



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:16 PM UTC

PDB ID : 8Y5O / pdb_00008y5o
EMDB ID : EMD-38944
Title : E.coli transcription translation coupling complex in TTC-B state 3 (subclass1) containing mRNA with 30-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-01-31
Resolution : 4.20 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:

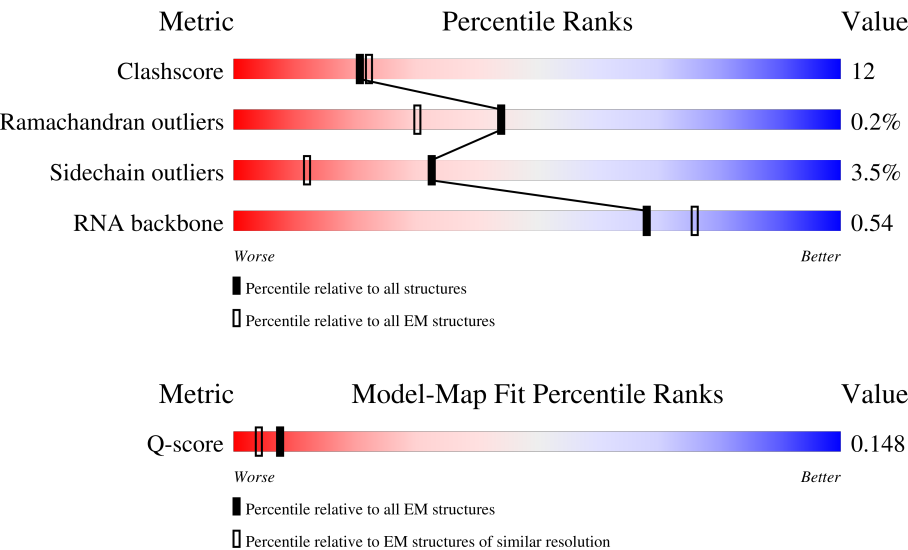
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.20 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.



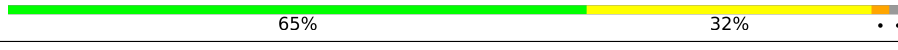
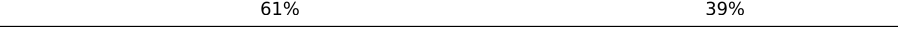
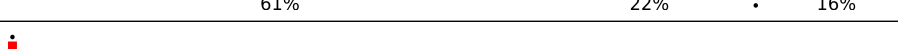
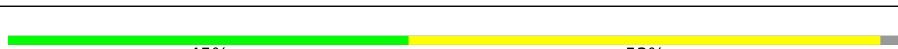
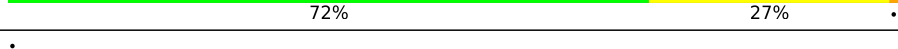
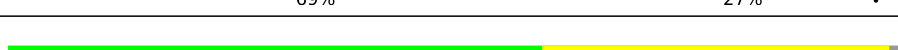
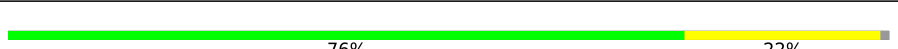
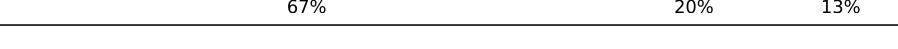
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	70	
2	B	57	
3	C	55	

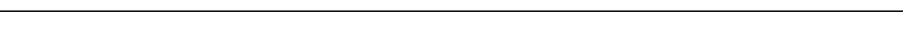
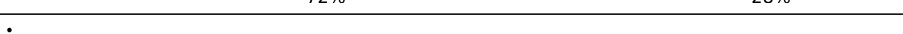
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Mol	Chain	Length	Quality of chain
4	D	46	
5	E	65	
6	F	38	
7	G	241	
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	
27	b	273	
28	c	209	

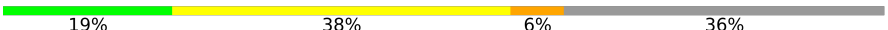
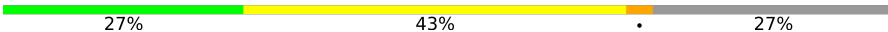
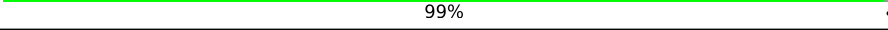
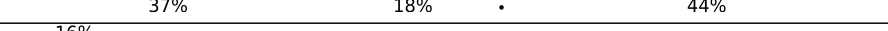
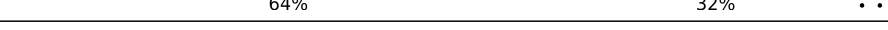
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Mol	Chain	Length	Quality of chain
29	d	201	
30	e	179	
31	f	177	
32	g	149	
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	

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Mol	Chain	Length	Quality of chain
54	4	47	
55	8	37	
56	9	37	
57	A1	329	
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
65	a	234	
66	0	716	
67	h	6	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 183377 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 L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	46	Total	C	N	O	S	0	0
			355	221	62	66	6		

- Molecule 2 is a protein called 50S ribosomal protein L32.

