



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 07:48 pm GMT

PDB ID : 7BL2
EMDB ID : EMD-12215
Title : pre-50S-ObgE particle state 1
Authors : Hilal, T.; Nikolay, R.; Schmidt, S.; Spahn, C.M.T.
Deposited on : 2021-01-18
Resolution : 3.70 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

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

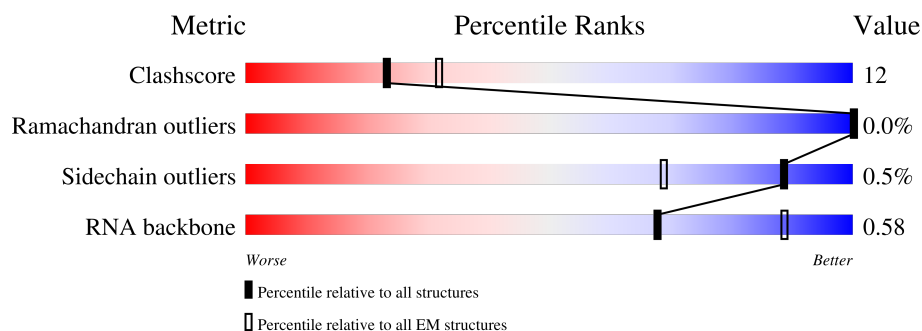
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2919	<div> <div>15%</div> <div>46%</div> <div>46%</div> <div>7%</div> <div>.</div> </div>
2	B	120	<div> <div>50%</div> <div>42%</div> <div>51%</div> <div>7%</div> <div>.</div> </div>
3	9P1	390	<div> <div>61%</div> <div>61%</div> <div>26%</div> <div>13%</div> </div>
4	C	273	<div> <div>19%</div> <div>64%</div> <div>35%</div> <div>.</div> </div>
5	D	209	<div> <div>17%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>
6	E	201	<div> <div>37%</div> <div>74%</div> <div>26%</div> </div>
7	G	177	<div> <div>64%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	J	142	
9	L	144	
10	N	127	
11	O	117	
12	Q	118	
13	R	103	
14	S	110	
15	T	100	
16	U	104	
17	V	94	
18	W	85	
19	X	78	
20	Y	63	
21	Z	59	
22	0	57	
23	1	55	
24	2	46	
25	I	142	
26	K	123	
27	P	115	
28	6	105	
29	H	149	
30	F	179	
31	b	70	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92831 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2902	Total	C	N	O	P	0	0
			62301	27793	11465	20141	2902		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 3 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9P1	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L20.

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

- Molecule 13 is a protein called 50S ribosomal protein L21.

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

- Molecule 14 is a protein called 50S ribosomal protein L22.

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

- Molecule 15 is a protein called 50S ribosomal protein L23.

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

- Molecule 16 is a protein called 50S ribosomal protein L24.

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

- Molecule 17 is a protein called 50S ribosomal protein L25.

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

- Molecule 18 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 19 is a protein called 50S ribosomal protein L28.

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

- Molecule 20 is a protein called 50S ribosomal protein L29.

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

- Molecule 21 is a protein called 50S ribosomal protein L30.

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

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L11.

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 28 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	Q	1	Total	Mg	0
			1	1	

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Zn	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	15	Total	O	0
			15	15	
34	B	1	Total	O	0
			1	1	
34	C	4	Total	O	0
			4	4	

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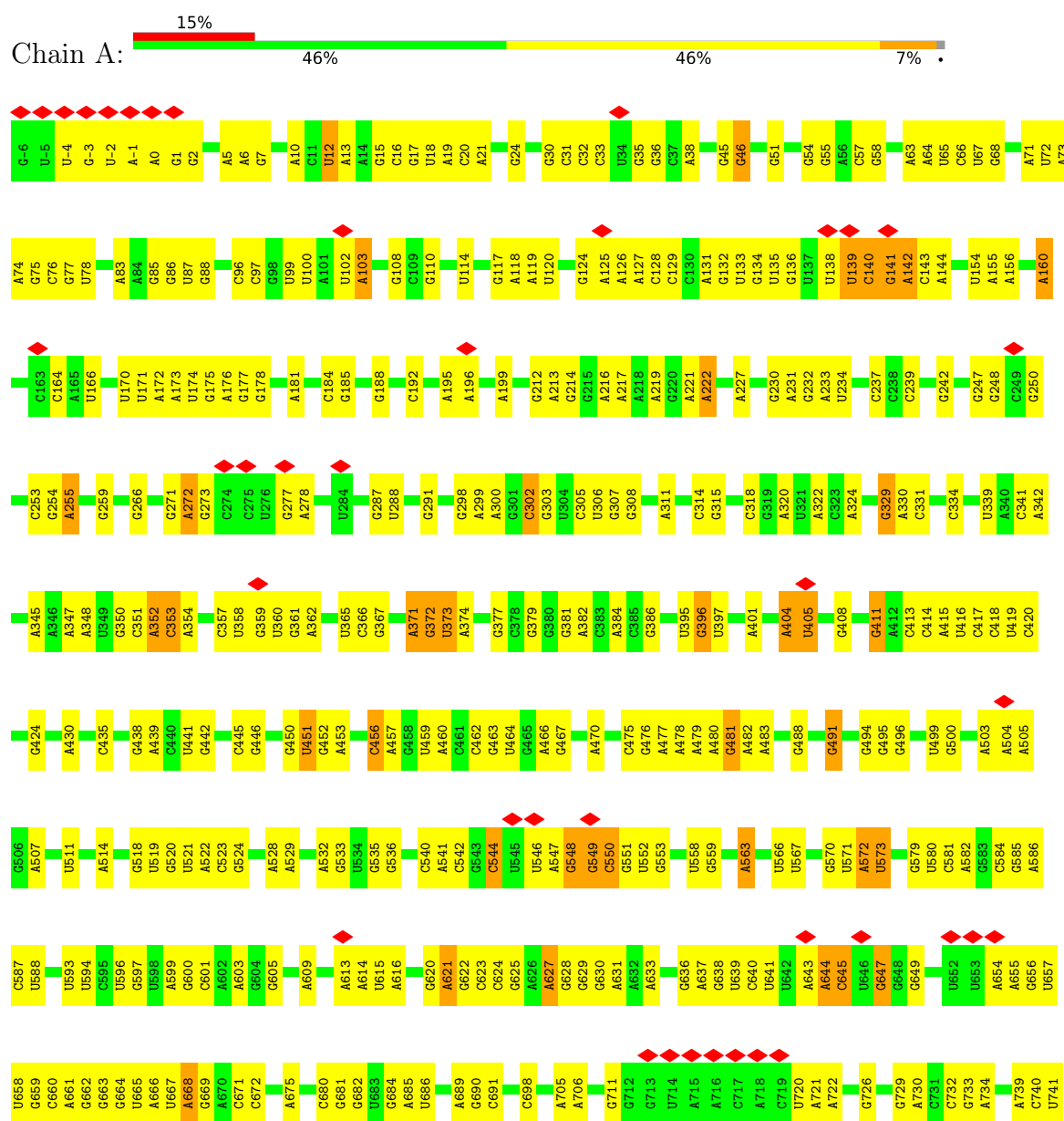
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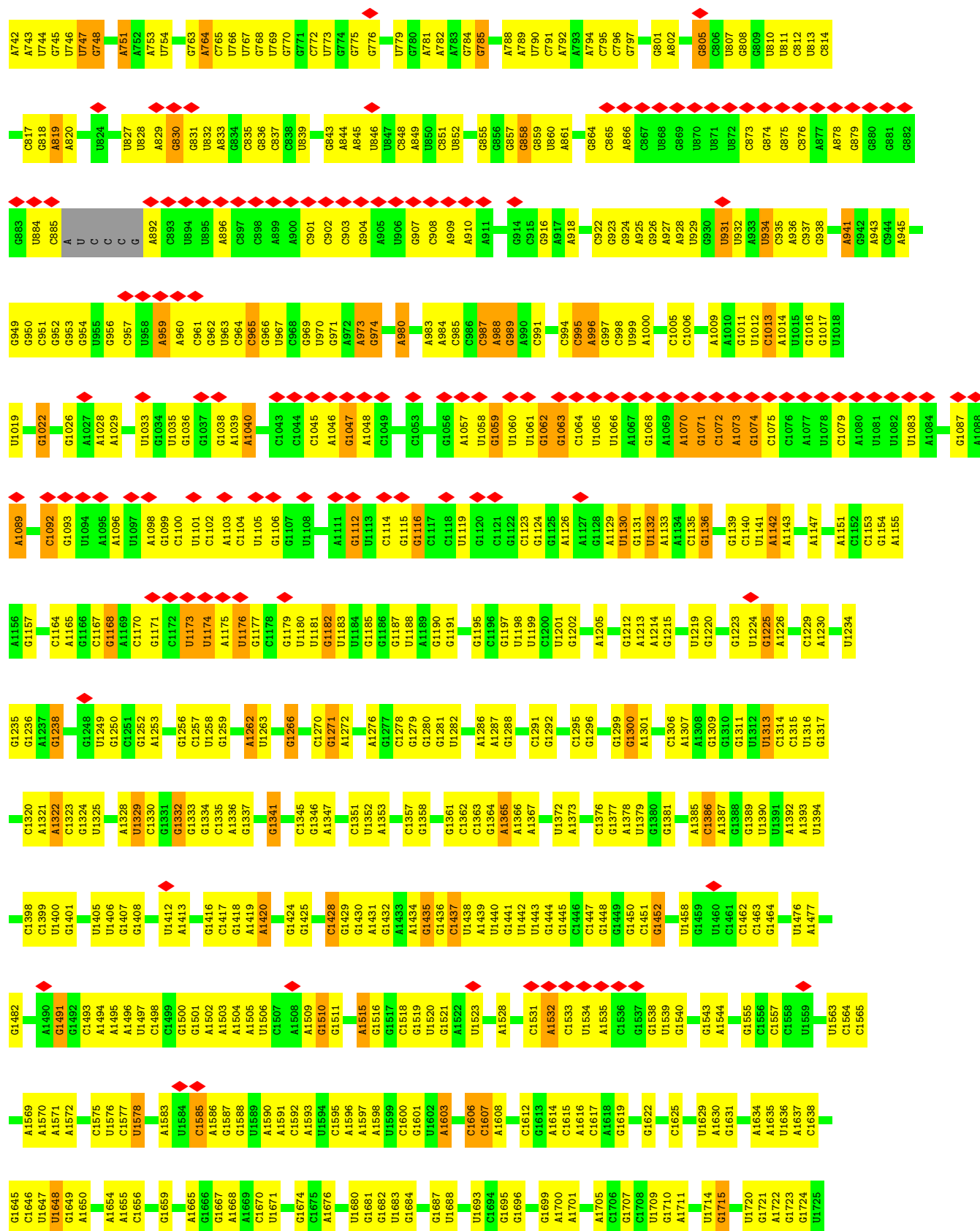
Mol	Chain	Residues	Atoms		AltConf
34	L	4	Total 4	O 4	0
34	N	2	Total 2	O 2	0
34	F	1	Total 1	O 1	0

