



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 12:33 AM JST

PDB ID : 5XXB  
EMDB ID : EMD-6778  
Title : Large subunit of Toxoplasma gondii ribosome  
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.  
Deposited on : 2017-07-03  
Resolution : 3.17 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

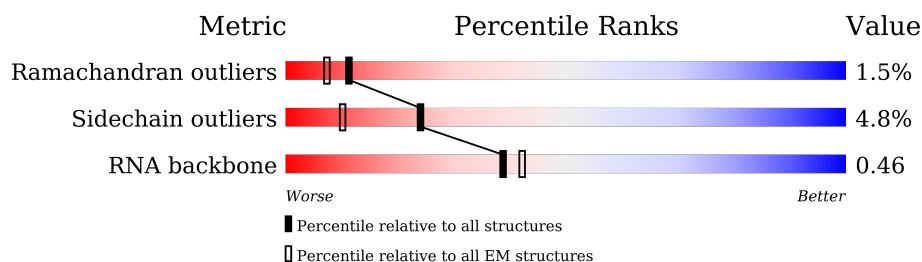
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.17 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	3477	
2	3	124	
3	4	158	
4	A	260	
5	B	389	
6	C	416	
7	D	310	
8	E	193	

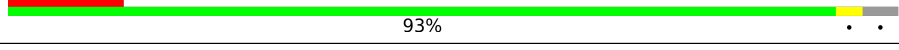
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Mol	Chain	Length	Quality of chain
9	F	258	
10	G	276	
11	H	190	
12	I	221	
13	J	175	
14	K	355	
15	L	134	
16	M	205	
17	N	269	
18	O	195	
19	P	187	
20	Q	187	
21	R	183	
22	S	157	
23	T	133	
24	U	139	
25	V	155	
26	W	167	
27	X	141	
28	Y	146	
29	Z	147	
30	a	54	
31	b	108	
32	c	120	
33	d	134	

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Mol	Chain	Length	Quality of chain
34	e	112	
35	f	134	
36	g	123	
37	h	101	
38	i	98	
39	j	84	
40	k	51	
41	l	129	
42	n	105	
43	o	96	
44	p	129	

## 2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 121433 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 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3077	Total	C	N	O	P	0	0
			65598	29312	11639	21570	3077		

- Molecule 2 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	118	Total	C	N	O	P	0	0
			2519	1123	452	826	118		

- Molecule 3 is a RNA chain called 5.8S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	157	Total	C	N	O	P	0	0
			3339	1493	586	1103	157		

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	246	Total	C	N	O	S	0	0
			1882	1170	379	324	9		

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	369	Total	C	N	O	S	0	0
			2942	1867	561	496	18		

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	394	Total	C	N	O	S	0	0
			3060	1897	621	528	14		

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	261	Total	C	N	O	S	0	0
			2123	1336	406	375	6		

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	124	Total	C	N	O	S	0	0
			971	621	177	170	3		

- Molecule 9 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	250	Total	C	N	O	S	0	0
			2059	1324	389	338	8		

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1877	1192	357	319	9		

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	187	Total	C	N	O	S	0	0
			1478	938	264	266	10		

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	193	Total	C	N	O	S	0	0
			1540	976	296	258	10		

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	166	Total	C	N	O	S	0	0
			1343	845	258	236	4		

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	199	Total	C	N	O	S	0	0
			1593	1006	321	262	4		

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total	C	N	O	S	0	0
			1063	674	203	180	6		

- Molecule 16 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	202	Total	C	N	O	S	0	0
			1683	1060	350	268	5		

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	200	Total	C	N	O	S	0	0
			1645	1034	330	272	9		

- Molecule 18 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	158	Total	C	N	O	S	0	0
			1286	805	249	222	10		

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	186	Total	C	N	O	S	0	0
			1477	918	306	246	7		

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	176	Total	C	N	O	S	0	0
			1473	918	309	236	10		

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	182	Total	C	N	O	S	0	0
			1492	953	282	250	7		

- Molecule 22 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	154	Total	C	N	O	S	0	0
			1231	775	242	208	6		

- Molecule 23 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	99	Total	C	N	O	S	0	0
			827	531	147	145	4		

- Molecule 24 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	129	Total	C	N	O	S	0	0
			968	613	178	168	9		

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	63	Total	C	N	O	S	0	0
			533	344	104	82	3		

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	127	Total	C	N	O	S	0	0
			1038	655	194	186	3		

- Molecule 27 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	124	Total	C	N	O	S	0	0
			1011	629	207	172	3		

- Molecule 28 is a protein called Ribosomal protein eL27.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	144	Total	C	N	O	S	0	0
			1163	751	214	191	7		

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	145	Total	C	N	O	S	0	0
			1136	724	221	186	5		

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	49	Total	C	N	O	S	0	0
			404	243	93	62	6		

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	96	Total	C	N	O	S	0	0
			725	450	134	134	7		

- Molecule 32 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	107	Total	C	N	O	S	0	0
			908	573	182	151	2		

- Molecule 33 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	122	Total	C	N	O	S	0	0
			1011	639	203	165	4		

- Molecule 34 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	105	Total	C	N	O	S	0	0
			854	546	167	140	1		

- Molecule 35 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	107	Total	C	N	O	S	0	0
			863	535	191	132	5		

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	121	Total	C	N	O	S	0	0
			981	615	199	165	2		

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	97	Total	C	N	O	S	0	0
			772	481	165	125	1		

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	87	Total	C	N	O	S	0	0
			688	418	152	112	6		

- Molecule 39 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	72	Total	C	N	O	S	0	0
			591	376	112	102	1		

- Molecule 40 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	49	Total	C	N	O	S	0	0
			419	264	94	59	2		

- Molecule 41 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	52	Total	C	N	O	S	0	0
			419	263	85	66	5		

- Molecule 42 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	97	Total	C	N	O	S	0	0
			790	503	157	125	5		

- Molecule 43 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	90	Total	C	N	O	S	0	0
			684	428	137	113	6		

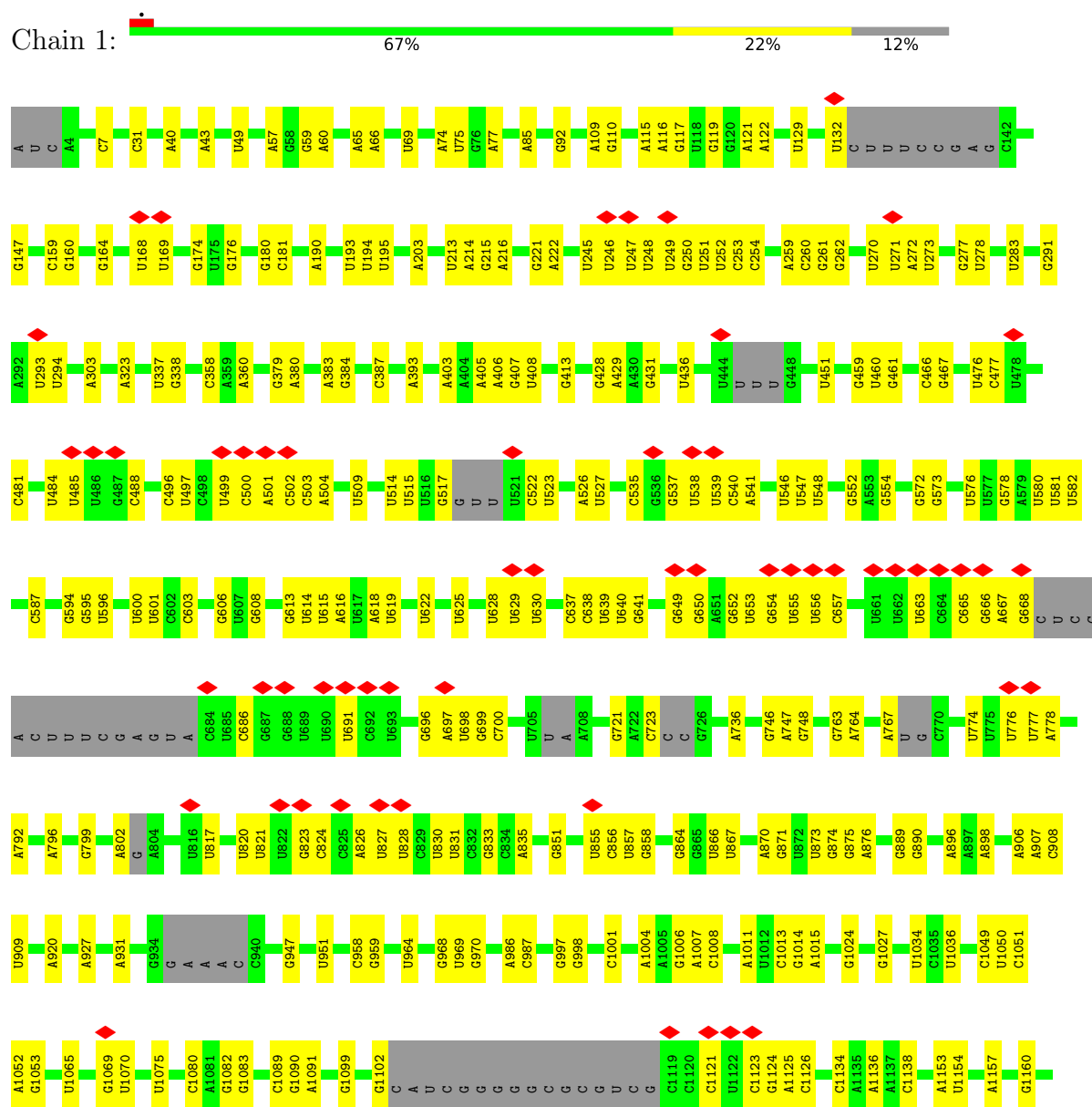
- Molecule 44 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	122	Total	C	N	O	S	0	0
			974	607	197	161	9		

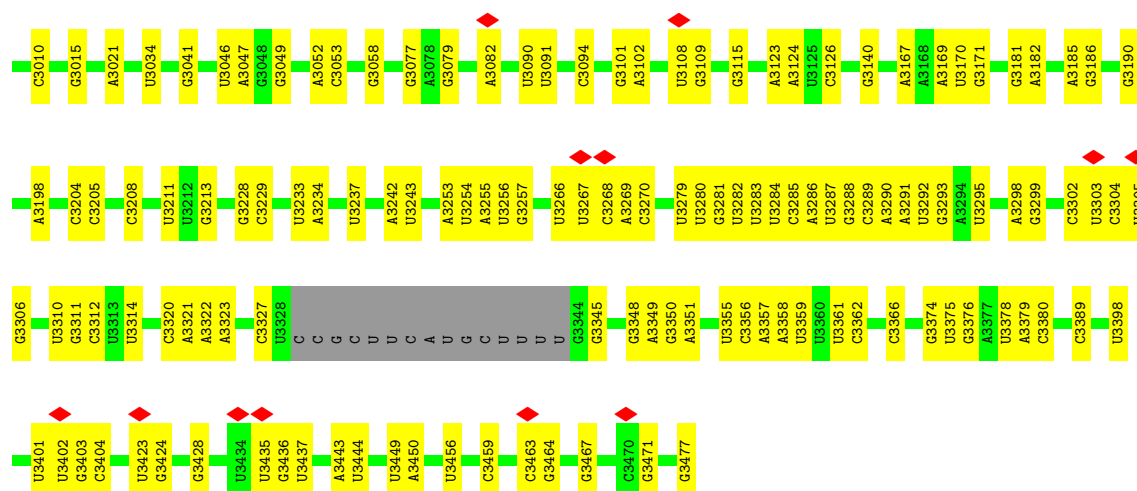
### 3 Residue-property plots

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.

