wwPDB EM Validation Summary Report

Nov 11, 2026 – 10:29 AM JST

PDB ID	:	24NS / pdb_000024ns
EMDB ID	:	EMD-69705
Title	:	M. smegmatis 50S ribosome in complex with RRF and EF-G1 (RRI IV)
Authors	:	Sengupta, J.; Dhur, A.; Baid, P.; Srinivasan, K.
Deposited on	:	2026-03-12
Resolution	:	6.60 Å(reported)
Based on initial model	:	5O61

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:

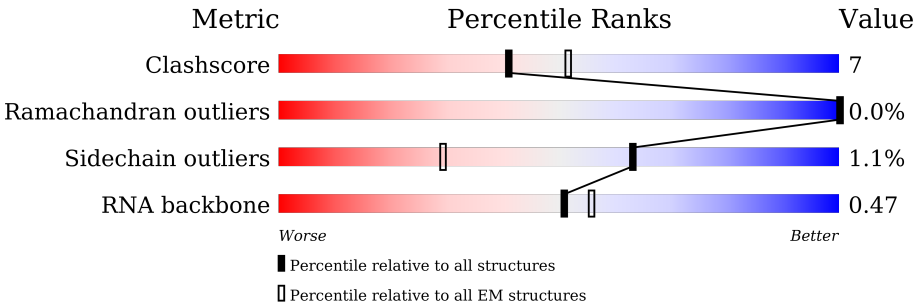
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

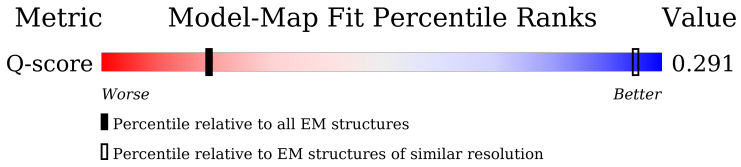
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.60 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.





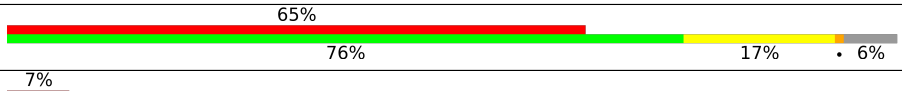
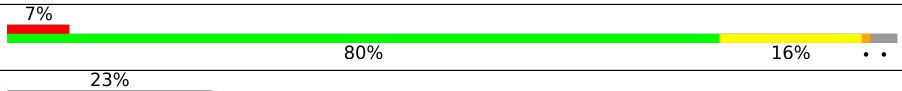
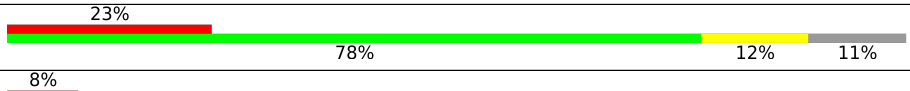
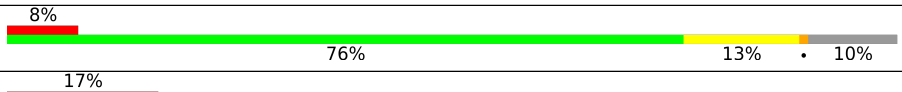
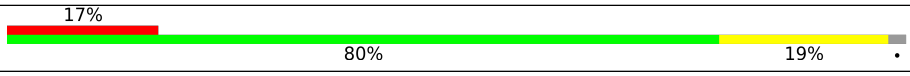
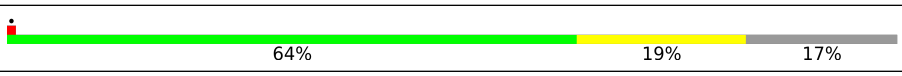
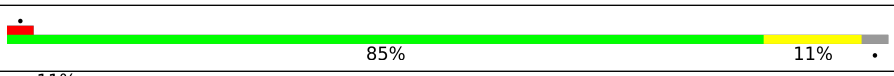
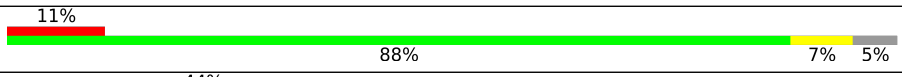
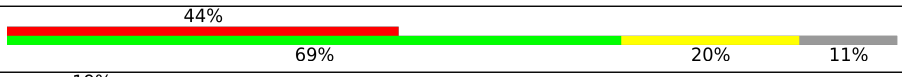
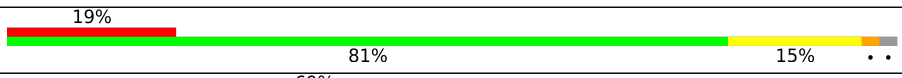
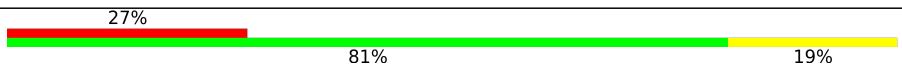
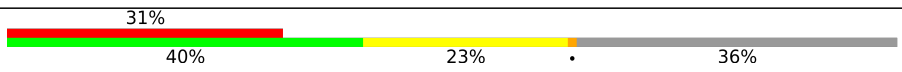
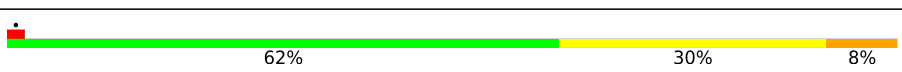
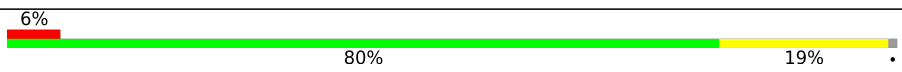
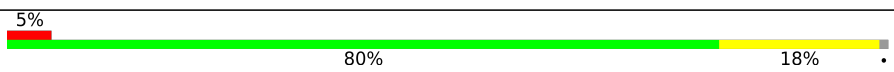
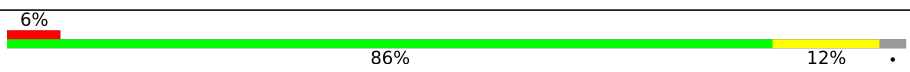
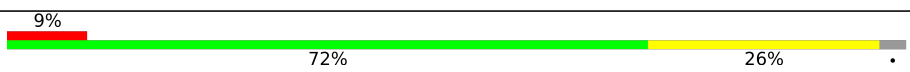
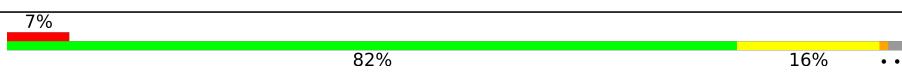
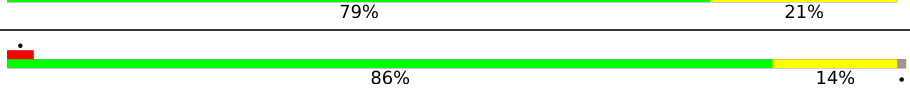
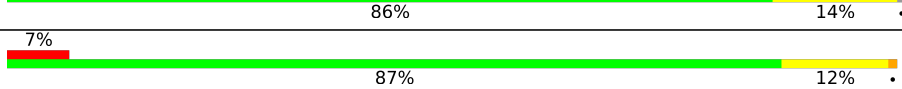
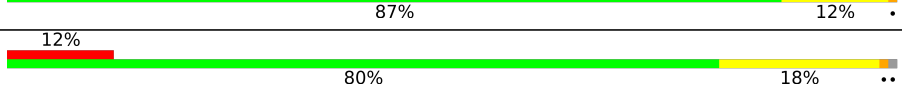
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	531 (6.10 - 7.10)

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 <=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	3	24	67% 92%
2	A	701	30% 70% 30%
3	B	118	66% 30%

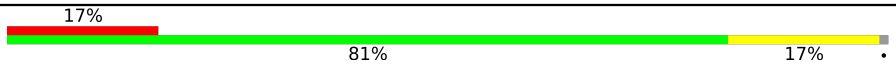
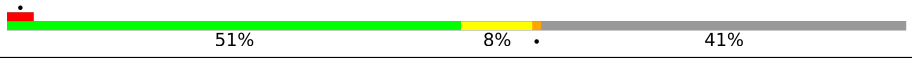
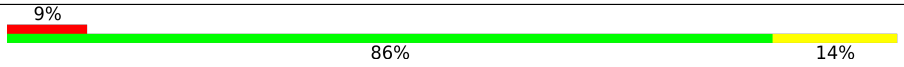
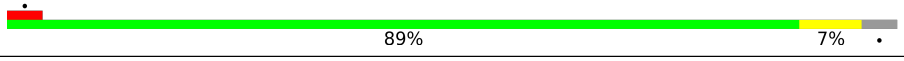
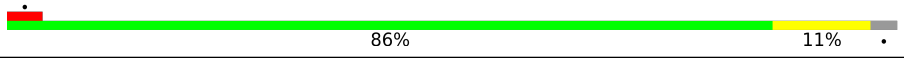
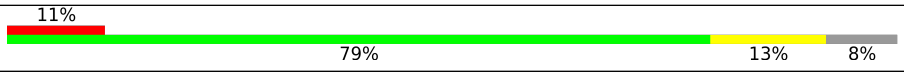
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Mol	Chain	Length	Quality of chain
4	C	185	
5	I	175	
6	J	142	
7	U	100	
8	W	215	
9	X	88	
10	Y	64	
11	Z	77	
12	a	61	
13	b	57	
14	c	55	
15	d	47	
16	e	64	
17	f	37	
18	g	75	
19	h	3120	
20	i	278	
21	j	217	
22	k	215	
23	l	187	
24	m	179	
25	n	151	
26	q	147	
27	r	122	
28	s	147	

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Mol	Chain	Length	Quality of chain
29	t	138	
30	u	199	
31	v	127	
32	w	113	
33	x	129	
34	y	103	
35	z	153	
36	1	105	

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 104614 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 bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	701	Total	C	N	O	S	0	0
			5441	3433	916	1071	21		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	185	Total	C	N	O	S	0	0
			1459	894	265	295	5		

- Molecule 5 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 6 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 7 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 8 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 9 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 10 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 11 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 12 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 13 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 14 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	49	Total 405	C 248	N 82	O 71	S 4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d	46	Total 377	C 225	N 97	O 54	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	e	63	Total 502	C 302	N 115	O 85	0	0

- Molecule 17 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	f	37	Total 299	C 181	N 66	O 47	S 5	0	0

- Molecule 18 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	g	48	Total 364	C 225	N 63	O 71	S 5	0	0

- Molecule 19 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	h	3119	Total 66981	C 29854	N 12313	O 21695	P 3119	0	0

- Molecule 20 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	275	Total 2110	C 1298	N 438	O 370	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	m	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 25 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	n	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 26 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 28 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	145	Total 1078	C 676	N 205	O 194	S 3	0	0

- Molecule 29 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	t	136	Total 1092	C 690	N 213	O 187	S 2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	u	118	Total 928	C 583	N 180	O 163	S 2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	v	126	Total 956	C 586	N 199	O 171	0	0

- Molecule 32 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	113	Total 907	C 570	N 171	O 165	S 1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	x	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 34 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	y	100	Total 754	C 478	N 137	O 139	0	0

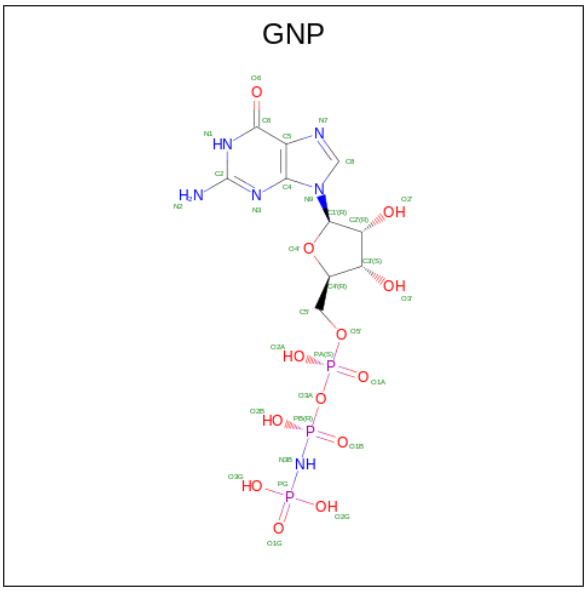
- Molecule 35 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	z	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 36 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 37 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	X	1	Total	Mg	0
			1	1	
38	h	2	Total	Mg	0
			2	2	
38	i	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms	AltConf
38	j	1	Total Mg 1 1	0
38	l	1	Total Mg 1 1	0
38	t	1	Total Mg 1 1	0
38	z	1	Total Mg 1 1	0

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

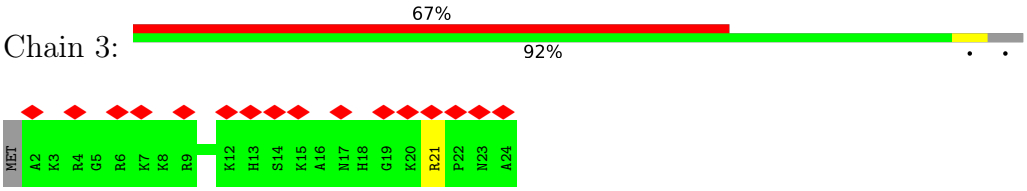
Mol	Chain	Residues	Atoms	AltConf
39	Y	1	Total Zn 1 1	0
39	c	1	Total Zn 1 1	0
39	f	1	Total Zn 1 1	0
39	g	1	Total Zn 1 1	0

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.

