



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:40 AM UTC

PDB ID : 7BL5 / pdb_00007b15
EMDB ID : EMD-12218
Title : pre-50S-ObgE particle
Authors : Hilal, T.; Nikolay, R.; Spahn, C.M.T.; Schmidt, S.
Deposited on : 2021-01-18
Resolution : 3.30 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:

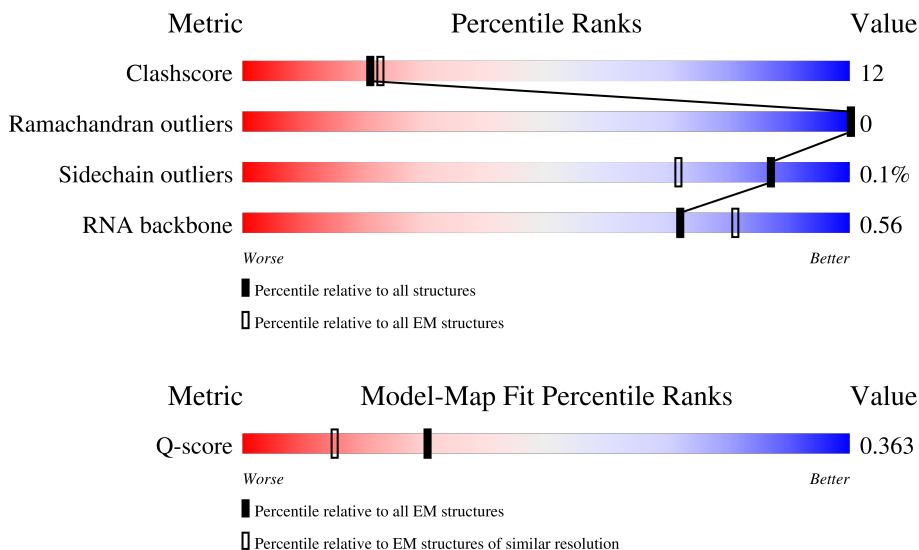
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	C	273	
2	D	209	
3	E	201	

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Mol	Chain	Length	Quality of chain
4	G	177	44% 66% 31%
5	J	142	10% 73% 27%
6	L	144	22% 68% 31%
7	N	127	64% 31% 6%
8	O	117	45% 68% 32%
9	Q	118	8% 76% 23%
10	R	103	9% 63% 37%
11	S	110	9% 74% 26%
12	T	100	14% 75% 18% 7%
13	U	104	13% 72% 26%
14	V	94	40% 69% 31%
15	W	85	15% 60% 29% 11%
16	X	78	10% 77% 22%
17	Y	63	25% 71% 29%
18	Z	59	7% 68% 31%
19	0	57	14% 72% 26%
20	1	55	53% 71% 20% 9%
21	2	46	11% 72% 28%
22	B	120	16% 50% 44% 5%
23	I	142	97% 76% 23%
24	K	123	8% 71% 28%
25	P	115	15% 61% 37%
26	6	105	41% 72% 25%
27	7	326	78% 68% 29%
28	8	183	43% 59% 27% 14%

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Mol	Chain	Length	Quality of chain
29	9	390	
30	M	136	
31	A	2919	
32	H	149	
33	e	165	
34	F	179	
35	b	70	

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 98927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

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

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

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

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

- Molecule 4 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	171	1281	806	235	238	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L13.

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

- Molecule 6 is a protein called 50S ribosomal protein L15.

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

- Molecule 7 is a protein called 50S ribosomal protein L17.

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

- Molecule 8 is a protein called 50S ribosomal protein L18.

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

- Molecule 9 is a protein called 50S ribosomal protein L20.

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

- Molecule 10 is a protein called 50S ribosomal protein L21.

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

- Molecule 11 is a protein called 50S ribosomal protein L22.

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

- Molecule 12 is a protein called 50S ribosomal protein L23.

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

- Molecule 13 is a protein called 50S ribosomal protein L24.

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

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L27.

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

- Molecule 16 is a protein called 50S ribosomal protein L28.

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

- Molecule 17 is a protein called 50S ribosomal protein L29.

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

- Molecule 18 is a protein called 50S ribosomal protein L30.

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

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 20 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 21 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 23 is a protein called 50S ribosomal protein L11.

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

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

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

- Molecule 26 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 27 is a protein called Ribosomal large subunit pseudouridine synthase D.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	317	Total	C	N	O	S	0	0
			2533	1593	471	457	12		

- Molecule 28 is a protein called UPF0307 protein YjgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	157	Total	C	N	O	S	0	0
			1281	792	251	237	1		

- Molecule 29 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 30 is a protein called 50S ribosomal protein L16.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	2913	Total	C	N	O	P	0	0
			62534	27897	11506	20218	2913		

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

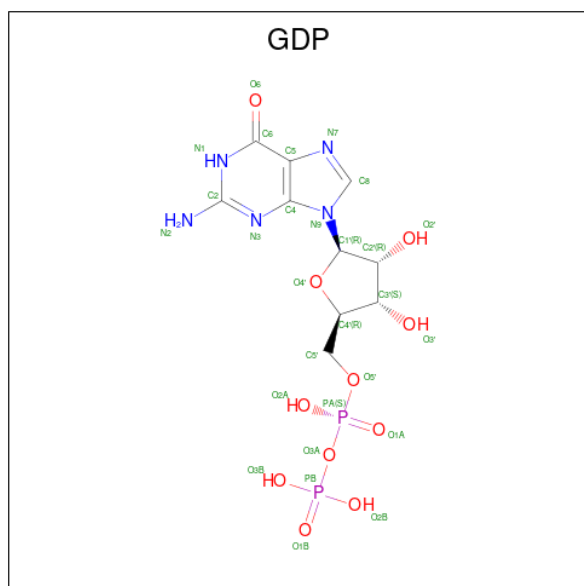
- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L31.

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

- Molecule 36 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

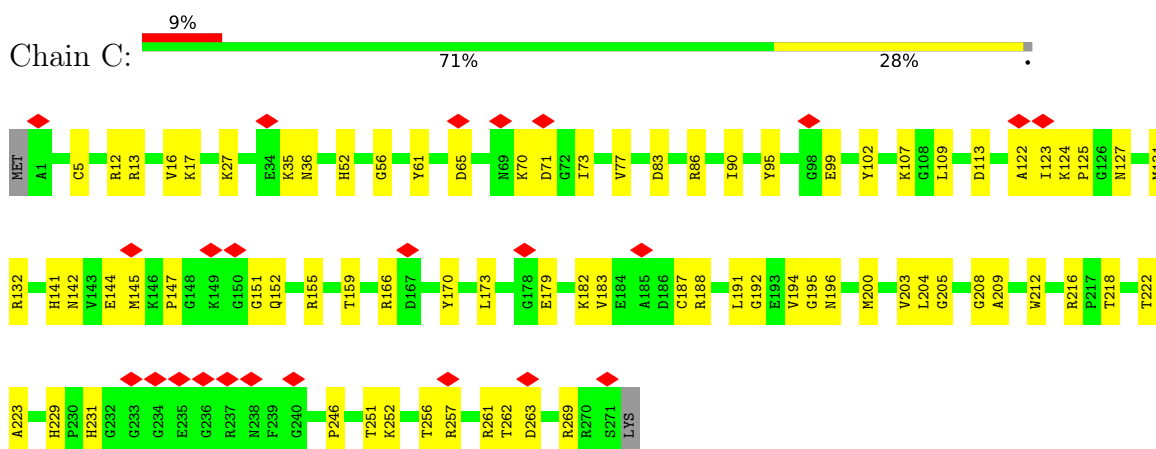


Mol	Chain	Residues	Atoms	AltConf
39	C	3	Total O 3 3	0
39	D	1	Total O 1 1	0
39	N	2	Total O 2 2	0
39	S	1	Total O 1 1	0
39	2	1	Total O 1 1	0
39	B	1	Total O 1 1	0
39	A	17	Total O 17 17	0
39	F	1	Total O 1 1	0

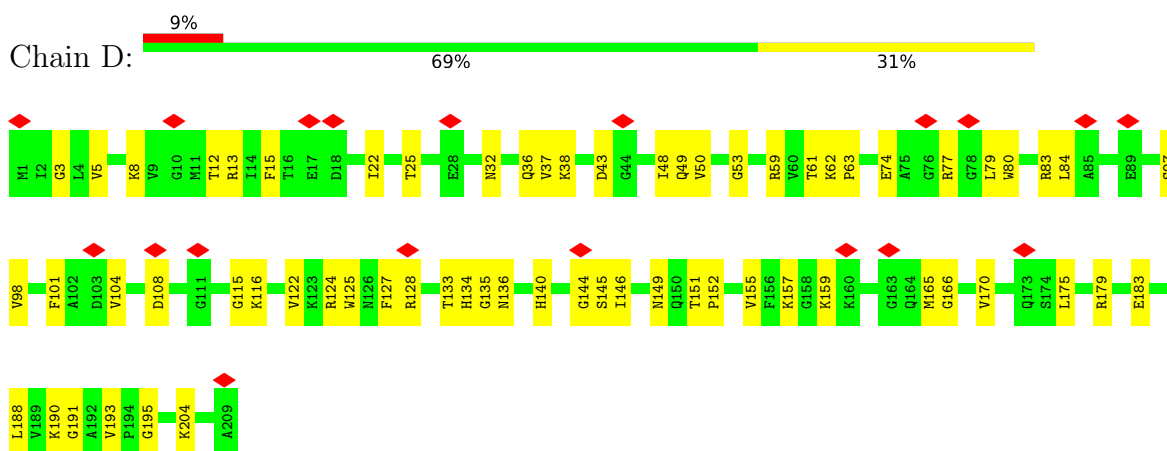
3 Residue-property plots [i](#)