3 Residue-property plots

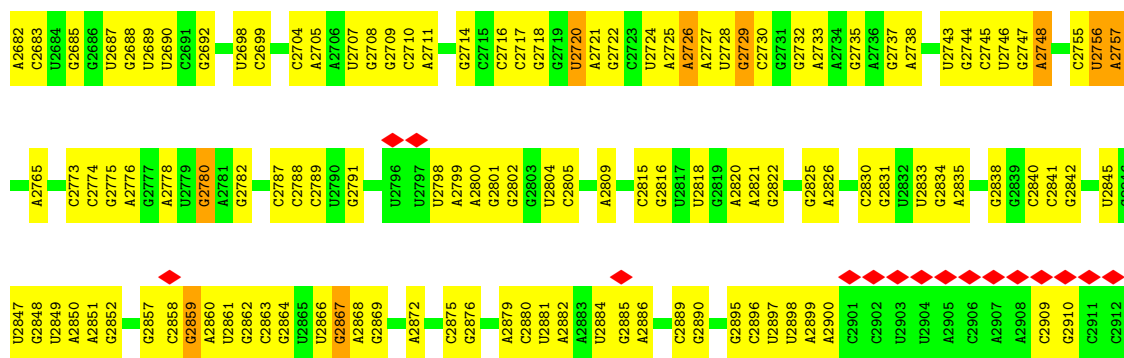
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