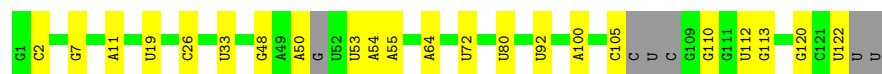
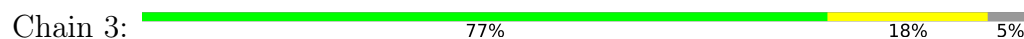
#### • Molecule 1: 25S RNA



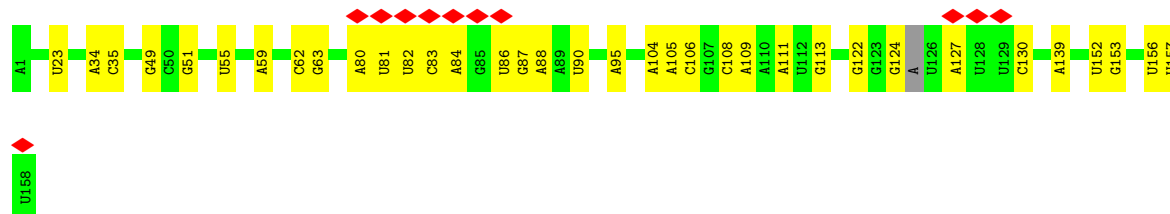
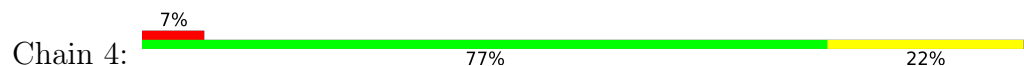




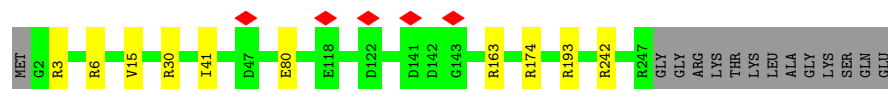
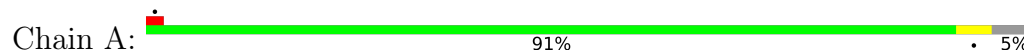
• Molecule 2: 5S RNA



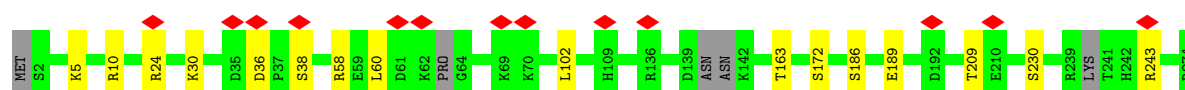
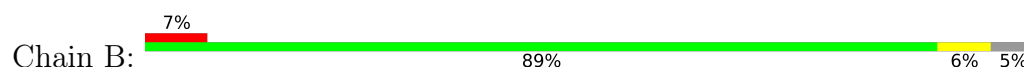
• Molecule 3: 5.8S RNA

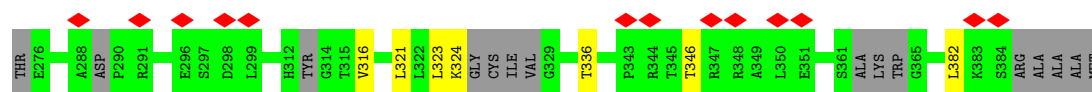


• Molecule 4: Ribosomal protein uL2

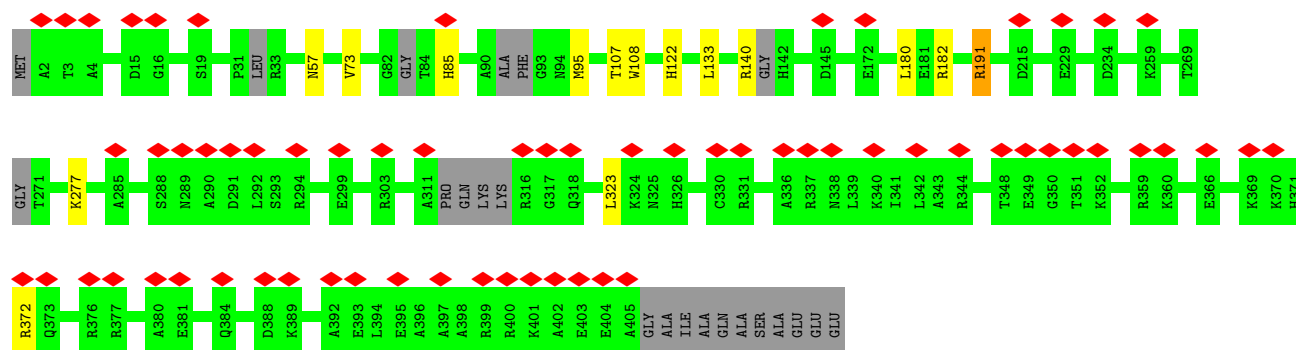
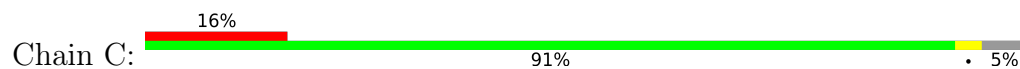


• Molecule 5: Ribosomal protein uL3

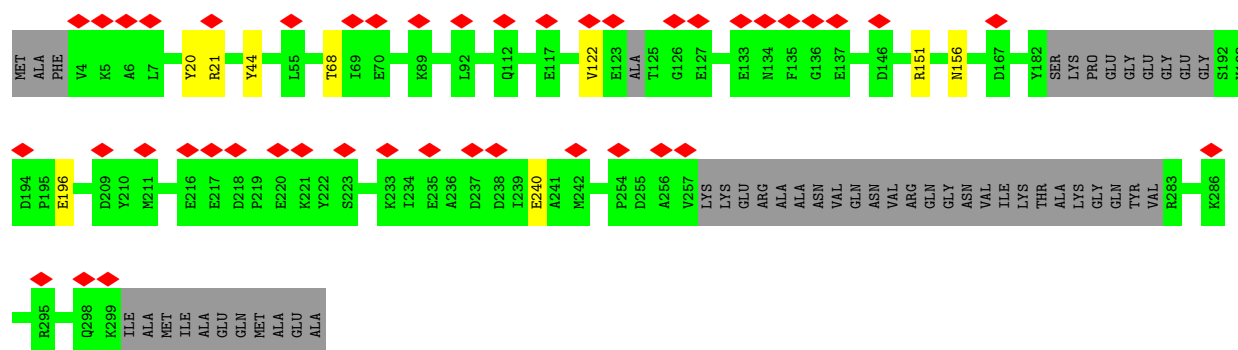
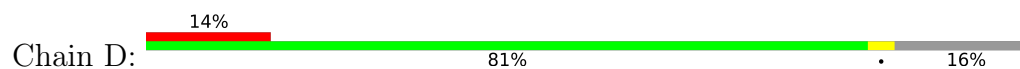