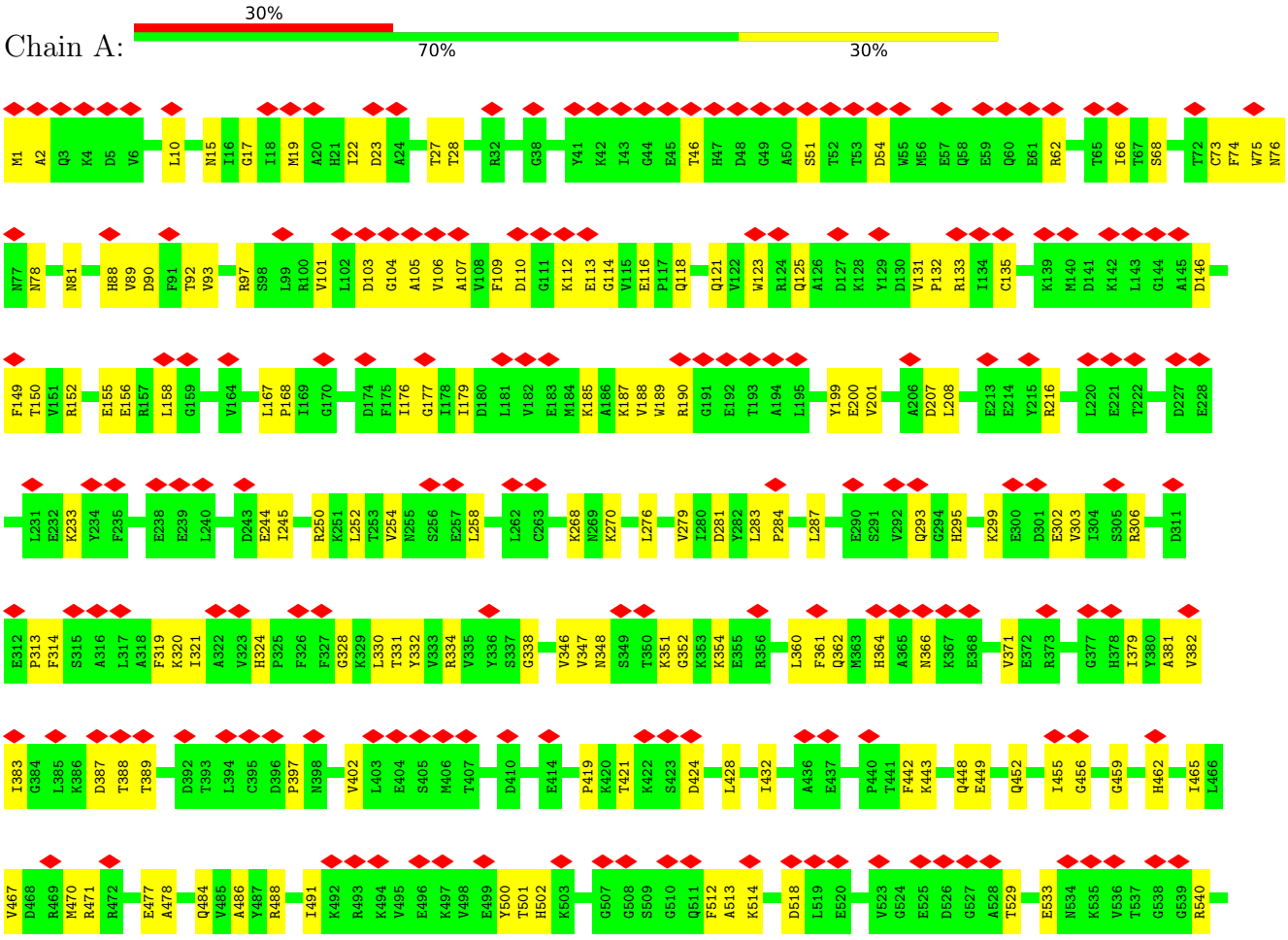
• Molecule 1: 50S ribosomal protein bL37

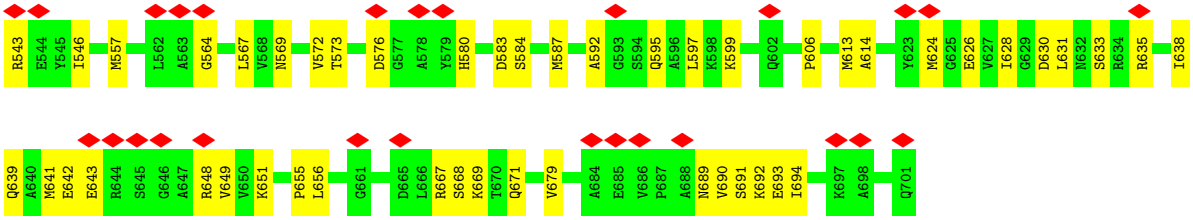
Chain 3:



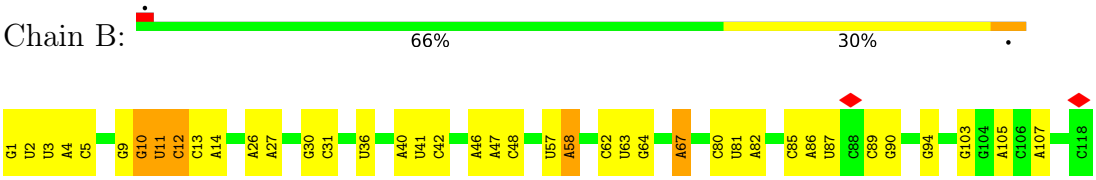
• Molecule 2: Elongation factor G

Chain A:

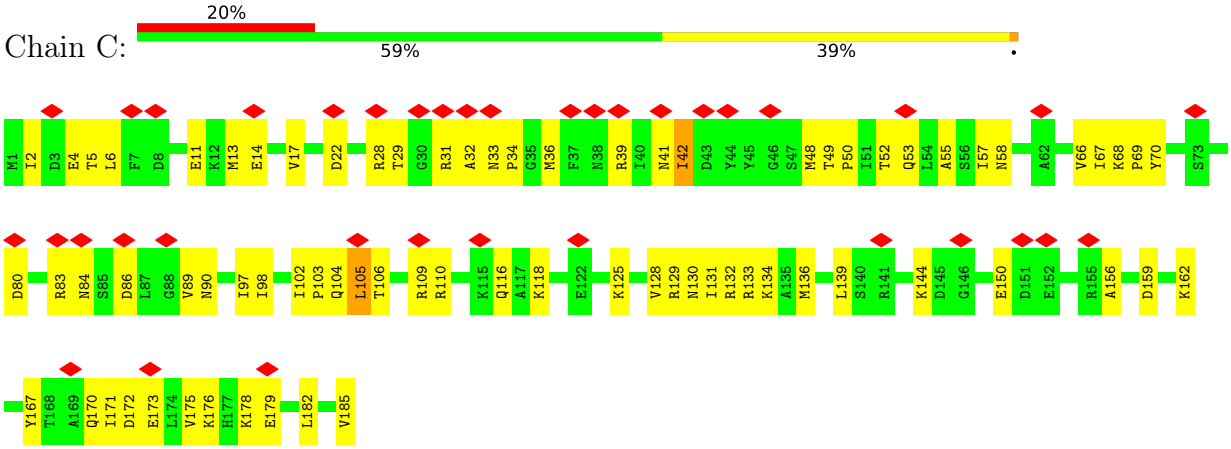




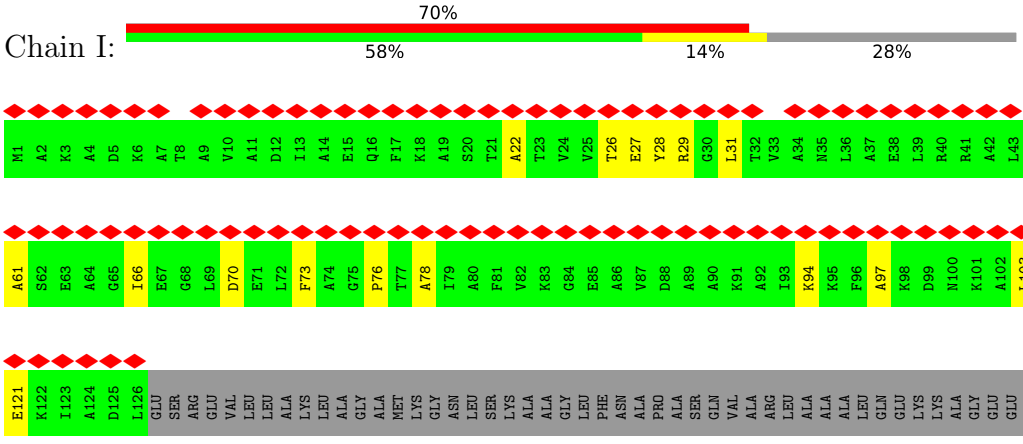
• Molecule 3: 5S ribosomal RNA



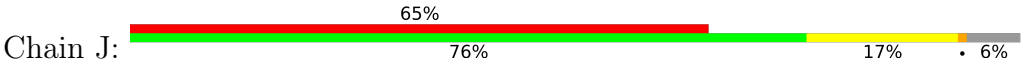
• Molecule 4: Ribosome-recycling factor



• Molecule 5: 50S ribosomal protein L10

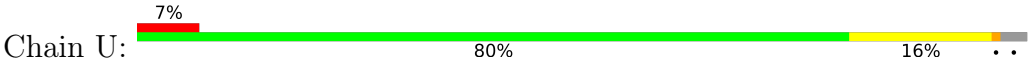


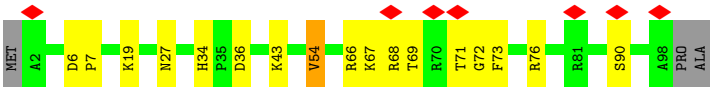
• Molecule 6: 50S ribosomal protein L11



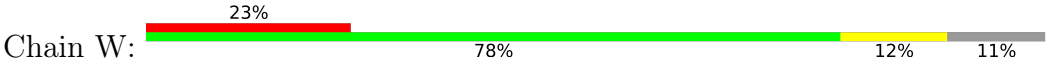


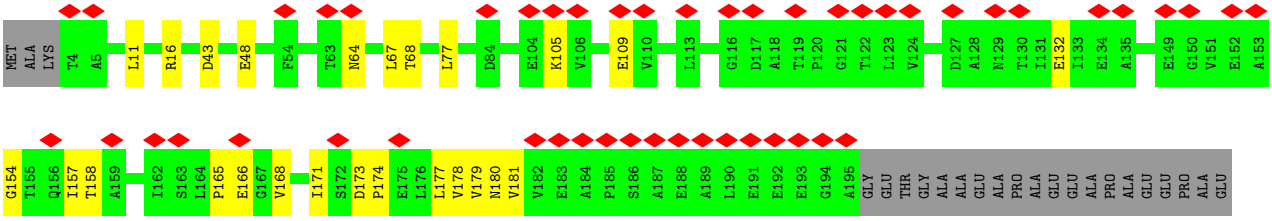
• Molecule 7: 50S ribosomal protein L23



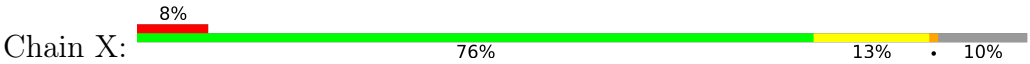


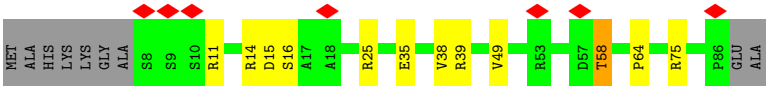
• Molecule 8: 50S ribosomal protein L25



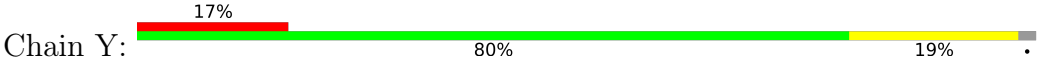


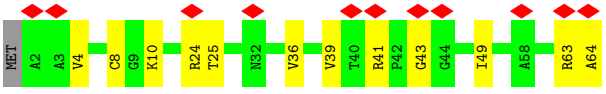
• Molecule 9: 50S ribosomal protein L27





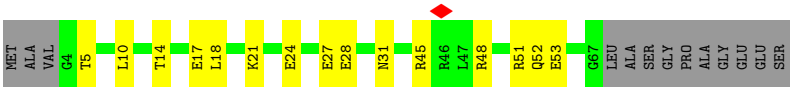
• Molecule 10: 50S ribosomal protein L28





• Molecule 11: 50S ribosomal protein L29





• Molecule 12: 50S ribosomal protein L30

Chain a:

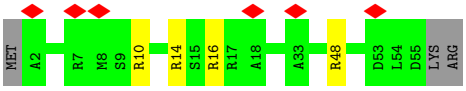




• Molecule 13: 50S ribosomal protein L32

Chain b:

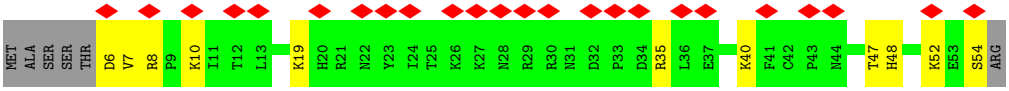




• Molecule 14: 50S ribosomal protein L33 1

Chain c:

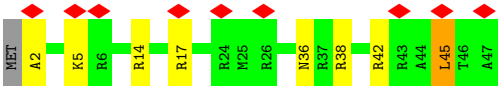




• Molecule 15: 50S ribosomal protein L34

Chain d:

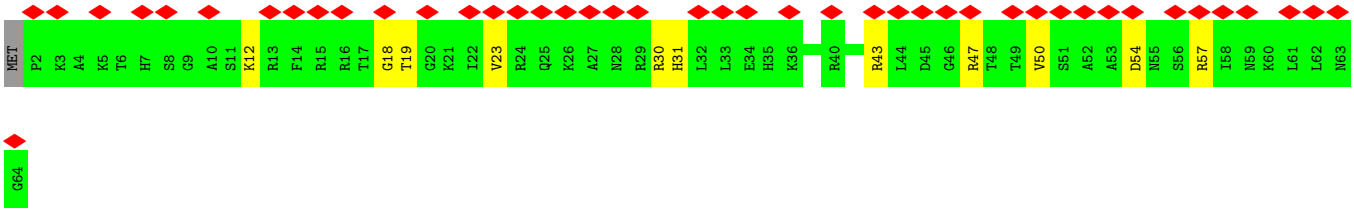




• Molecule 16: 50S ribosomal protein L35

Chain e:

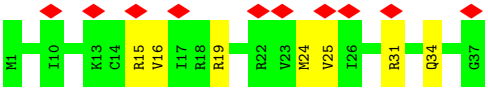




• Molecule 17: 50S ribosomal protein L36

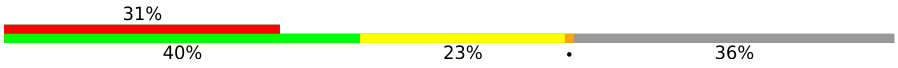
Chain f:

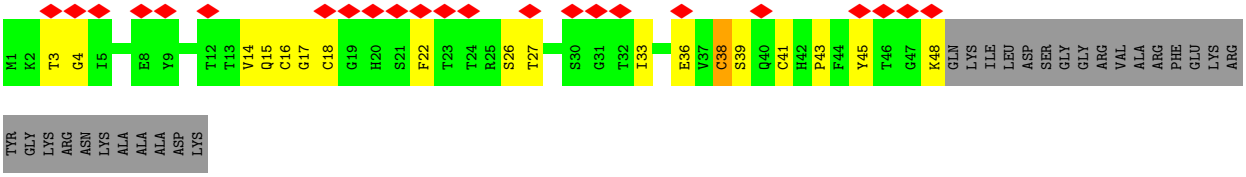




• Molecule 18: 50S ribosomal protein L31

Chain g:

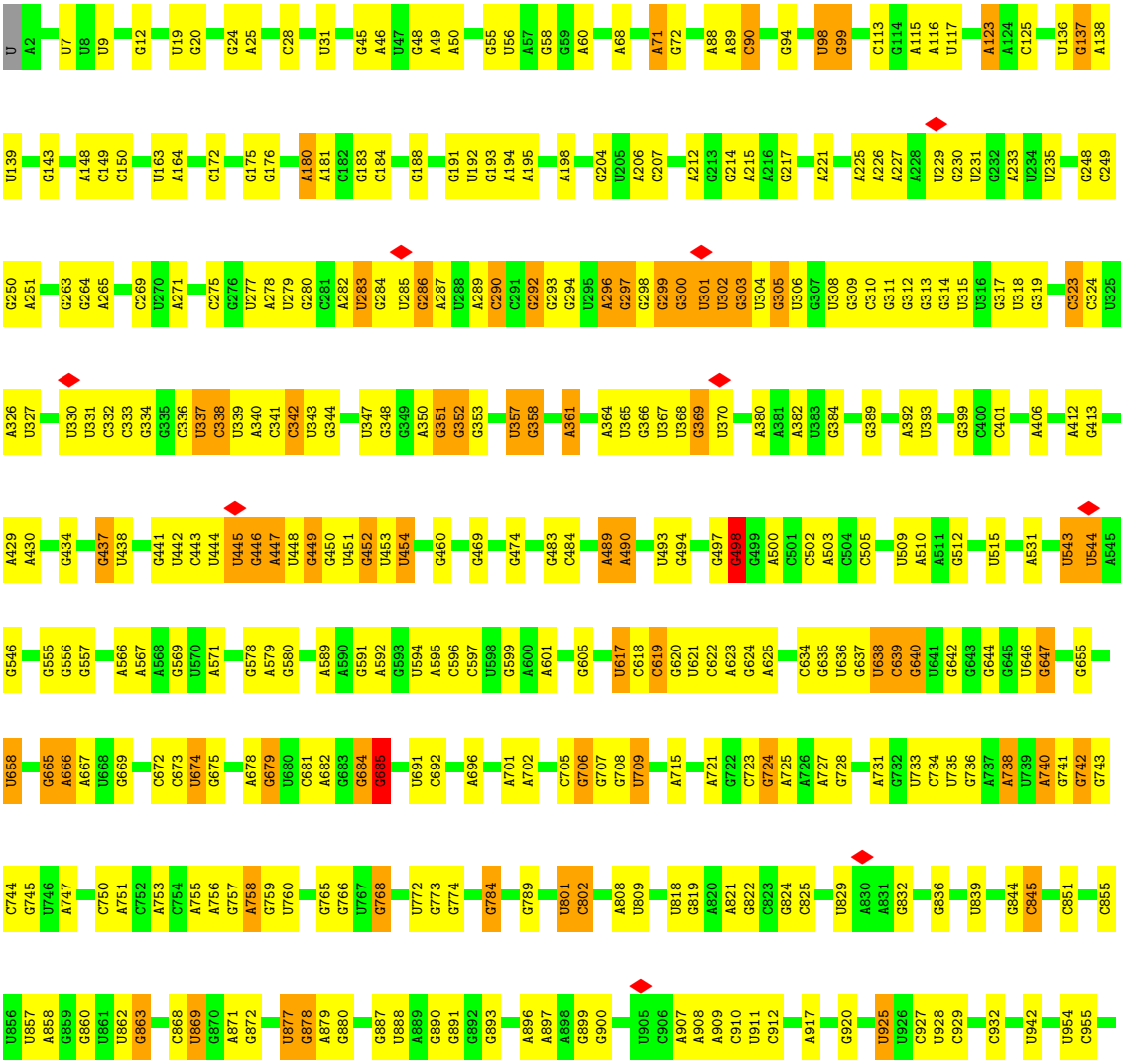


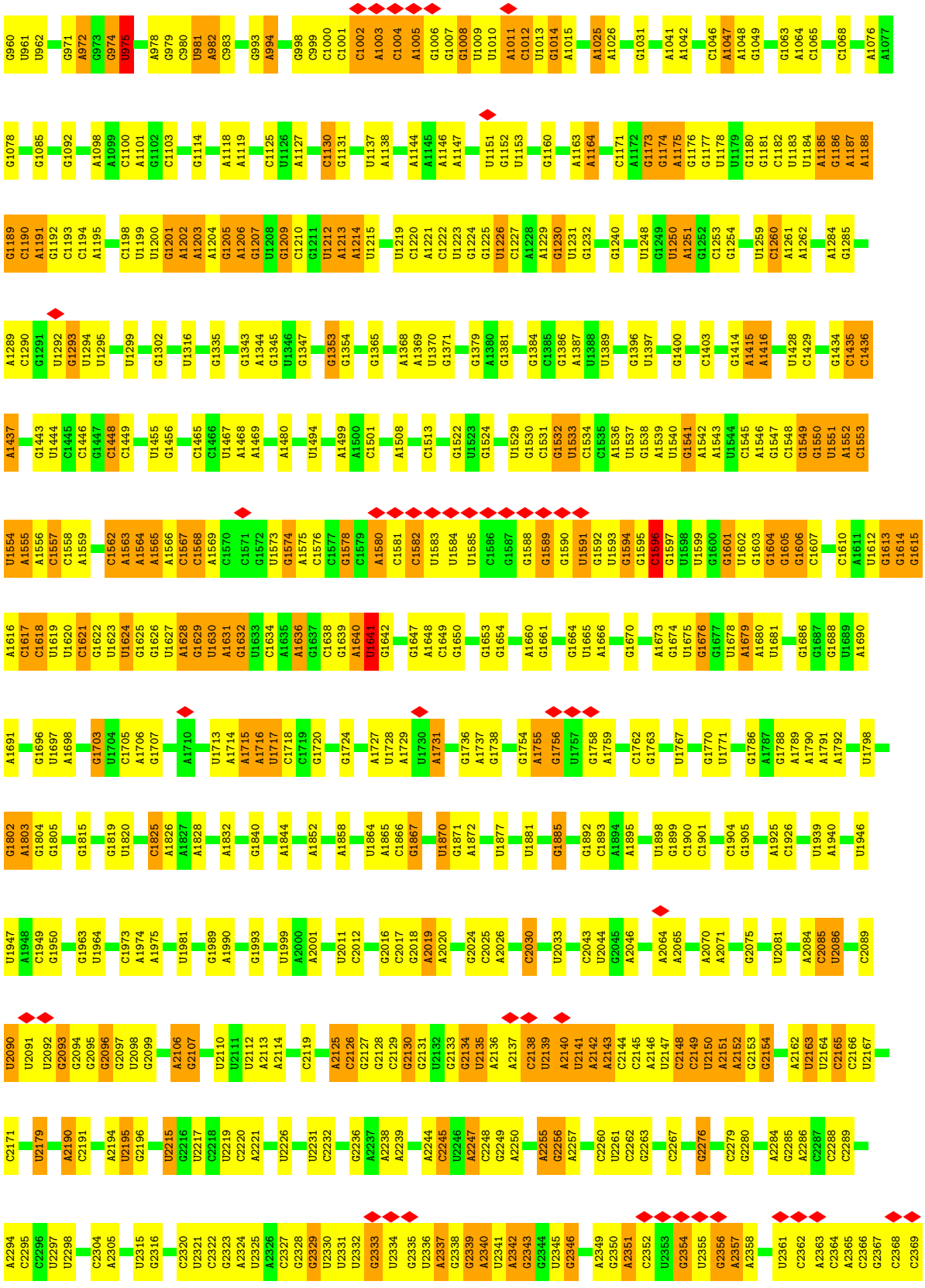


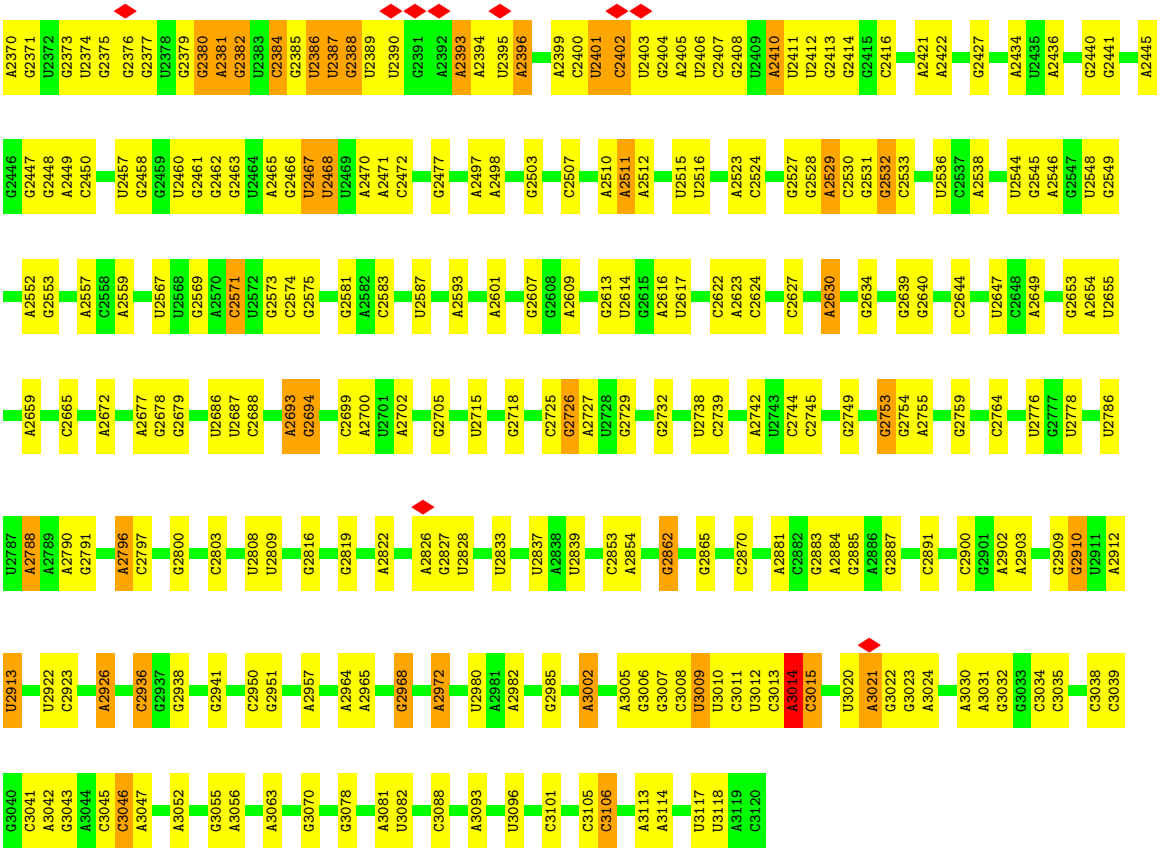
• Molecule 19: 23S ribosomal RNA

Chain h:





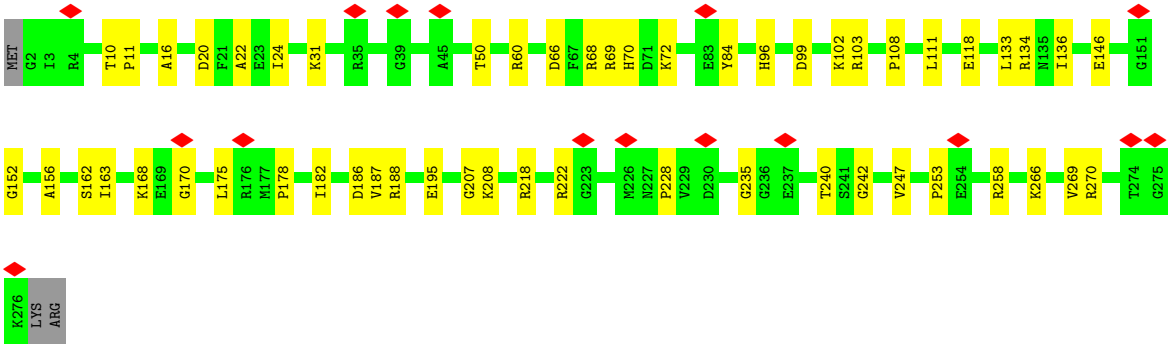




• Molecule 20: 50S ribosomal protein L2

Chain i:

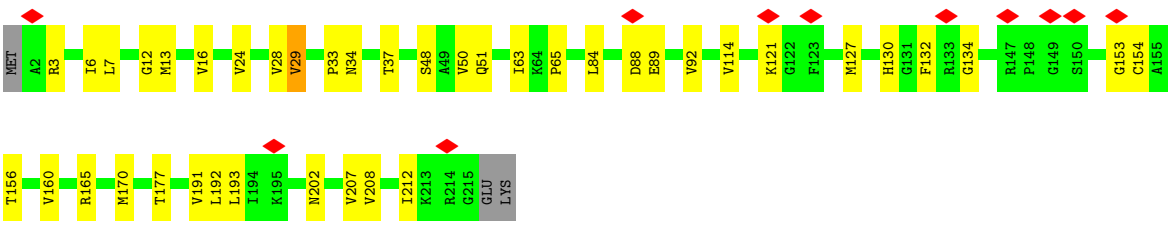




• Molecule 21: 50S ribosomal protein L3

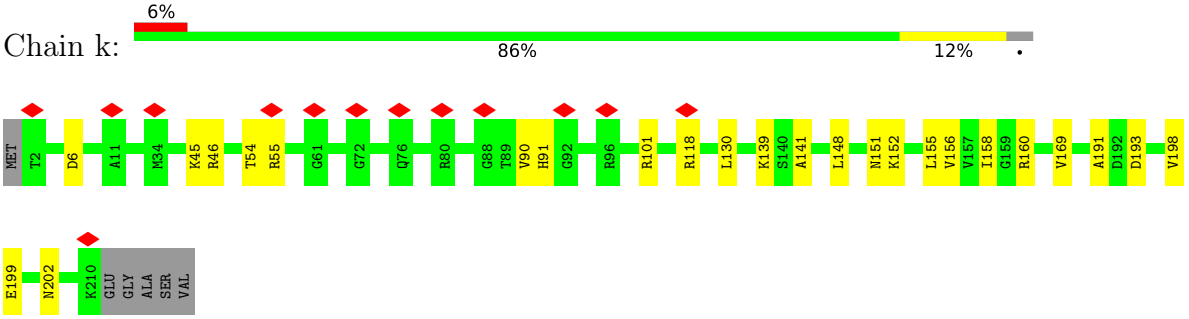
Chain j:





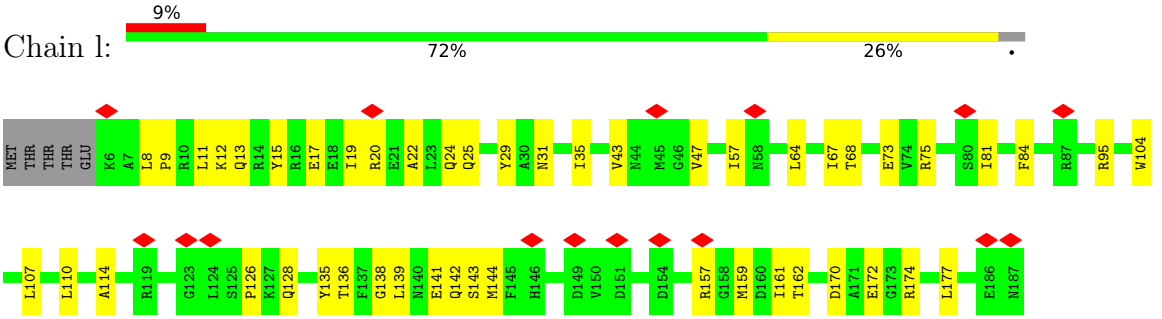
• Molecule 22: 50S ribosomal protein L4

Chain k:



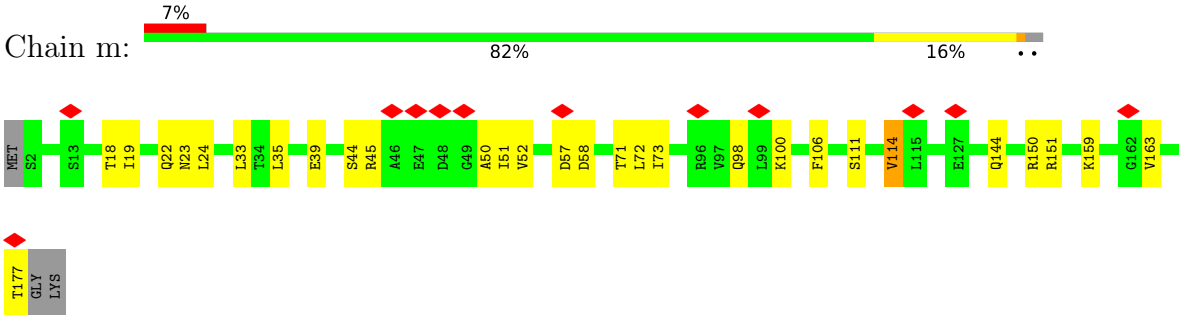
• Molecule 23: 50S ribosomal protein L5

Chain l:



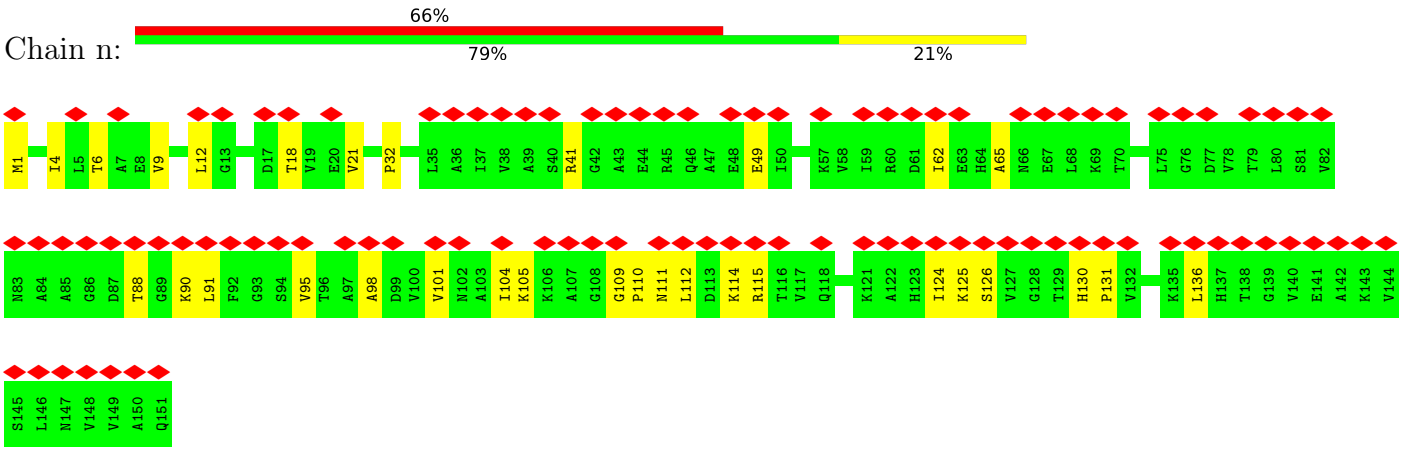
• Molecule 24: 50S ribosomal protein L6

Chain m:



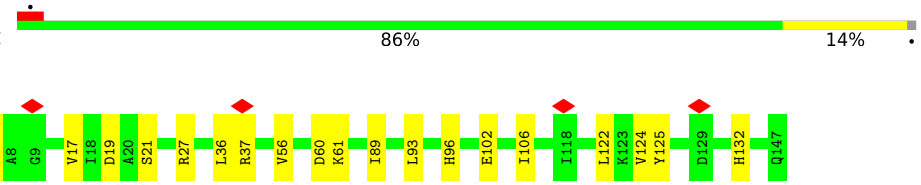
• Molecule 25: 50S ribosomal protein L9

Chain n:



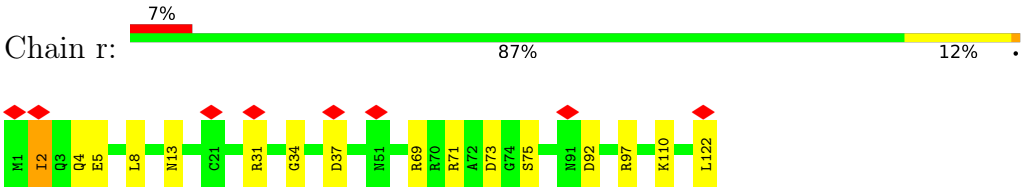
• Molecule 26: 50S ribosomal protein L13

Chain q:



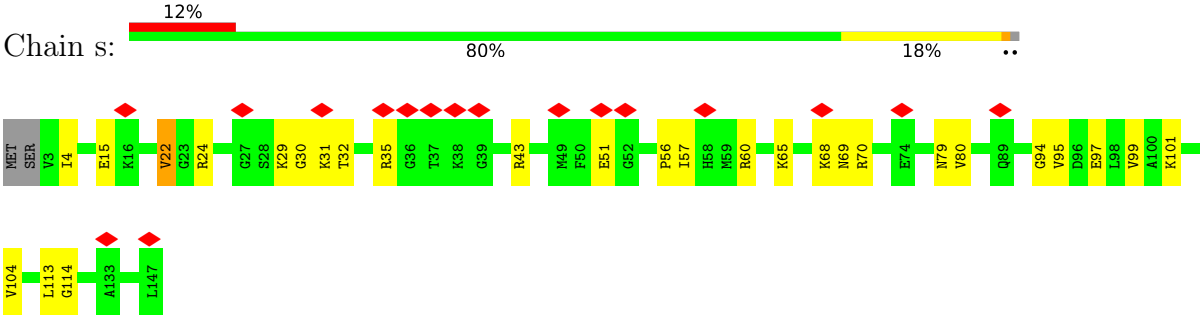
• Molecule 27: 50S ribosomal protein L14

Chain r:



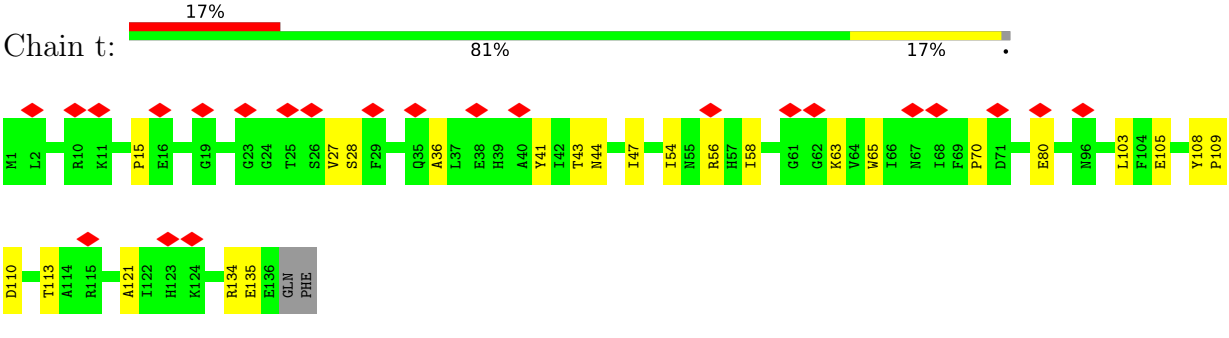
• Molecule 28: 50S ribosomal protein L15

Chain s:



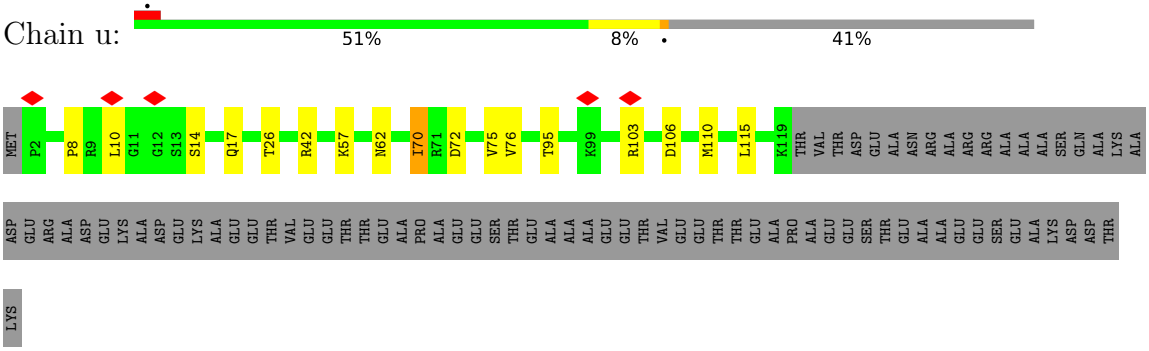
• Molecule 29: 50S ribosomal protein L16

Chain t:



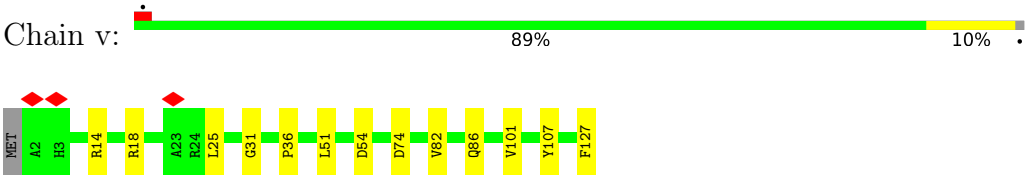
• Molecule 30: 50S ribosomal protein L17

Chain u:



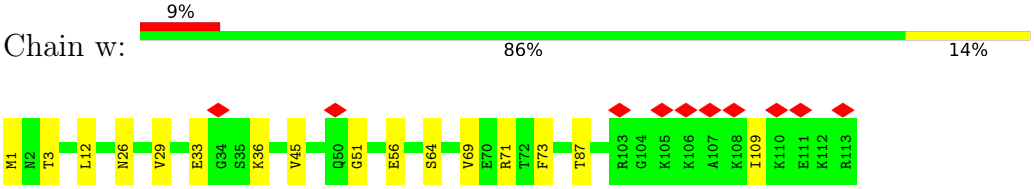
• Molecule 31: 50S ribosomal protein L18

Chain v:



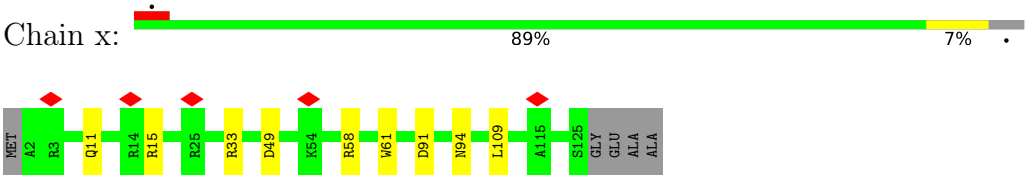
• Molecule 32: 50S ribosomal protein L19

