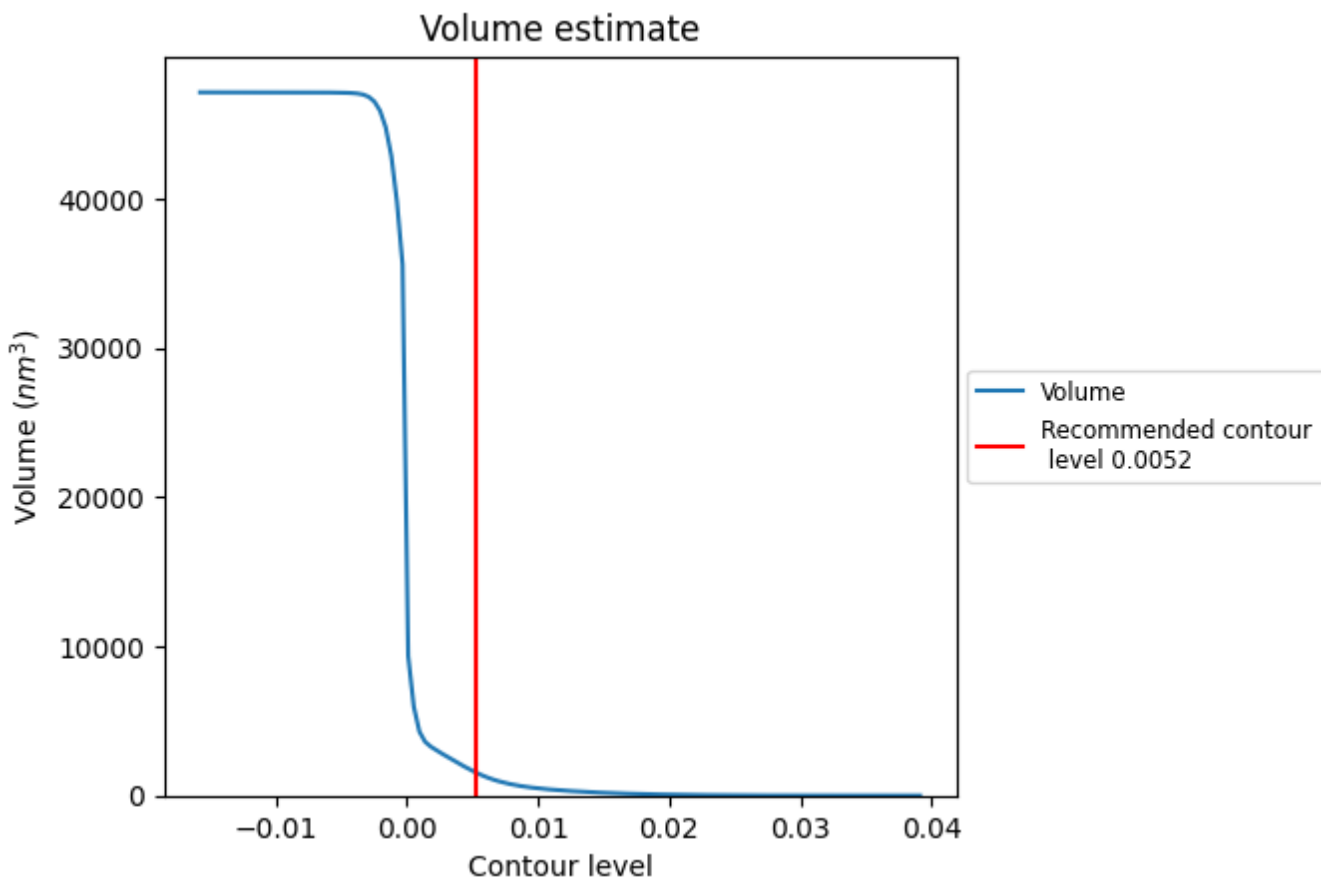
This section contains the results of statistical analysis of the map.