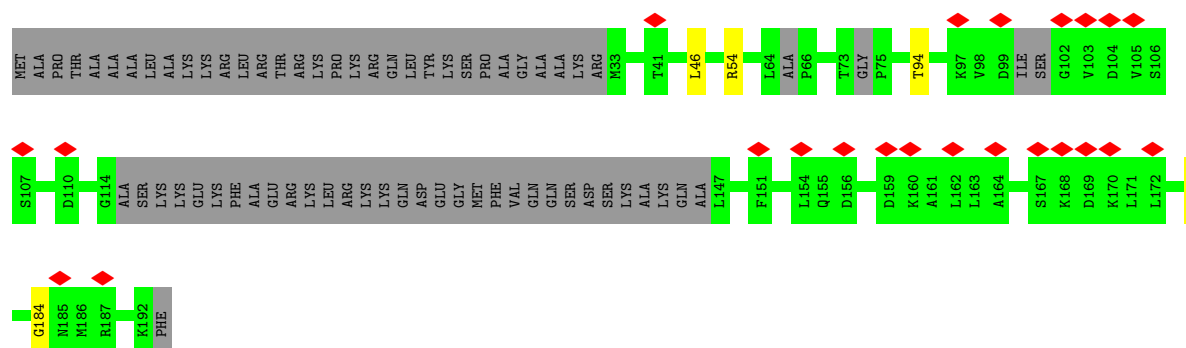
• Molecule 6: Ribosomal protein uL4



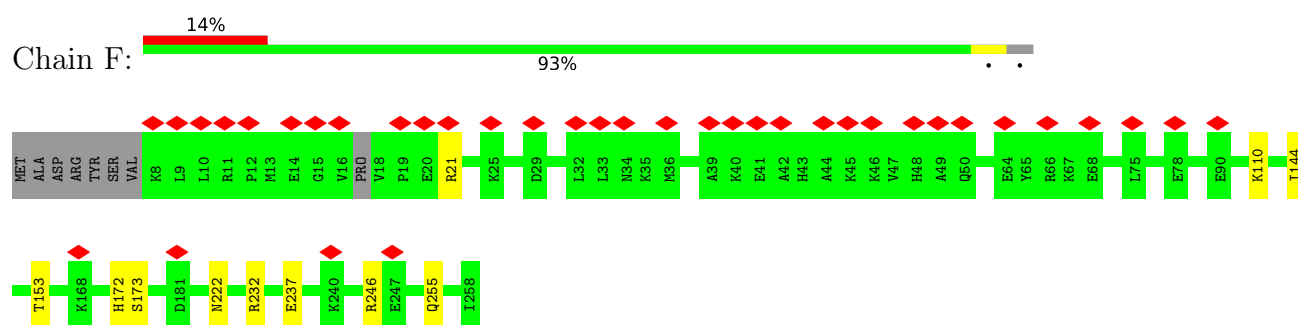
• Molecule 7: Ribosomal protein uL18



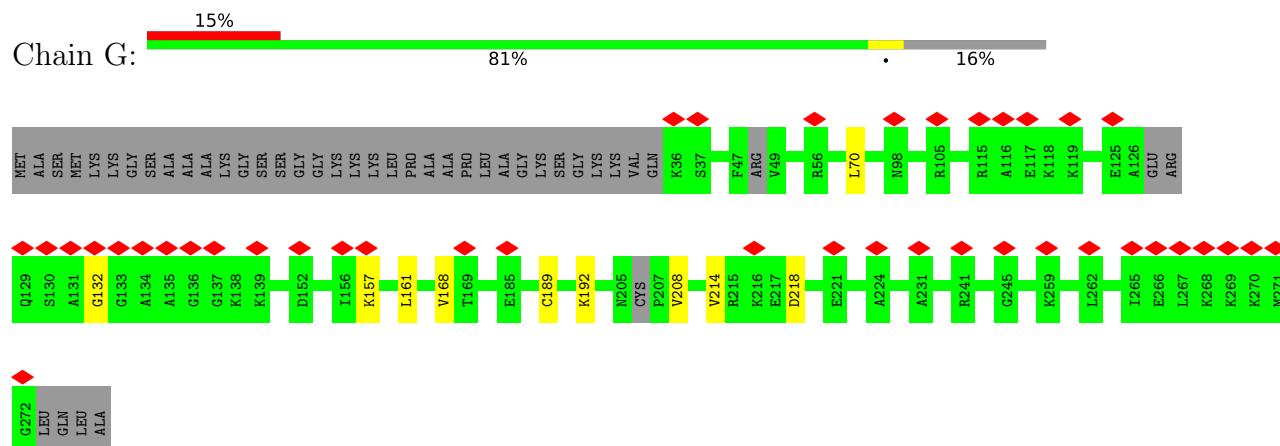
• Molecule 8: Ribosomal protein eL6



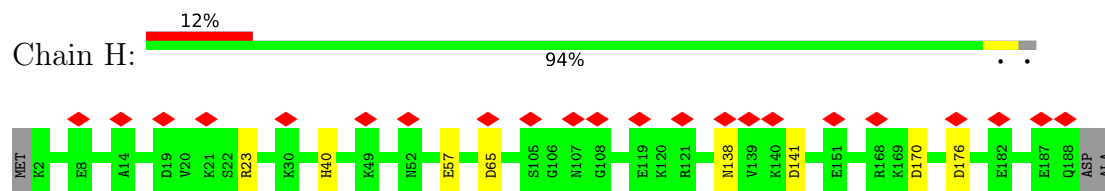
• Molecule 9: Ribosomal protein uL30



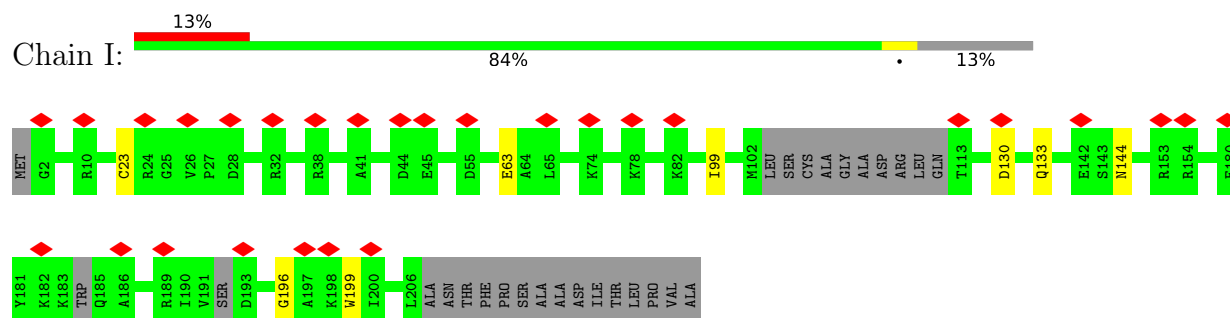
• Molecule 10: Ribosomal protein eL8



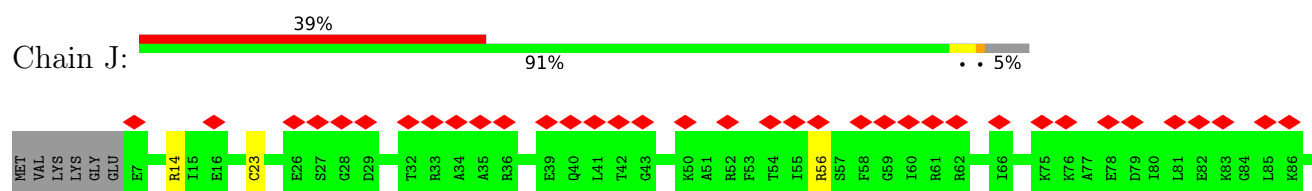
• Molecule 11: Ribosomal protein uL6



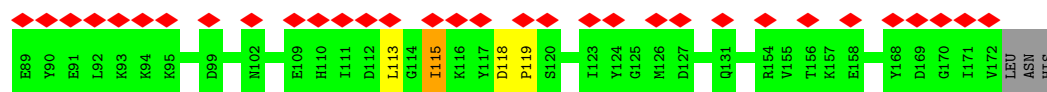
• Molecule 12: Ribosomal protein uL16



• Molecule 13: Ribosomal protein uL5

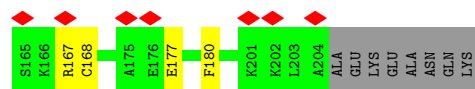
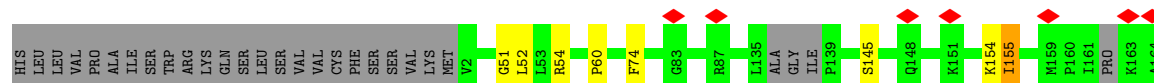
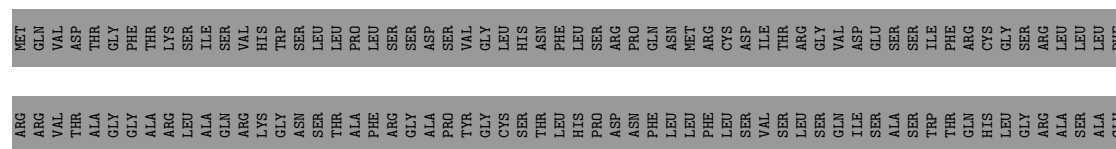






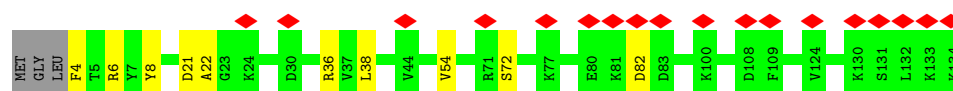
• Molecule 14: Ribosomal protein eL13

Chain K: 53% 44%



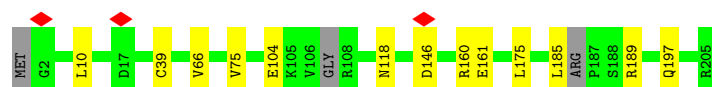
• Molecule 15: Ribosomal protein eL14

Chain L: 13% 90% 7%



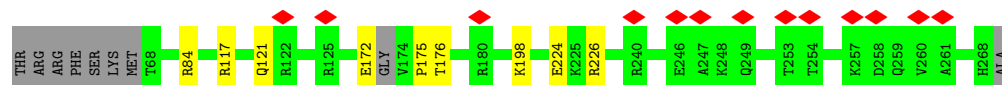
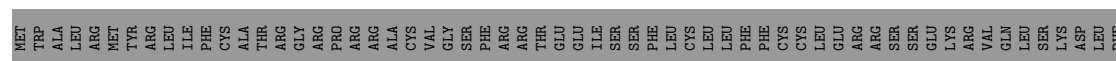
• Molecule 16: Ribosomal protein eL15

Chain M: 92% 6%



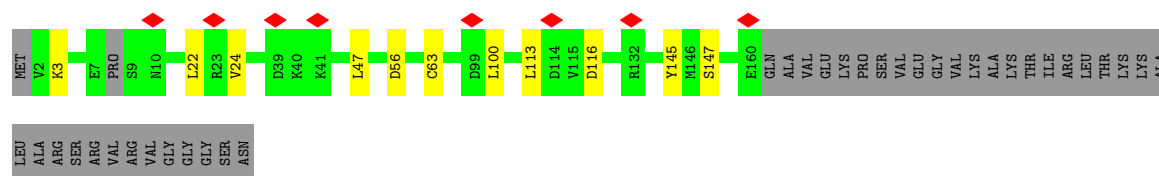
• Molecule 17: Ribosomal protein uL13

Chain N: 5% 71% 26%

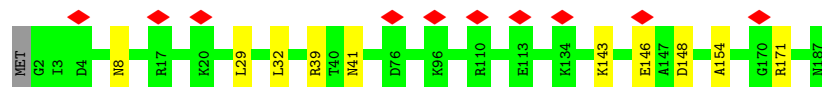


• Molecule 18: Ribosomal protein uL22

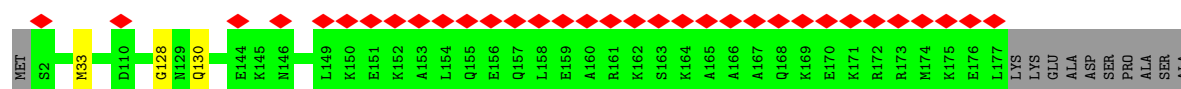
Chain O: 75% 6% 19%



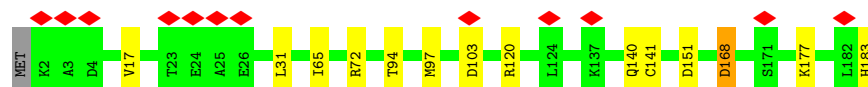
- Molecule 19: Ribosomal protein eL18



- Molecule 20: Ribosomal protein eL19



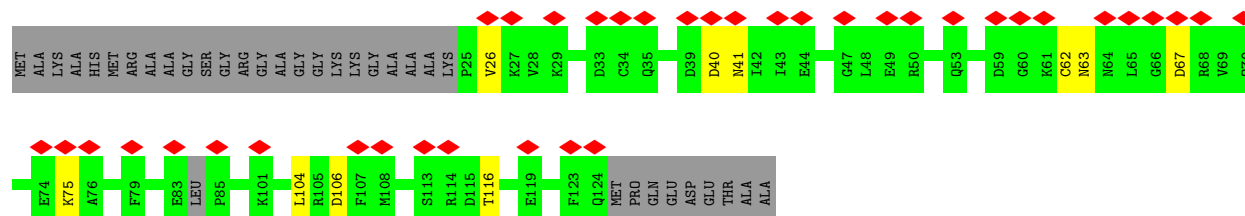
- Molecule 21: Ribosomal protein eL20



- Molecule 22: Ribosomal protein eL21

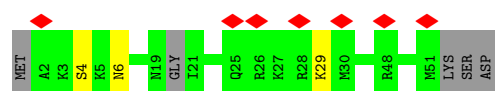
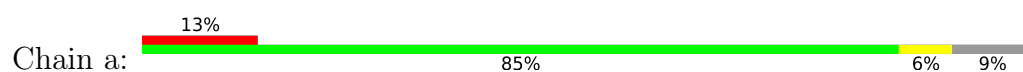