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

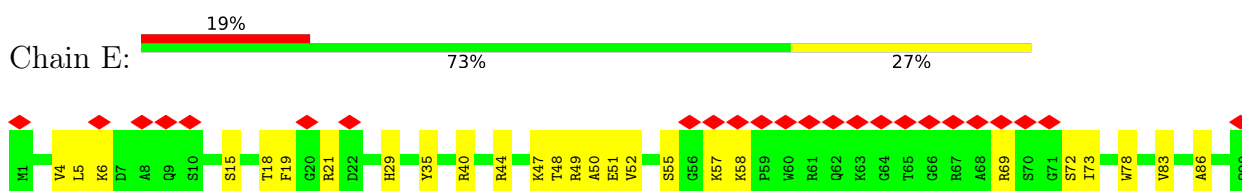
- Molecule 1: 50S ribosomal protein L2

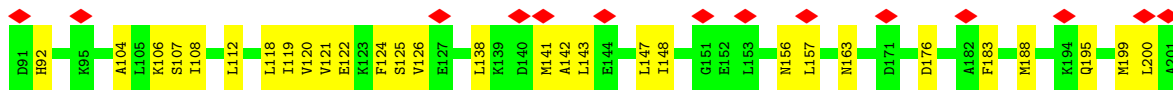


- Molecule 2: 50S ribosomal protein L3

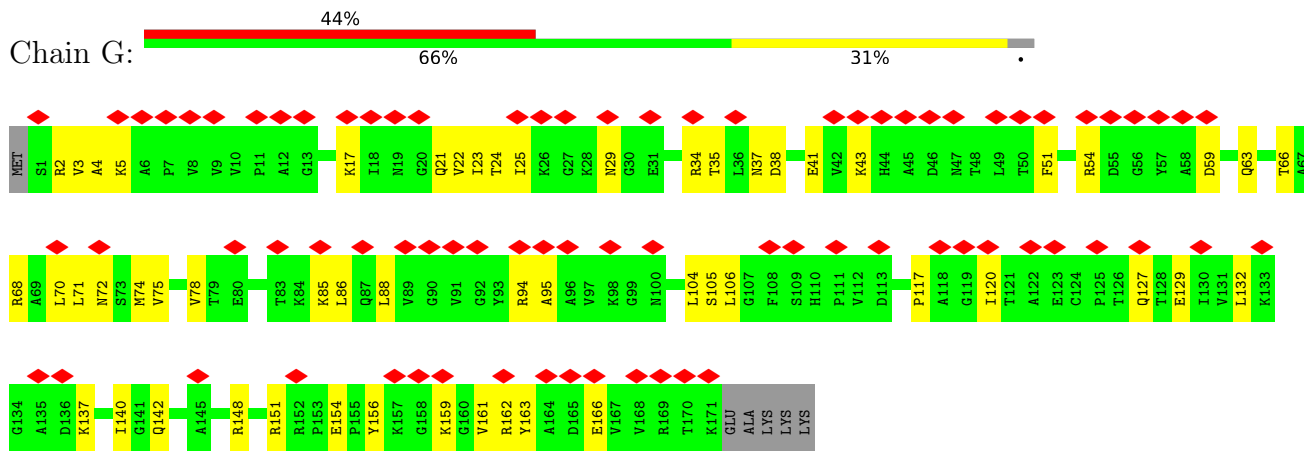


- Molecule 3: 50S ribosomal protein L4

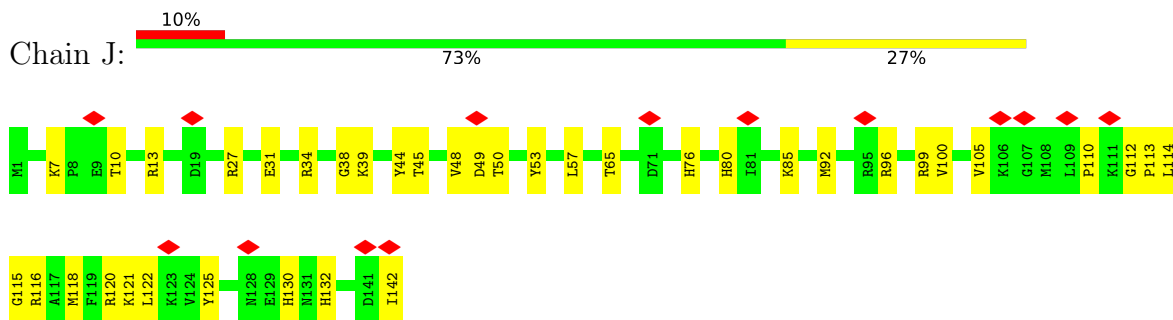




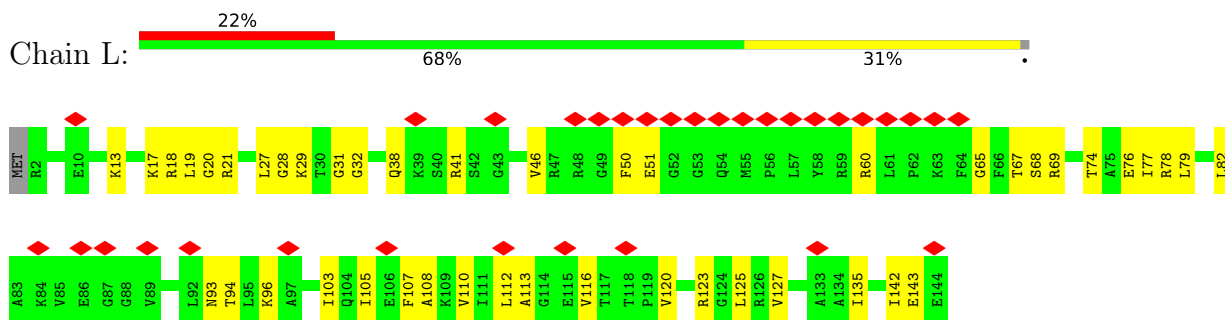
• Molecule 4: 50S ribosomal protein L6



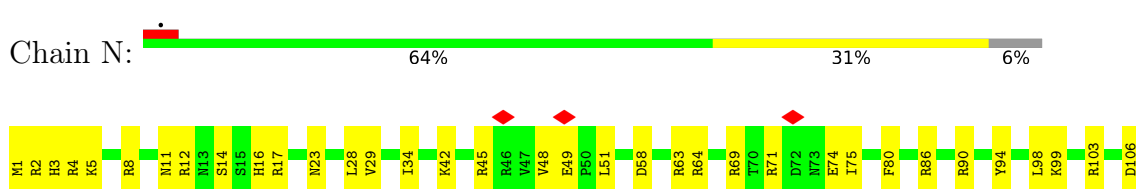
• Molecule 5: 50S ribosomal protein L13

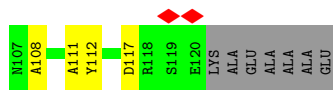


• Molecule 6: 50S ribosomal protein L15

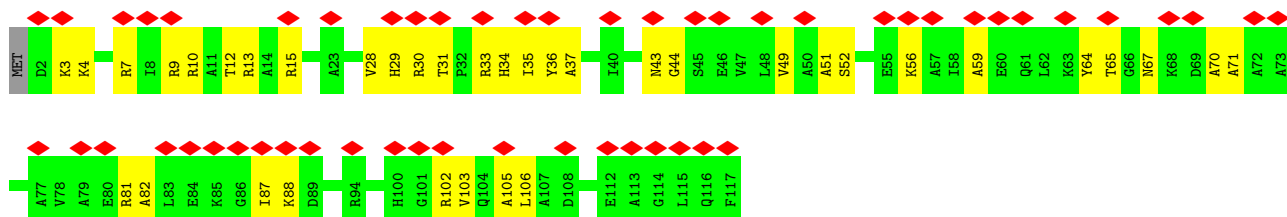
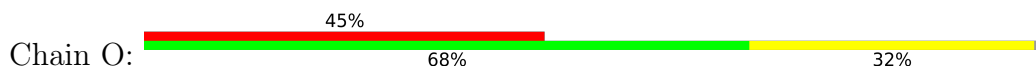


• Molecule 7: 50S ribosomal protein L17

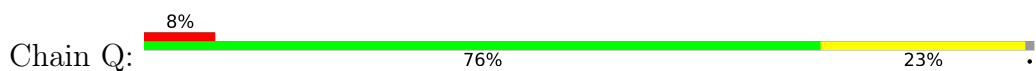




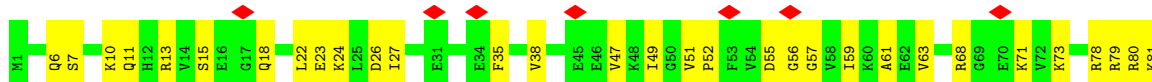
- Molecule 8: 50S ribosomal protein L18



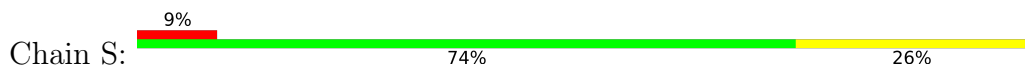
- Molecule 9: 50S ribosomal protein L20



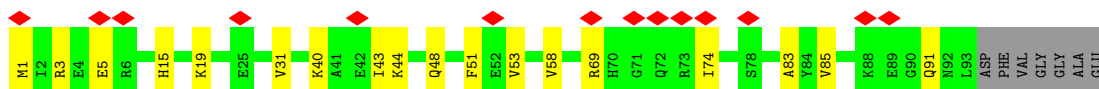
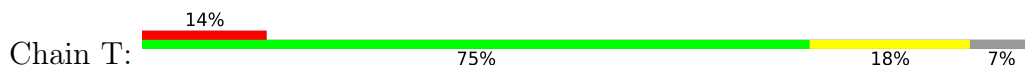
- Molecule 10: 50S ribosomal protein L21



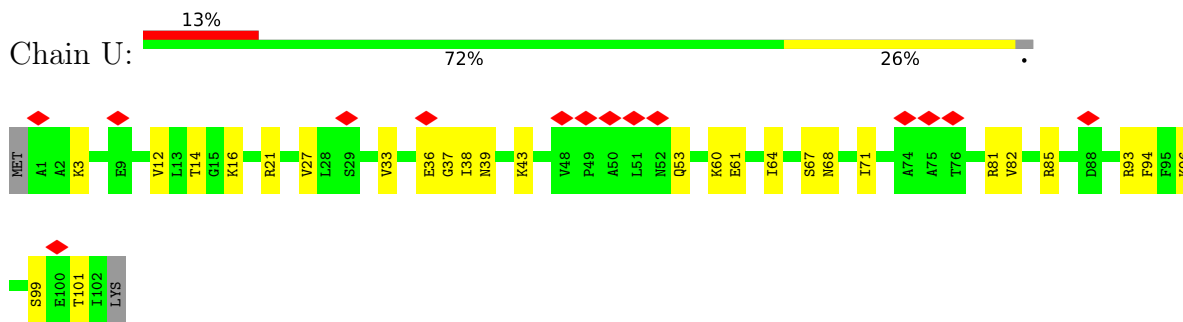
- Molecule 11: 50S ribosomal protein L22



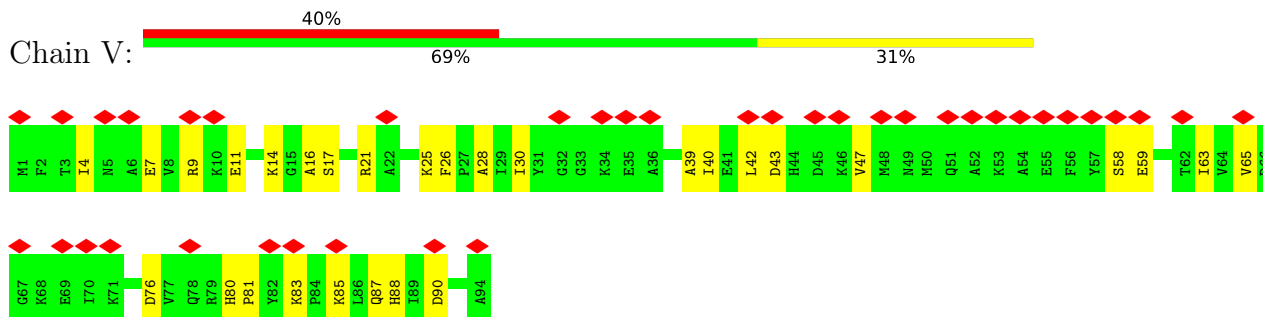
- Molecule 12: 50S ribosomal protein L23



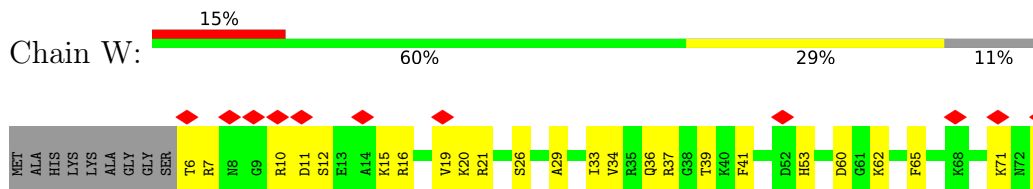
- Molecule 13: 50S ribosomal protein L24



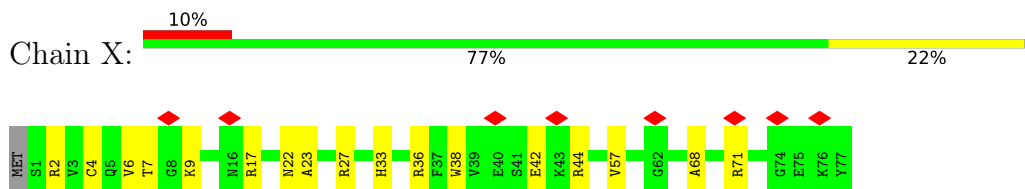
• Molecule 14: 50S ribosomal protein L25



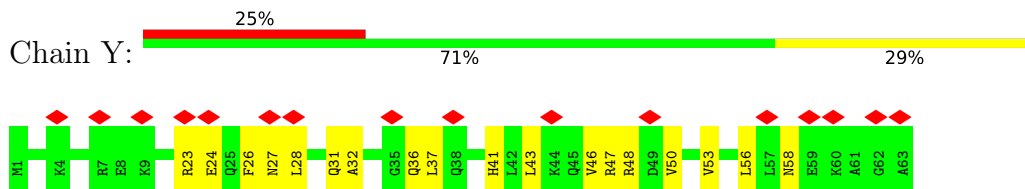
• Molecule 15: 50S ribosomal protein L27



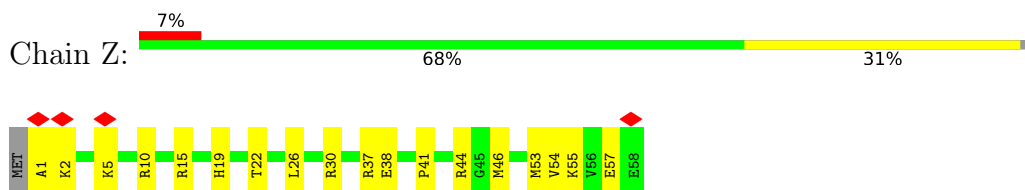
• Molecule 16: 50S ribosomal protein L28



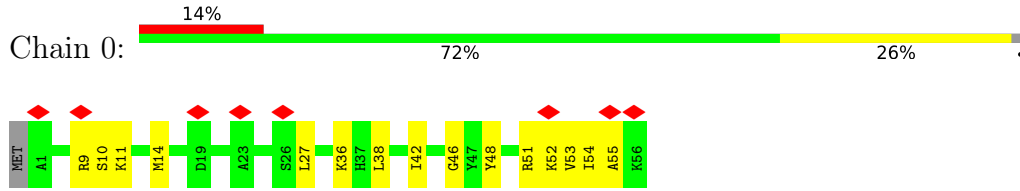
• Molecule 17: 50S ribosomal protein L29