### 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.

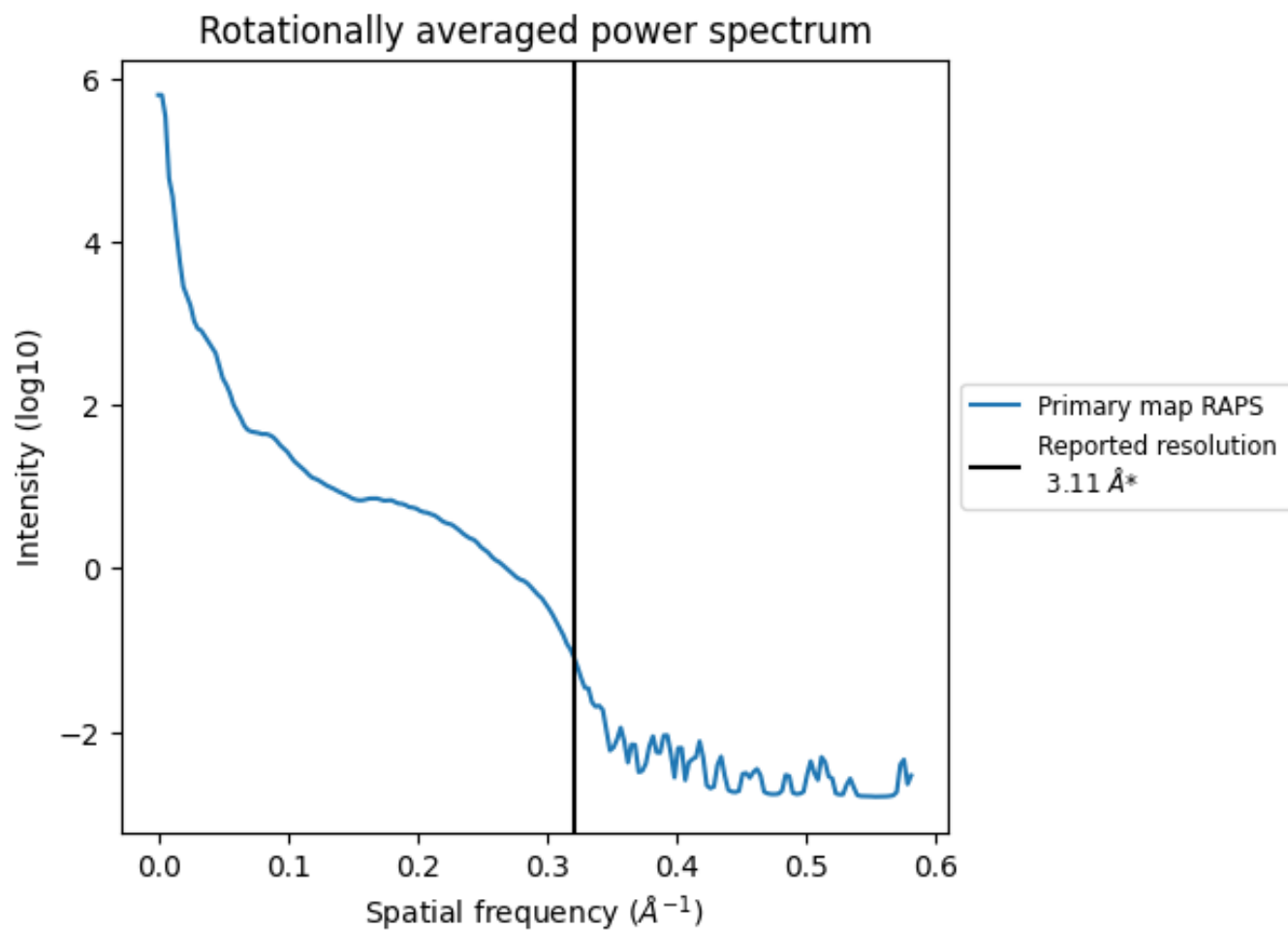
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1571 nm<sup>3</sup>; this corresponds to an approximate mass of 1419 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 0.322 Å<sup>-1</sup>