- Molecule 23: Ribosomal protein eL22

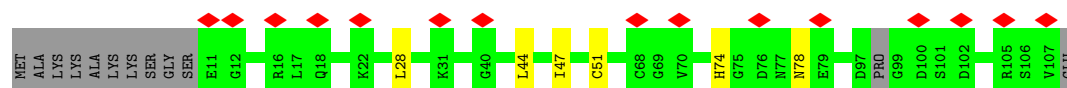
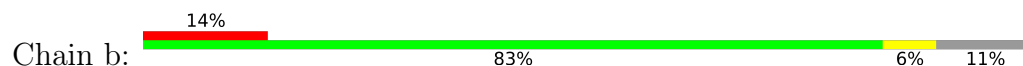


- Molecule 24: Ribosomal protein uL14

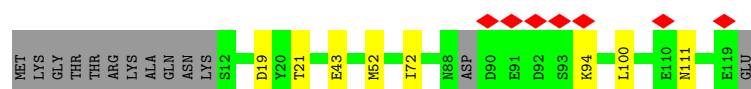
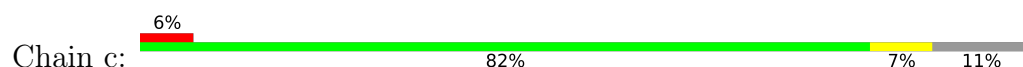




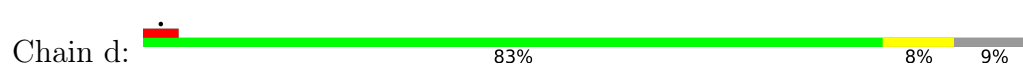
- Molecule 31: Ribosomal protein eL30



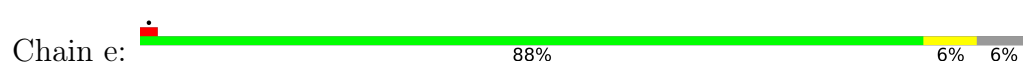
- Molecule 32: Ribosomal protein eL31



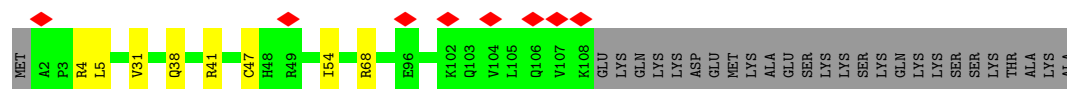
- Molecule 33: Ribosomal protein eL32



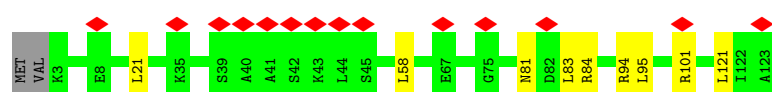
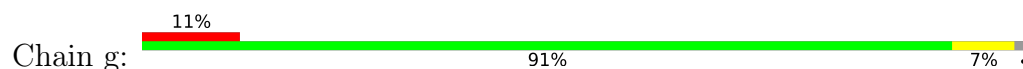
- Molecule 34: Ribosomal protein eL33



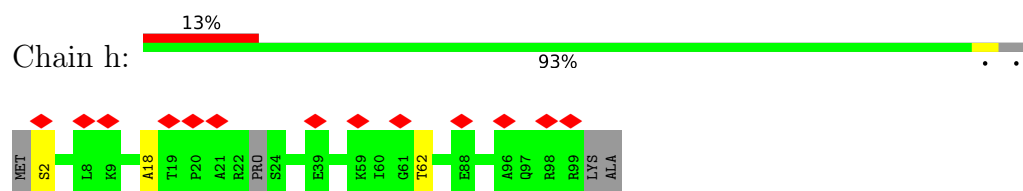
- Molecule 35: Ribosomal protein eL34



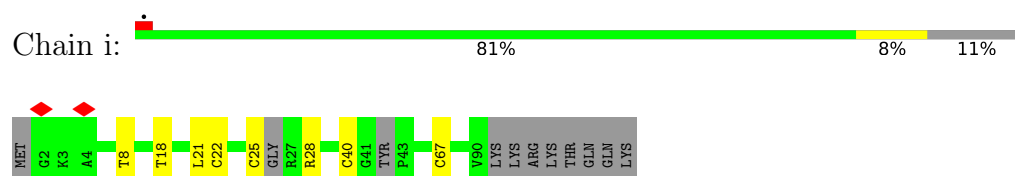
- Molecule 36: Ribosomal protein uL29



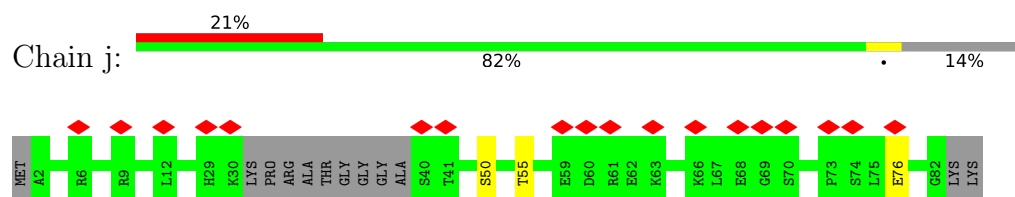
- Molecule 37: Ribosomal protein eL36



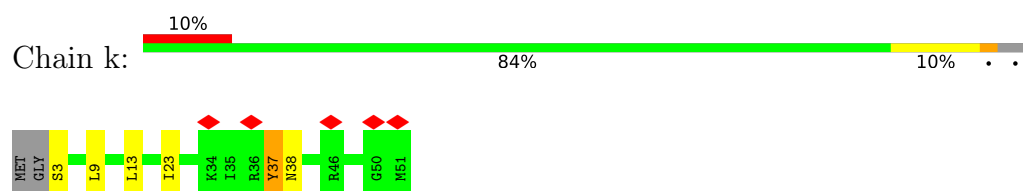
- Molecule 38: Ribosomal protein eL37



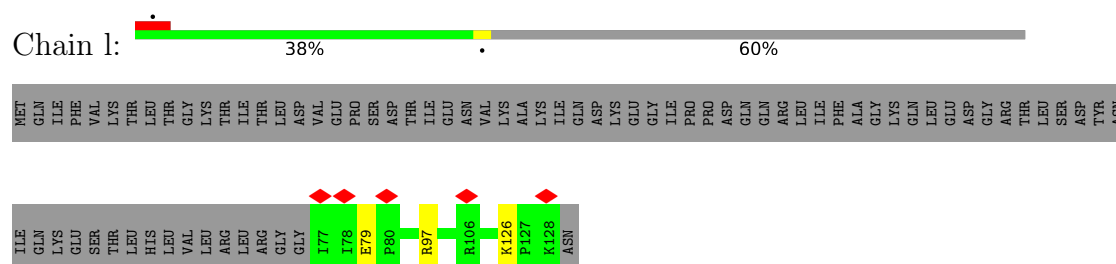
- Molecule 39: Ribosomal protein eL38



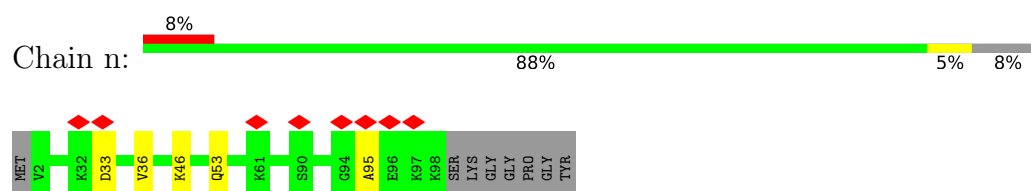
- Molecule 40: Ribosomal protein eL39



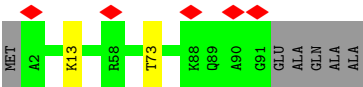
- Molecule 41: Ribosomal protein eL40



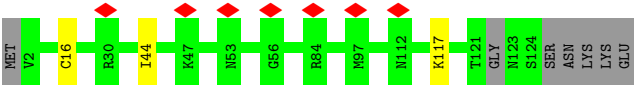
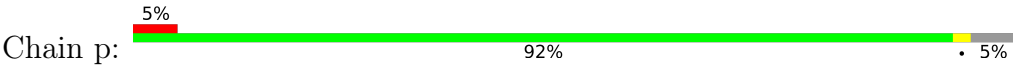
- Molecule 42: Ribosomal protein eL42



- Molecule 43: Ribosomal protein eL43



• Molecule 44: Ribosomal protein eL28



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	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	0.354	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1	0.22	0/73347	0.68	0/114257
2	3	0.20	0/2813	0.66	0/4379
3	4	0.23	0/3731	0.67	0/5808
4	A	0.33	0/1918	0.61	0/2572
5	B	0.37	0/3006	0.58	0/4023
6	C	0.35	0/3104	0.59	0/4164
7	D	0.35	0/2158	0.56	0/2891
8	E	0.35	0/981	0.54	0/1311
9	F	0.36	0/2102	0.55	0/2811
10	G	0.37	0/1905	0.57	0/2546
11	H	0.35	0/1500	0.53	0/2019
12	I	0.40	0/1570	0.62	0/2099
13	J	0.37	0/1366	0.54	0/1823
14	K	0.34	0/1621	0.60	0/2172
15	L	0.39	0/1077	0.63	0/1438
16	M	0.39	0/1715	0.65	0/2289
17	N	0.36	0/1671	0.59	0/2233
18	O	0.42	0/1308	0.66	0/1744
19	P	0.34	0/1498	0.62	0/1992
20	Q	0.34	0/1491	0.57	0/1970
21	R	0.37	0/1523	0.61	0/2043
22	S	0.40	0/1257	0.59	0/1685
23	T	0.39	0/840	0.59	0/1120
24	U	0.36	0/984	0.58	0/1326
25	V	0.37	0/547	0.59	0/728
26	W	0.36	0/1054	0.62	0/1420
27	X	0.38	0/1026	0.63	0/1367
28	Y	0.40	0/1182	0.59	0/1573
29	Z	0.48	0/1161	0.72	0/1549
30	a	0.30	0/408	0.59	0/531
31	b	0.39	0/732	0.56	0/980
32	c	0.38	0/925	0.65	0/1239
33	d	0.36	0/1029	0.71	0/1370
34	e	0.35	0/872	0.60	0/1170