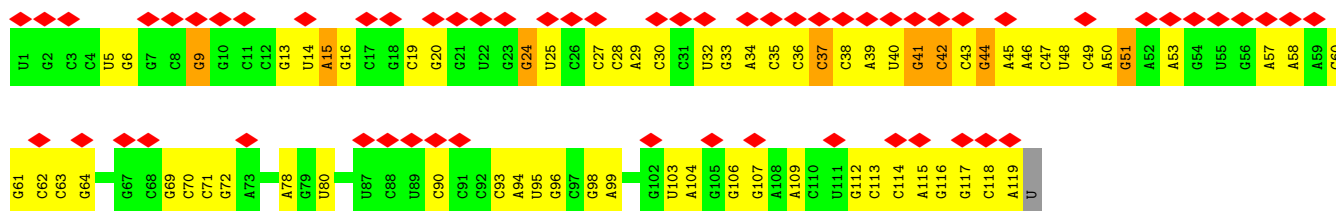




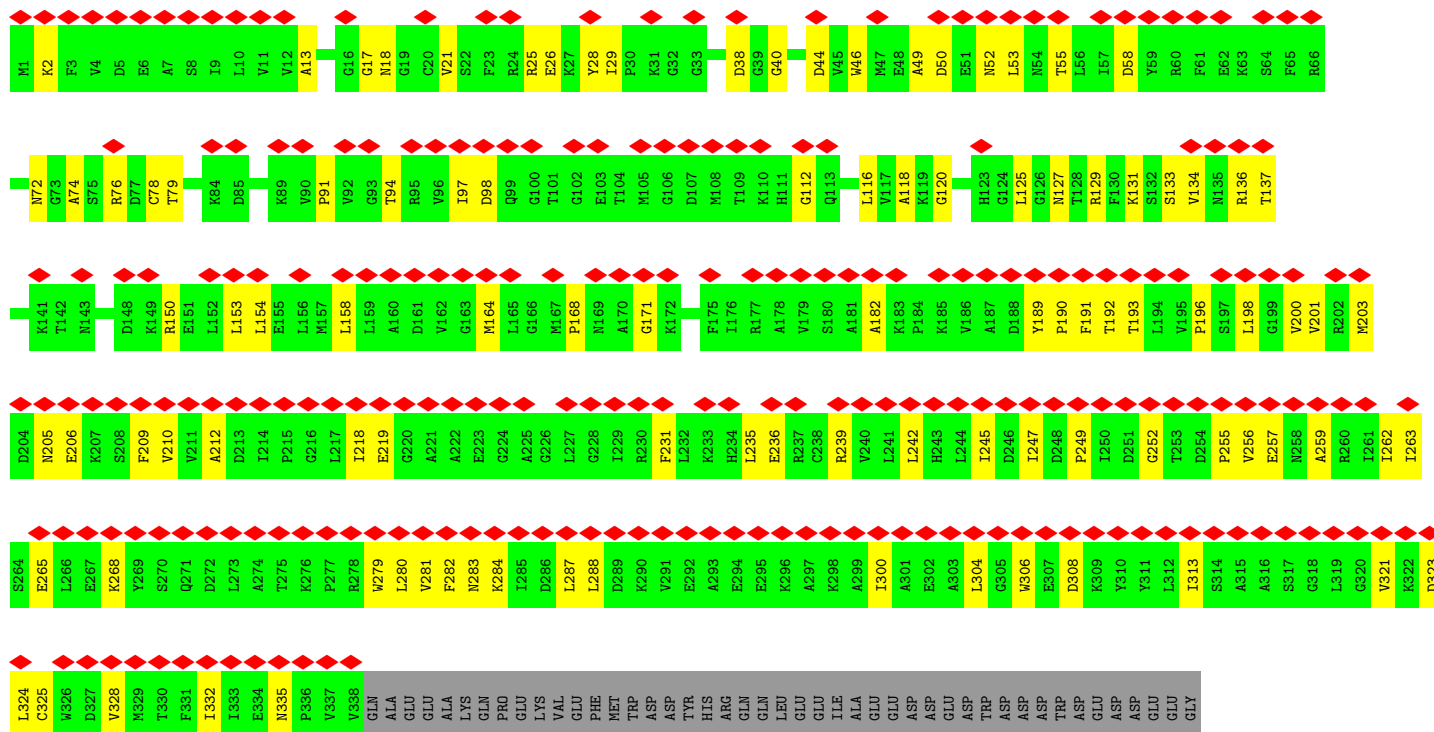




• Molecule 2: 5S ribosomal RNA

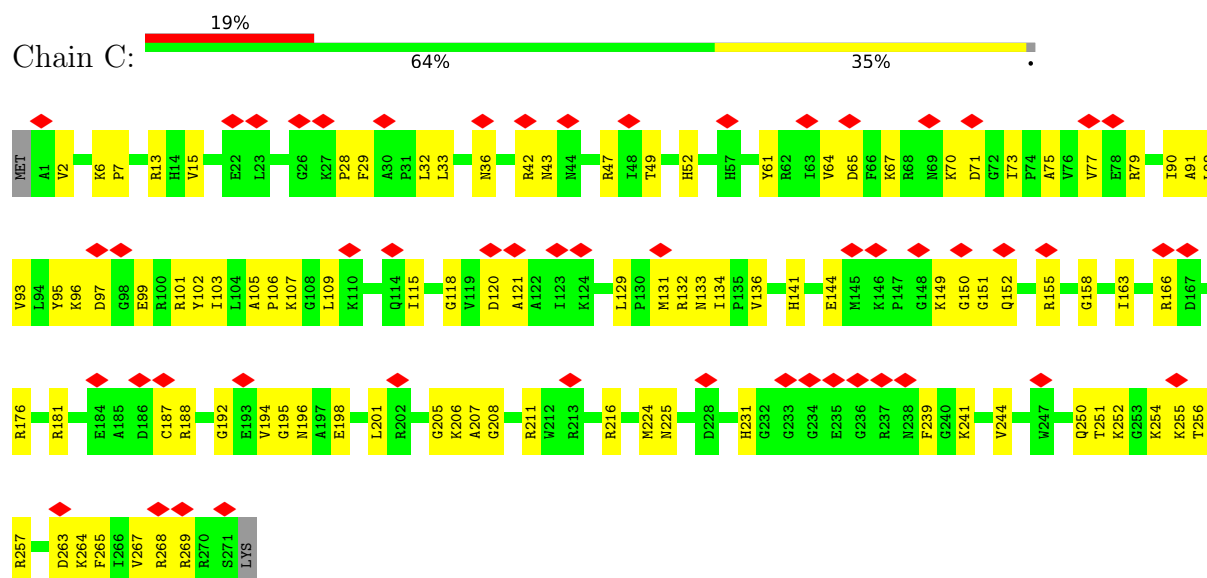


• Molecule 3: GTPase ObgE/CgtA

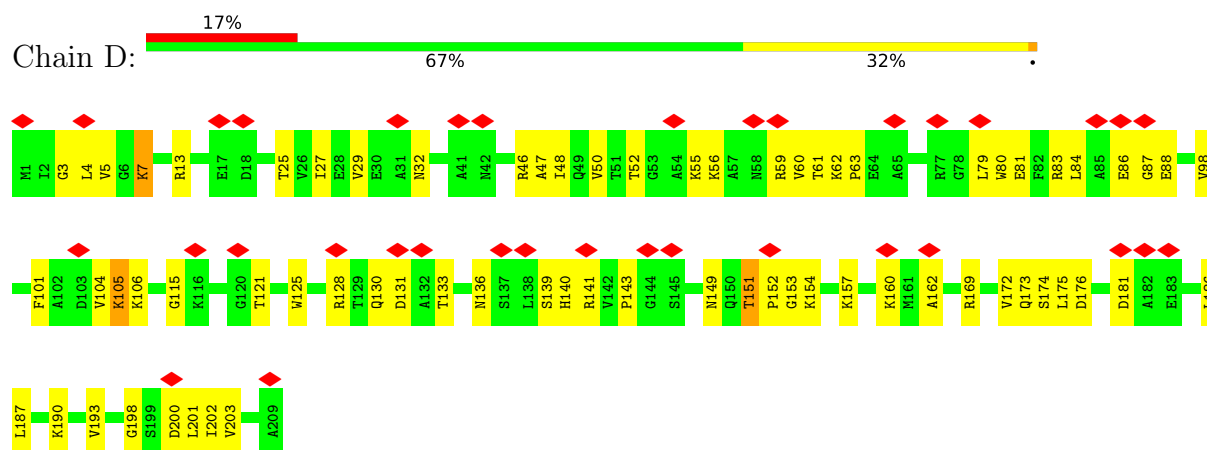


VAL
GLU
PHE
ILE
TYR
LYS
ARG

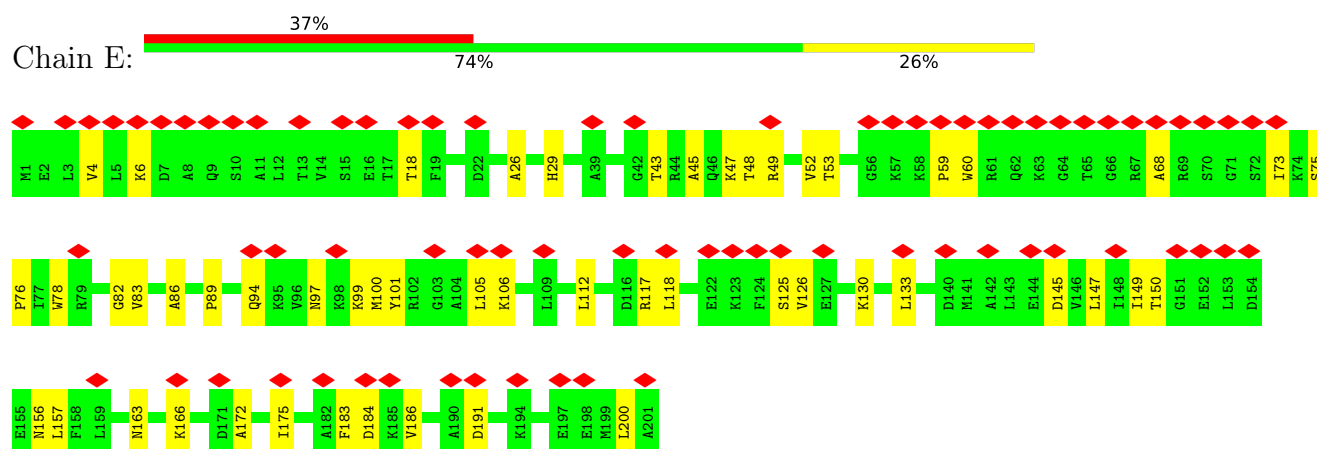
- Molecule 4: 50S ribosomal protein L2



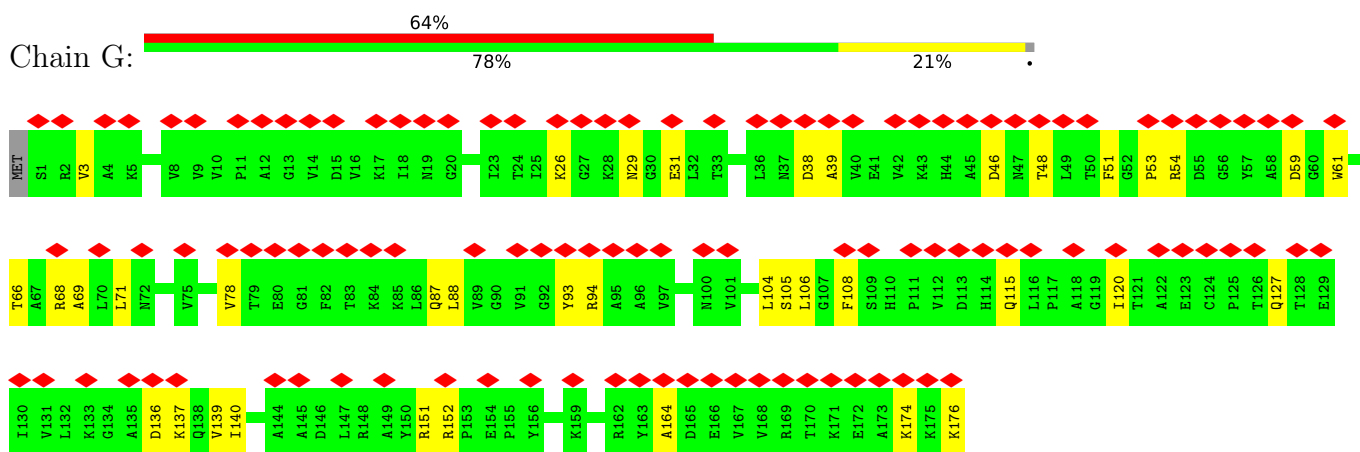
- Molecule 5: 50S ribosomal protein L3



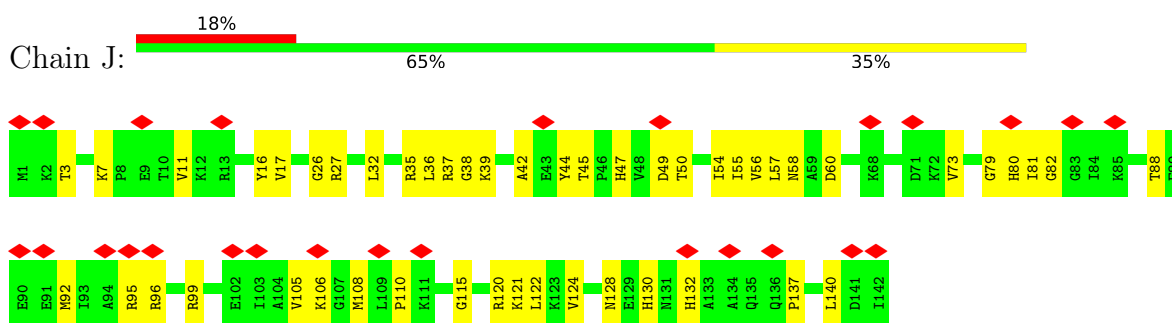
- Molecule 6: 50S ribosomal protein L4



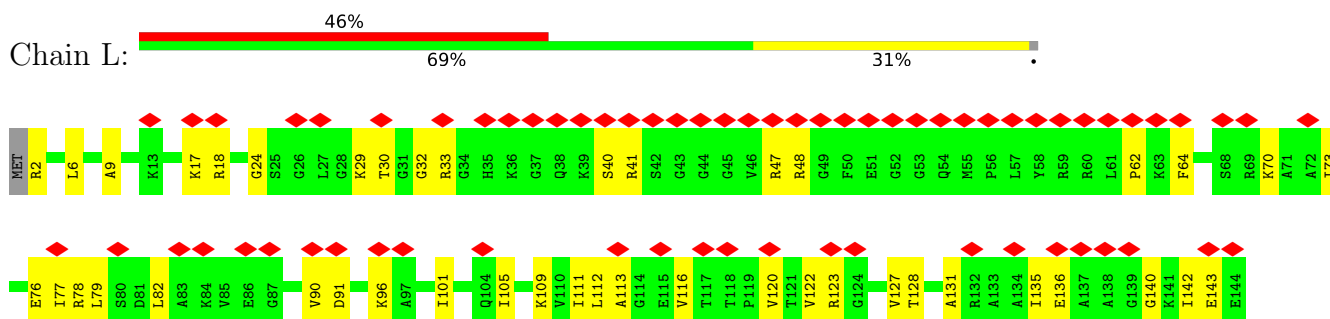
- Molecule 7: 50S ribosomal protein L6



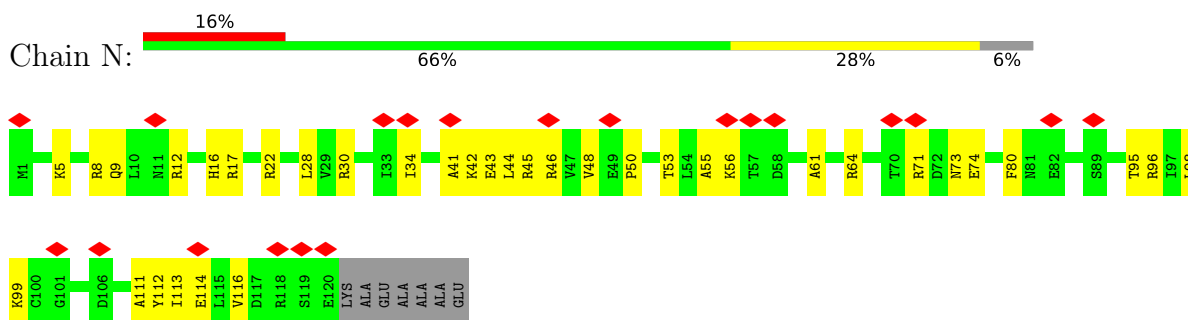
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L15

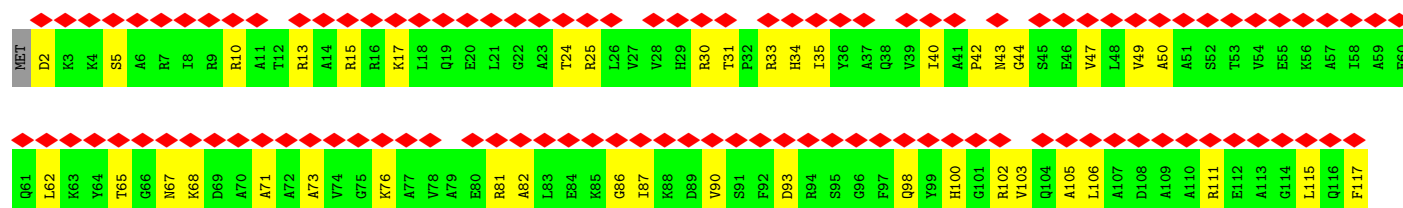


• Molecule 10: 50S ribosomal protein L17

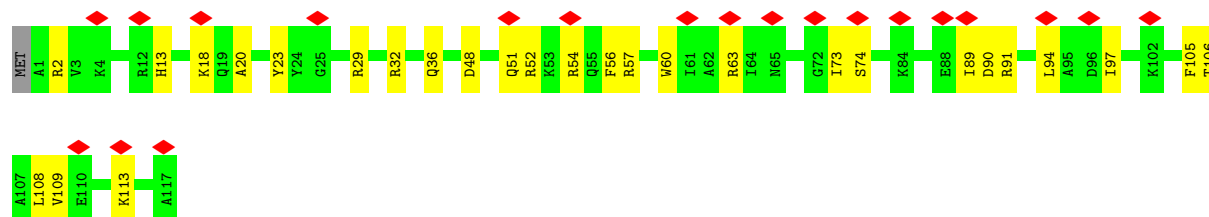
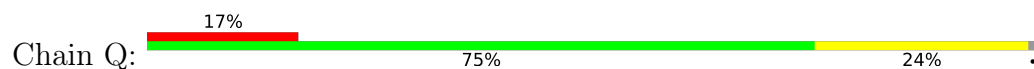


• Molecule 11: 50S ribosomal protein L18

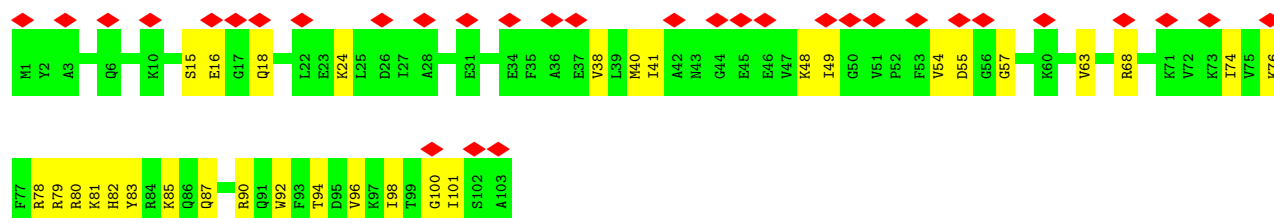




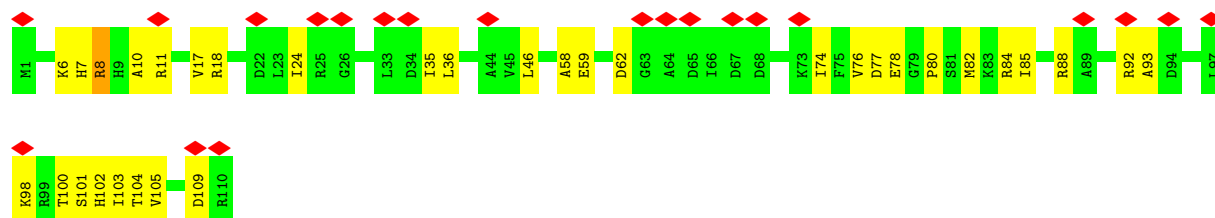
• Molecule 12: 50S ribosomal protein L20



• Molecule 13: 50S ribosomal protein L21

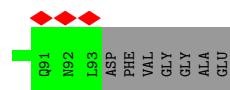


• Molecule 14: 50S ribosomal protein L22

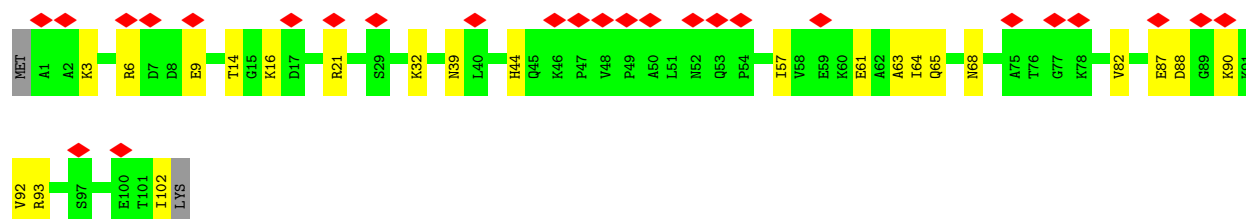
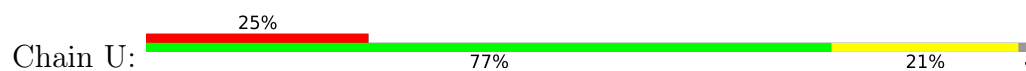