Chain w:



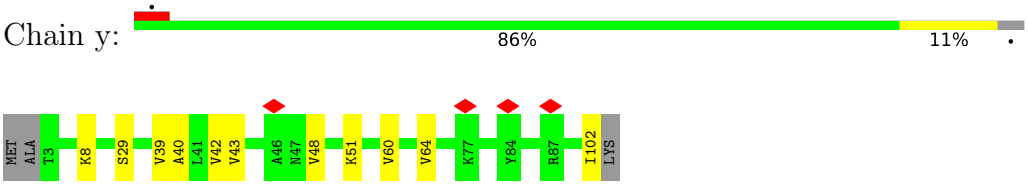
• Molecule 33: 50S ribosomal protein L20

Chain x:



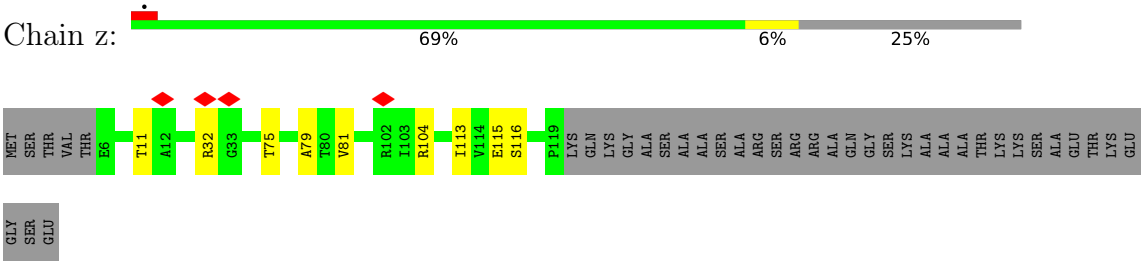
• Molecule 34: 50S ribosomal protein L21

Chain y:



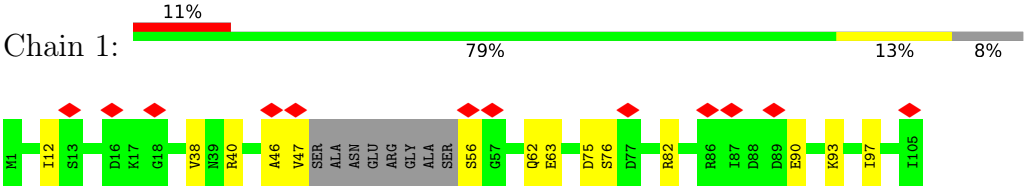
• Molecule 35: 50S ribosomal protein L22

Chain z:



• Molecule 36: Large ribosomal subunit protein uL24

Chain 1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15686	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20.82	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0203	Depositor
Map size (Å)	449.40002, 449.40002, 449.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 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	3	0.44	0/191	0.51	0/247
2	A	0.15	0/5536	0.30	0/7489
3	B	0.73	0/2821	0.82	2/4396 (0.0%)
4	C	0.28	0/1472	0.42	0/1976
5	I	0.12	0/925	0.29	0/1246
6	J	0.15	0/1006	0.33	0/1364
7	U	0.40	0/766	0.43	0/1030
8	W	0.23	0/1443	0.33	0/1970
9	X	0.45	0/595	0.40	0/798
10	Y	0.41	0/478	0.44	0/641
11	Z	0.36	0/534	0.37	0/713
12	a	0.42	0/477	0.38	0/640
13	b	0.41	0/427	0.36	0/572
14	c	0.20	0/413	0.36	0/553
15	d	0.44	0/380	0.38	0/500
16	e	0.20	0/507	0.36	0/672
17	f	0.40	0/303	0.37	0/401
18	g	0.15	0/372	0.32	0/503
19	h	1.01	1/75001 (0.0%)	0.92	58/117027 (0.0%)
20	i	0.44	0/2153	0.43	0/2895
21	j	0.45	0/1609	0.46	0/2165
22	k	0.41	0/1592	0.44	0/2153
23	l	0.20	0/1467	0.39	0/1973
24	m	0.25	0/1369	0.37	0/1848
25	n	0.14	0/1027	0.34	0/1398
26	q	0.41	0/1157	0.40	0/1567
27	r	0.39	0/946	0.42	0/1268
28	s	0.37	0/1091	0.50	2/1457 (0.1%)
29	t	0.38	0/1118	0.38	0/1506
30	u	0.44	0/945	0.50	0/1267
31	v	0.28	0/966	0.34	0/1298
32	w	0.39	0/921	0.42	0/1236

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	x	0.45	0/1000	0.40	0/1341
34	y	0.42	0/764	0.37	0/1030
35	z	0.40	0/887	0.44	0/1204
36	1	0.35	0/738	0.36	0/987
All	All	0.85	1/113397 (0.0%)	0.81	62/169331 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	1302	G	C8-N7	-5.06	1.27	1.30

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	h	338	C	N3-C2-O2	-8.53	115.93	121.90
19	h	2245	C	N1-C2-O2	8.48	123.99	118.90
19	h	617	U	C2-N1-C1'	8.35	127.72	117.70
19	h	1012	C	C2-N1-C1'	8.08	127.69	118.80
19	h	1596	C	N1-C2-O2	8.00	123.70	118.90

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	3	189	0	205	1	0
2	A	5441	0	5422	141	0
3	B	2522	0	1285	16	0
4	C	1459	0	1478	53	0
5	I	918	0	959	18	0
6	J	990	0	1021	19	0
7	U	756	0	802	10	0
8	W	1428	0	1443	15	0
9	X	586	0	601	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	470	0	480	10	0
11	Z	531	0	541	12	0
12	a	474	0	500	5	0
13	b	423	0	463	7	0
14	c	405	0	407	6	0
15	d	377	0	411	8	0
16	e	502	0	541	11	0
17	f	299	0	321	7	0
18	g	364	0	348	12	0
19	h	66981	0	33700	670	0
20	i	2110	0	2165	37	0
21	j	1587	0	1630	27	0
22	k	1569	0	1607	22	0
23	l	1445	0	1476	33	0
24	m	1348	0	1399	19	0
25	n	1018	0	988	20	0
26	q	1130	0	1167	14	0
27	r	938	0	1000	13	0
28	s	1078	0	1151	22	0
29	t	1092	0	1128	13	0
30	u	928	0	972	13	0
31	v	956	0	991	7	0
32	w	907	0	938	10	0
33	x	988	0	1038	6	0
34	y	754	0	802	6	0
35	z	873	0	909	5	0
36	1	732	0	782	9	0
37	A	32	0	13	4	0
38	X	1	0	0	0	0
38	h	2	0	0	0	0
38	i	3	0	0	0	0
38	j	1	0	0	0	0
38	l	1	0	0	0	0
38	t	1	0	0	0	0
38	z	1	0	0	0	0
39	Y	1	0	0	0	0
39	c	1	0	0	0	0
39	f	1	0	0	0	0
39	g	1	0	0	0	0
All	All	104614	0	71084	1178	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 7.

The worst 5 of 1178 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)
19:h:1541:G:H1	19:h:1631:A:N6	1.46	1.12
19:h:1541:G:N1	19:h:1631:A:N6	2.05	1.02
19:h:365:U:H3	19:h:437:G:H1	1.00	0.96
18:g:18:CYS:HB3	18:g:41:CYS:SG	2.09	0.93
19:h:1540:U:H3	19:h:1632:G:H1	1.15	0.90

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	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
2	A	699/701 (100%)	674 (96%)	25 (4%)	0	100	100
4	C	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
5	I	124/175 (71%)	118 (95%)	6 (5%)	0	100	100
6	J	131/142 (92%)	124 (95%)	7 (5%)	0	100	100
7	U	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
8	W	190/215 (88%)	187 (98%)	3 (2%)	0	100	100
9	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
10	Y	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
11	Z	62/77 (80%)	62 (100%)	0	0	100	100
12	a	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
13	b	52/57 (91%)	52 (100%)	0	0	100	100
14	c	47/55 (86%)	45 (96%)	1 (2%)	1 (2%)	5	30
15	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	e	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
17	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
18	g	46/75 (61%)	43 (94%)	3 (6%)	0	100	100
20	i	273/278 (98%)	262 (96%)	11 (4%)	0	100	100
21	j	212/217 (98%)	201 (95%)	11 (5%)	0	100	100
22	k	207/215 (96%)	198 (96%)	9 (4%)	0	100	100
23	l	180/187 (96%)	173 (96%)	7 (4%)	0	100	100
24	m	174/179 (97%)	169 (97%)	5 (3%)	0	100	100
25	n	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
26	q	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
27	r	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
28	s	143/147 (97%)	129 (90%)	14 (10%)	0	100	100
29	t	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
30	u	116/199 (58%)	112 (97%)	4 (3%)	0	100	100
31	v	124/127 (98%)	124 (100%)	0	0	100	100
32	w	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
33	x	122/129 (95%)	120 (98%)	2 (2%)	0	100	100
34	y	98/103 (95%)	97 (99%)	1 (1%)	0	100	100
35	z	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
36	1	93/105 (89%)	92 (99%)	1 (1%)	0	100	100
All	All	4497/4877 (92%)	4327 (96%)	169 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	c	7	VAL

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	3	18/19 (95%)	18 (100%)	0	100	100
2	A	587/587 (100%)	585 (100%)	2 (0%)	86	86
4	C	160/160 (100%)	157 (98%)	3 (2%)	50	67
5	I	89/120 (74%)	89 (100%)	0	100	100
6	J	102/108 (94%)	101 (99%)	1 (1%)	68	78
7	U	83/85 (98%)	82 (99%)	1 (1%)	63	75
8	W	155/168 (92%)	153 (99%)	2 (1%)	61	74
9	X	58/63 (92%)	55 (95%)	3 (5%)	21	42
10	Y	50/51 (98%)	49 (98%)	1 (2%)	48	66
11	Z	58/66 (88%)	58 (100%)	0	100	100
12	a	52/54 (96%)	52 (100%)	0	100	100
13	b	43/46 (94%)	43 (100%)	0	100	100
14	c	47/52 (90%)	46 (98%)	1 (2%)	47	65
15	d	35/36 (97%)	34 (97%)	1 (3%)	37	58
16	e	53/54 (98%)	53 (100%)	0	100	100
17	f	35/35 (100%)	35 (100%)	0	100	100
18	g	43/63 (68%)	42 (98%)	1 (2%)	44	64
20	i	215/218 (99%)	214 (100%)	1 (0%)	81	83
21	j	160/163 (98%)	158 (99%)	2 (1%)	61	74
22	k	169/173 (98%)	167 (99%)	2 (1%)	63	75
23	l	151/156 (97%)	150 (99%)	1 (1%)	76	81
24	m	148/150 (99%)	145 (98%)	3 (2%)	48	66
25	n	90/116 (78%)	88 (98%)	2 (2%)	45	64
26	q	119/120 (99%)	117 (98%)	2 (2%)	53	69
27	r	100/100 (100%)	99 (99%)	1 (1%)	68	78
28	s	112/114 (98%)	111 (99%)	1 (1%)	70	79
29	t	114/116 (98%)	112 (98%)	2 (2%)	51	68
30	u	97/158 (61%)	96 (99%)	1 (1%)	68	78
31	v	93/94 (99%)	91 (98%)	2 (2%)	45	64
32	w	100/100 (100%)	97 (97%)	3 (3%)	36	57
33	x	97/99 (98%)	97 (100%)	0	100	100
34	y	81/83 (98%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	z	90/117 (77%)	90 (100%)	0	100 100
36	1	81/86 (94%)	79 (98%)	2 (2%)	42 63
All	All	3685/3930 (94%)	3644 (99%)	41 (1%)	63 76

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	q	96	HIS
31	v	101	VAL
27	r	2	ILE
29	t	58	ILE
32	w	64	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
21	j	99	GLN
32	w	76	HIS
22	k	91	HIS
30	u	62	ASN
21	j	183	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	h	3118/3120 (99%)	637 (20%)	0
3	B	117/118 (99%)	18 (15%)	1 (0%)
All	All	3235/3238 (99%)	655 (20%)	1 (0%)

5 of 655 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	B	4	A
3	B	9	G
3	B	11	U
3	B	12	C
3	B	13	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B	10	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 15 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
37	GNP	A	801	-	33,34,34	1.01	5 (15%)	46,54,54	1.10	3 (6%)

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
37	GNP	A	801	-	-	7/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	A	801	GNP	PG-O1G	3.06	1.51	1.46
37	A	801	GNP	PB-O1B	2.57	1.50	1.46
37	A	801	GNP	PB-O2B	-2.16	1.50	1.56
37	A	801	GNP	PG-O3G	-2.05	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	A	801	GNP	PG-O2G	-2.05	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	801	GNP	O2B-PB-O1B	4.22	118.78	109.92
37	A	801	GNP	PB-O3A-PA	-3.16	121.49	132.62
37	A	801	GNP	O3G-PG-O1G	-2.01	108.40	113.45

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	A	801	GNP	C5'-O5'-PA-O1A
37	A	801	GNP	C5'-O5'-PA-O2A
37	A	801	GNP	O4'-C4'-C5'-O5'
37	A	801	GNP	C4'-C5'-O5'-PA
37	A	801	GNP	C3'-C4'-C5'-O5'