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	f	0.37	0/881	0.68	0/1183
36	g	0.37	0/987	0.62	0/1306
37	h	0.37	0/779	0.66	0/1033
38	i	0.47	0/700	0.79	0/923
39	j	0.37	0/599	0.55	0/800
40	k	0.47	0/428	0.77	0/566
41	l	0.42	0/426	0.64	0/566
42	n	0.33	0/802	0.54	0/1057
43	o	0.36	0/693	0.60	0/923
44	p	0.34	0/984	0.60	0/1307
All	All	0.29	0/130701	0.66	0/192306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	
4	A	244/260 (94%)	228 (93%)	15 (6%)	1 (0%)	30	62
5	B	351/389 (90%)	312 (89%)	33 (9%)	6 (2%)	7	33
6	C	380/416 (91%)	345 (91%)	30 (8%)	5 (1%)	10	39
7	D	253/310 (82%)	225 (89%)	24 (10%)	4 (2%)	8	35
8	E	114/193 (59%)	101 (89%)	12 (10%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	246/258 (95%)	226 (92%)	19 (8%)	1 (0%)	30	62
10	G	225/276 (82%)	209 (93%)	12 (5%)	4 (2%)	7	32
11	H	185/190 (97%)	169 (91%)	16 (9%)	0	100	100
12	I	185/221 (84%)	168 (91%)	15 (8%)	2 (1%)	12	42
13	J	164/175 (94%)	145 (88%)	16 (10%)	3 (2%)	7	32
14	K	193/355 (54%)	167 (86%)	20 (10%)	6 (3%)	3	20
15	L	129/134 (96%)	118 (92%)	8 (6%)	3 (2%)	5	27
16	M	196/205 (96%)	180 (92%)	15 (8%)	1 (0%)	25	58
17	N	196/269 (73%)	187 (95%)	6 (3%)	3 (2%)	8	36
18	O	154/195 (79%)	140 (91%)	13 (8%)	1 (1%)	22	55
19	P	184/187 (98%)	172 (94%)	10 (5%)	2 (1%)	12	42
20	Q	174/187 (93%)	165 (95%)	7 (4%)	2 (1%)	12	42
21	R	180/183 (98%)	159 (88%)	16 (9%)	5 (3%)	4	22
22	S	152/157 (97%)	141 (93%)	6 (4%)	5 (3%)	3	18
23	T	95/133 (71%)	85 (90%)	7 (7%)	3 (3%)	3	19
24	U	127/139 (91%)	117 (92%)	10 (8%)	0	100	100
25	V	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
26	W	125/167 (75%)	107 (86%)	16 (13%)	2 (2%)	8	35
27	X	122/141 (86%)	111 (91%)	10 (8%)	1 (1%)	16	49
28	Y	140/146 (96%)	123 (88%)	11 (8%)	6 (4%)	2	14
29	Z	141/147 (96%)	126 (89%)	11 (8%)	4 (3%)	4	22
30	a	45/54 (83%)	42 (93%)	1 (2%)	2 (4%)	2	14
31	b	92/108 (85%)	83 (90%)	9 (10%)	0	100	100
32	c	103/120 (86%)	93 (90%)	7 (7%)	3 (3%)	3	21
33	d	120/134 (90%)	111 (92%)	6 (5%)	3 (2%)	4	25
34	e	101/112 (90%)	94 (93%)	6 (6%)	1 (1%)	13	45
35	f	105/134 (78%)	98 (93%)	6 (6%)	1 (1%)	13	45
36	g	119/123 (97%)	113 (95%)	4 (3%)	2 (2%)	7	33
37	h	93/101 (92%)	89 (96%)	2 (2%)	2 (2%)	5	27
38	i	81/98 (83%)	77 (95%)	3 (4%)	1 (1%)	11	41
39	j	68/84 (81%)	63 (93%)	4 (6%)	1 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	47/51 (92%)	45 (96%)	1 (2%)	1 (2%)	5	29
41	l	50/129 (39%)	48 (96%)	1 (2%)	1 (2%)	6	29
42	n	95/105 (90%)	86 (90%)	7 (7%)	2 (2%)	5	29
43	o	88/96 (92%)	82 (93%)	5 (6%)	1 (1%)	12	42
44	p	118/129 (92%)	107 (91%)	10 (8%)	1 (1%)	16	49
All	All	6041/7166 (84%)	5517 (91%)	431 (7%)	93 (2%)	11	36

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	5	LYS
6	C	191	ARG
7	D	156	ASN
14	K	60	PRO
20	Q	130	GLN

### 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	
4	A	190/200 (95%)	181 (95%)	9 (5%)	22	52
5	B	315/330 (96%)	298 (95%)	17 (5%)	18	48
6	C	313/326 (96%)	302 (96%)	11 (4%)	31	60
7	D	218/253 (86%)	213 (98%)	5 (2%)	45	70
8	E	110/163 (68%)	106 (96%)	4 (4%)	30	59
9	F	216/223 (97%)	206 (95%)	10 (5%)	23	53
10	G	204/233 (88%)	198 (97%)	6 (3%)	37	65
11	H	167/169 (99%)	159 (95%)	8 (5%)	21	52
12	I	159/180 (88%)	153 (96%)	6 (4%)	28	58
13	J	141/151 (93%)	136 (96%)	5 (4%)	31	60
14	K	170/303 (56%)	163 (96%)	7 (4%)	26	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	116/118 (98%)	109 (94%)	7 (6%)	16	44
16	M	171/176 (97%)	159 (93%)	12 (7%)	12	39
17	N	178/240 (74%)	172 (97%)	6 (3%)	32	61
18	O	139/168 (83%)	129 (93%)	10 (7%)	12	38
19	P	154/155 (99%)	146 (95%)	8 (5%)	19	49
20	Q	154/162 (95%)	153 (99%)	1 (1%)	84	92
21	R	162/163 (99%)	152 (94%)	10 (6%)	15	44
22	S	134/137 (98%)	128 (96%)	6 (4%)	23	53
23	T	93/111 (84%)	86 (92%)	7 (8%)	11	37
24	U	100/105 (95%)	96 (96%)	4 (4%)	27	56
25	V	56/131 (43%)	54 (96%)	2 (4%)	30	59
26	W	116/139 (84%)	110 (95%)	6 (5%)	19	49
27	X	113/128 (88%)	106 (94%)	7 (6%)	15	44
28	Y	128/130 (98%)	119 (93%)	9 (7%)	12	39
29	Z	116/118 (98%)	110 (95%)	6 (5%)	19	49
30	a	44/48 (92%)	43 (98%)	1 (2%)	45	70
31	b	80/89 (90%)	74 (92%)	6 (8%)	11	37
32	c	99/110 (90%)	94 (95%)	5 (5%)	20	49
33	d	112/122 (92%)	104 (93%)	8 (7%)	12	38
34	e	91/97 (94%)	85 (93%)	6 (7%)	14	41
35	f	91/115 (79%)	84 (92%)	7 (8%)	10	36
36	g	103/105 (98%)	96 (93%)	7 (7%)	13	40
37	h	79/82 (96%)	78 (99%)	1 (1%)	65	82
38	i	69/79 (87%)	62 (90%)	7 (10%)	6	23
39	j	66/73 (90%)	64 (97%)	2 (3%)	36	64
40	k	44/45 (98%)	38 (86%)	6 (14%)	3	14
41	l	47/116 (40%)	45 (96%)	2 (4%)	25	54
42	n	88/93 (95%)	85 (97%)	3 (3%)	32	61
43	o	68/71 (96%)	67 (98%)	1 (2%)	60	79
44	p	108/114 (95%)	106 (98%)	2 (2%)	52	74
All	All	5322/6071 (88%)	5069 (95%)	253 (5%)	24	52

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	47	LEU
35	f	54	ILE
22	S	67	VAL
35	f	41	ARG
38	i	67	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	147	GLN
29	Z	25	HIS
42	n	53	GLN
22	S	13	GLN
23	T	63	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3053/3477 (87%)	732 (23%)	91 (2%)
2	3	115/124 (92%)	21 (18%)	1 (0%)
3	4	155/158 (98%)	35 (22%)	2 (1%)
All	All	3323/3759 (88%)	788 (23%)	94 (2%)

5 of 788 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	31	C
1	1	40	A
1	1	43	A
1	1	49	U

5 of 94 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2224	G
1	1	2806	A
1	1	2258	A
1	1	2663	U

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Mol	Chain	Res	Type
1	1	3167	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 oligosaccharides 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](#)

There are no chain breaks in this entry.

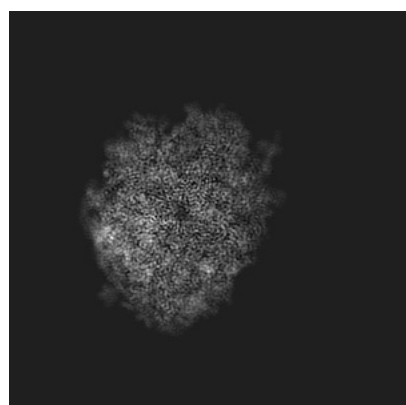
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6778. These allow visual inspection of the internal detail of the map and identification of artifacts.

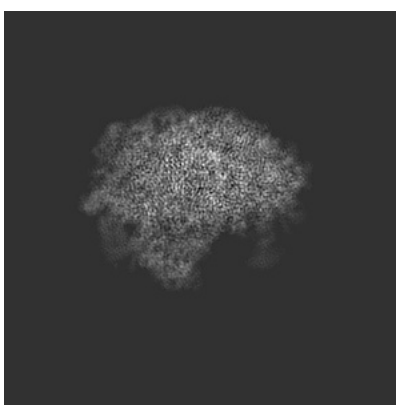
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

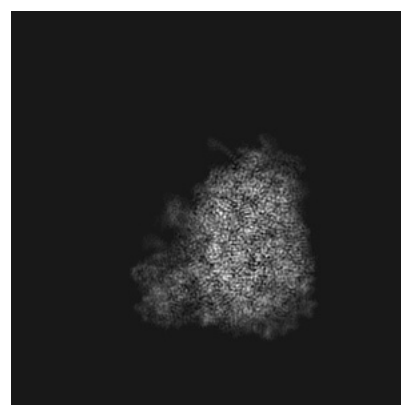
#### 6.1.1 Primary map



X



Y

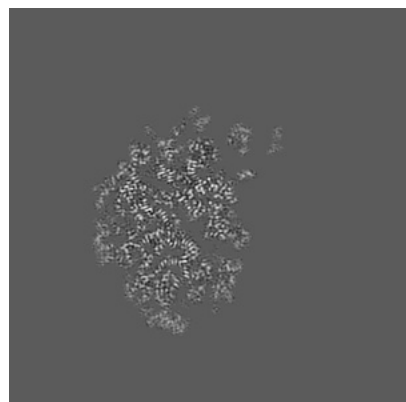


Z

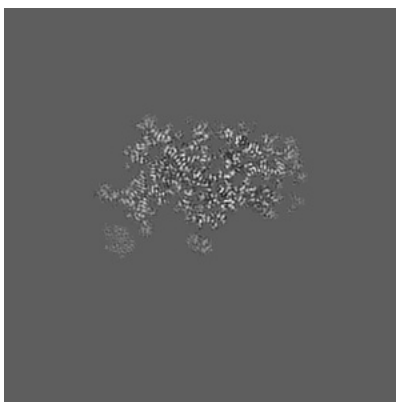
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 160



Y Index: 160

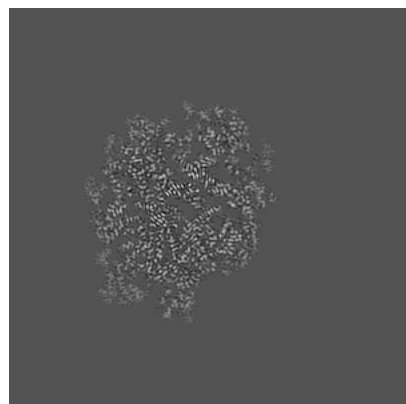


Z Index: 160

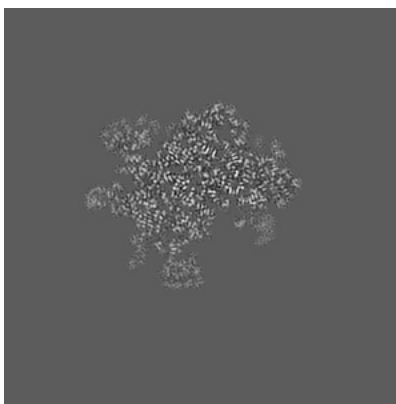
The images above show central slices of the map in three orthogonal directions.