• Molecule 15: 50S ribosomal protein L23

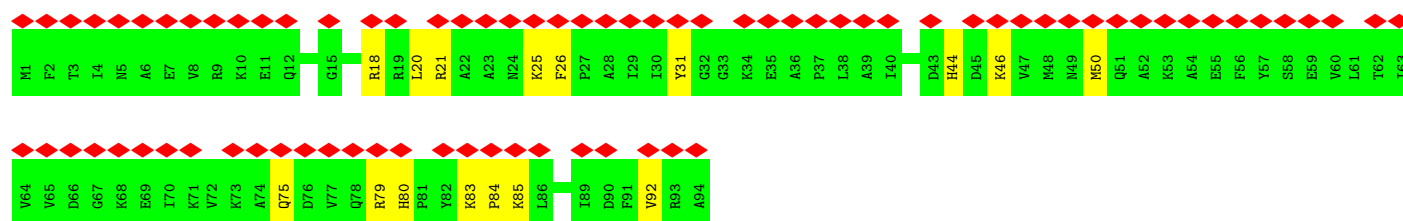
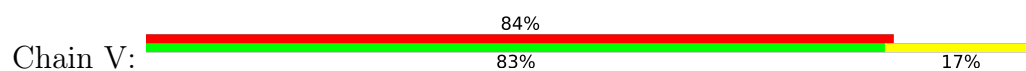




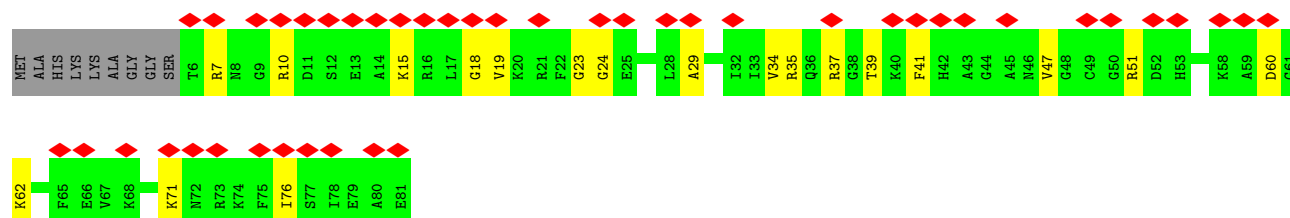
- Molecule 16: 50S ribosomal protein L24



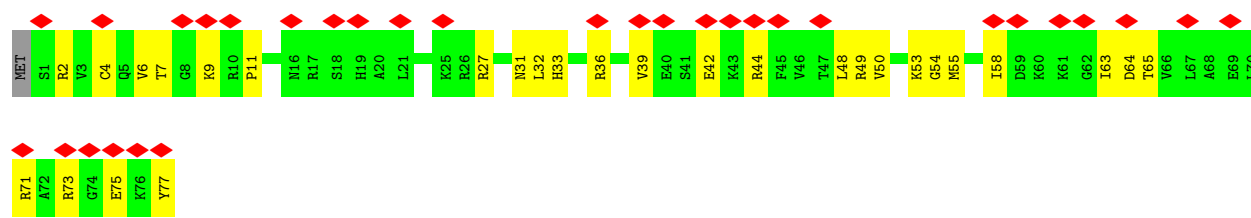
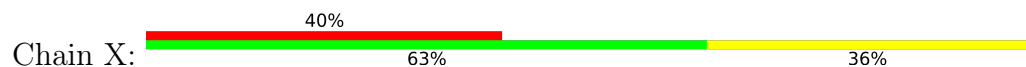
- Molecule 17: 50S ribosomal protein L25



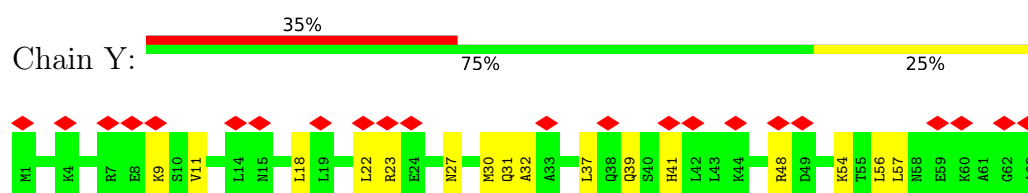
- Molecule 18: 50S ribosomal protein L27



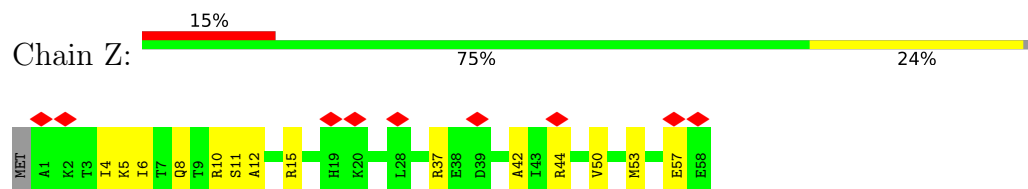
- Molecule 19: 50S ribosomal protein L28



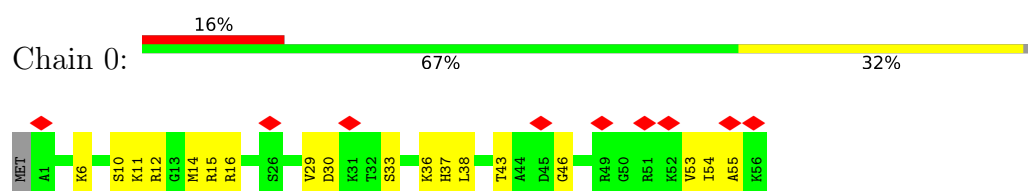
- Molecule 20: 50S ribosomal protein L29



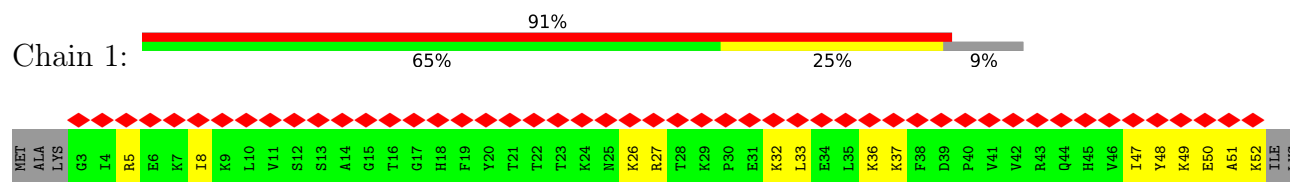
- Molecule 21: 50S ribosomal protein L30



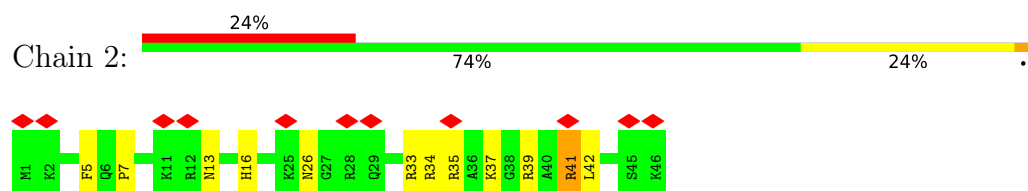
- Molecule 22: 50S ribosomal protein L32



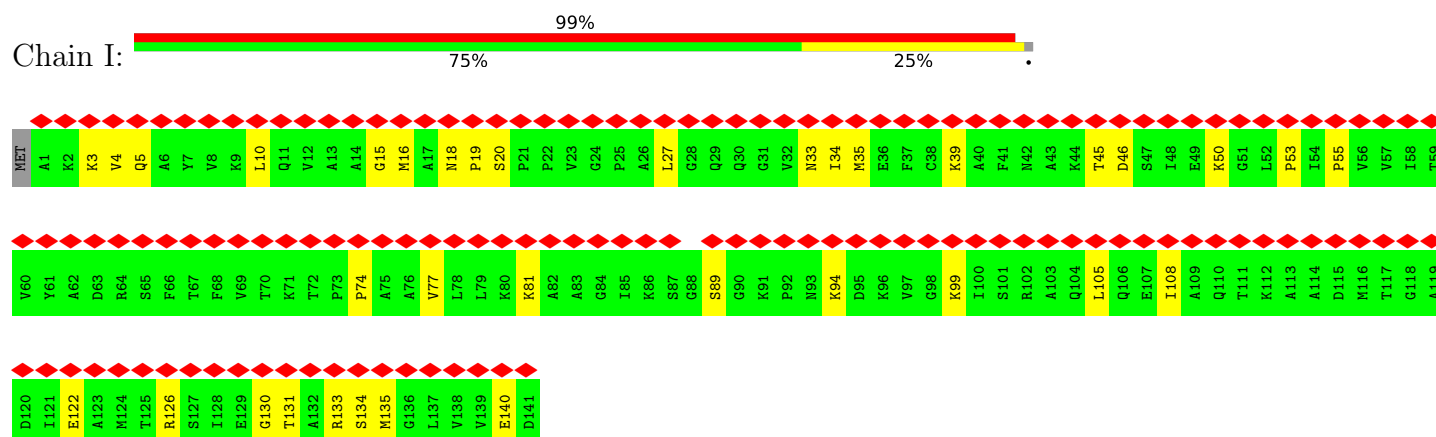
- Molecule 23: 50S ribosomal protein L33



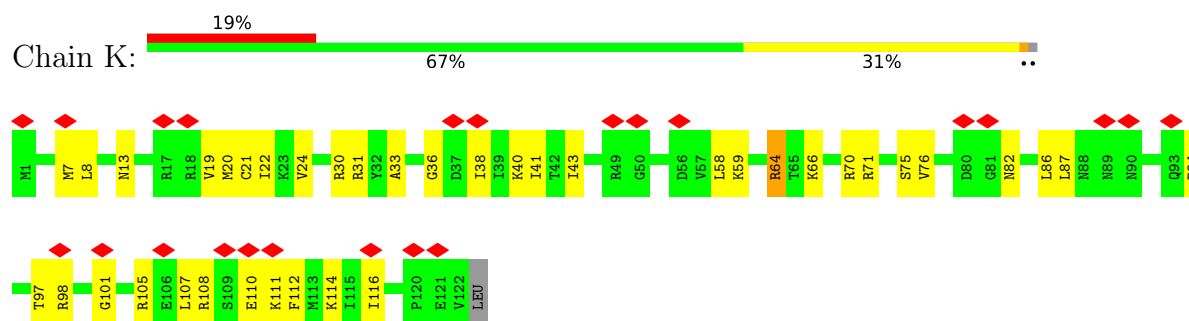
- Molecule 24: 50S ribosomal protein L34



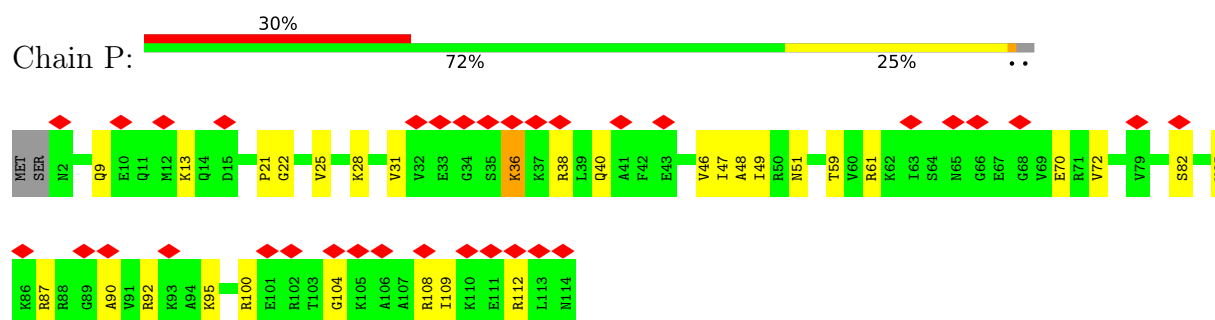
- Molecule 25: 50S ribosomal protein L11