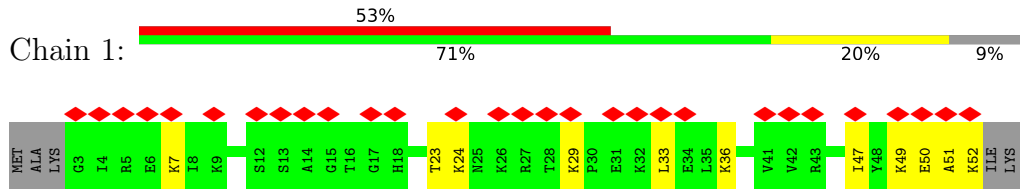
• Molecule 18: 50S ribosomal protein L30



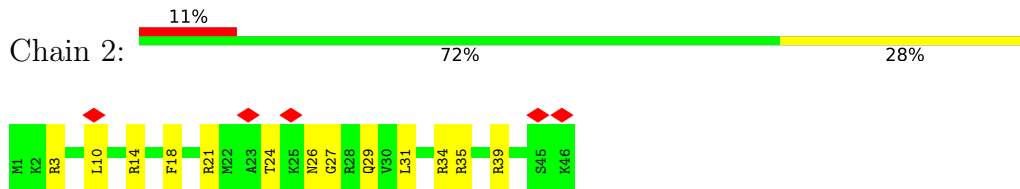
• Molecule 19: 50S ribosomal protein L32



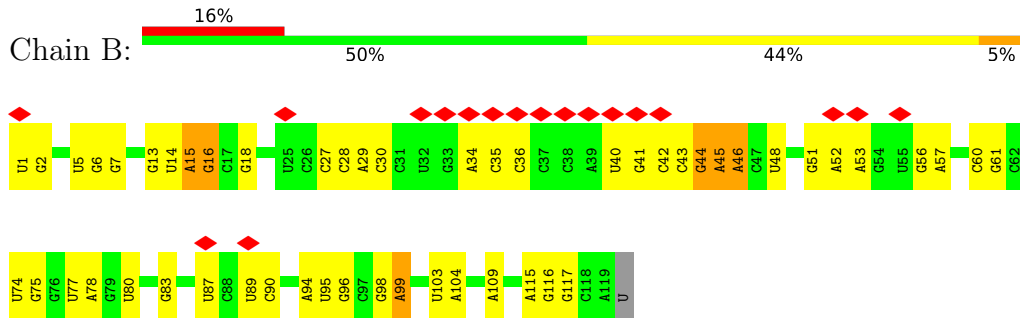
• Molecule 20: 50S ribosomal protein L33



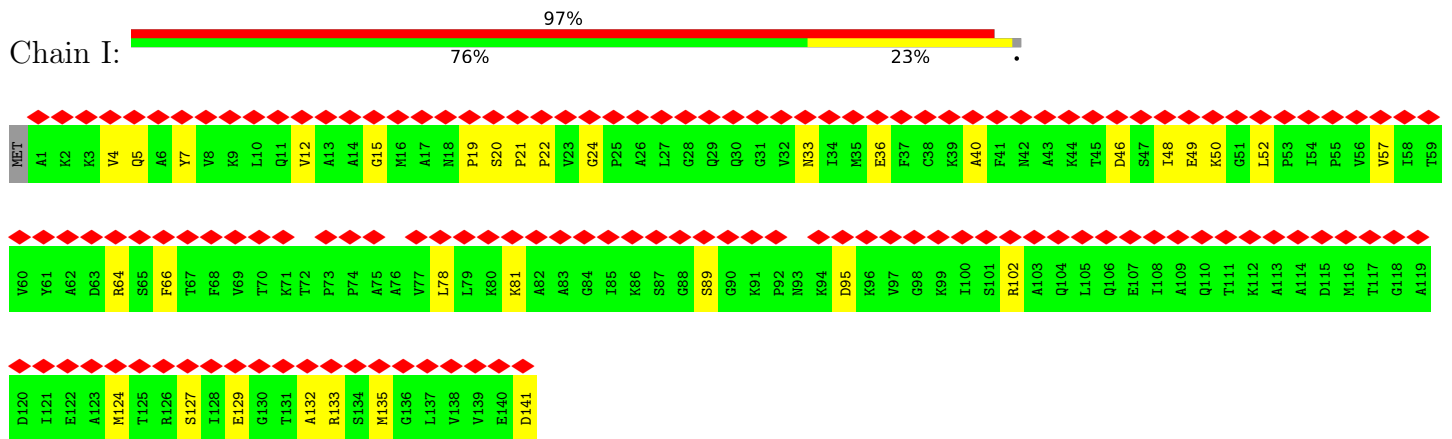
• Molecule 21: 50S ribosomal protein L34



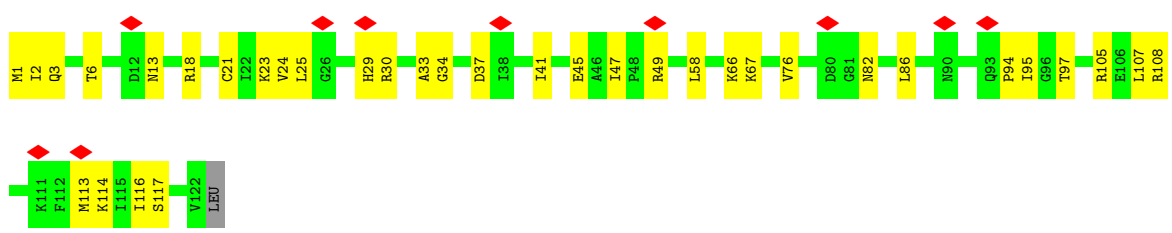
• Molecule 22: 5S ribosomal RNA



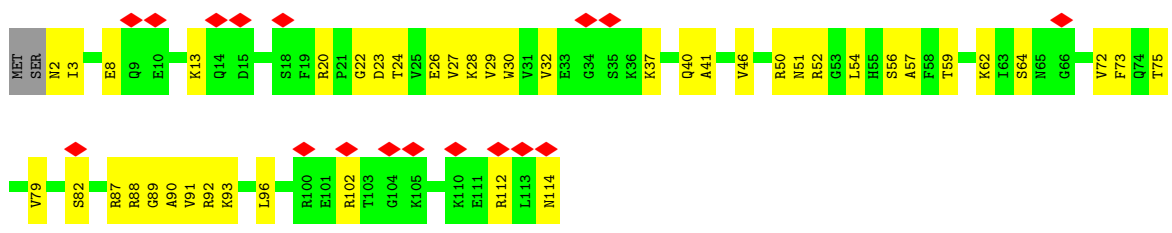
• Molecule 23: 50S ribosomal protein L11



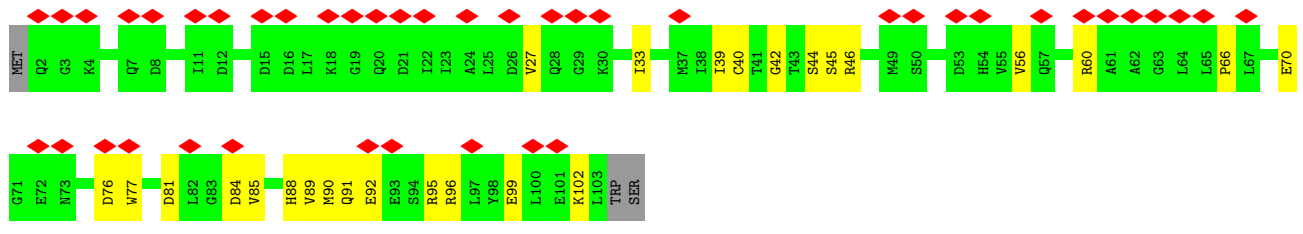
• Molecule 24: 50S ribosomal protein L14



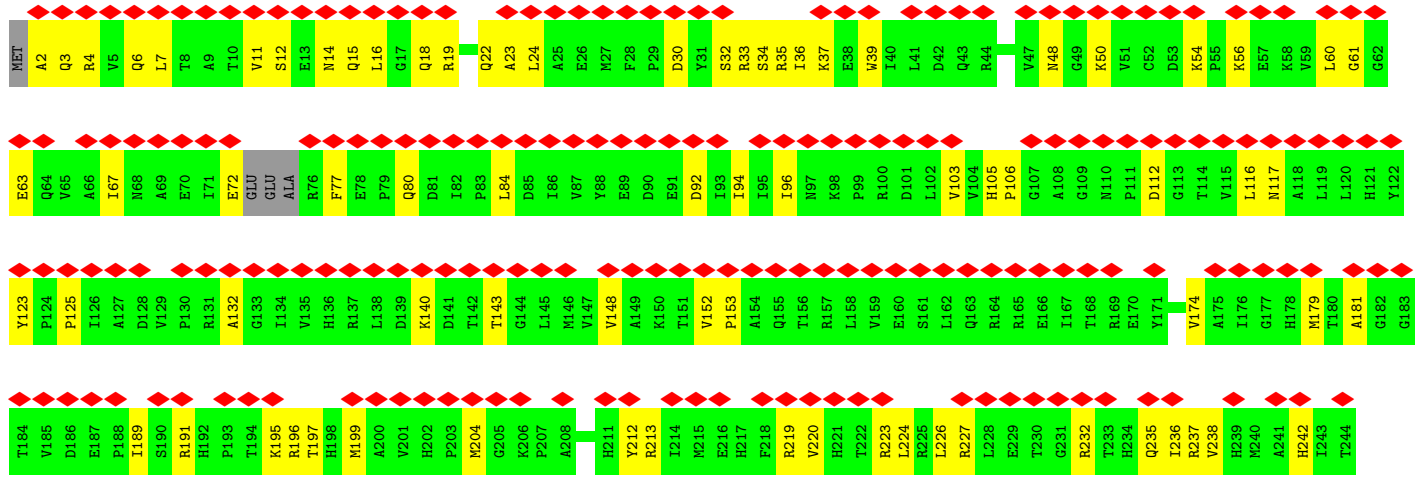
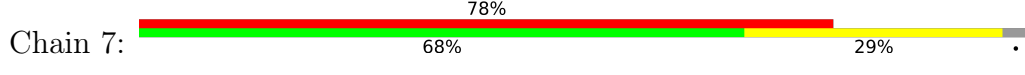
• Molecule 25: 50S ribosomal protein L19

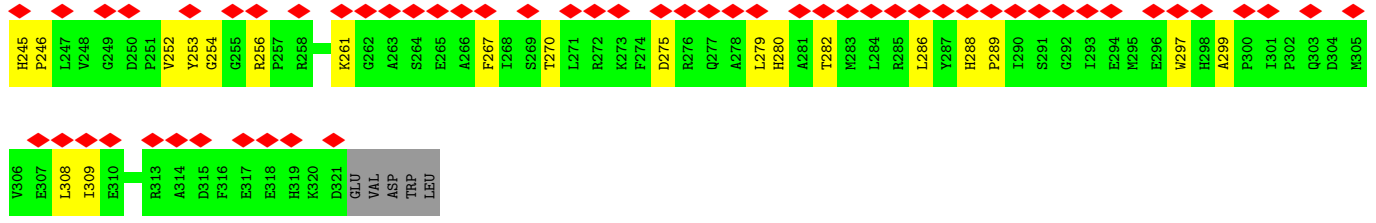


• Molecule 26: Ribosomal silencing factor RsfS

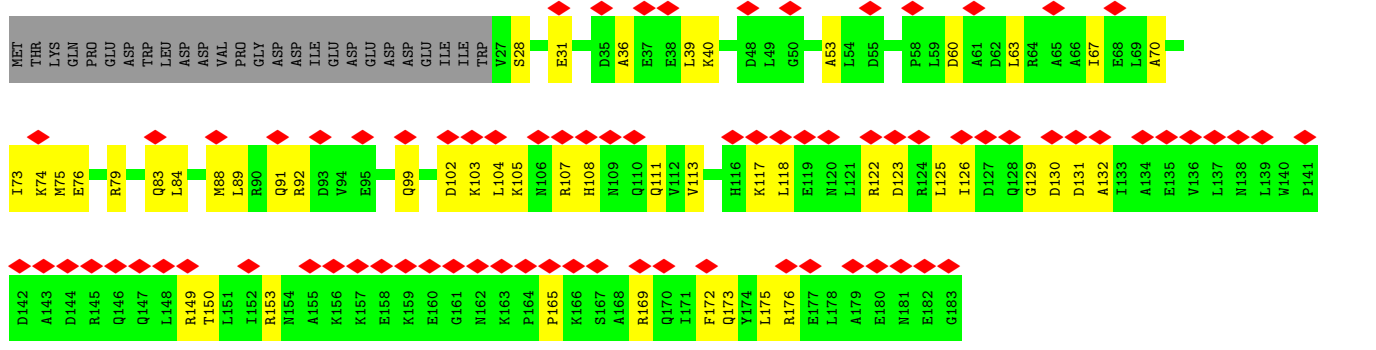
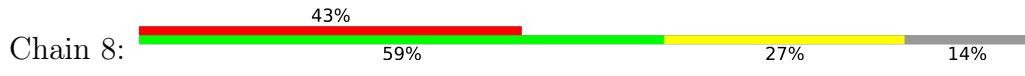