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

- Molecule 3 is a protein called 50S ribosomal protein L33.

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

- Molecule 4 is a protein called 50S ribosomal protein L34.

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

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1929590828

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	U	conflict	GB NR_103249

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	30	Total	C	N	O	P	0	0
			627	280	92	225	30		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	301	Total	C	N	O	S	0	0
			2088	1293	380	409	6		
57	A2	288	Total	C	N	O	S	0	0
			2029	1257	366	400	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10546	6616	1839	2048	43		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NA	492	Total	C	N	O	0	0
			2432	1448	492	492		

- Molecule 62 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	NG	154	Total	C	N	O	0	0
			758	450	154	154		

- Molecule 63 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 64 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 65 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	a	132	Total	C	N	O	S	0	0
			1013	638	183	190	2		

- Molecule 66 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	0	697	Total	C	N	O	S	0	0
			5399	3403	929	1042	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8

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Chain	Residue	Modelled	Actual	Comment	Reference
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

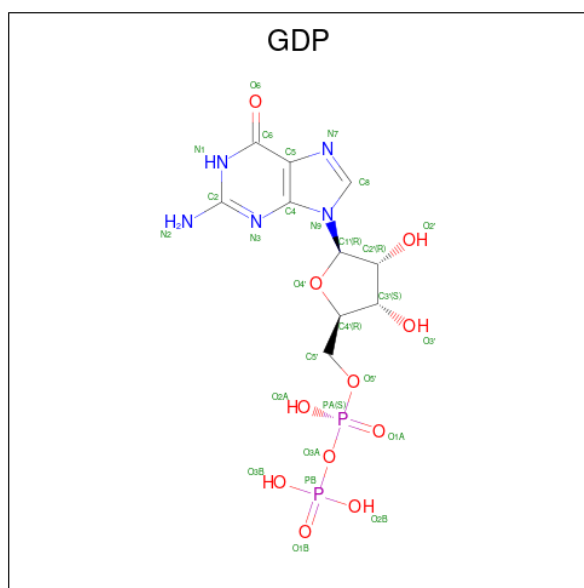
- Molecule 67 is a protein (with D amino acids) called Viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

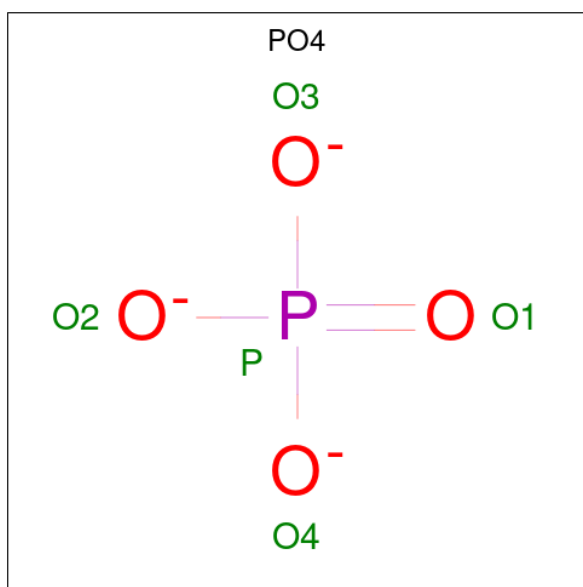
Mol	Chain	Residues	Atoms		AltConf
68	B1	1	Total	Mg	0
			1	1	

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
69	0	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 70 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