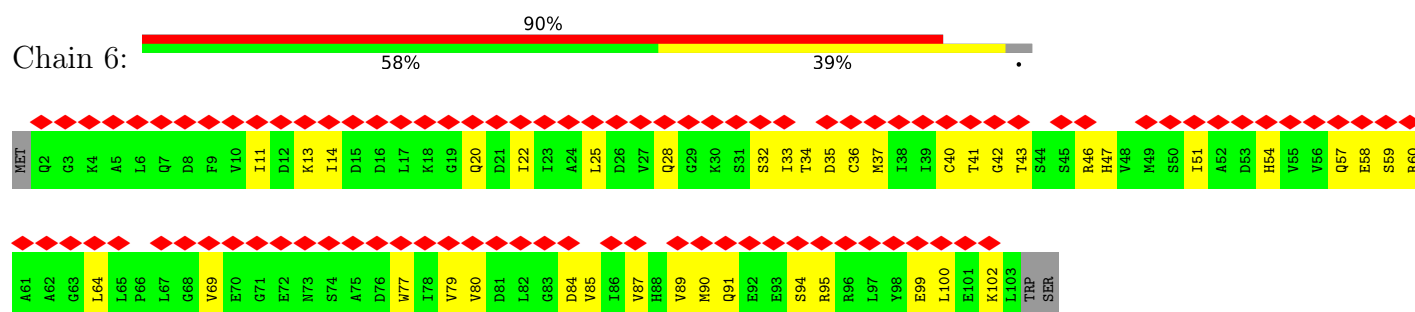
- Molecule 26: 50S ribosomal protein L14



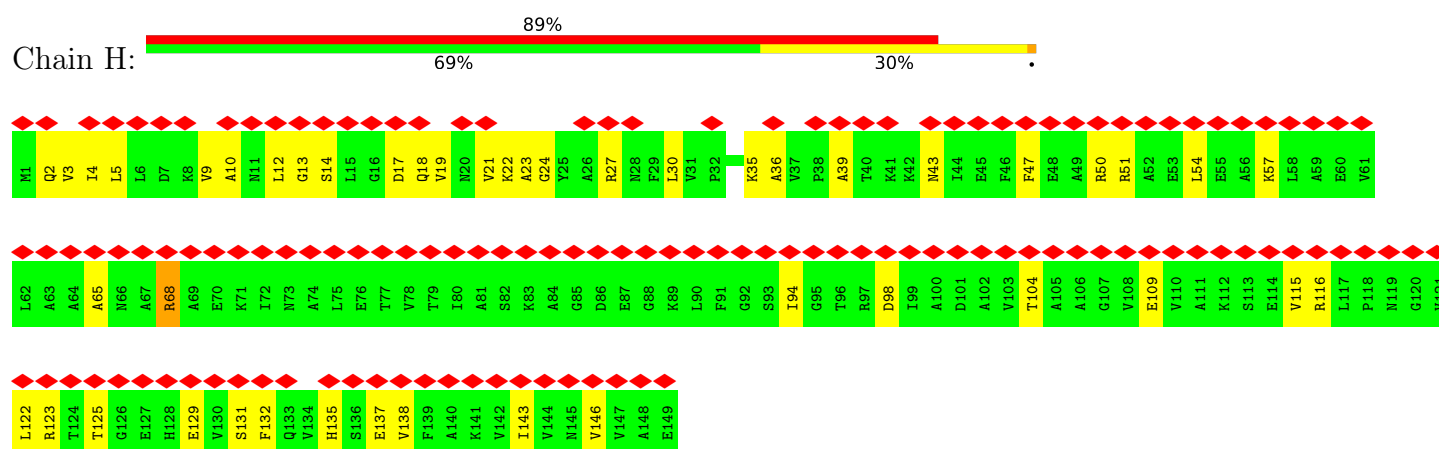
- Molecule 27: 50S ribosomal protein L19



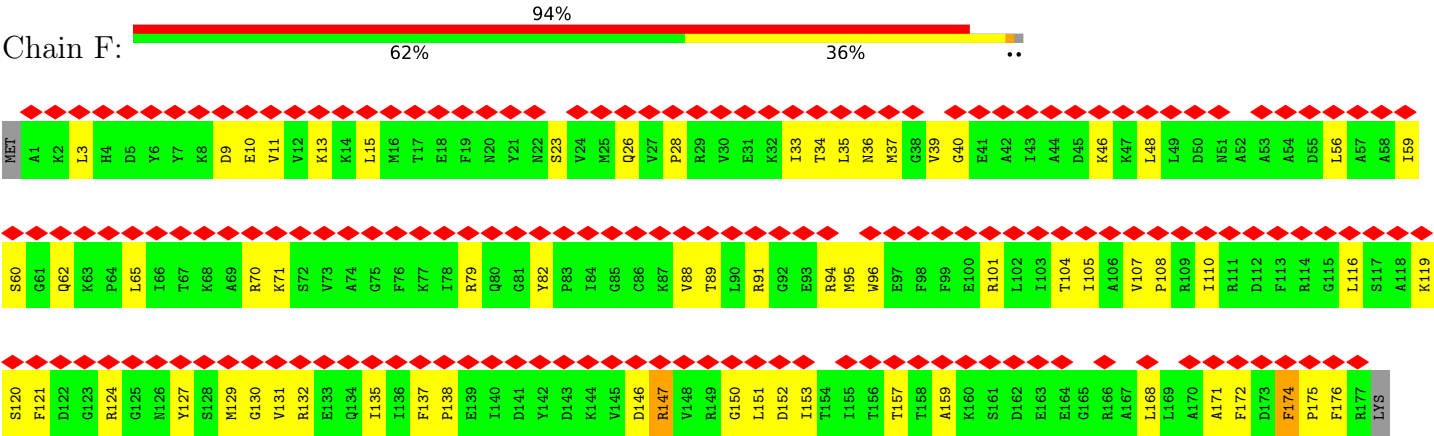
- Molecule 28: Ribosomal silencing factor RsfS



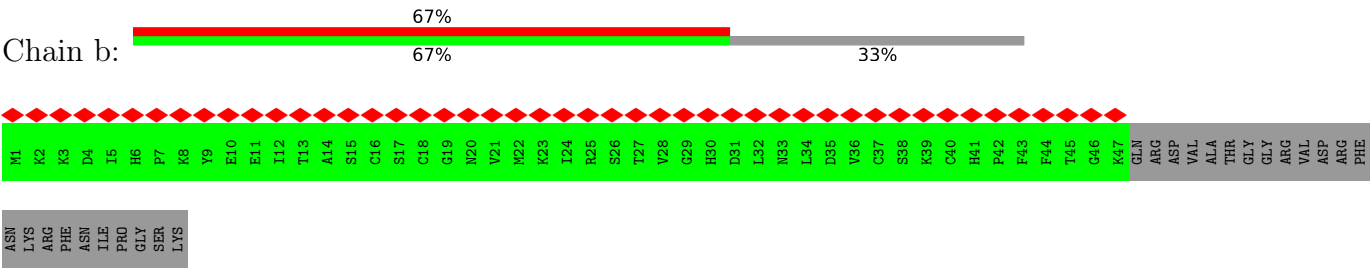
- Molecule 29: 50S ribosomal protein L9



- Molecule 30: 50S ribosomal protein L5



● Molecule 31: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16873	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.453	Depositor
Minimum map value	-6.939	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.777	Depositor
Recommended contour level	2.8	Depositor
Map size (\AA)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.24, 1.24, 1.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/69777	0.74	9/108853 (0.0%)
2	B	0.15	0/2847	0.72	0/4440
3	9P1	0.25	0/2626	0.48	0/3542
4	C	0.25	0/2121	0.45	0/2852
5	D	0.27	0/1586	0.50	0/2134
6	E	0.24	0/1571	0.43	0/2113
7	G	0.24	0/1343	0.45	0/1816
8	J	0.25	0/1152	0.46	0/1551
9	L	0.25	0/1054	0.51	0/1403
10	N	0.24	0/973	0.46	0/1301
11	O	0.25	0/902	0.48	0/1209
12	Q	0.25	0/960	0.40	0/1278
13	R	0.25	0/829	0.49	0/1107
14	S	0.24	0/864	0.47	0/1156
15	T	0.25	0/744	0.50	0/994
16	U	0.26	0/787	0.51	0/1051
17	V	0.24	0/766	0.42	0/1025
18	W	0.25	0/582	0.45	0/769
19	X	0.24	0/635	0.48	0/848
20	Y	0.24	0/510	0.51	0/677
21	Z	0.23	0/453	0.46	0/605
22	0	0.23	0/450	0.45	0/599
23	1	0.25	0/416	0.46	0/554
24	2	0.25	0/380	0.47	0/498
25	I	0.25	0/1046	0.48	0/1410
26	K	0.26	0/947	0.53	0/1268
27	P	0.25	0/923	0.44	0/1234
28	6	0.24	0/787	0.46	0/1062
29	H	0.24	0/1121	0.46	0/1515
30	F	0.25	0/1434	0.48	0/1926
31	b	0.22	0/371	0.43	0/496
All	All	0.20	0/100957	0.68	9/151286 (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
5	D	0	1
30	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2063	C	C2-N1-C1'	7.93	127.52	118.80
1	A	1625	C	N1-C2-O2	6.88	123.03	118.90
1	A	1625	C	N3-C2-O2	-6.77	117.16	121.90
1	A	1313	U	C2-N1-C1'	6.14	125.07	117.70
1	A	2063	C	C6-N1-C1'	-5.83	113.81	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	151	THR	Peptide
30	F	174	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62301	0	31334	1145	0
2	B	2548	0	1292	65	0
3	9P1	2582	0	2607	75	0
4	C	2082	0	2157	87	0
5	D	1565	0	1616	64	0
6	E	1552	0	1619	39	0
7	G	1323	0	1374	35	0
8	J	1129	0	1162	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1045	0	1117	42	0
10	N	960	0	1000	32	0
11	O	892	0	923	33	0
12	Q	947	0	1022	34	0
13	R	816	0	839	25	0
14	S	857	0	922	30	0
15	T	738	0	807	30	0
16	U	779	0	834	16	0
17	V	753	0	780	13	0
18	W	575	0	589	16	0
19	X	625	0	655	26	0
20	Y	509	0	543	11	0
21	Z	449	0	491	11	0
22	0	444	0	461	15	0
23	1	409	0	440	8	0
24	2	377	0	418	13	0
25	I	1032	0	1088	25	0
26	K	938	0	1012	38	0
27	P	911	0	957	22	0
28	6	780	0	783	32	0
29	H	1110	0	1148	31	0
30	F	1410	0	1447	46	0
31	b	364	0	362	0	0
32	Q	1	0	0	0	0
33	b	1	0	0	0	0
34	A	15	0	0	1	0
34	B	1	0	0	0	0
34	C	4	0	0	0	0
34	F	1	0	0	0	0
34	L	4	0	0	0	0
34	N	2	0	0	0	0
All	All	92831	0	61799	1836	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1836 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:A:H62	2:B:98:G:H21	0.97	0.96
2:B:78:A:H62	2:B:98:G:N2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:A:H61	1:A:1116:G:H1	1.22	0.88
1:A:1800:C:H42	1:A:1817:G:H22	1.15	0.88
1:A:954:G:H1	1:A:963:U:H3	1.18	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	9P1	336/390 (86%)	307 (91%)	28 (8%)	1 (0%)	41	74
4	C	269/273 (98%)	251 (93%)	18 (7%)	0	100	100
5	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
6	E	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
7	G	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
8	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
9	L	141/144 (98%)	122 (86%)	19 (14%)	0	100	100
10	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
11	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
12	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
13	R	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
14	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
15	T	91/100 (91%)	79 (87%)	12 (13%)	0	100	100
16	U	100/104 (96%)	86 (86%)	14 (14%)	0	100	100
17	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
18	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
19	X	75/78 (96%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
21	Z	56/59 (95%)	56 (100%)	0	0	100	100
22	0	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
23	1	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
24	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
25	I	139/142 (98%)	113 (81%)	26 (19%)	0	100	100
26	K	120/123 (98%)	107 (89%)	13 (11%)	0	100	100
27	P	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
28	6	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
29	H	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
30	F	175/179 (98%)	160 (91%)	15 (9%)	0	100	100
31	b	45/70 (64%)	42 (93%)	3 (7%)	0	100	100
All	All	3554/3735 (95%)	3298 (93%)	255 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	9P1	192	THR