• Molecule 27: Ribosomal large subunit pseudouridine synthase D

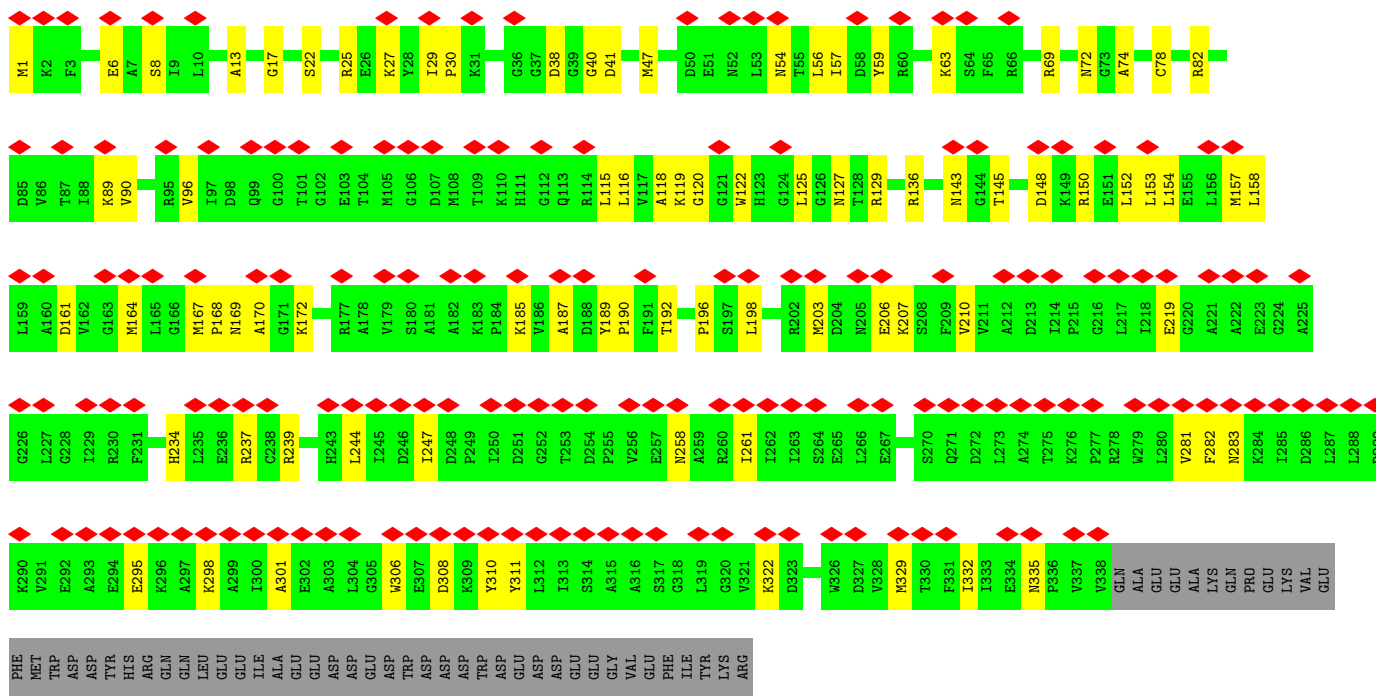
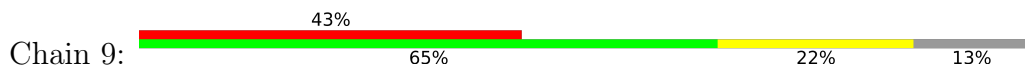




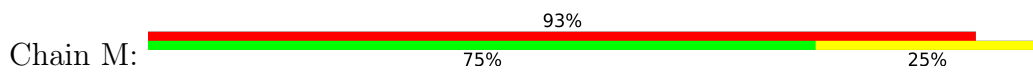
• Molecule 28: UPF0307 protein YjgA

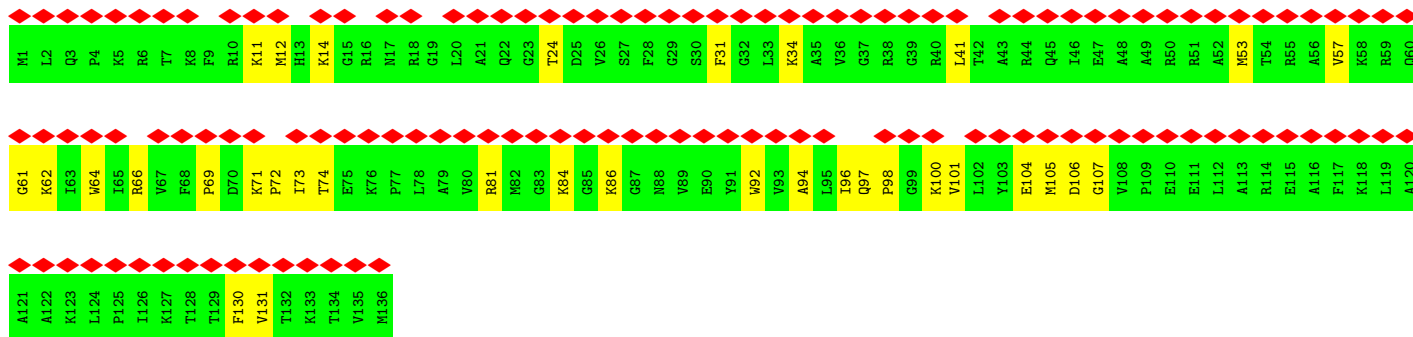


• Molecule 29: GTPase ObgE/CgtA

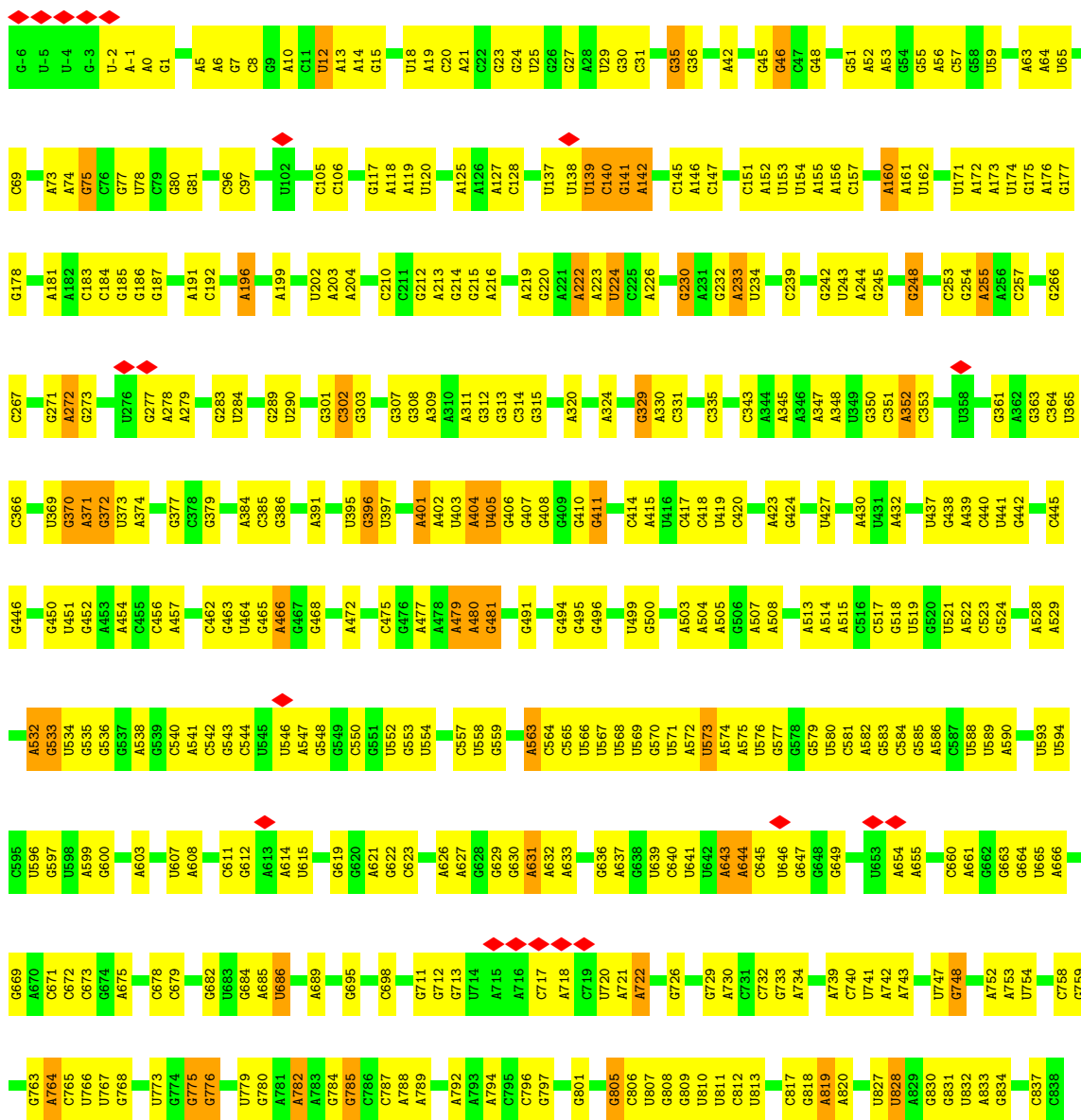


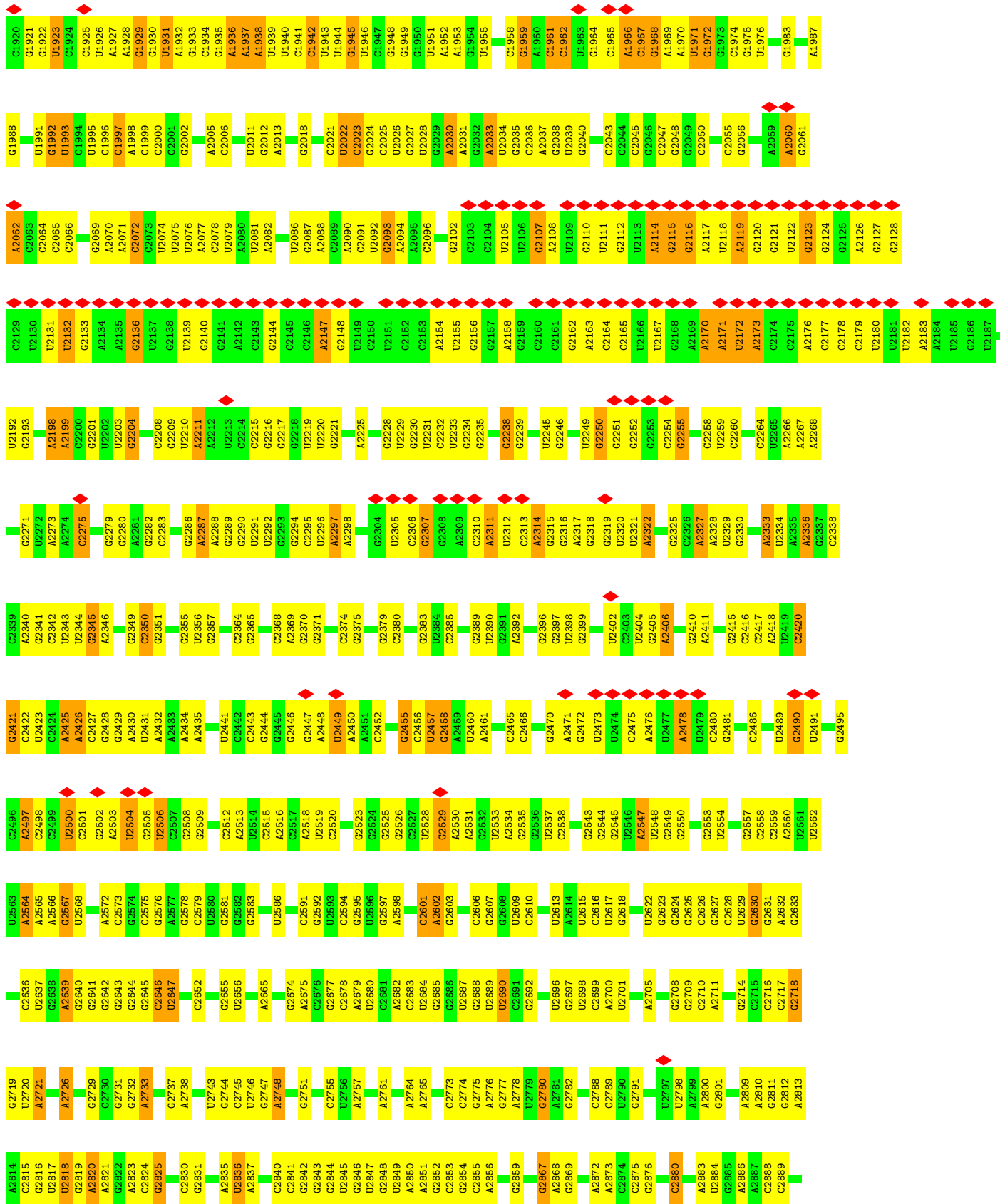
• Molecule 30: 50S ribosomal protein L16