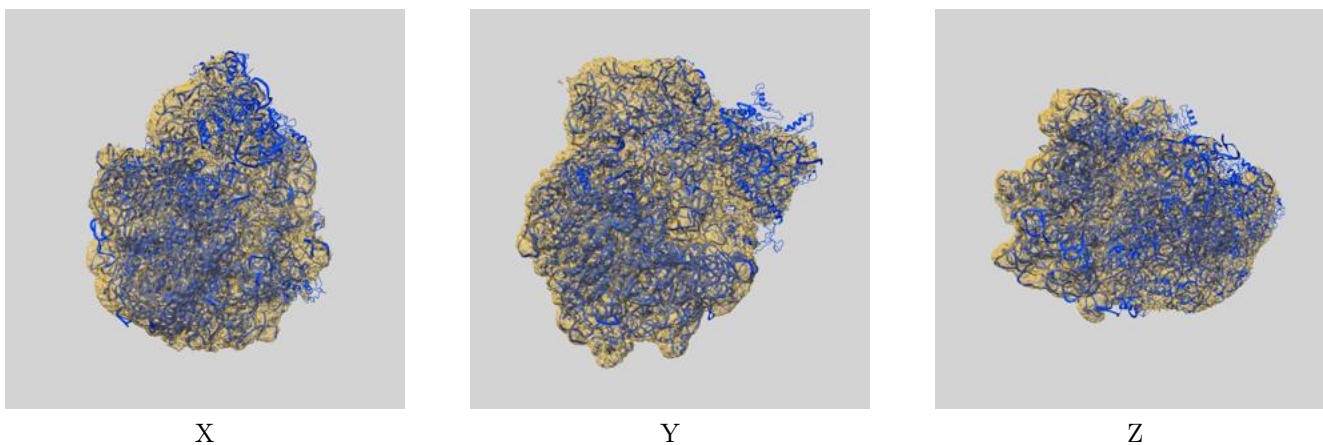
## 8 Fourier-Shell correlation

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

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

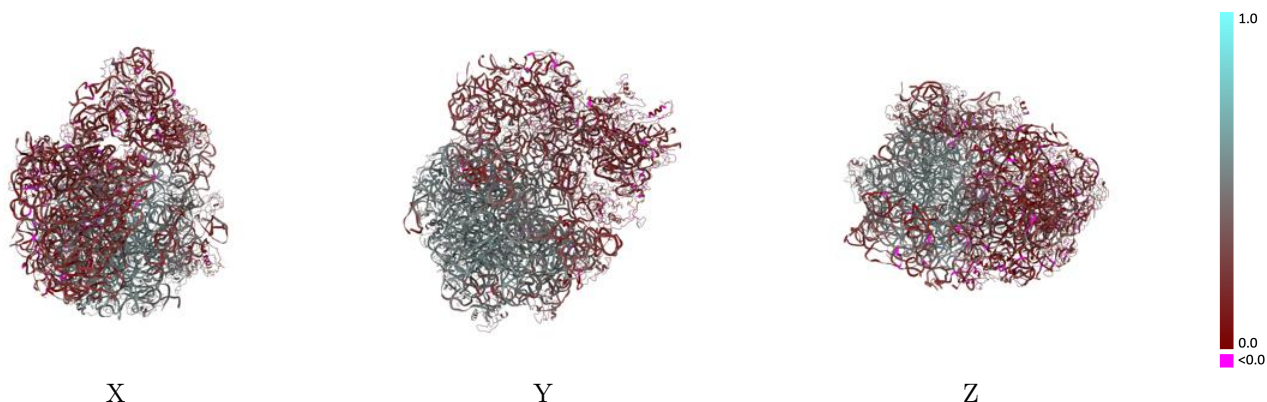
This section contains information regarding the fit between EMDB map EMD-11902 and PDB model 7ASO. Per-residue inclusion information can be found in section 3 on page 12.

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



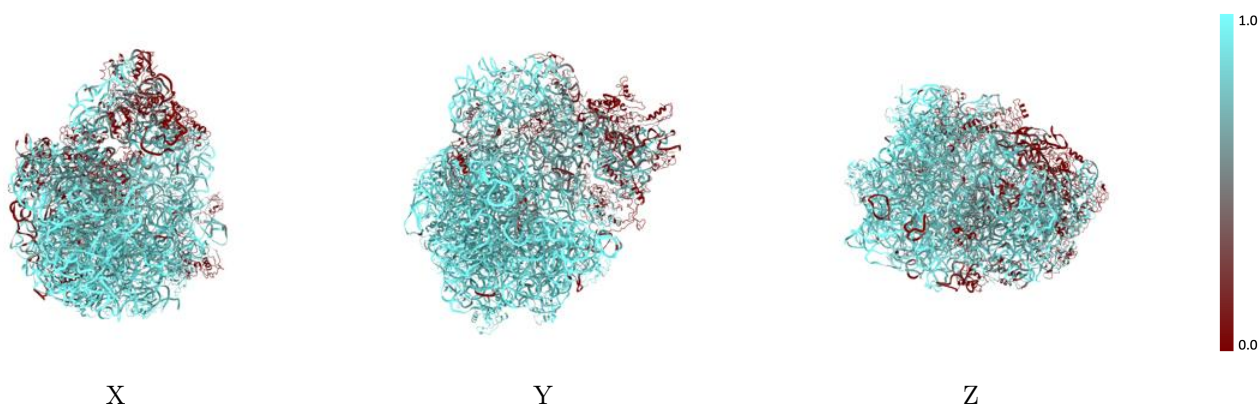
The images above show the 3D surface view of the map at the recommended contour level 0.0052 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