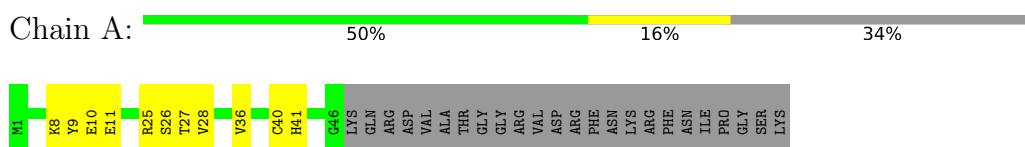


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

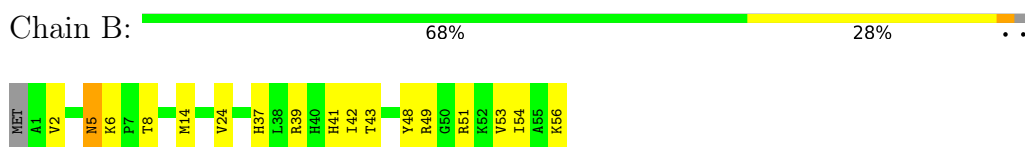
3 Residue-property plots

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

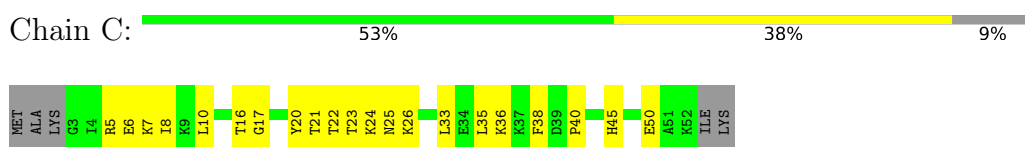
- Molecule 1: 50S ribosomal protein L31



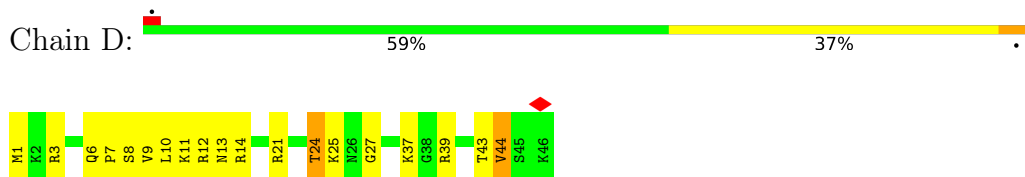
- Molecule 2: 50S ribosomal protein L32



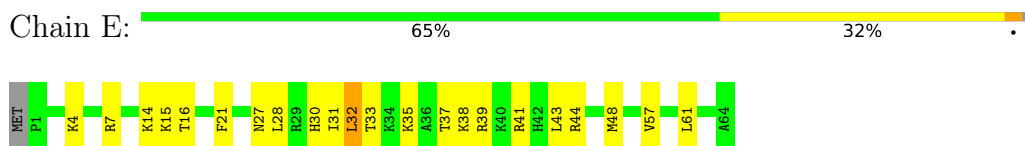
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34

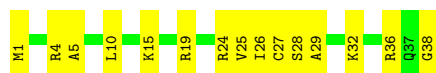


- Molecule 5: 50S ribosomal protein L35



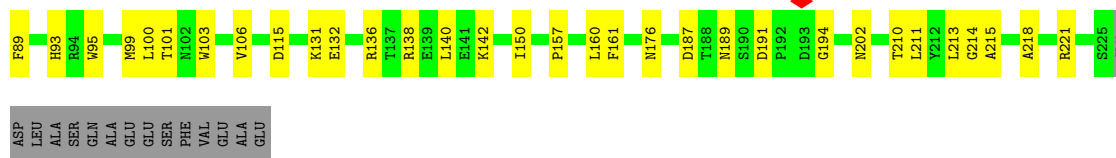
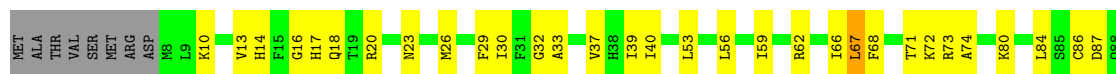
- Molecule 6: 50S ribosomal protein L36

Chain F:  61% 39%



• Molecule 7: 30S ribosomal protein S2

Chain G:  64% 26% 10%



• Molecule 8: 30S ribosomal protein S3

Chain H:  63% 24% 12%



• Molecule 9: 30S ribosomal protein S4

Chain I:  71% 27%



• Molecule 10: 30S ribosomal protein S5

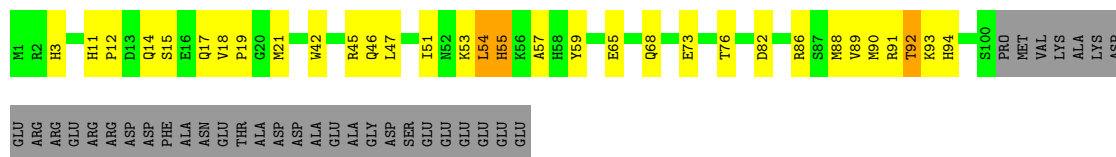
Chain J:  66% 28% 6%





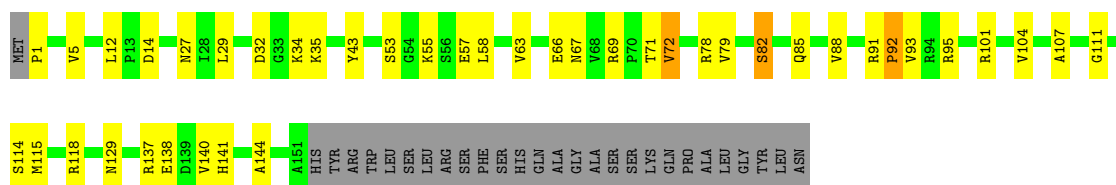
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K: 50% 21% 26%