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

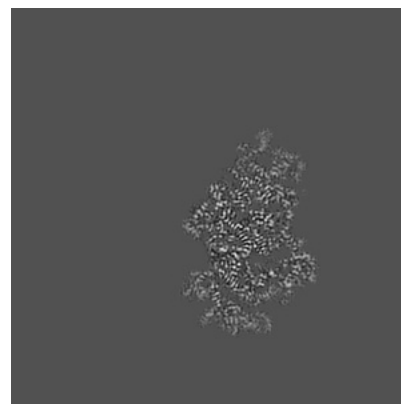
### 6.3.1 Primary map



X Index: 187



Y Index: 111

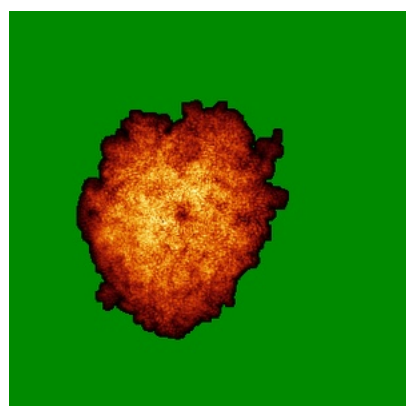


Z Index: 171

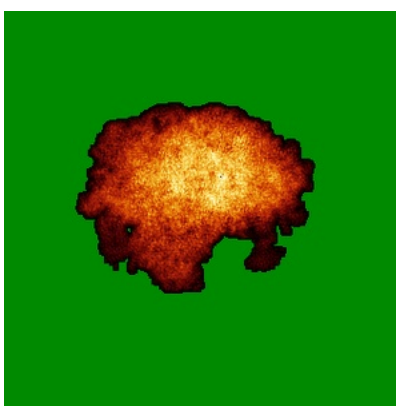
The images above show the largest variance slices of the map in three orthogonal directions.

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

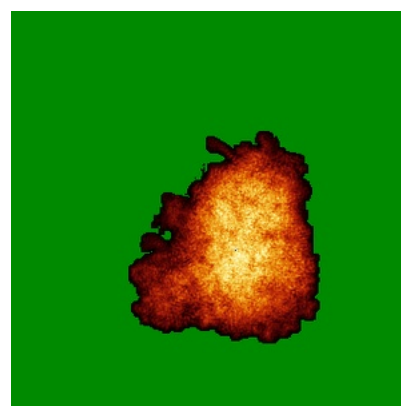
### 6.4.1 Primary map



X



Y



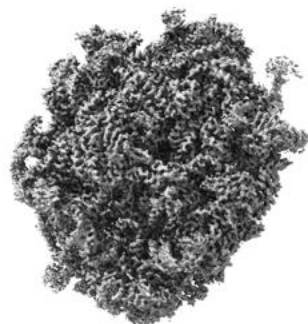
Z

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



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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

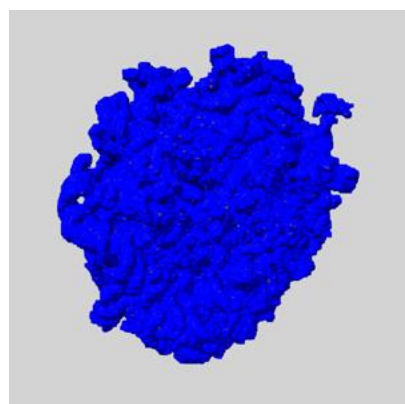
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

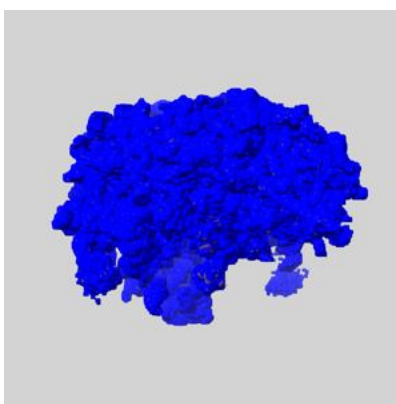
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

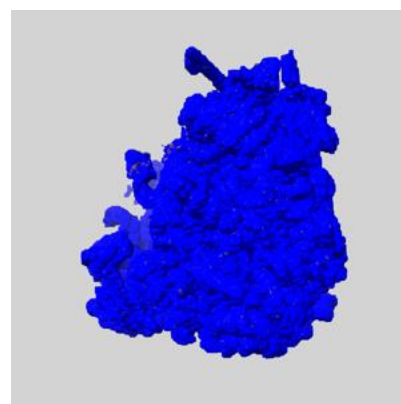
### 6.6.1 emd\_6778\_msk\_1.map [i](#)