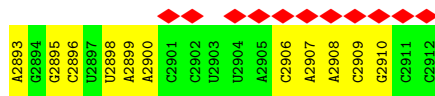




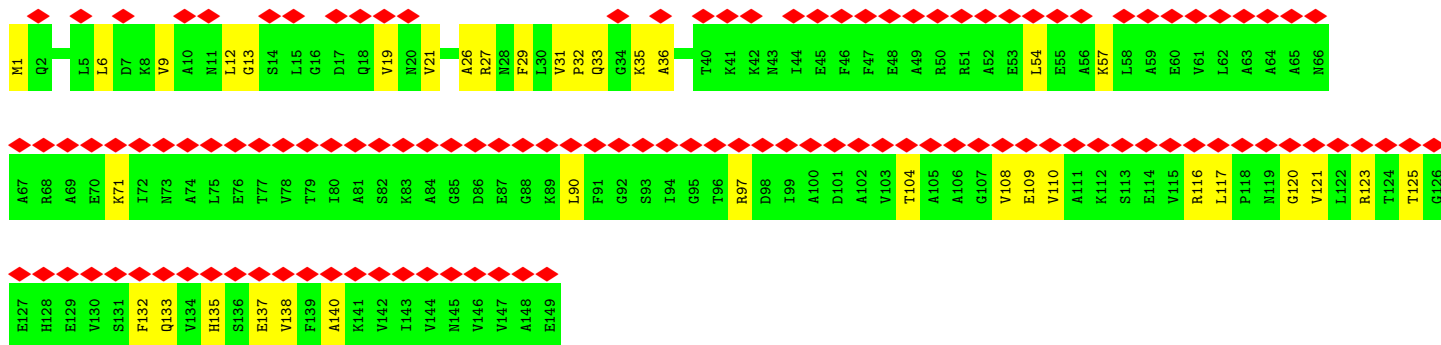
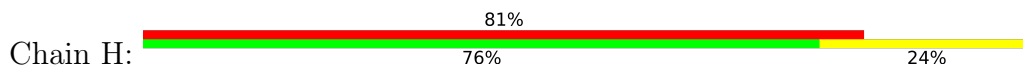
• Molecule 31: 23S ribosomal RNA



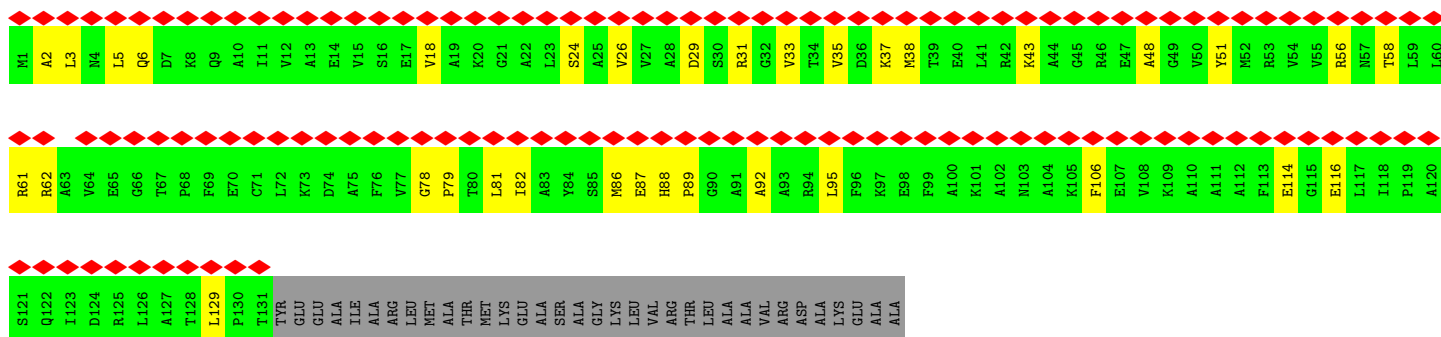
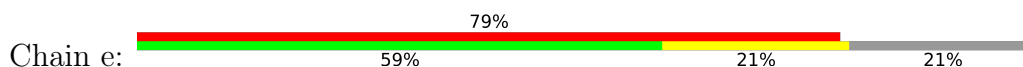




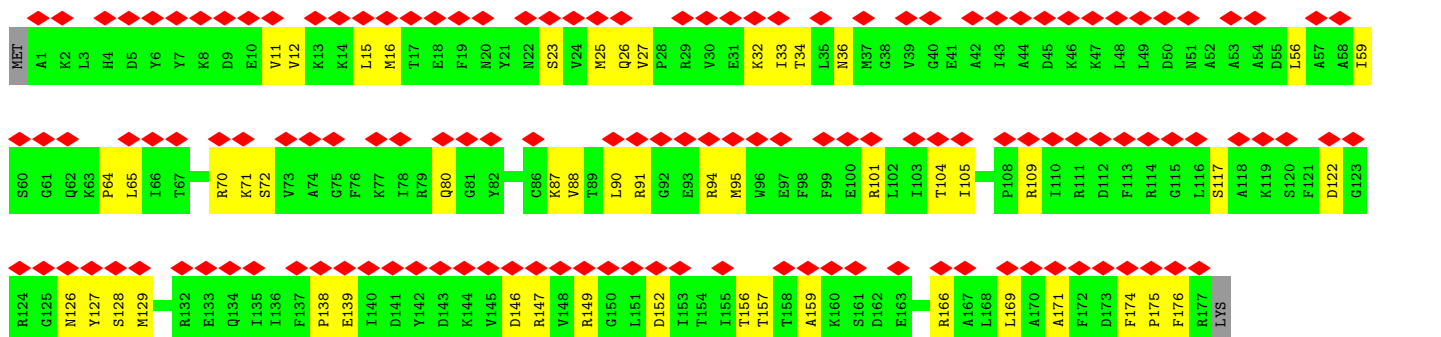
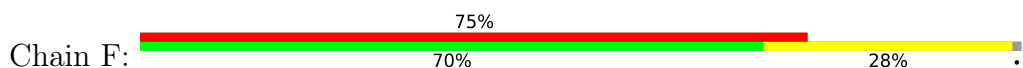
• Molecule 32: 50S ribosomal protein L9



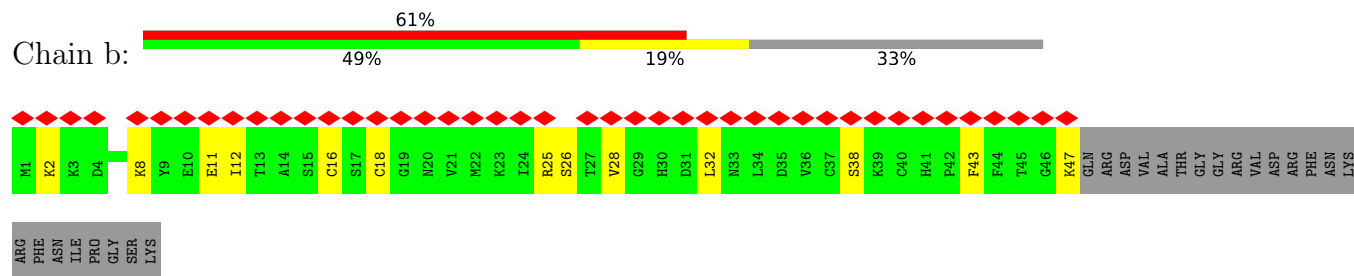
• Molecule 33: 50S ribosomal protein L10



• Molecule 34: 50S ribosomal protein L5



• Molecule 35: 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	22282	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	13.174	Depositor
Minimum map value	-5.976	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.789	Depositor
Recommended contour level	2.5	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: GDP, MG, ZN

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	0.12	0/2121	0.33	0/2852
2	D	0.12	0/1586	0.35	0/2134
3	E	0.09	0/1571	0.28	0/2113
4	G	0.11	0/1301	0.31	0/1764
5	J	0.10	0/1152	0.28	0/1551
6	L	0.13	0/1054	0.44	0/1403
7	N	0.13	0/973	0.37	0/1301
8	O	0.11	0/902	0.32	0/1209
9	Q	0.10	0/960	0.30	0/1278
10	R	0.14	0/829	0.39	0/1107
11	S	0.11	0/864	0.30	0/1156
12	T	0.11	0/744	0.32	0/994
13	U	0.12	0/787	0.36	0/1051
14	V	0.12	0/766	0.38	0/1025
15	W	0.13	0/582	0.39	0/769
16	X	0.11	0/635	0.30	0/848
17	Y	0.12	0/510	0.41	0/677
18	Z	0.12	0/453	0.36	0/605
19	0	0.12	0/450	0.38	0/599
20	1	0.12	0/416	0.32	0/554
21	2	0.12	0/380	0.36	0/498
22	B	0.07	0/2847	0.16	0/4440
23	I	0.12	0/1046	0.37	0/1410
24	K	0.13	0/947	0.37	0/1268
25	P	0.11	0/923	0.34	0/1234
26	6	0.14	0/787	0.40	0/1062
27	7	0.12	0/2590	0.33	0/3513
28	8	0.12	0/1292	0.34	0/1727
29	9	0.12	0/2626	0.36	0/3542
30	M	0.12	0/1093	0.34	0/1460
31	A	0.08	0/70038	0.19	0/109262
32	H	0.11	0/1121	0.34	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.11	0/1001	0.36	0/1350
34	F	0.12	0/1434	0.35	0/1926
35	b	0.11	0/371	0.30	0/496
All	All	0.09	0/107152	0.25	0/159693

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 [\(i\)](#)