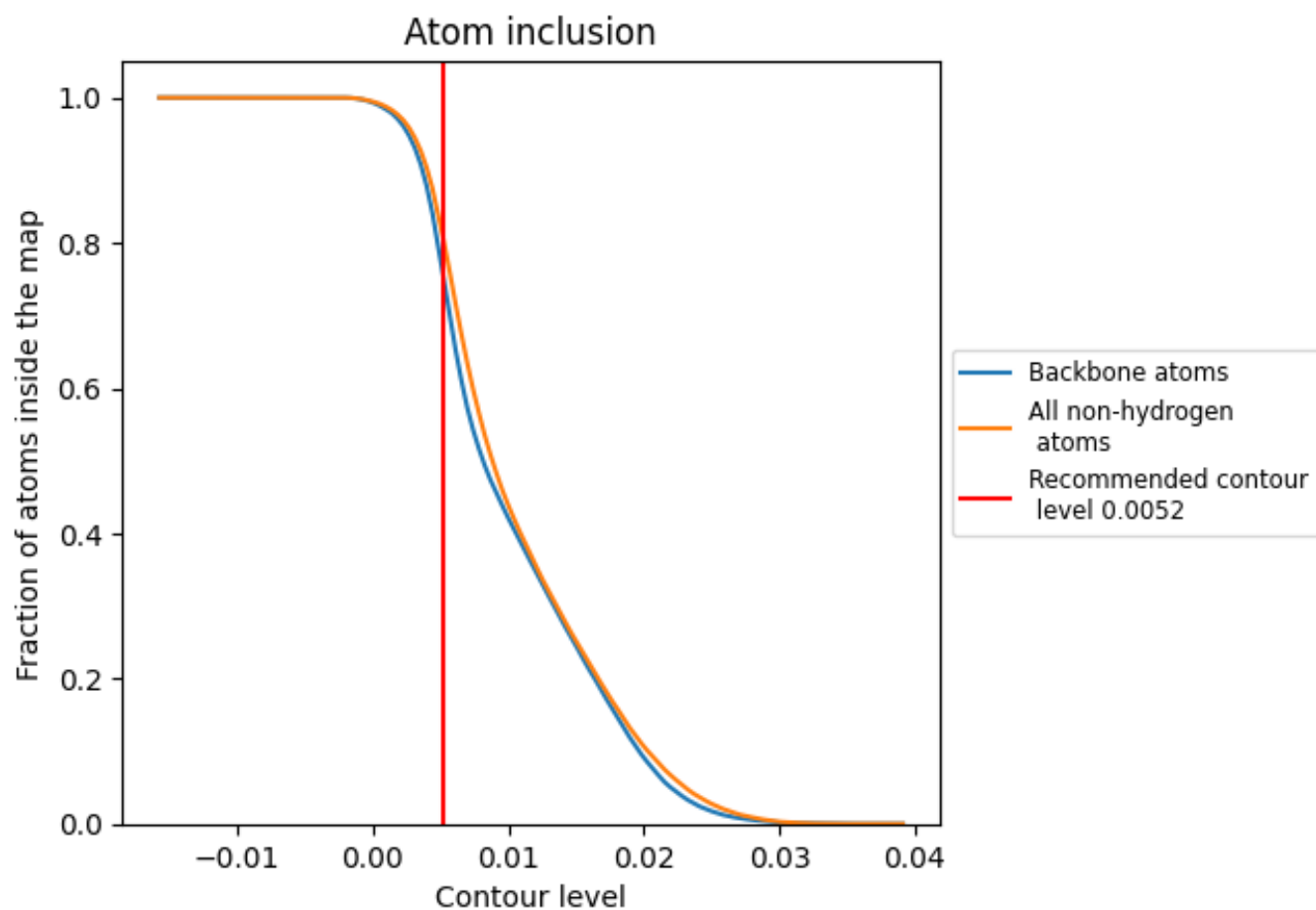
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0052).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 81% 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 (0.0052) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8055	 0.3580
1	 0.1166	 0.1950
2	 0.0890	 0.2510
3	 0.1017	 0.2140
4	 0.3153	 0.2170
5	 0.1366	 0.2110
6	 0.3921	 0.2180
7	 0.4753	 0.1430
8	 0.4384	 0.2580
9	 0.3447	 0.2210
A	 0.2716	 0.2000
B	 0.0886	 0.2520
C	 0.9444	 0.2810
D	 0.2923	 0.2540
E	 0.2536	 0.1940
F	 0.4136	 0.2310
G	 0.4516	 0.1910
H	 0.2699	 0.2470
I	 0.1676	 0.2250
J	 0.9084	 0.4850
K	 0.6093	 0.2410
L	 0.2190	 0.2550
M	 0.9100	 0.5130
N	 0.8492	 0.5230
O	 0.9037	 0.4810
P	 0.8366	 0.4750
Q	 0.8999	 0.5110
R	 0.8636	 0.3240
S	 0.9285	 0.5410
T	 0.4278	 0.3970
U	 0.9349	 0.5160
V	 0.8933	 0.5300
W	 0.8628	 0.4550
X	 0.8044	 0.1890
Y	 0.9410	 0.4510



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Z	 0.7717	 0.4180
a	 0.3598	 0.3440
b	 0.8507	 0.5050
c	 0.7328	 0.4770
d	 0.8351	 0.3850
e	 0.9367	 0.5280
f	 0.9136	 0.5110
g	 0.8630	 0.4480
h	 0.0519	 0.2470
i	 0.9104	 0.5490
j	 0.8876	 0.5200
k	 0.5263	 0.3340
l	 0.2662	 0.2720