X



Y

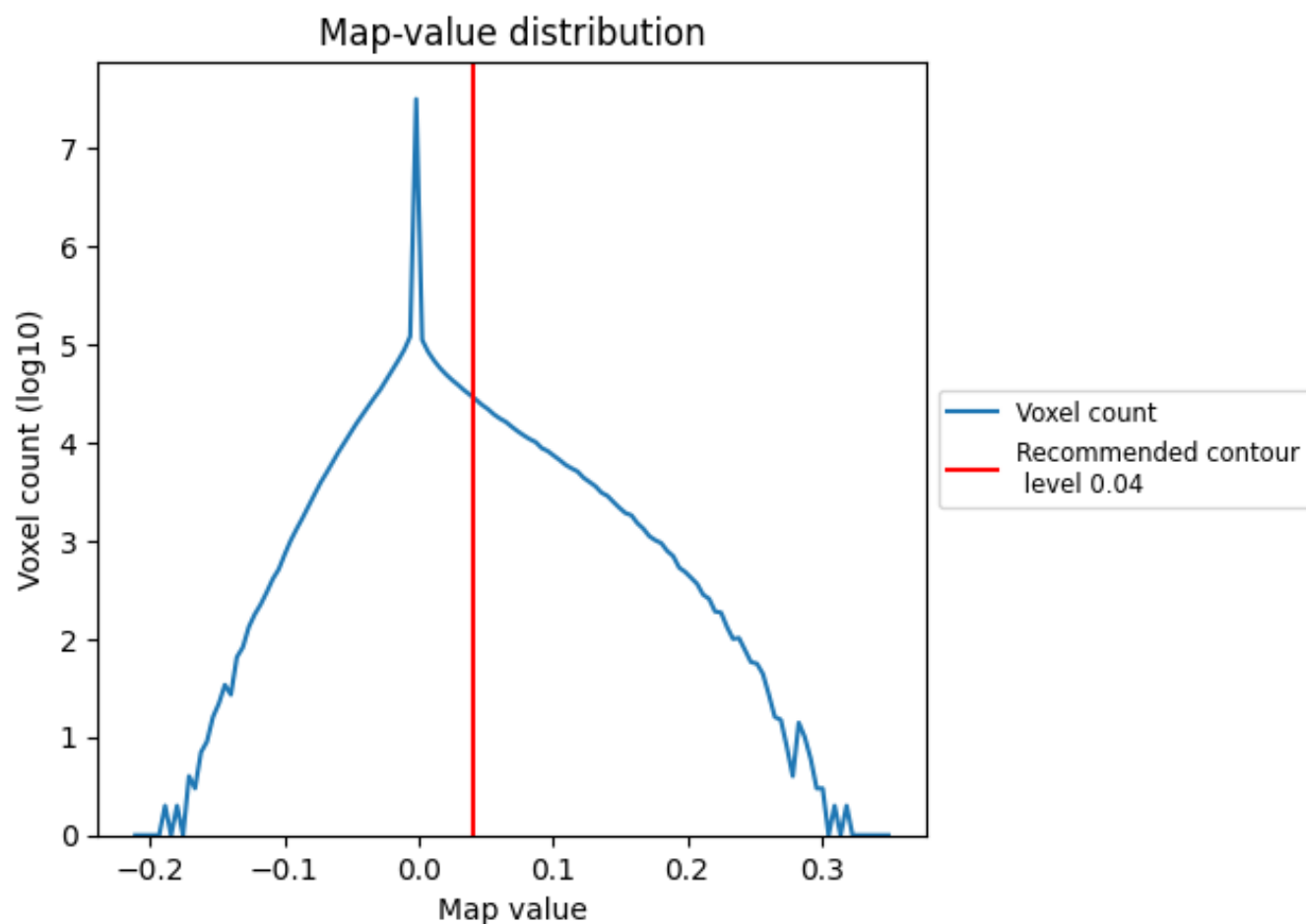


Z

## 7 Map analysis [i](#)

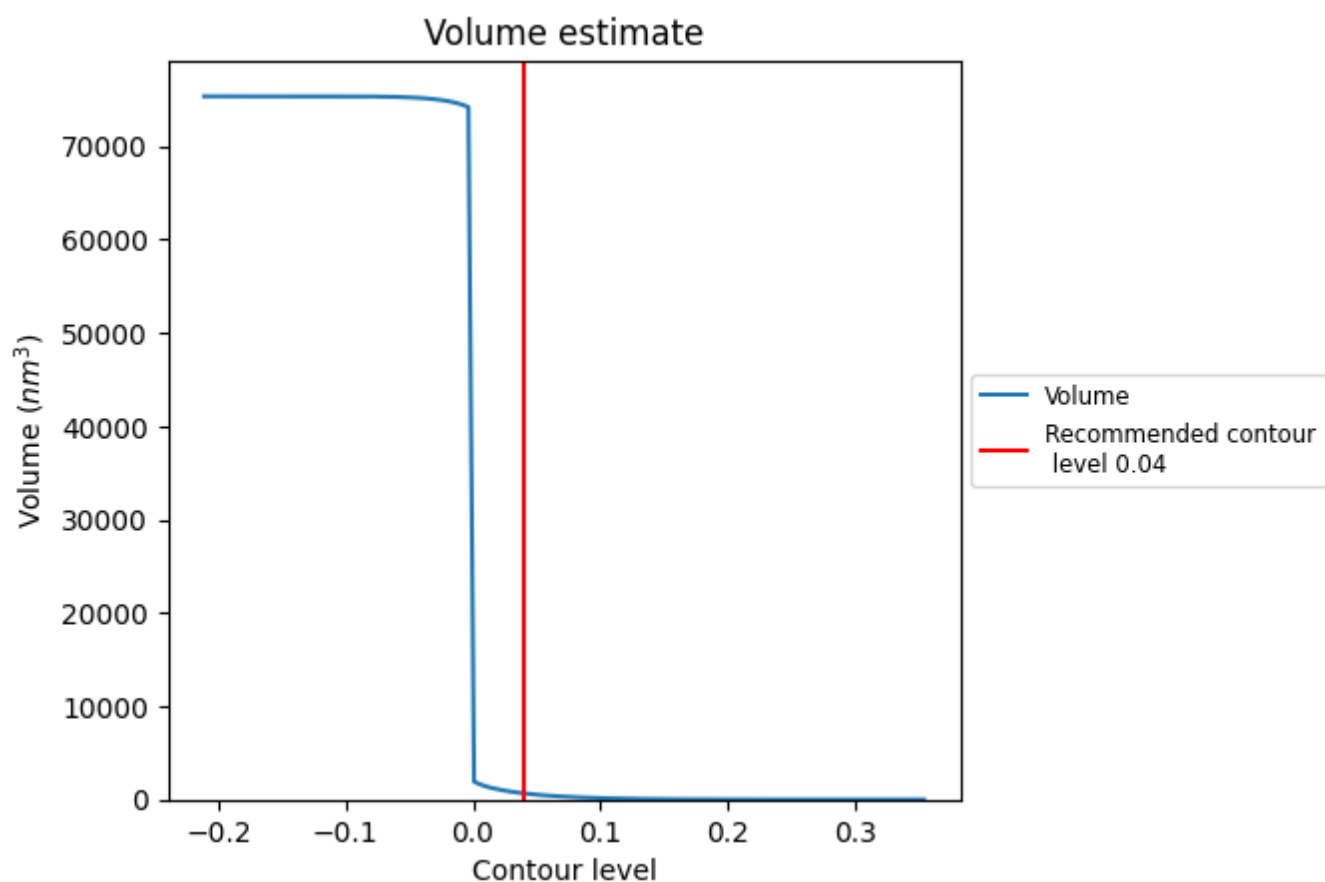
This section contains the results of statistical analysis of the map.

### 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.

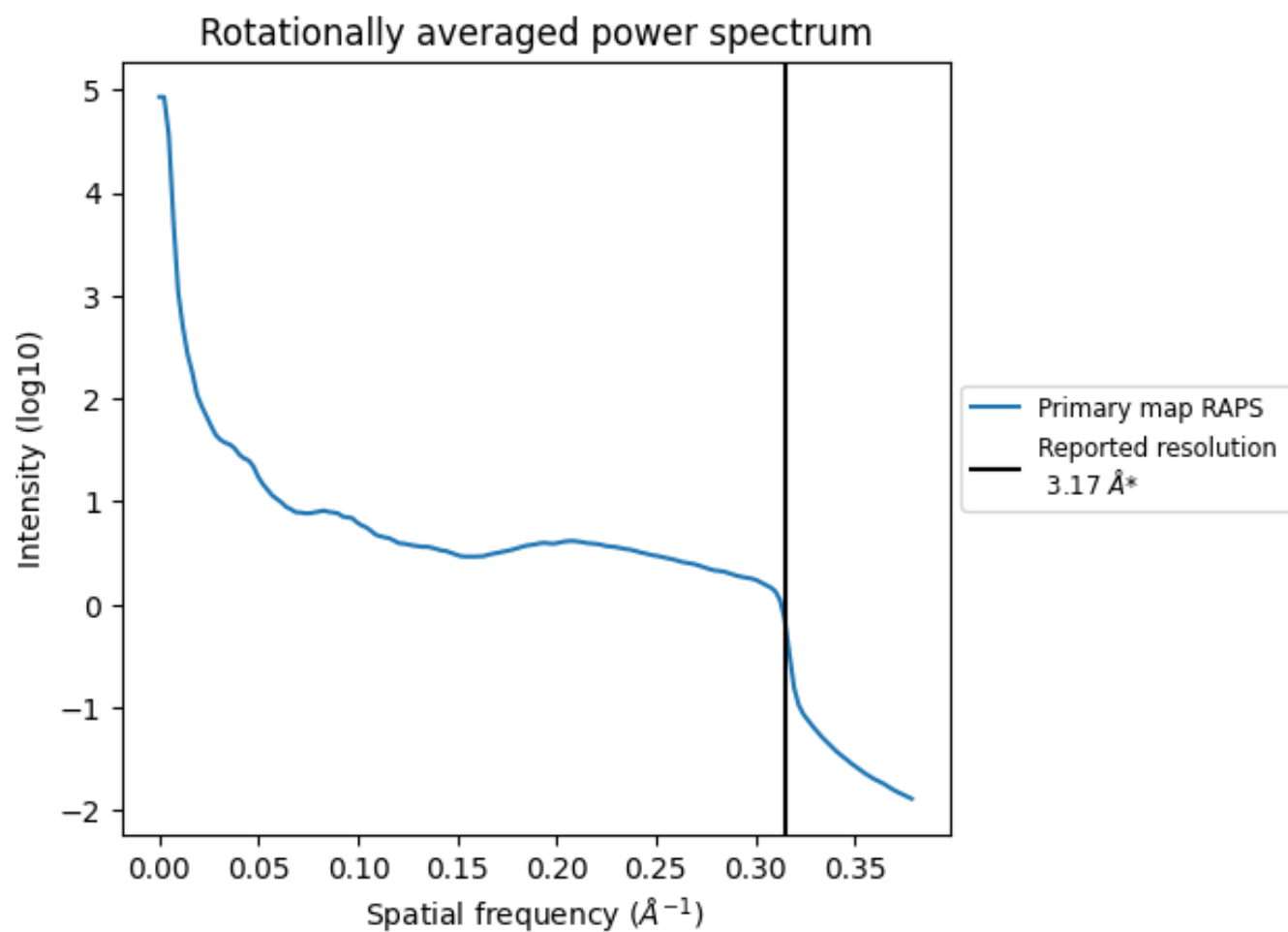
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 664 nm<sup>3</sup>; this corresponds to an approximate mass of 600 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 ⓘ

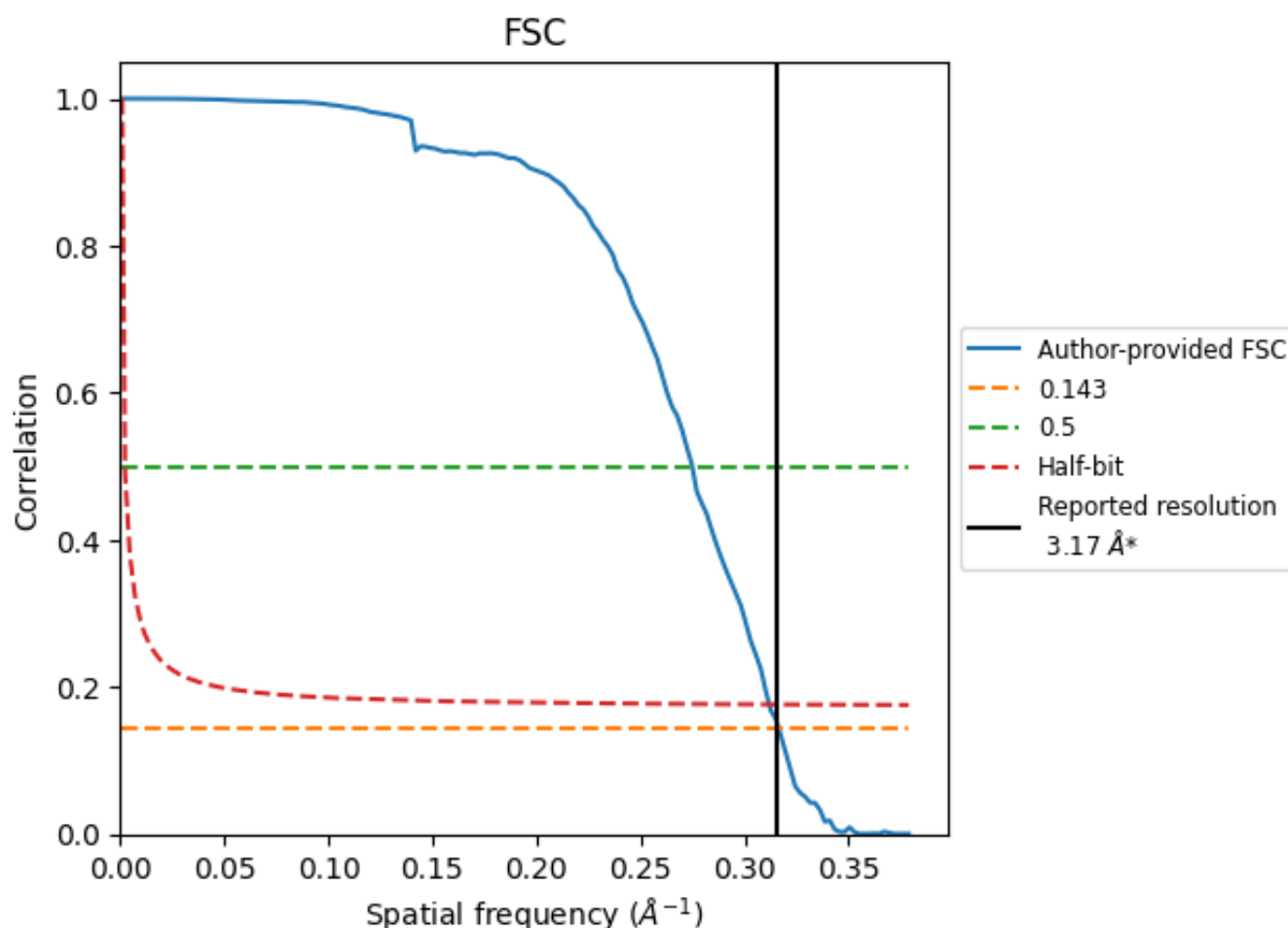


\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

## 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 0.315 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

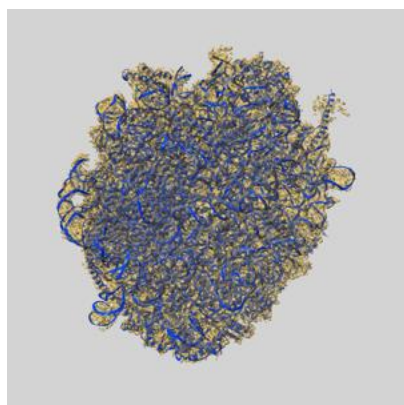
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.16	3.64	3.21
Unmasked-calculated*	-	-	-

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

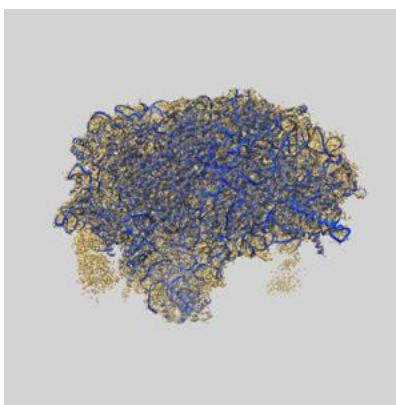
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6778 and PDB model 5XXB. Per-residue inclusion information can be found in section [3](#) on page [12](#).