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	C	2082	0	2157	57	0
2	D	1565	0	1616	51	0
3	E	1552	0	1619	41	0
4	G	1281	0	1324	38	0
5	J	1129	0	1162	26	0
6	L	1045	0	1117	36	0
7	N	960	0	1000	34	0
8	O	892	0	923	26	0
9	Q	947	0	1022	24	0
10	R	816	0	839	28	0
11	S	857	0	922	23	0
12	T	738	0	807	15	0
13	U	779	0	834	19	0
14	V	753	0	780	22	0
15	W	575	0	589	20	0
16	X	625	0	655	12	0
17	Y	509	0	543	11	0
18	Z	449	0	491	13	0
19	0	444	0	461	11	0
20	1	409	0	440	9	0
21	2	377	0	418	10	0
22	B	2548	0	1292	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	I	1032	0	1088	23	0
24	K	938	0	1012	27	0
25	P	911	0	957	32	0
26	6	780	0	783	19	0
27	7	2533	0	2549	72	0
28	8	1281	0	1335	35	0
29	9	2582	0	2606	60	0
30	M	1074	0	1157	30	0
31	A	62534	0	31452	1171	0
32	H	1110	0	1148	25	0
33	e	988	0	1025	22	0
34	F	1410	0	1447	38	0
35	b	364	0	362	12	0
36	9	28	0	12	0	0
37	9	1	0	0	0	0
37	A	1	0	0	0	0
38	b	1	0	0	0	0
39	2	1	0	0	0	0
39	A	17	0	0	0	0
39	B	1	0	0	0	0
39	C	3	0	0	0	0
39	D	1	0	0	1	0
39	F	1	0	0	1	0
39	N	2	0	0	0	0
39	S	1	0	0	0	0
All	All	98927	0	67944	1915	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 1915 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)
31:A:1093:G:N2	31:A:1098:A:H62	1.48	1.12
31:A:377:G:H1	31:A:397:U:H3	1.04	0.97
31:A:713:G:H21	31:A:718:A:H62	1.12	0.95
31:A:196:A:H61	31:A:831:G:H21	1.14	0.95
31:A:1093:G:H21	31:A:1098:A:N6	1.64	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
2	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
3	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
4	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100
5	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
6	L	141/144 (98%)	119 (84%)	22 (16%)	0	100	100
7	N	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
8	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
9	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
10	R	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
11	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
12	T	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
13	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
14	V	92/94 (98%)	92 (100%)	0	0	100	100
15	W	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
16	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
17	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
18	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
19	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
20	1	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
21	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
23	I	139/142 (98%)	116 (84%)	23 (16%)	0	100	100
24	K	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
25	P	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
26	6	100/105 (95%)	94 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	7	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
28	8	155/183 (85%)	152 (98%)	3 (2%)	0	100	100
29	9	336/390 (86%)	312 (93%)	24 (7%)	0	100	100
30	M	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
32	H	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
33	e	129/165 (78%)	113 (88%)	16 (12%)	0	100	100
34	F	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	b	45/70 (64%)	41 (91%)	4 (9%)	0	100	100
All	All	4280/4545 (94%)	4035 (94%)	245 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	216/218 (99%)	216 (100%)	0	100	100
2	D	164/164 (100%)	163 (99%)	1 (1%)	78	81
3	E	165/165 (100%)	165 (100%)	0	100	100
4	G	133/138 (96%)	133 (100%)	0	100	100
5	J	116/116 (100%)	116 (100%)	0	100	100
6	L	102/103 (99%)	102 (100%)	0	100	100
7	N	100/103 (97%)	100 (100%)	0	100	100
8	O	86/87 (99%)	86 (100%)	0	100	100
9	Q	89/90 (99%)	89 (100%)	0	100	100
10	R	84/84 (100%)	84 (100%)	0	100	100
11	S	93/93 (100%)	93 (100%)	0	100	100
12	T	80/84 (95%)	80 (100%)	0	100	100
13	U	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	V	78/78 (100%)	78 (100%)	0	100	100
15	W	56/63 (89%)	56 (100%)	0	100	100
16	X	67/68 (98%)	66 (98%)	1 (2%)	57	72
17	Y	55/55 (100%)	55 (100%)	0	100	100
18	Z	48/49 (98%)	48 (100%)	0	100	100
19	0	47/48 (98%)	47 (100%)	0	100	100
20	1	45/49 (92%)	45 (100%)	0	100	100
21	2	38/38 (100%)	38 (100%)	0	100	100
23	I	109/110 (99%)	109 (100%)	0	100	100
24	K	103/104 (99%)	103 (100%)	0	100	100
25	P	98/100 (98%)	98 (100%)	0	100	100
26	6	88/91 (97%)	88 (100%)	0	100	100
27	7	274/282 (97%)	273 (100%)	1 (0%)	84	84
28	8	135/161 (84%)	135 (100%)	0	100	100
29	9	273/321 (85%)	272 (100%)	1 (0%)	84	84
30	M	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	e	100/123 (81%)	100 (100%)	0	100	100
34	F	148/150 (99%)	148 (100%)	0	100	100
35	b	43/62 (69%)	43 (100%)	0	100	100
All	All	3539/3705 (96%)	3535 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	36	GLN
16	X	22	ASN
27	7	15	GLN
29	9	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
29	9	52	ASN

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Mol	Chain	Res	Type
29	9	113	GLN
33	e	9	GLN
10	R	18	GLN
10	R	11	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	B	118/120 (98%)	18 (15%)	0
31	A	2911/2919 (99%)	474 (16%)	17 (0%)
All	All	3029/3039 (99%)	492 (16%)	17 (0%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	B	15	A
22	B	16	G
22	B	30	C
22	B	35	C
22	B	36	C

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	2249	U
31	A	2425	A
31	A	1224	U
31	A	1606	C
31	A	1666	G

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	GDP	9	1001	37	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GDP	9	1001	37	-	3/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	1001	GDP	C5-C4	3.18	1.47	1.38
36	9	1001	GDP	C6-N1	-2.41	1.34	1.38
36	9	1001	GDP	C5-N7	-2.04	1.35	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	9	1001	GDP	C5-C4-N3	-6.18	118.55	128.39
36	9	1001	GDP	C2-N3-C4	5.05	121.01	112.30
36	9	1001	GDP	N9-C4-N3	4.53	135.01	125.95
36	9	1001	GDP	C6-C5-N7	3.26	136.23	130.29
36	9	1001	GDP	C4-C5-N7	-2.64	106.48	110.67

There are no chirality outliers.

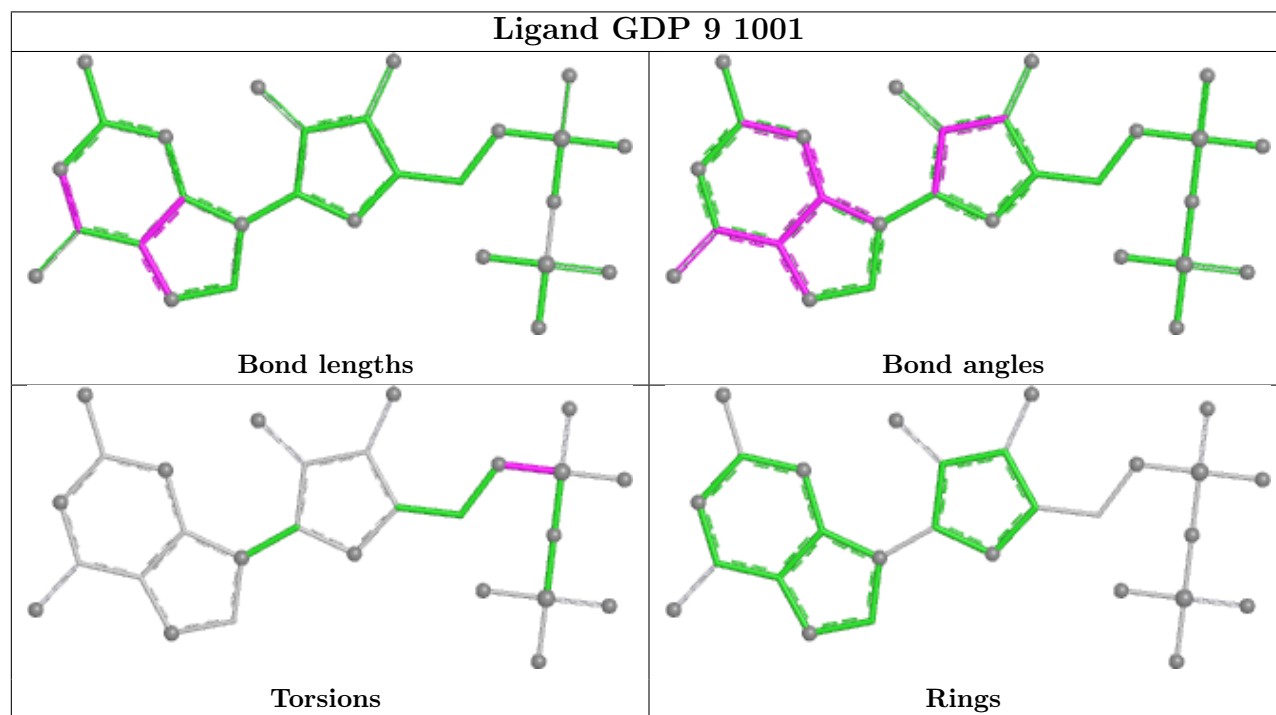
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	9	1001	GDP	C5'-O5'-PA-O3A
36	9	1001	GDP	C5'-O5'-PA-O1A
36	9	1001	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

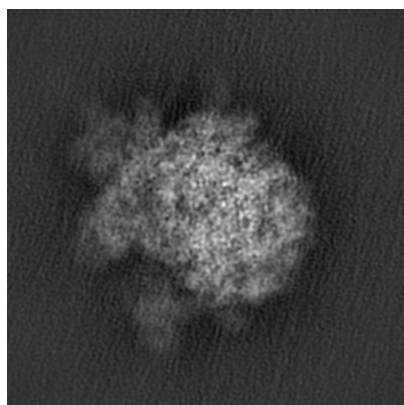
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12218. These allow visual inspection of the internal detail of the map and identification of artifacts.

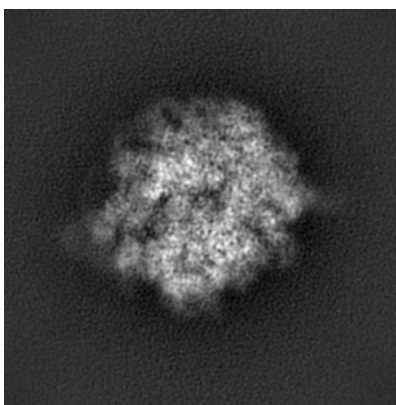
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

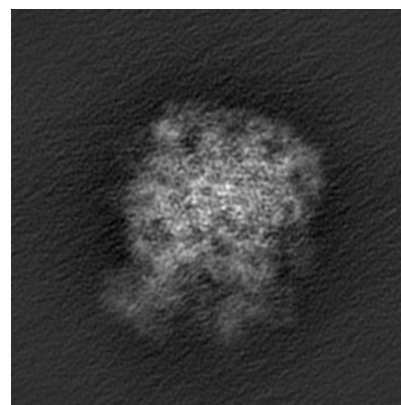
6.1.1 Primary map



X



Y

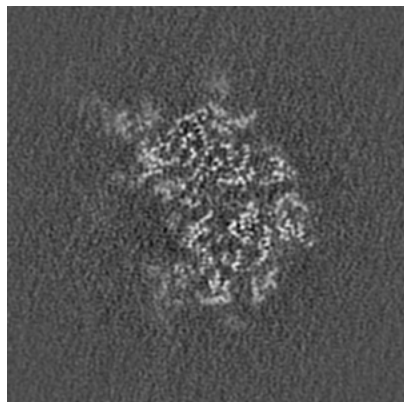


Z

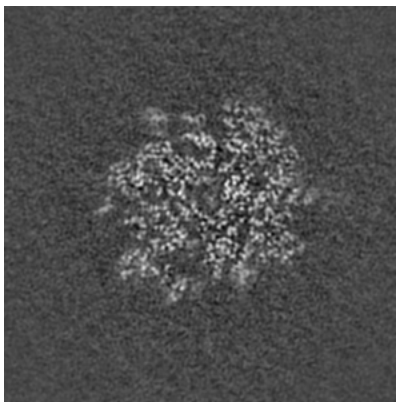
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

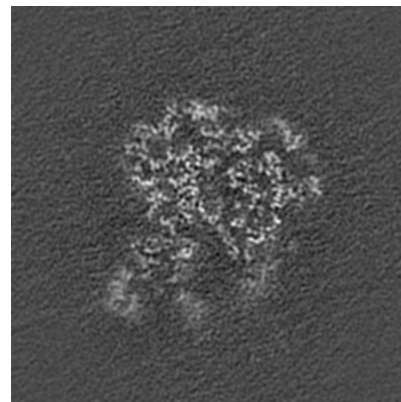
6.2.1 Primary map



X Index: 135



Y Index: 135

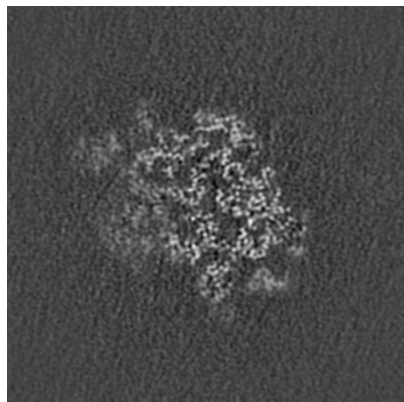


Z Index: 135

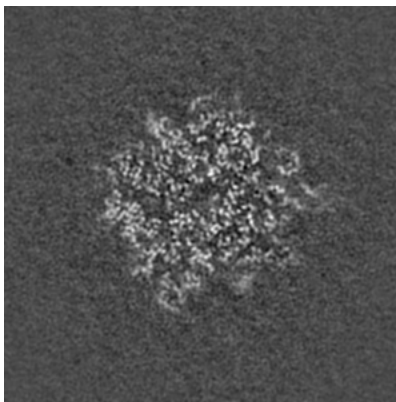
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

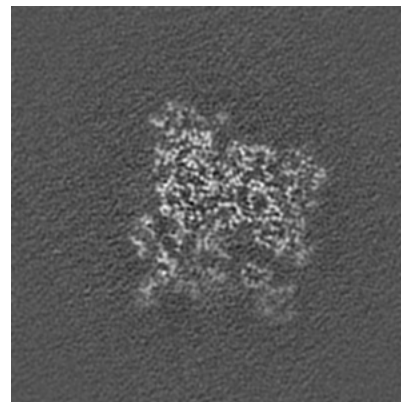
6.3.1 Primary map



X Index: 157



Y Index: 142

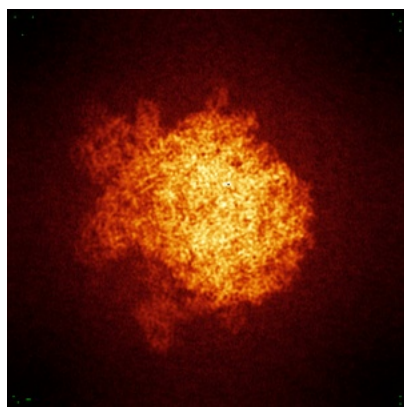


Z Index: 151

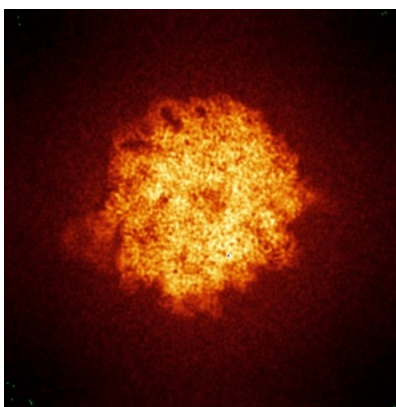
The images above show the largest variance slices of the map in three orthogonal directions.