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	
3	9P1	273/321 (85%)	273 (100%)	0	100	100
4	C	216/218 (99%)	215 (100%)	1 (0%)	88	94
5	D	164/164 (100%)	162 (99%)	2 (1%)	71	84
6	E	165/165 (100%)	165 (100%)	0	100	100
7	G	137/138 (99%)	136 (99%)	1 (1%)	84	91
8	J	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L	102/103 (99%)	102 (100%)	0	100	100
10	N	100/103 (97%)	100 (100%)	0	100	100
11	O	86/87 (99%)	86 (100%)	0	100	100
12	Q	89/90 (99%)	89 (100%)	0	100	100
13	R	84/84 (100%)	84 (100%)	0	100	100
14	S	93/93 (100%)	92 (99%)	1 (1%)	73	85
15	T	80/84 (95%)	80 (100%)	0	100	100
16	U	83/85 (98%)	83 (100%)	0	100	100
17	V	78/78 (100%)	78 (100%)	0	100	100
18	W	56/63 (89%)	56 (100%)	0	100	100
19	X	67/68 (98%)	67 (100%)	0	100	100
20	Y	55/55 (100%)	55 (100%)	0	100	100
21	Z	48/49 (98%)	48 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	45 (100%)	0	100	100
24	2	38/38 (100%)	37 (97%)	1 (3%)	46	69
25	I	109/110 (99%)	108 (99%)	1 (1%)	78	88
26	K	103/104 (99%)	102 (99%)	1 (1%)	76	86
27	P	98/100 (98%)	97 (99%)	1 (1%)	76	86
28	6	88/91 (97%)	88 (100%)	0	100	100
29	H	114/114 (100%)	113 (99%)	1 (1%)	78	88
30	F	148/150 (99%)	144 (97%)	4 (3%)	44	68
31	b	43/62 (69%)	43 (100%)	0	100	100
All	All	2925/3030 (96%)	2911 (100%)	14 (0%)	89	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	K	64	ARG
27	P	36	LYS
30	F	147	ARG
30	F	71	LYS
30	F	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	130	GLN
7	G	127	GLN
17	V	75	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2899/2919 (99%)	455 (15%)	15 (0%)
2	B	118/120 (98%)	14 (11%)	0
All	All	3017/3039 (99%)	469 (15%)	15 (0%)

5 of 469 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	35	G
1	A	46	G
1	A	51	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2058	A
1	A	2756	U
1	A	2127	G
1	A	2858	C
1	A	2425	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

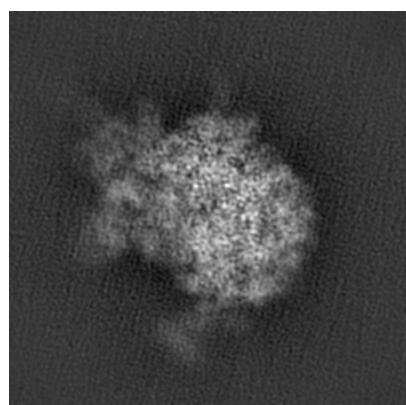
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12215. These allow visual inspection of the internal detail of the map and identification of artifacts.

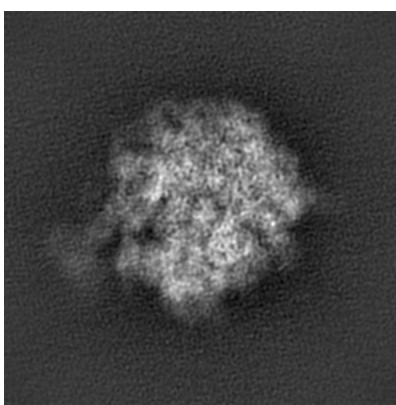
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

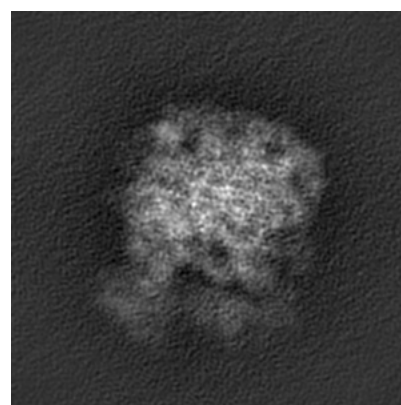
6.1.1 Primary map



X



Y

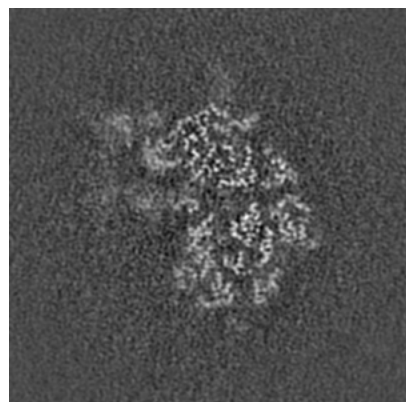


Z

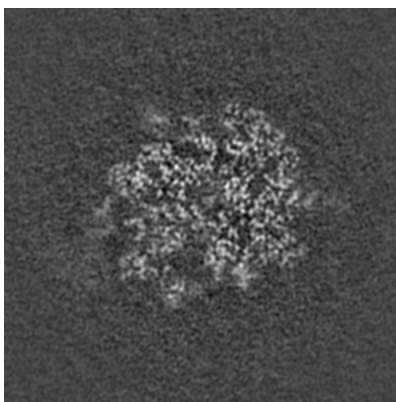
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

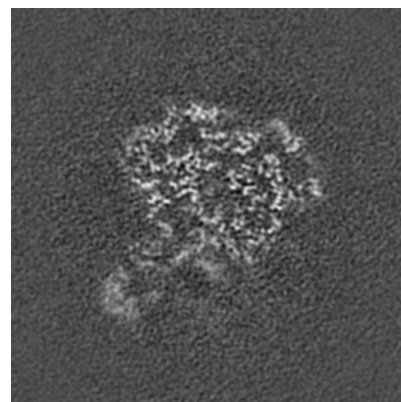
6.2.1 Primary map



X Index: 135



Y Index: 135

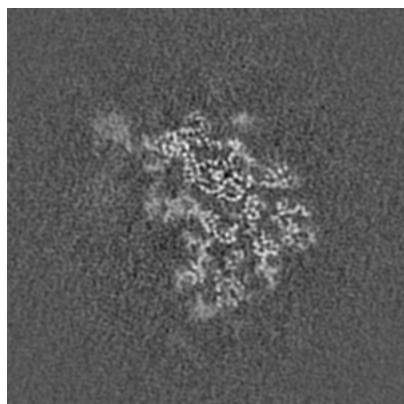


Z Index: 135

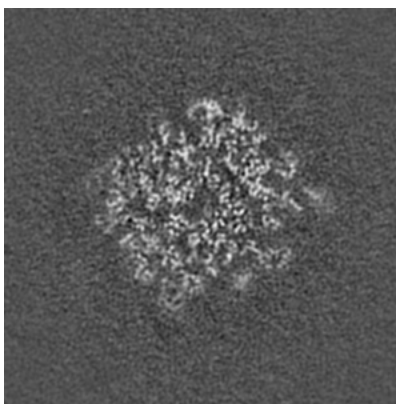
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

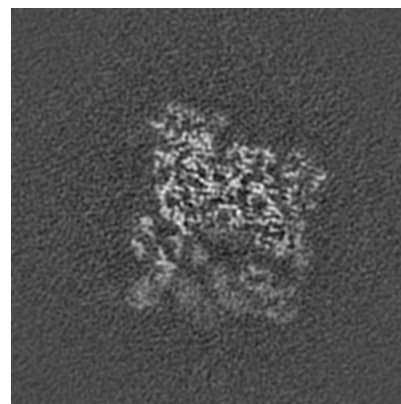
6.3.1 Primary map



X Index: 130



Y Index: 145



Z Index: 151

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

6.4 Orthogonal surface views [i](#)

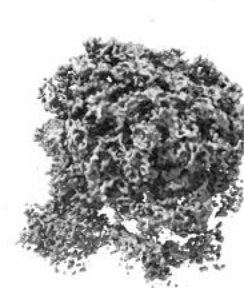
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