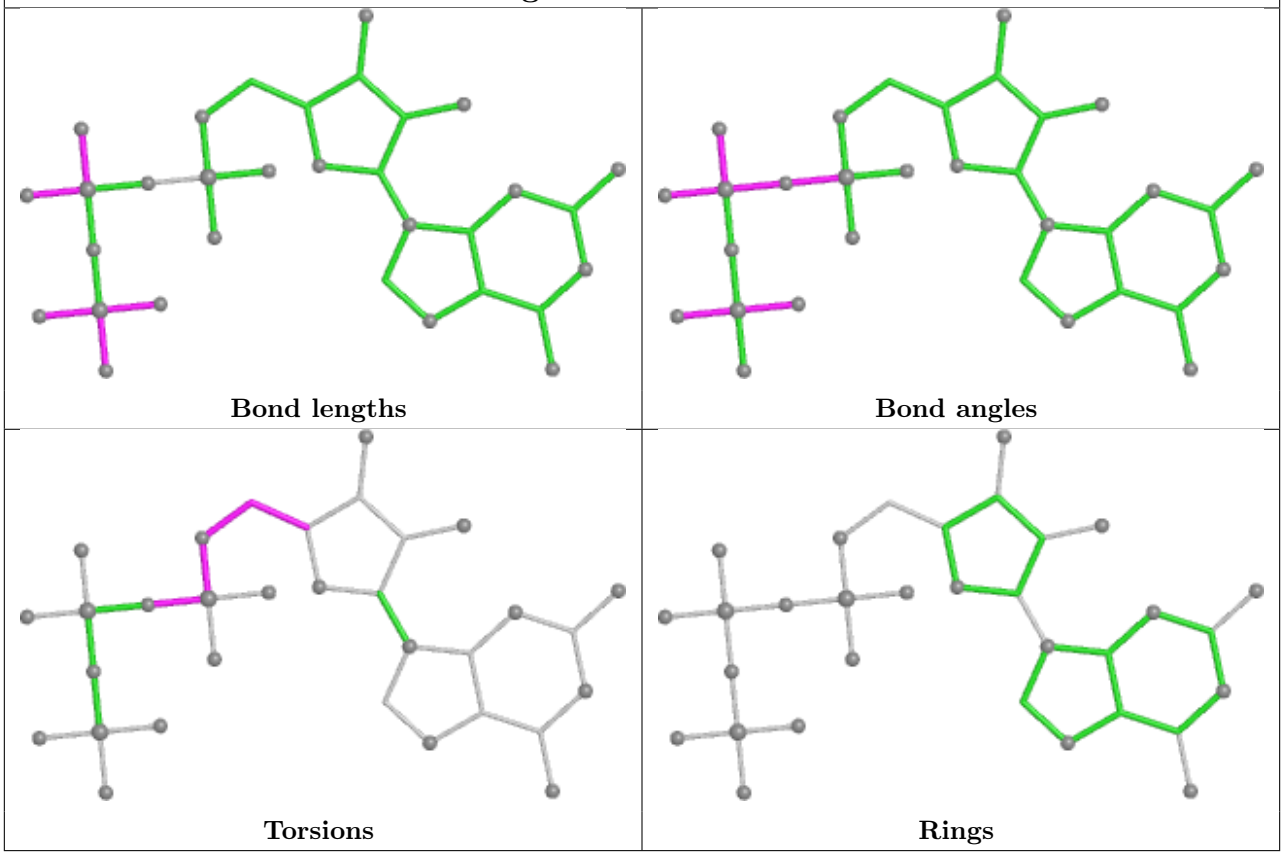
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A	801	GNP	4	0

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 then 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.

Ligand GNP A 801



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.

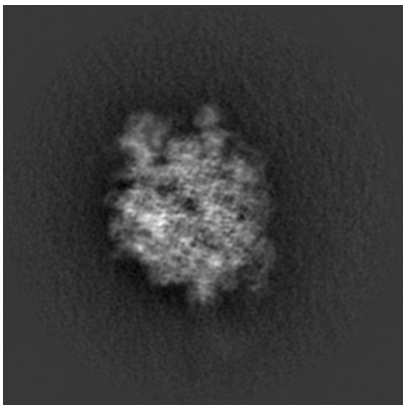
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69705. These allow visual inspection of the internal detail of the map and identification of artifacts.

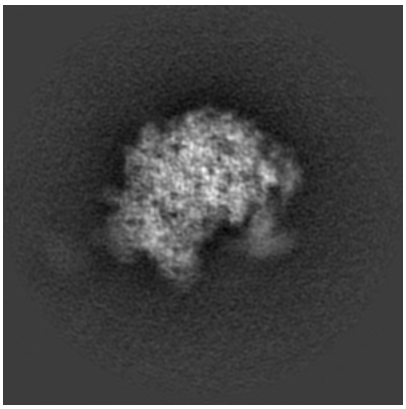
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

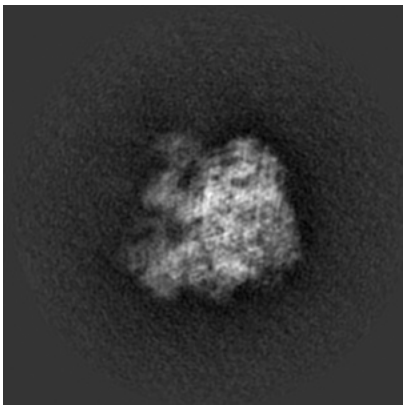
6.1.1 Primary map



X

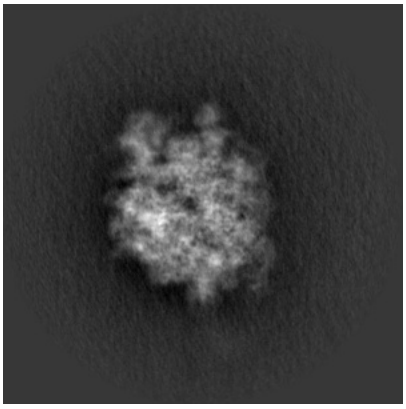


Y

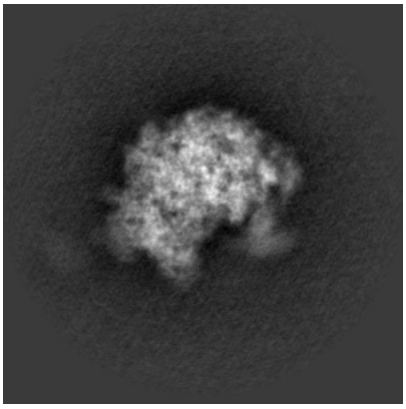


Z

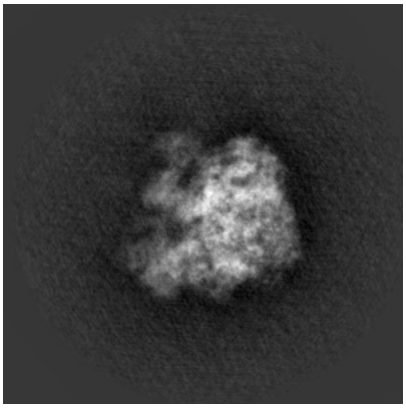
6.1.2 Raw map



X



Y

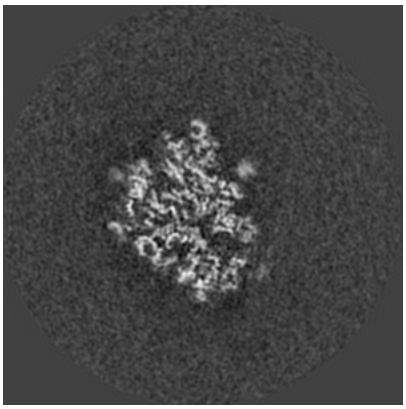


Z

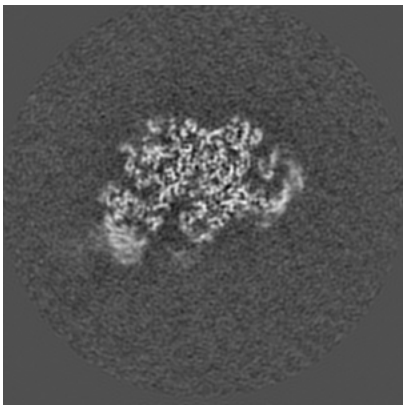
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

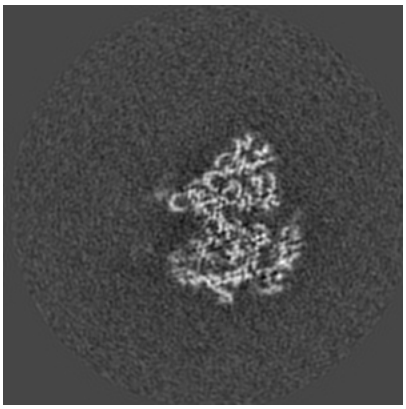
6.2.1 Primary map



X Index: 210

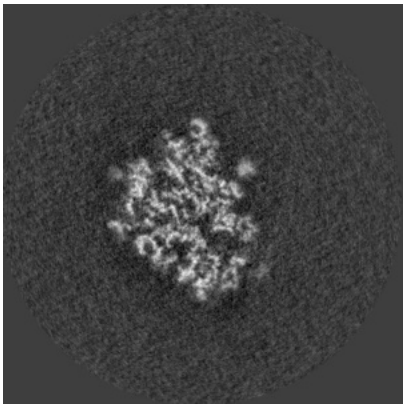


Y Index: 210

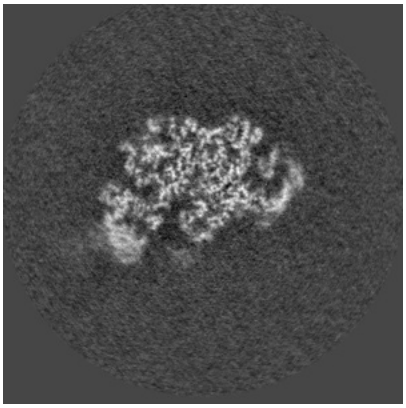


Z Index: 210

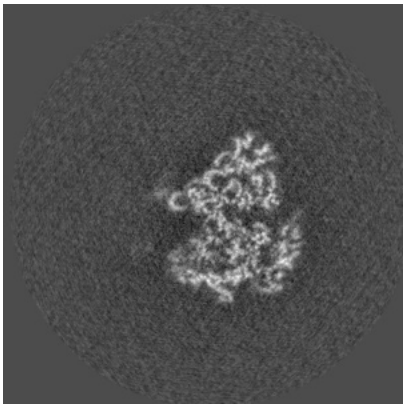
6.2.2 Raw map



X Index: 210



Y Index: 210

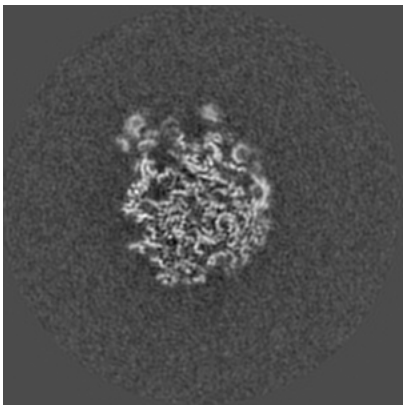


Z Index: 210

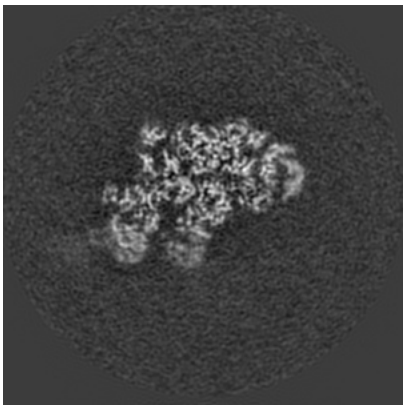
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

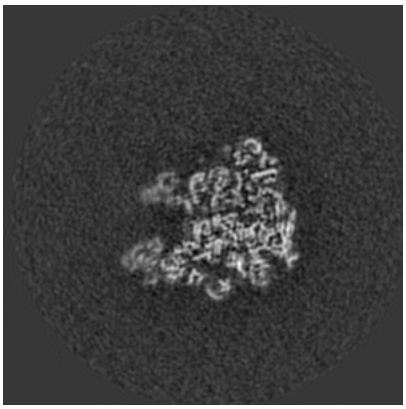
6.3.1 Primary map



X Index: 247

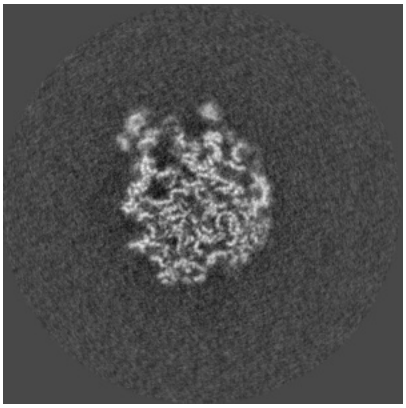


Y Index: 218

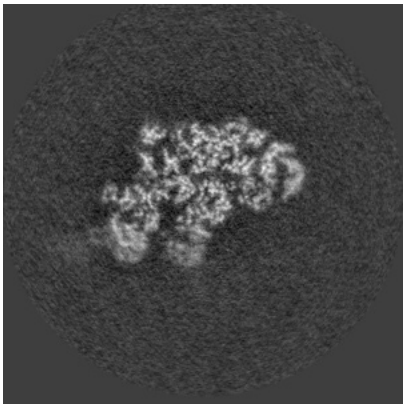


Z Index: 198

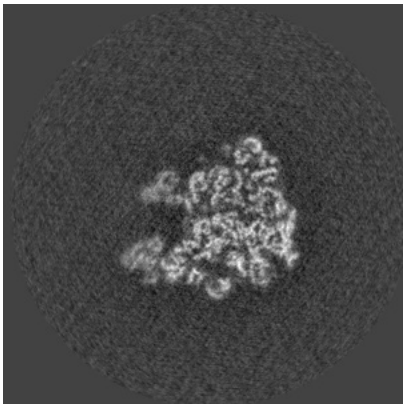
6.3.2 Raw map



X Index: 246



Y Index: 218

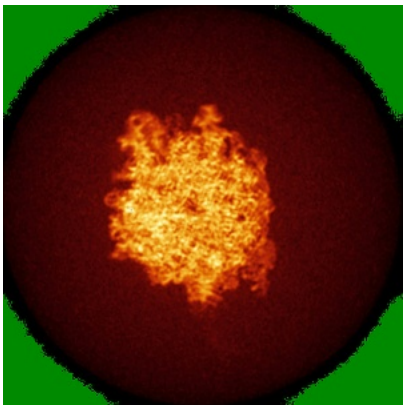


Z Index: 198

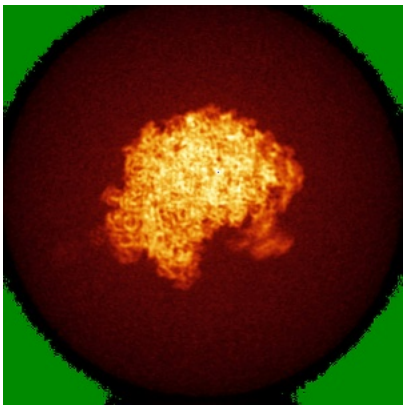
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