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

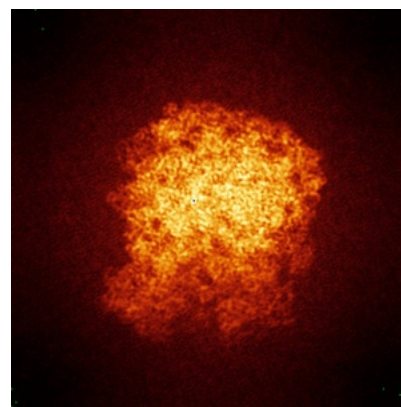
6.4.1 Primary map



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

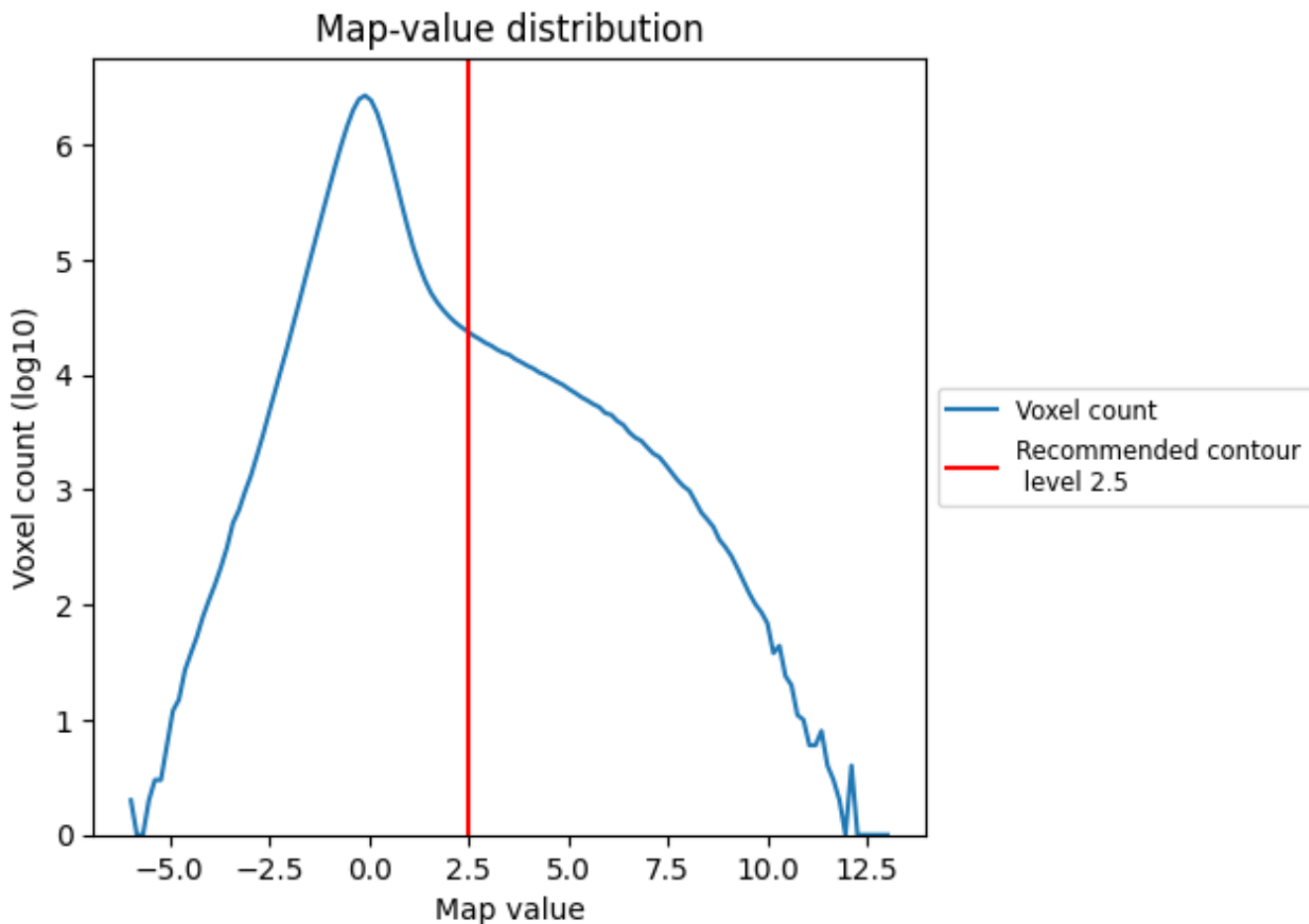
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

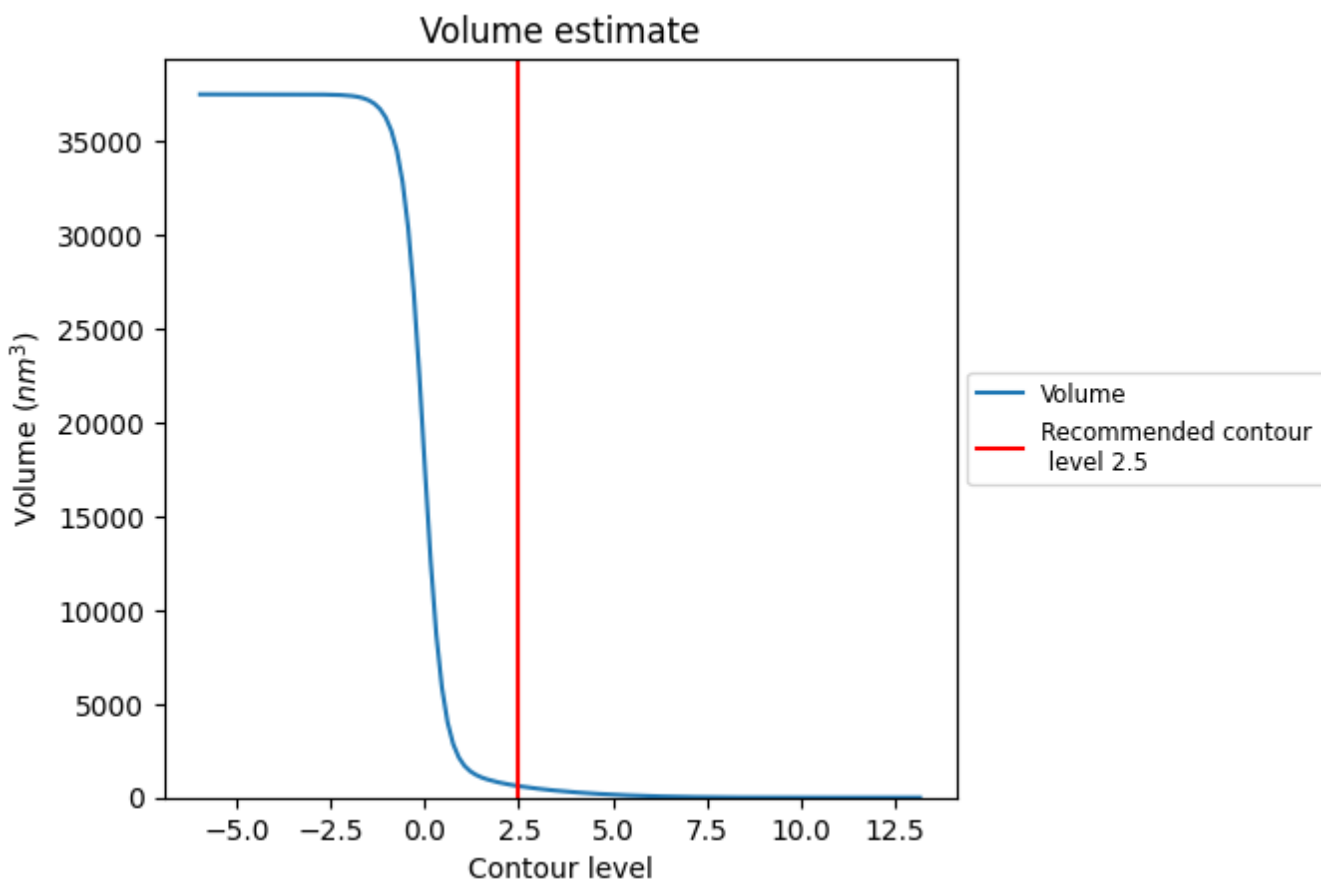
This section contains the results of statistical analysis of the map.

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.

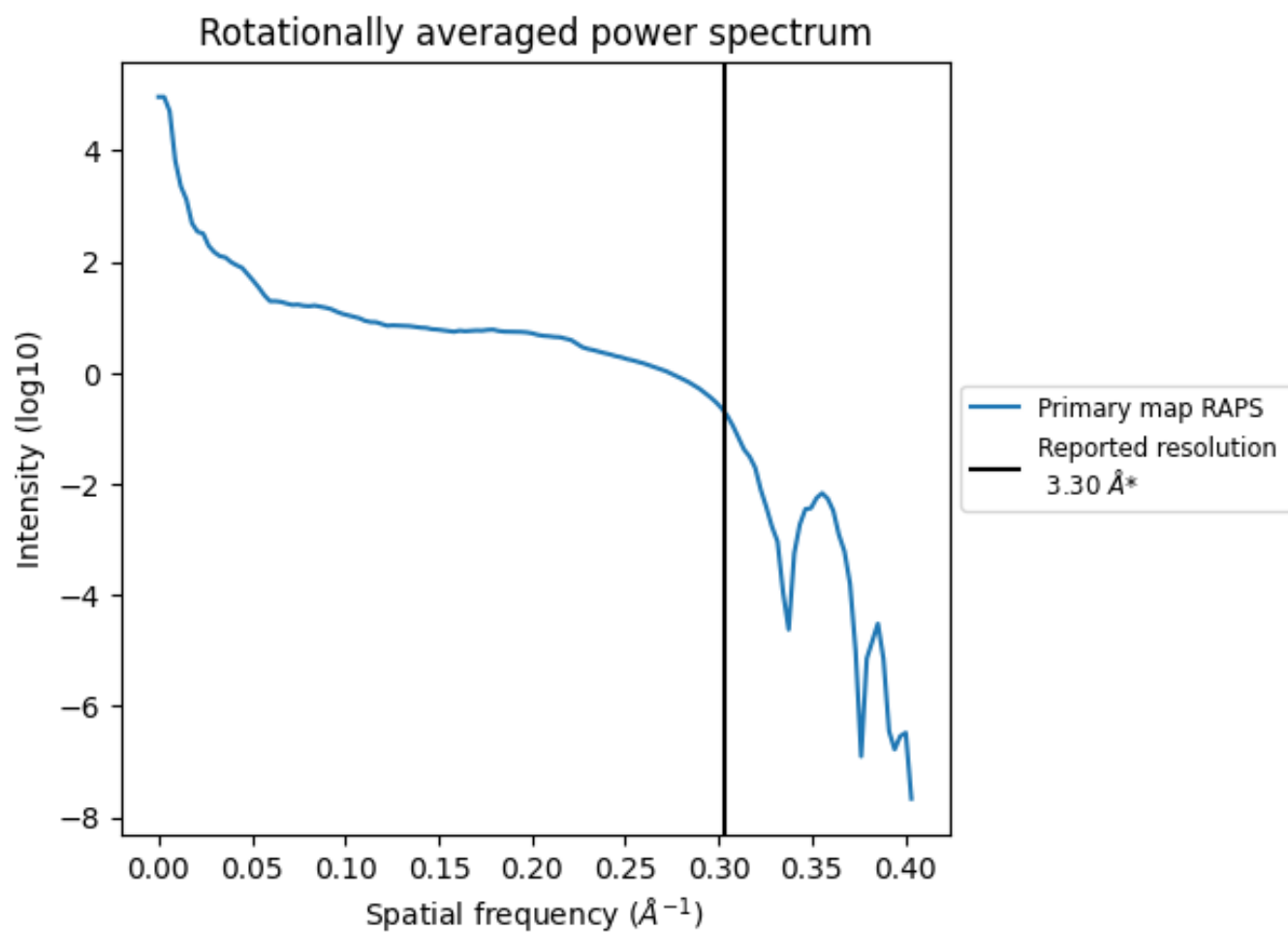
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 613 nm³; this corresponds to an approximate mass of 554 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](#)