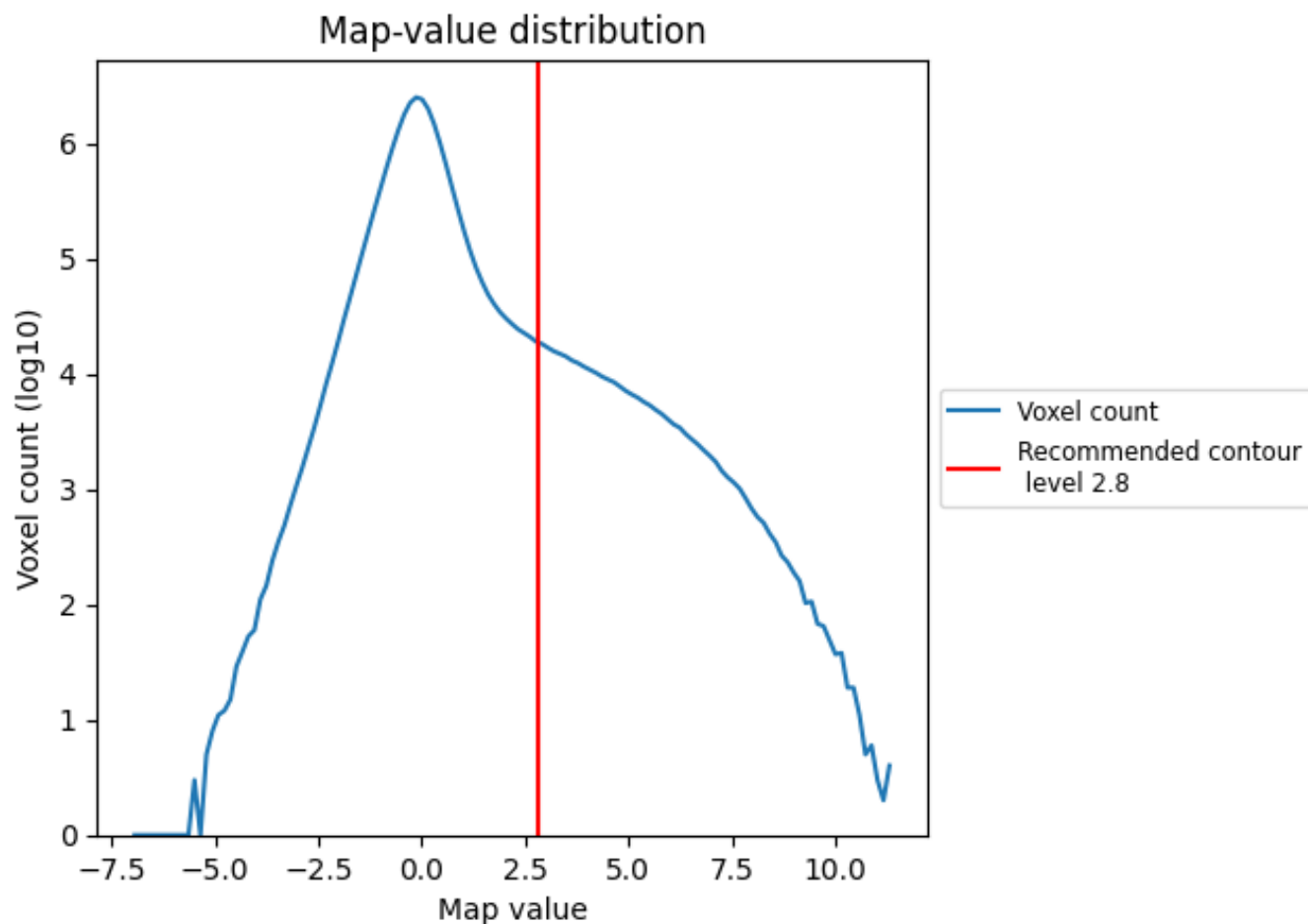
6.5 Mask visualisation

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

7 Map analysis [i](#)

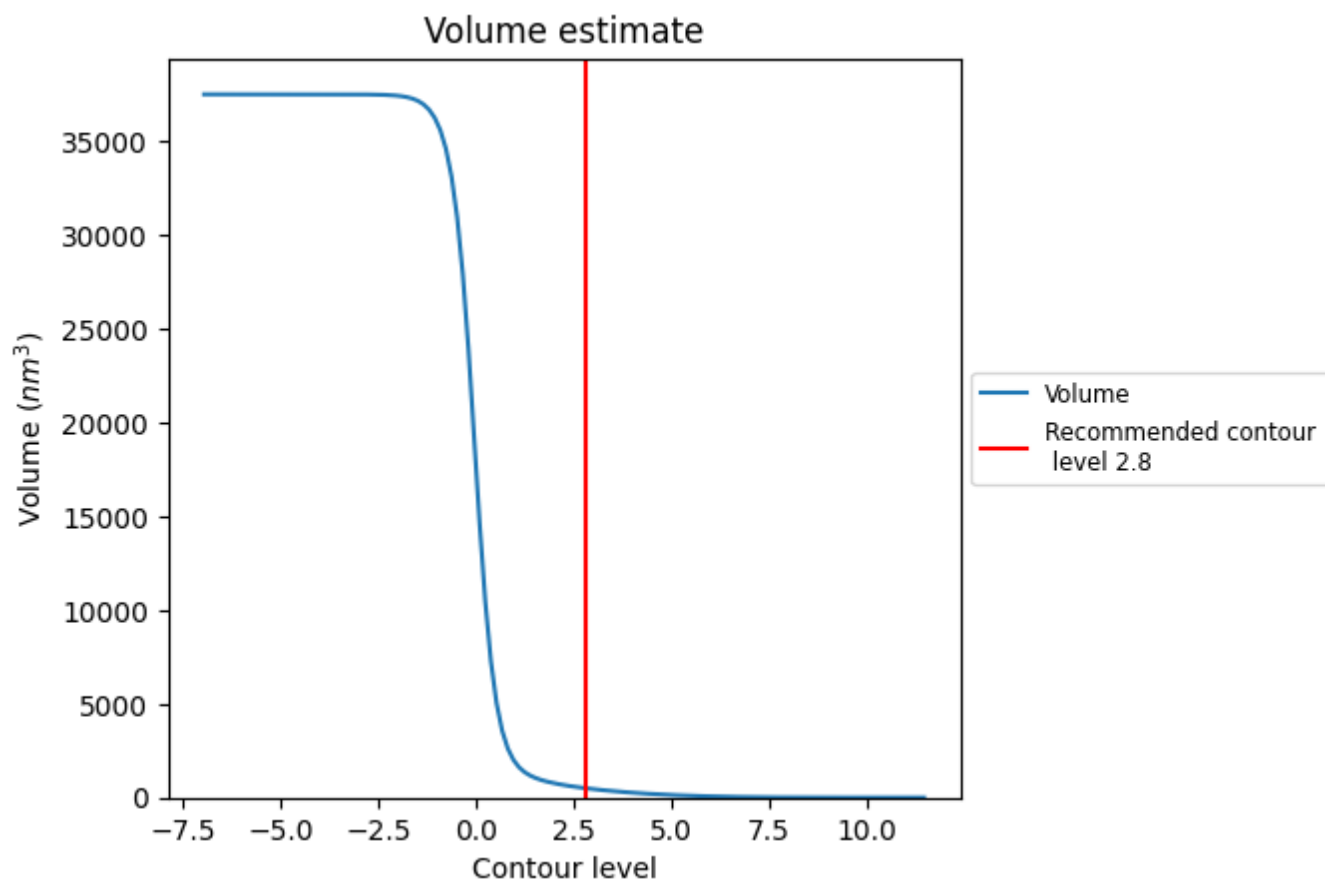
This section contains the results of statistical analysis of the map.

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.

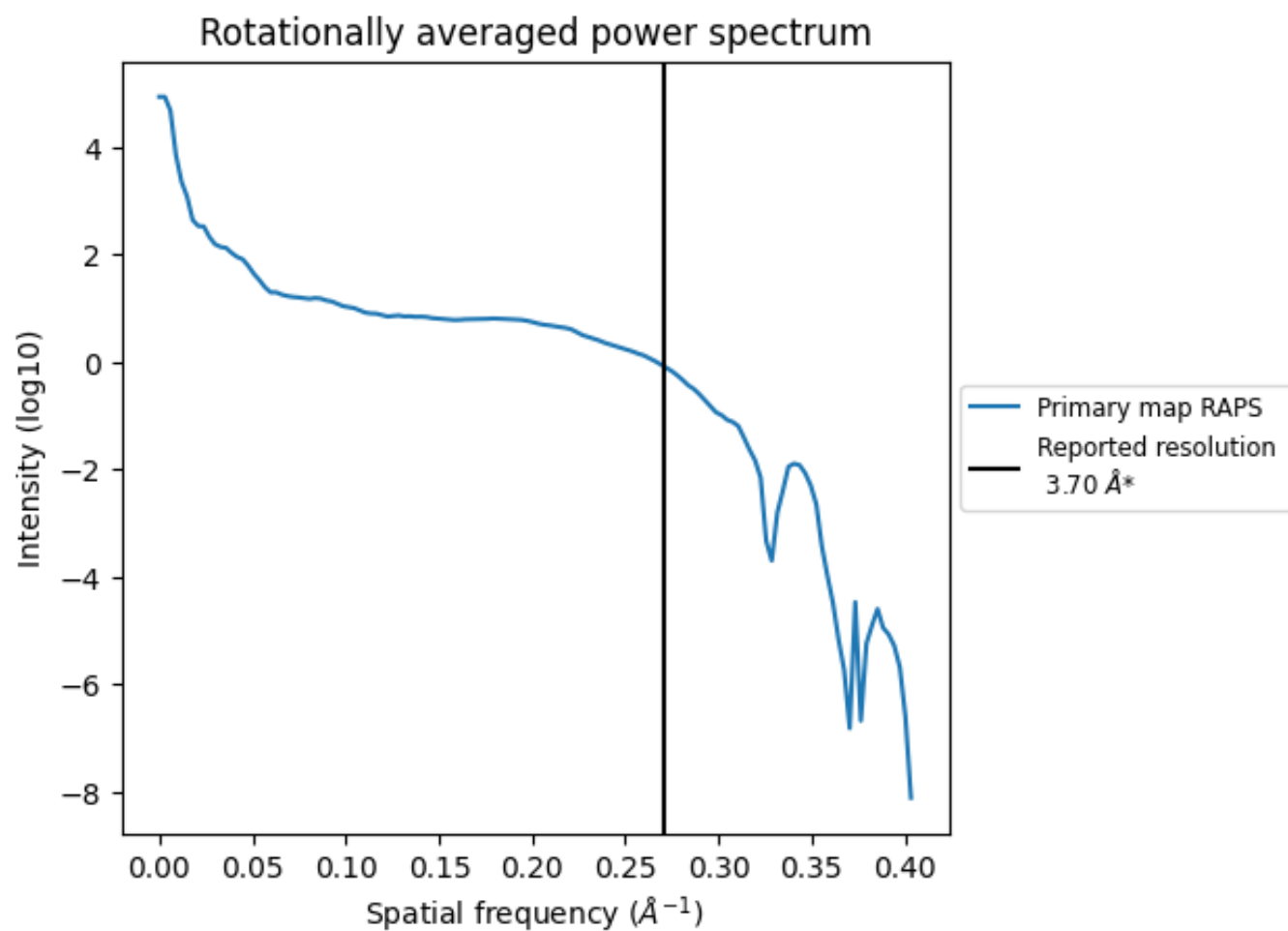
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 501 nm³; this corresponds to an approximate mass of 453 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 ⓘ