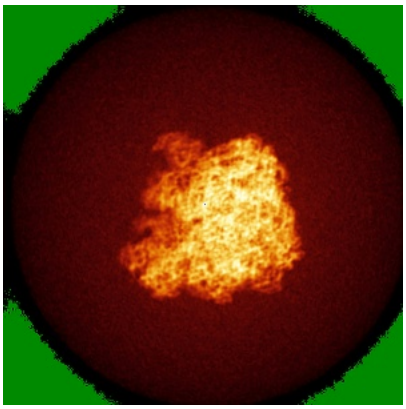
6.4.1 Primary map



X

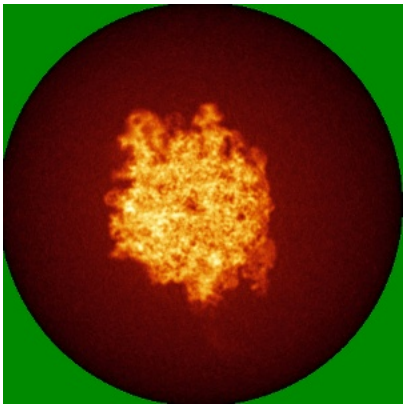


Y

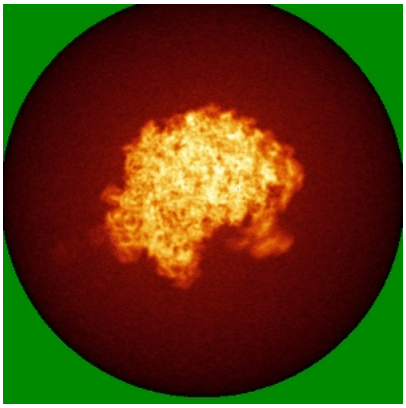


Z

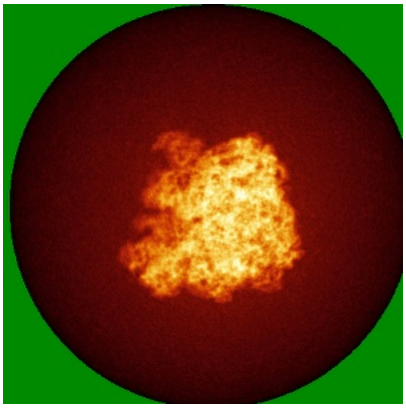
6.4.2 Raw map



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 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

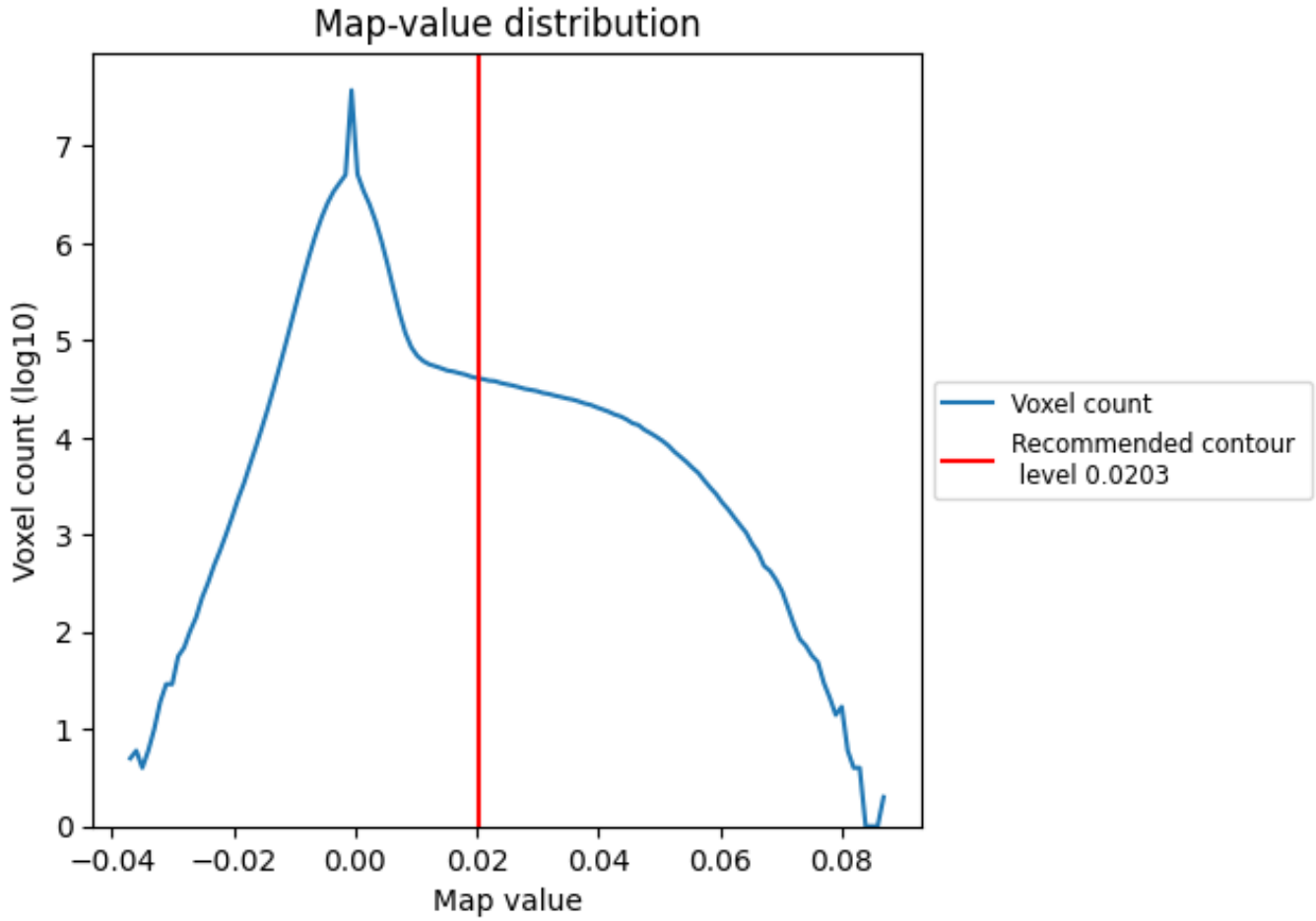
6.6 Mask visualisation (i)

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

7 Map analysis

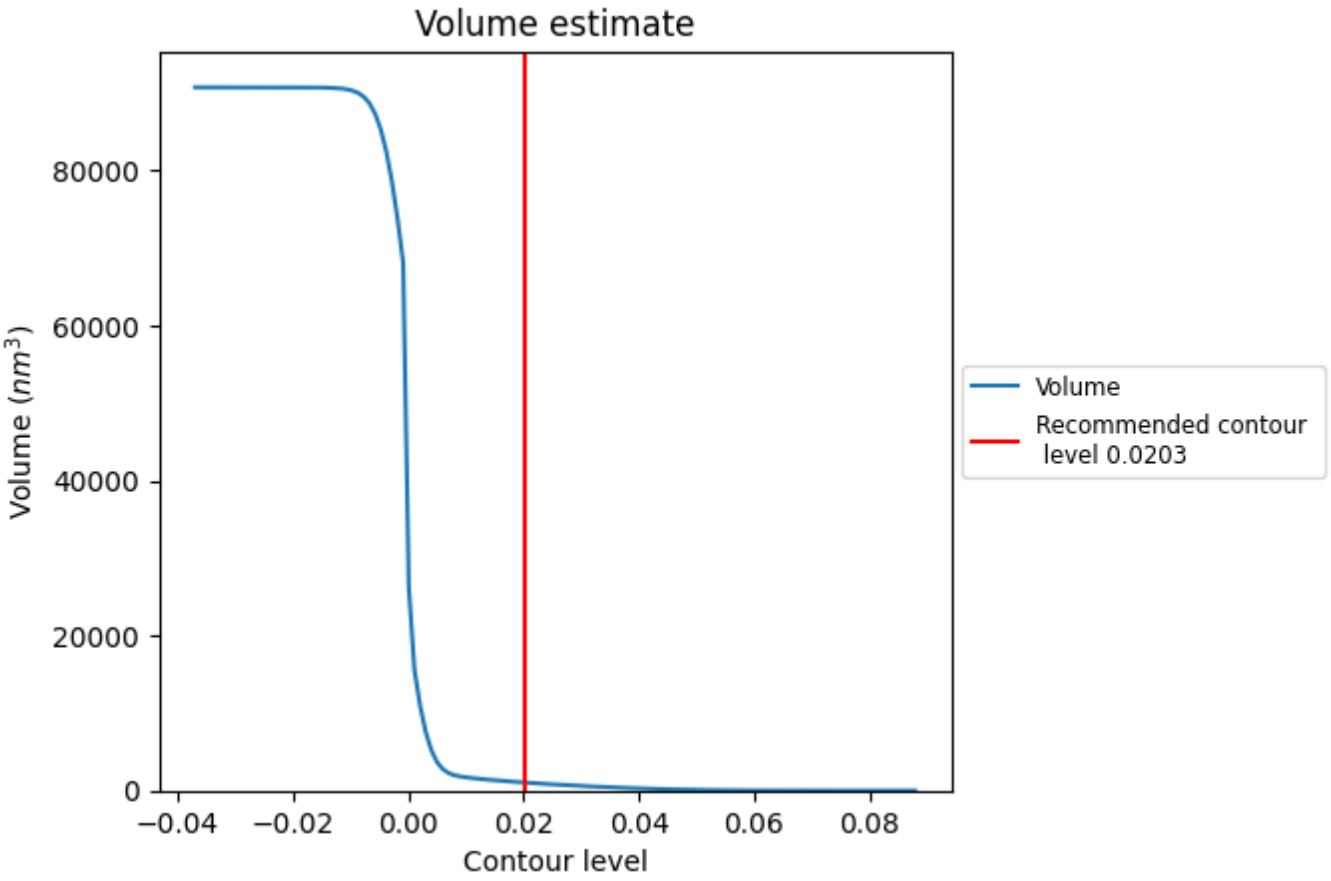
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

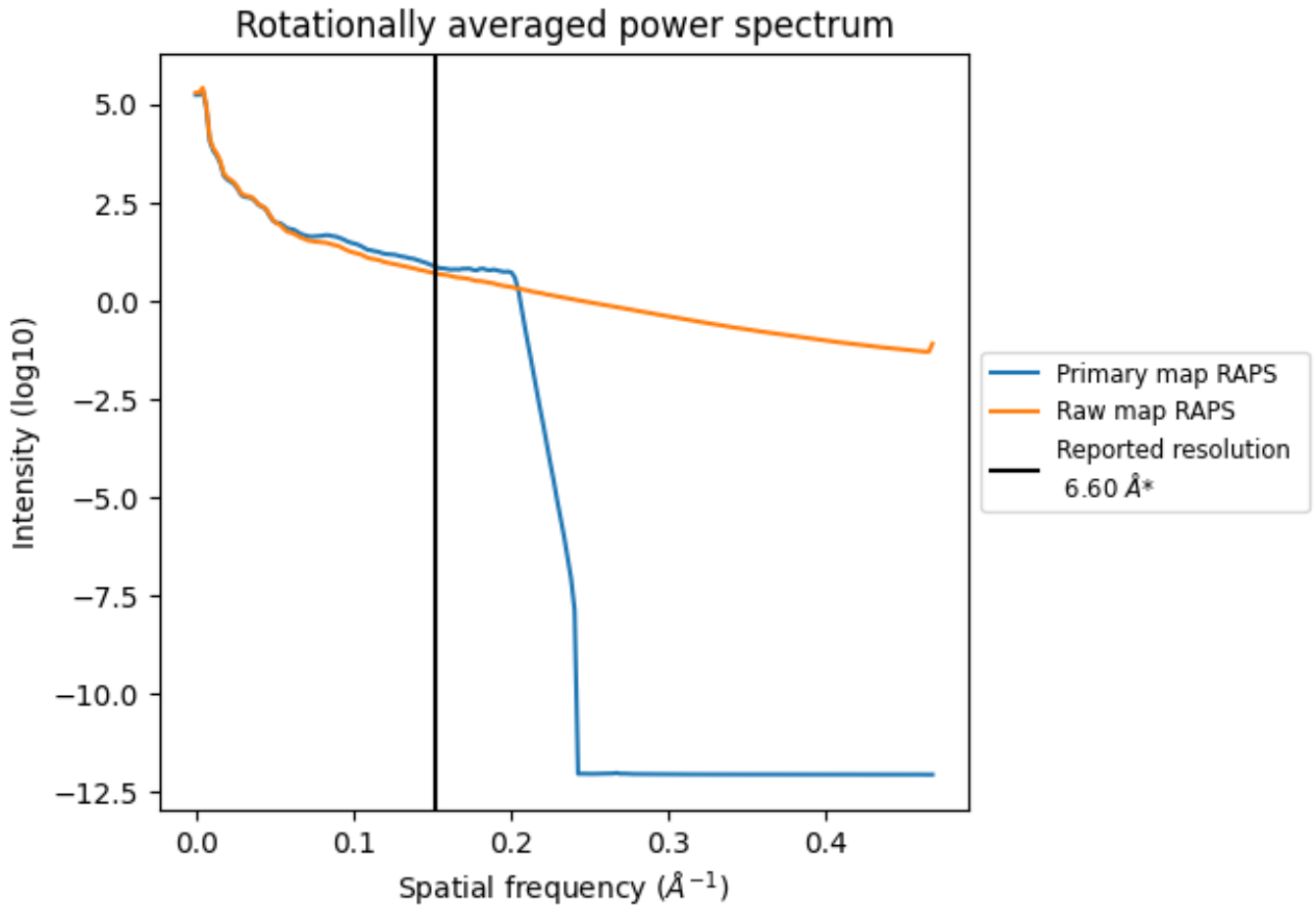
7.2 Volume estimate (i)