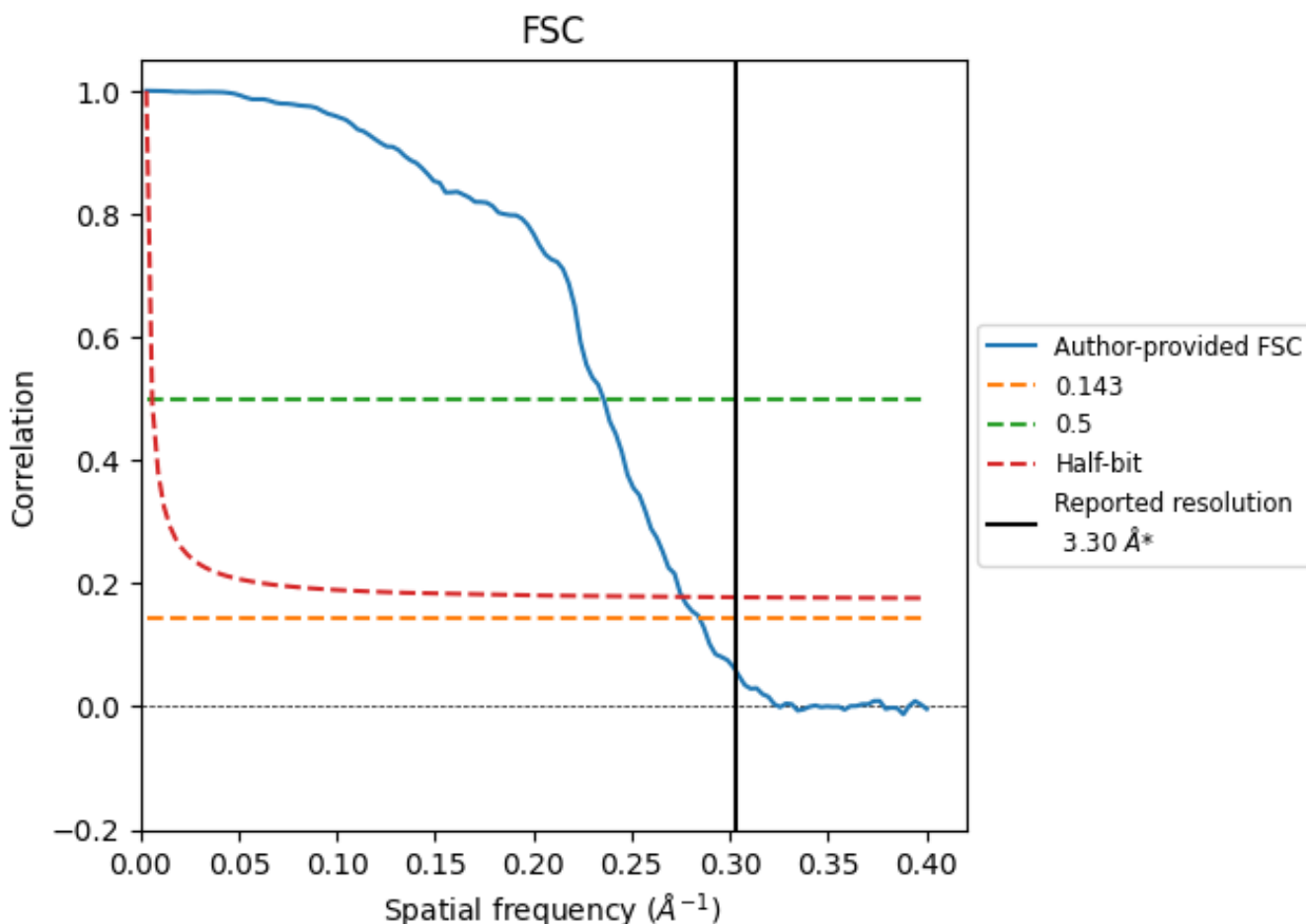


*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

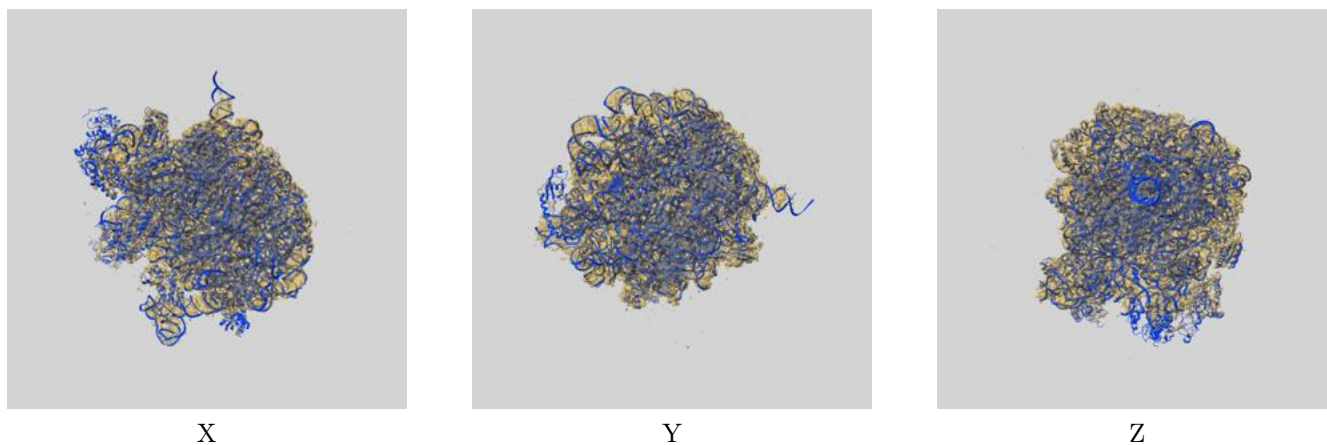
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.51	4.24	3.63
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

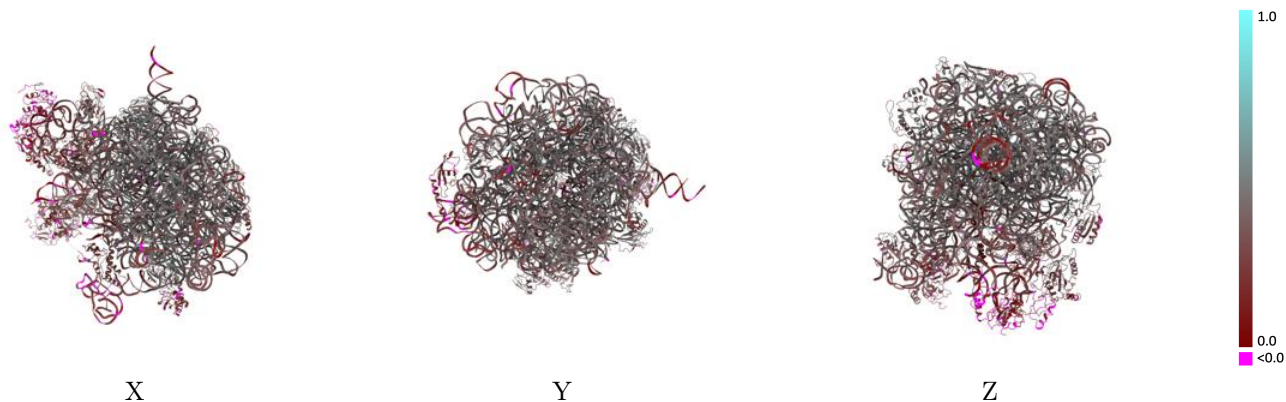
This section contains information regarding the fit between EMDB map EMD-12218 and PDB model 7BL5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.5 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](#)

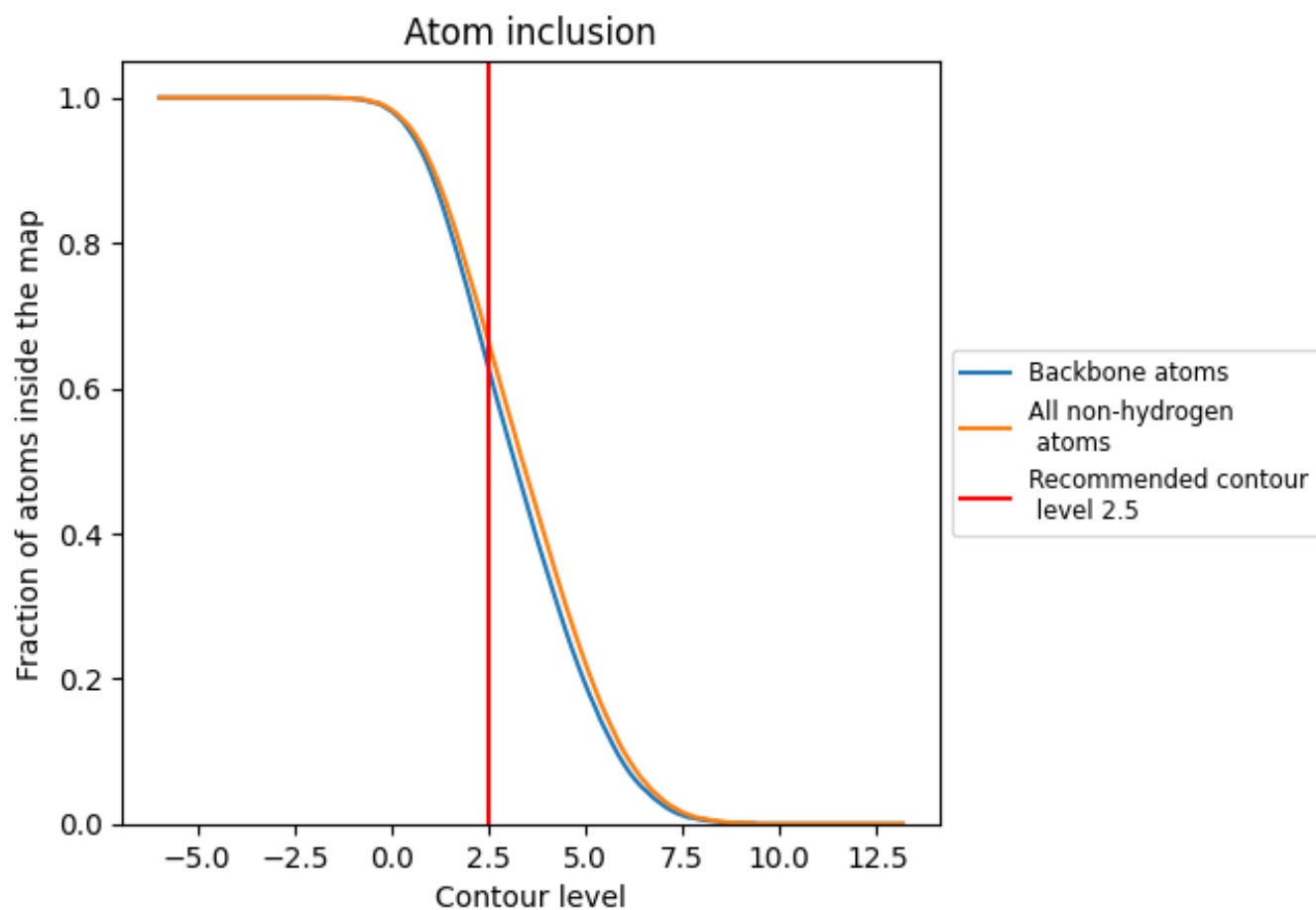


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 66% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3630
0	 0.6470	 0.4120
1	 0.3540	 0.3060
2	 0.6650	 0.4390
6	 0.4120	 0.3080
7	 0.2520	 0.2880
8	 0.3920	 0.3140
9	 0.3890	 0.3330
A	 0.7730	 0.3750
B	 0.6600	 0.3140
C	 0.6770	 0.4390
D	 0.6660	 0.4400
E	 0.5830	 0.3860
F	 0.2420	 0.2380
G	 0.4300	 0.3270
H	 0.1590	 0.1980
I	 0.0440	 0.0980
J	 0.6640	 0.4410
K	 0.6470	 0.4360
L	 0.5570	 0.3700
M	 0.1360	 0.2670
N	 0.6970	 0.4440
O	 0.4370	 0.3040
P	 0.6470	 0.4240
Q	 0.6720	 0.4340
R	 0.6610	 0.4270
S	 0.6720	 0.4340
T	 0.6150	 0.4050
U	 0.6150	 0.4020
V	 0.4490	 0.3160
W	 0.6080	 0.4200
X	 0.6640	 0.4450
Y	 0.5730	 0.3310
Z	 0.6640	 0.4210
b	 0.0910	 0.1770
e	 0.0240	 0.0660