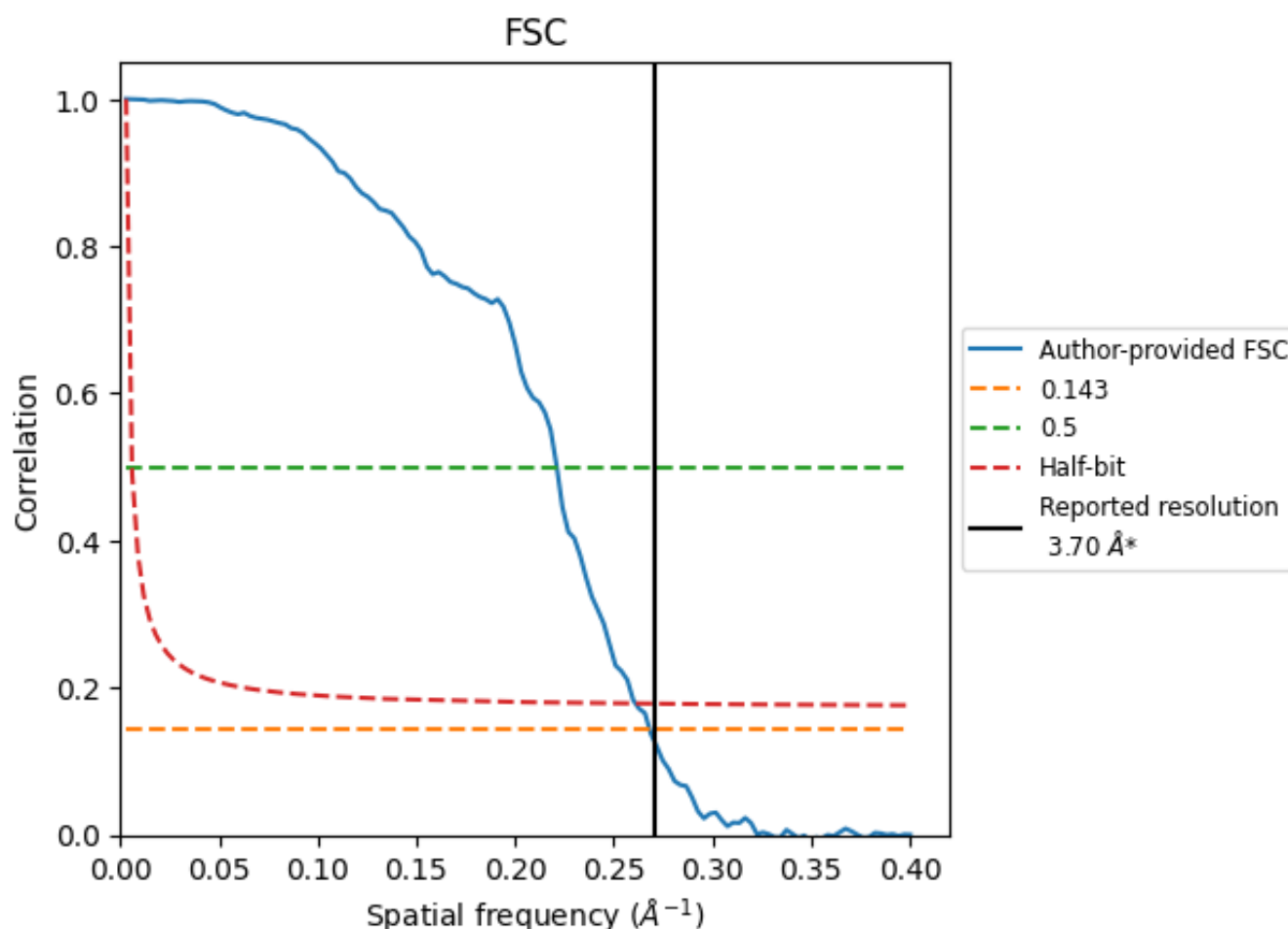


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

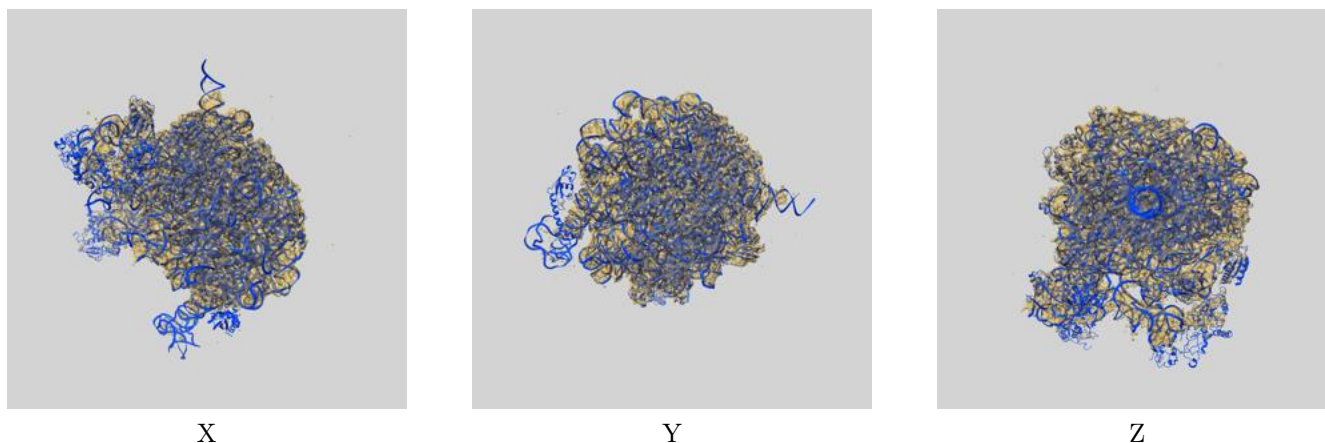
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.52	3.83
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

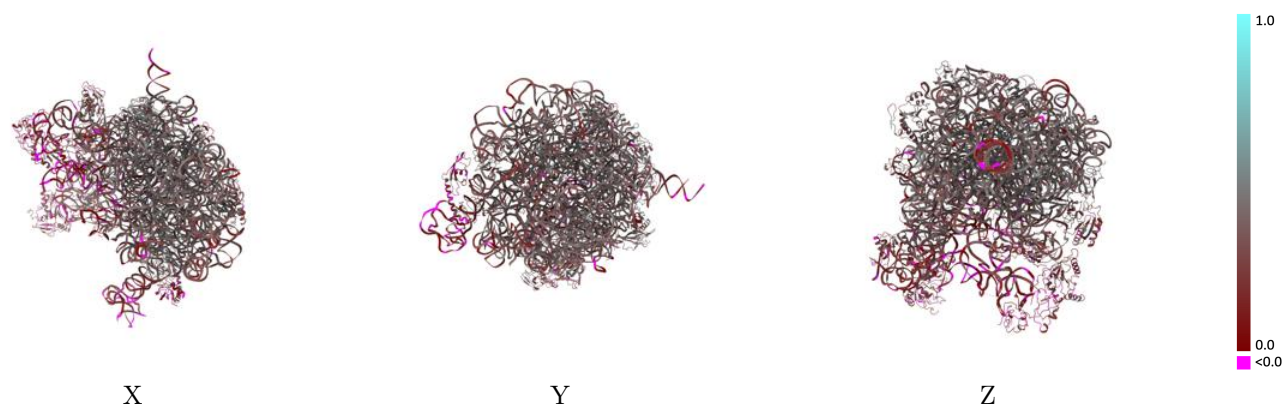
This section contains information regarding the fit between EMDB map EMD-12215 and PDB model 7BL2. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



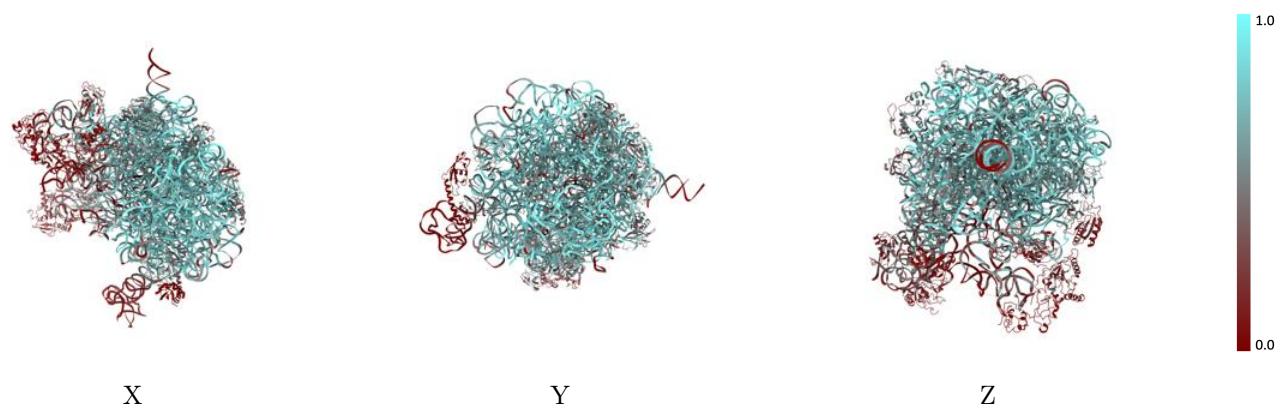
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



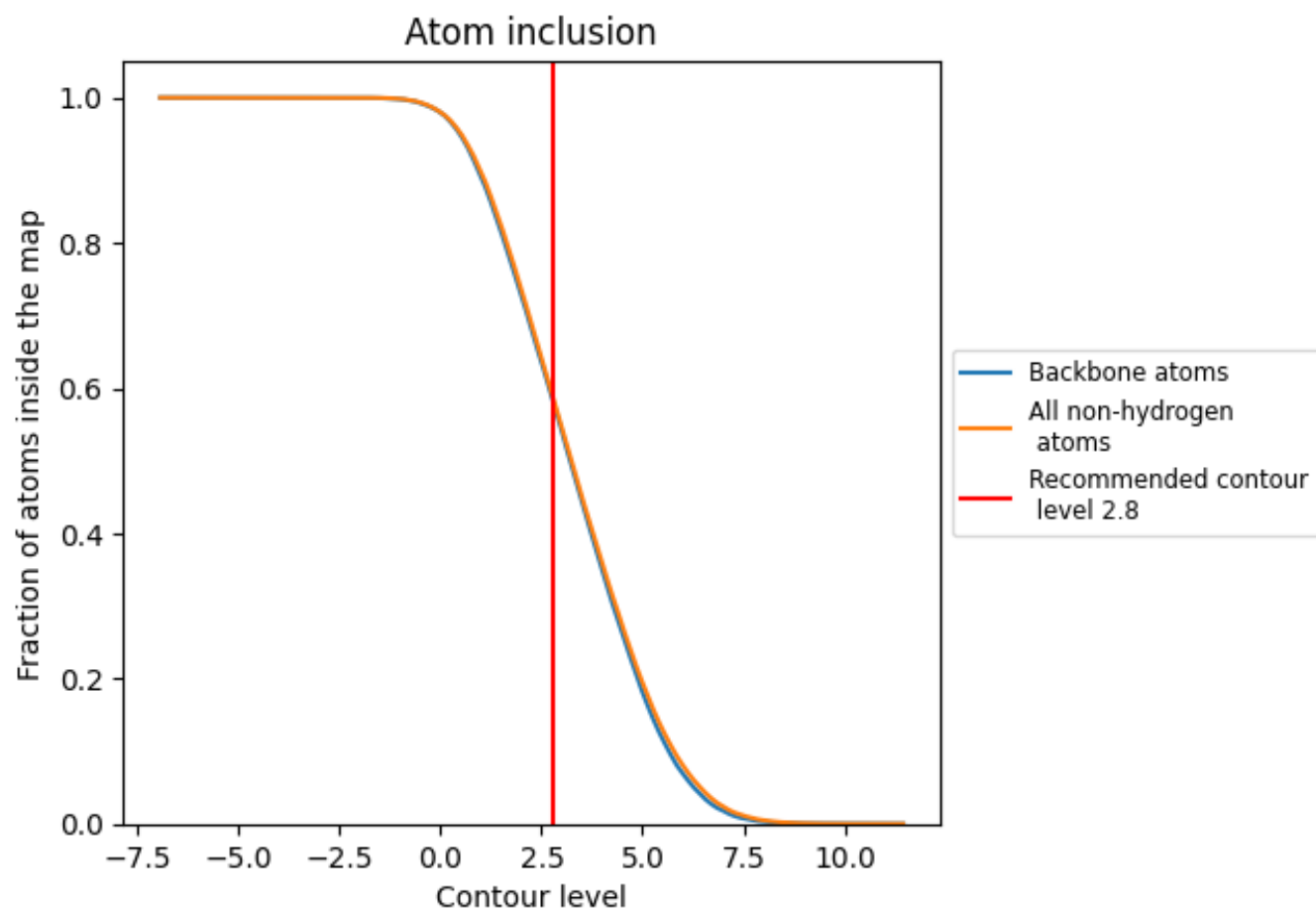
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5847	 0.3280
0	 0.5888	 0.3900
1	 0.0175	 0.1500
2	 0.5887	 0.4250
6	 0.1429	 0.2700
9P1	 0.2631	 0.2510
A	 0.6797	 0.3350
B	 0.4195	 0.2200
C	 0.5838	 0.4050
D	 0.5819	 0.4190
E	 0.4770	 0.3470
F	 0.0626	 0.1630
G	 0.3084	 0.2960
H	 0.1032	 0.1940
I	 0.0059	 0.1190
J	 0.5836	 0.4150
K	 0.5487	 0.3940
L	 0.4045	 0.2910
N	 0.6009	 0.4030
O	 0.1518	 0.2180
P	 0.5272	 0.4000
Q	 0.5930	 0.4030
R	 0.5295	 0.3840
S	 0.5921	 0.4290
T	 0.5249	 0.3910
U	 0.5359	 0.3930
V	 0.1694	 0.2400
W	 0.3453	 0.3140
X	 0.4859	 0.3770
Y	 0.4748	 0.3130
Z	 0.5217	 0.4040
b	 0.0000	 0.1500