The volume at the recommended contour level is 1030 nm^3; this corresponds to an approximate mass of 930 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)

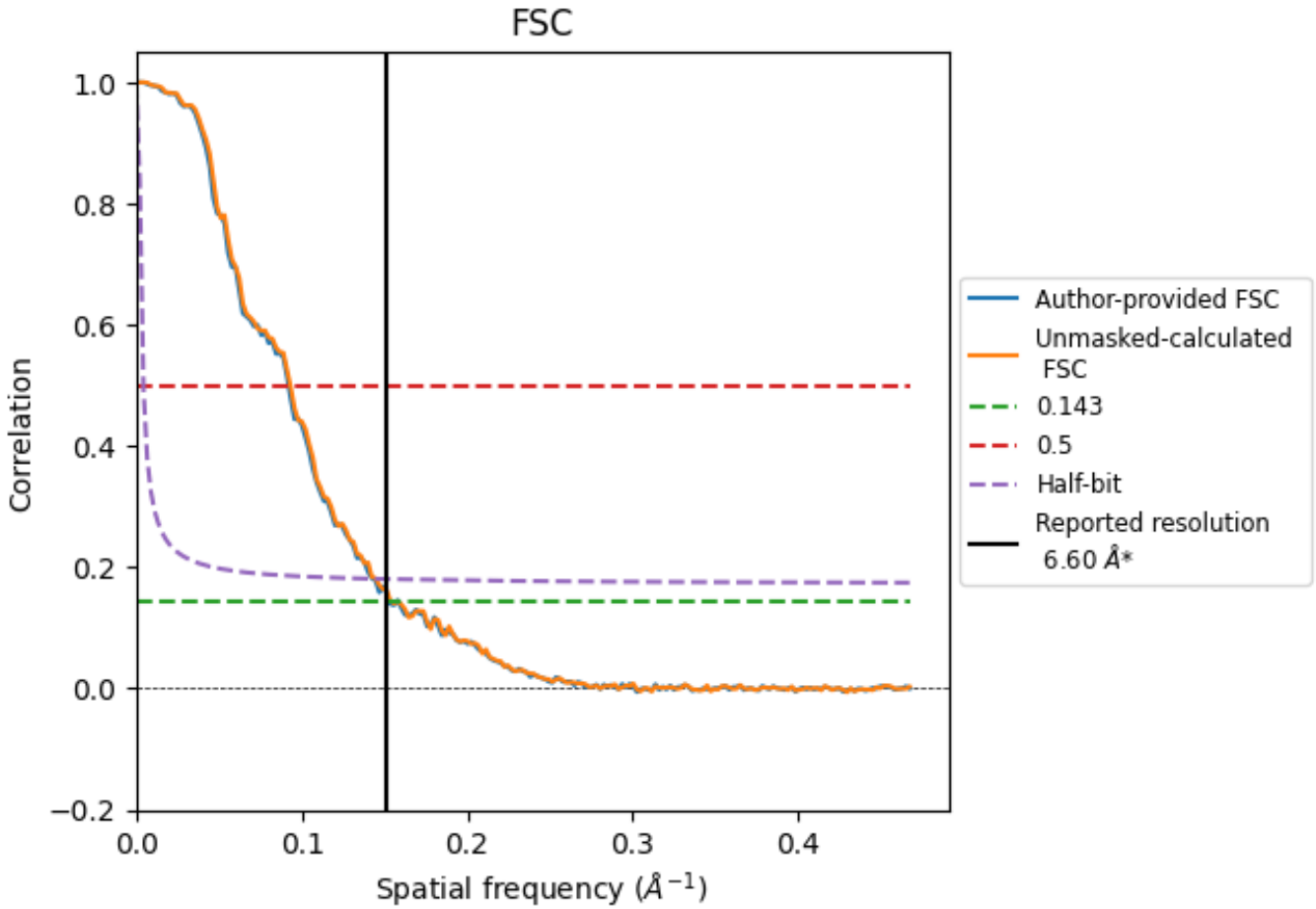


*Reported resolution corresponds to spatial frequency of 0.152 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

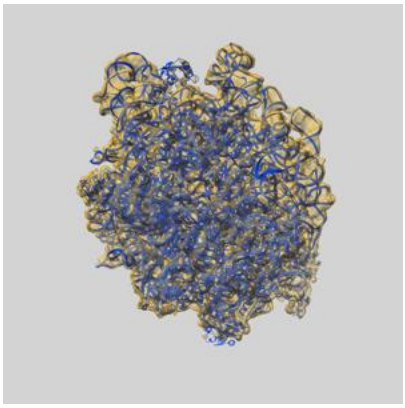
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.53	10.87	6.99
Unmasked-calculated*	6.48	10.74	6.90

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

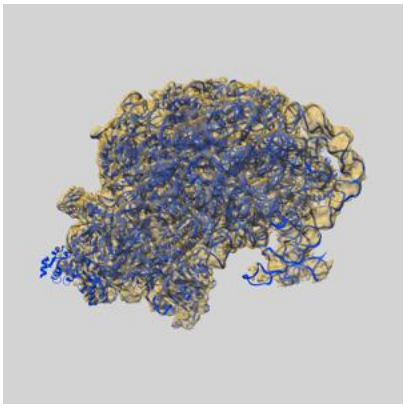
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69705 and PDB model 24NS. Per-residue inclusion information can be found in section 3 on page 12.

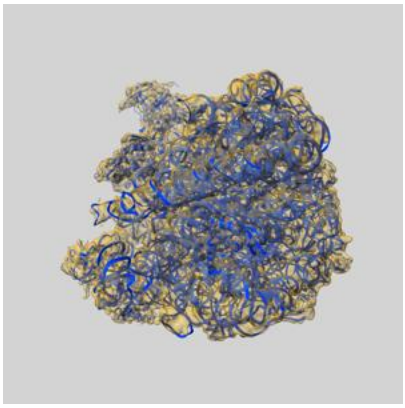
9.1 Map-model overlay



X



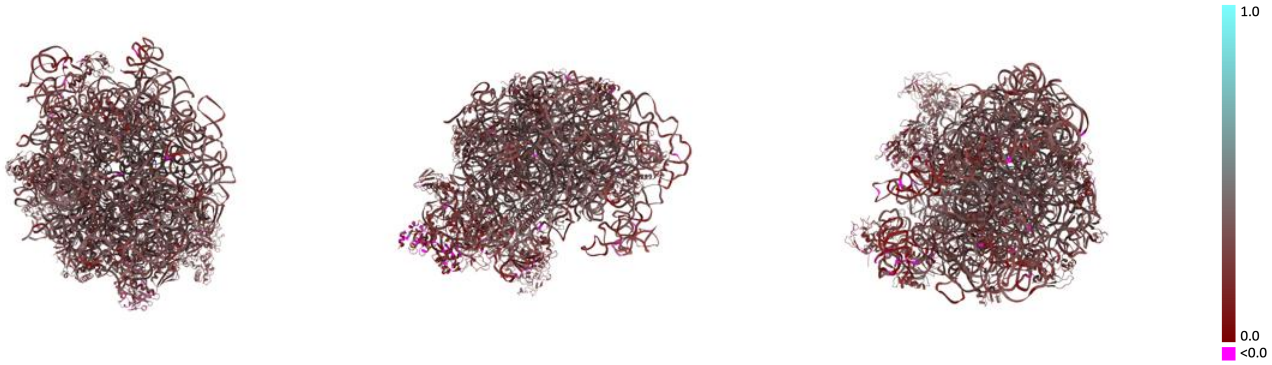
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0203 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.

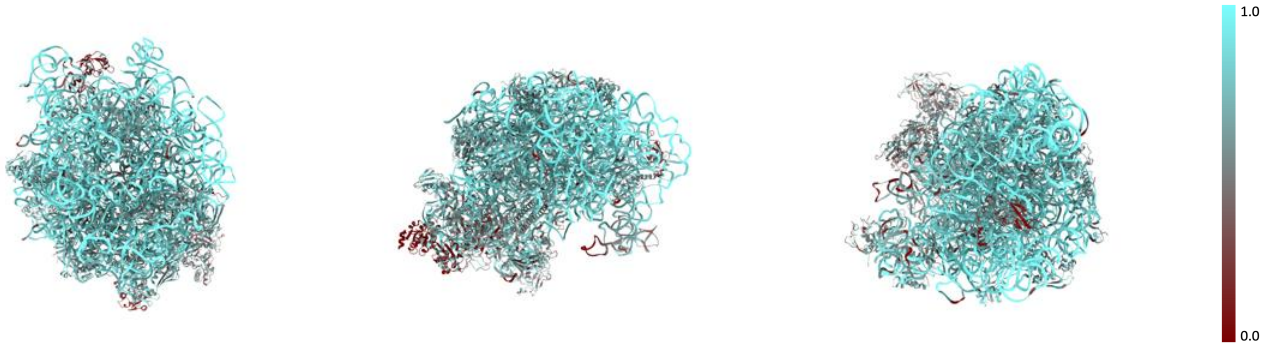
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

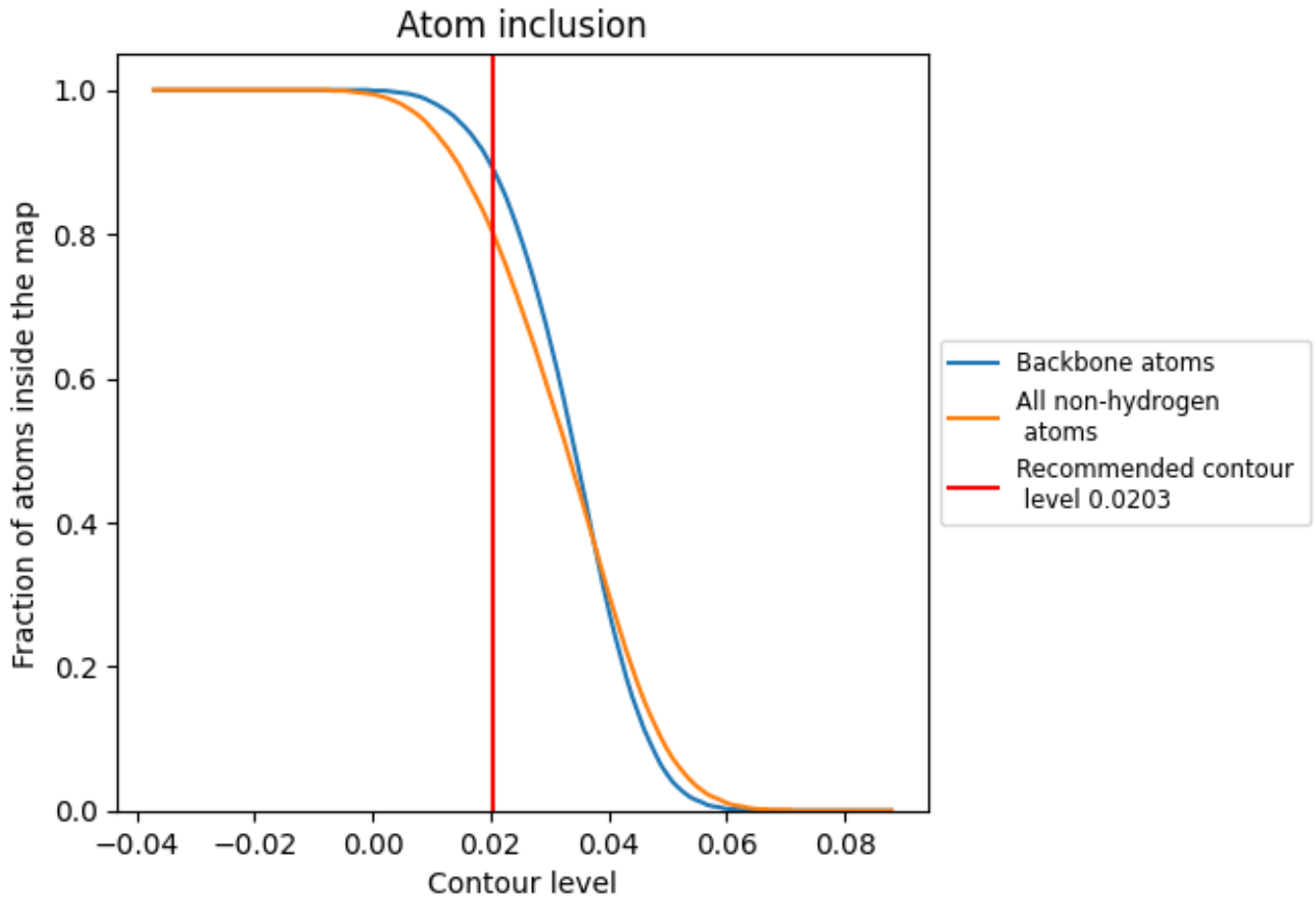
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0203).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.2910
1	0.6360	0.2610
3	0.3070	0.2060
A	0.4990	0.2540
B	0.9430	0.3090
C	0.5760	0.2680
I	0.0440	0.0990
J	0.2630	0.1210
U	0.6280	0.2880
W	0.5380	0.2760
X	0.6610	0.2770
Y	0.6830	0.2970
Z	0.6960	0.2460
a	0.6620	0.2710
b	0.6590	0.2940
c	0.4130	0.2390
d	0.5960	0.2690
e	0.3500	0.2580
f	0.5730	0.2690
g	0.4320	0.2030
h	0.9110	0.3060
i	0.6850	0.2910
j	0.6980	0.2920
k	0.6650	0.2820
l	0.6850	0.2240
m	0.6850	0.2810
n	0.2970	0.2460
q	0.6920	0.2920
r	0.6470	0.2810
s	0.6690	0.2860
t	0.6100	0.2890
u	0.6810	0.2540
v	0.7300	0.2630
w	0.6890	0.2820
x	0.6670	0.2560



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Chain	Atom inclusion	Q-score
y	0.6790	0.3160
z	0.6830	0.2900