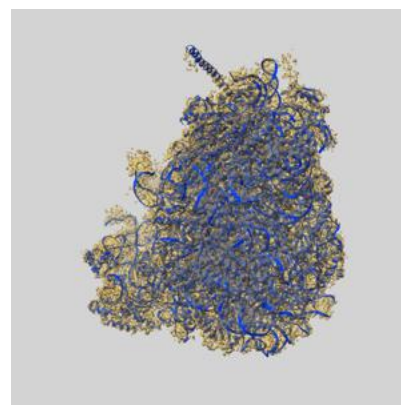
### 9.1 Map-model overlay [i](#)



X



Y

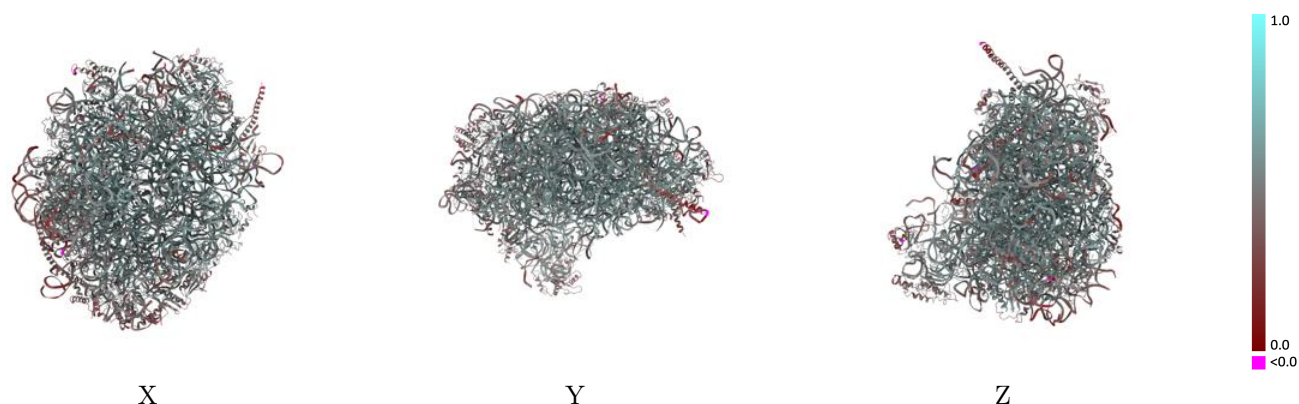


Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

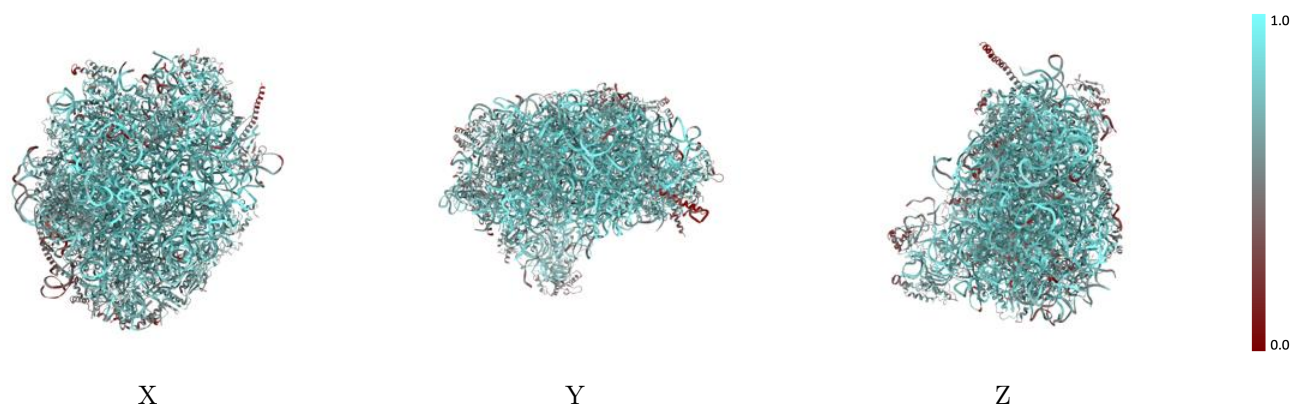


## 9.2 Q-score mapped to coordinate model [i](#)



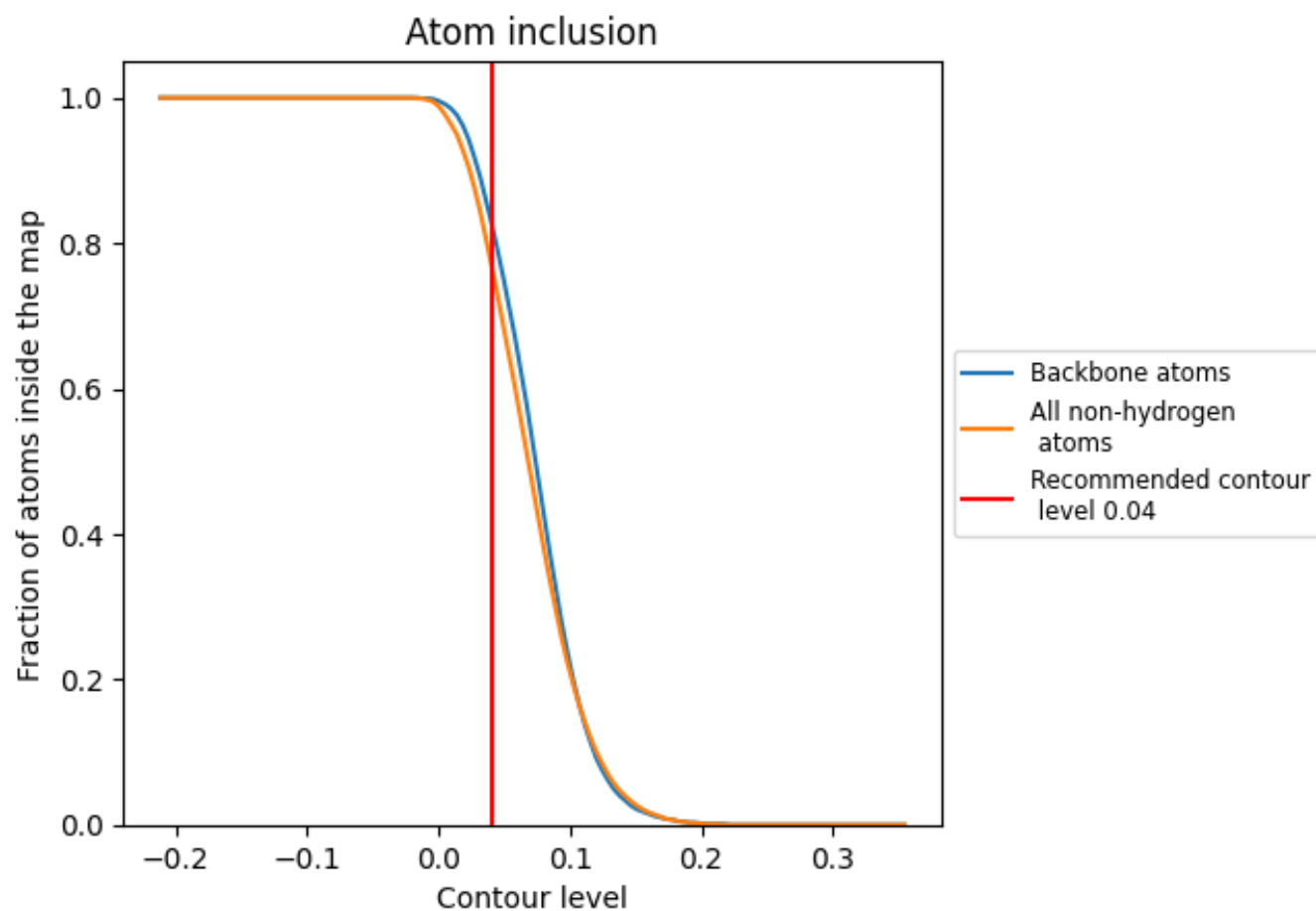
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5070
1	 0.8450	 0.5240
3	 0.8350	 0.4940
4	 0.8480	 0.5300
A	 0.7680	 0.5420
B	 0.7140	 0.5060
C	 0.6490	 0.4720
D	 0.5930	 0.4270
E	 0.5770	 0.4330
F	 0.6460	 0.4740
G	 0.6260	 0.4550
H	 0.6130	 0.4500
I	 0.6260	 0.4630
J	 0.4530	 0.3490
K	 0.7050	 0.4850
L	 0.6380	 0.4410
M	 0.7980	 0.5520
N	 0.6840	 0.5000
O	 0.7190	 0.5180
P	 0.7030	 0.5080
Q	 0.6200	 0.4670
R	 0.6760	 0.4990
S	 0.6710	 0.4930
T	 0.4880	 0.4010
U	 0.6650	 0.5060
V	 0.6580	 0.4900
W	 0.6940	 0.4930
X	 0.6930	 0.4980
Y	 0.6560	 0.4730
Z	 0.7840	 0.5380
a	 0.6990	 0.5310
b	 0.6050	 0.4520
c	 0.6990	 0.4980
d	 0.7250	 0.5210
e	 0.7640	 0.5270



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Chain	Atom inclusion	Q-score
f	 0.7420	 0.5120
g	 0.6680	 0.4930
h	 0.6370	 0.4530
i	 0.8110	 0.5500
j	 0.5380	 0.4240
k	 0.7690	 0.5400
l	 0.6730	 0.4910
n	 0.6530	 0.4910
o	 0.7120	 0.5210
p	 0.6550	 0.4710