- Molecule 12: 30S ribosomal protein S7

Chain L: 61% 22% 16%



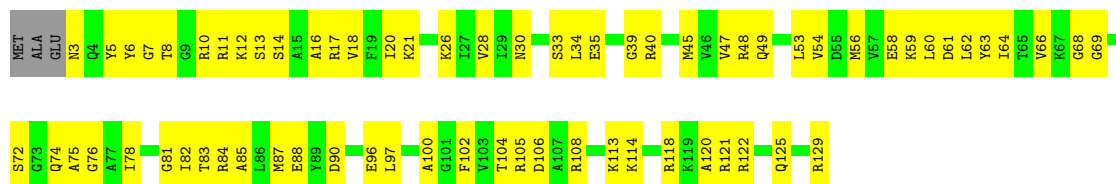
- Molecule 13: 30S ribosomal protein S8

Chain M: 66% 33% 1%



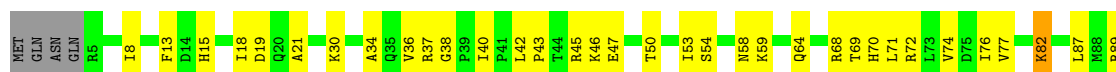
- Molecule 14: 30S ribosomal protein S9

Chain N: 45% 53% 2%



- Molecule 15: 30S ribosomal protein S10

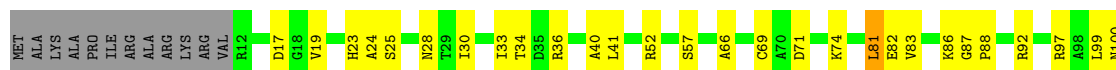
Chain O: 56% 38% 5%





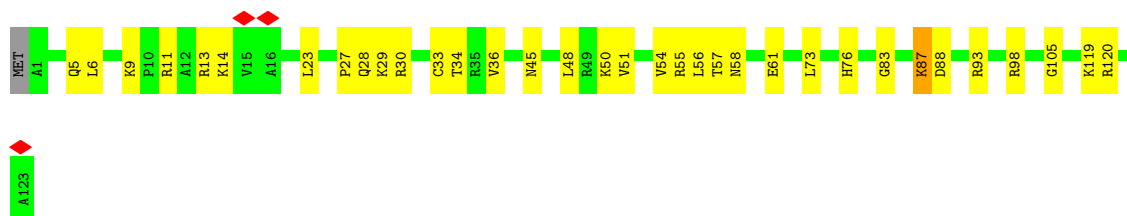
- Molecule 16: 30S ribosomal protein S11

Chain P: 61% 28% 10%



- Molecule 17: 30S ribosomal protein S12

Chain Q: 72% 27% 1%



- Molecule 18: 30S ribosomal protein S13

Chain R: 69% 27% 4%



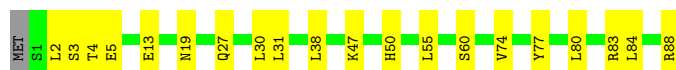
- Molecule 19: 30S ribosomal protein S14

Chain S: 60% 39% 1%



- Molecule 20: 30S ribosomal protein S15

Chain T: 76% 22% 2%



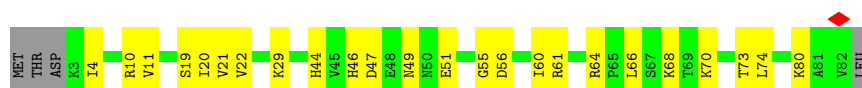
- Molecule 21: 30S ribosomal protein S16

Chain U:  72% 28%



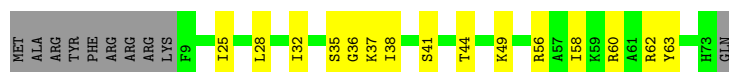
- Molecule 22: 30S ribosomal protein S17

Chain V:  67% 29% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  67% 20% 13%



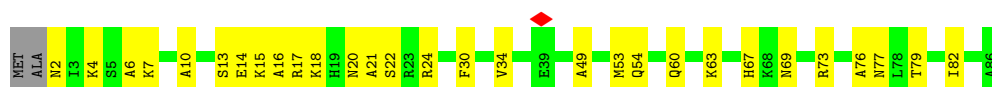
- Molecule 24: 30S ribosomal protein S19

Chain X:  64% 22% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  64% 33% 3%



- Molecule 26: 30S ribosomal protein S21

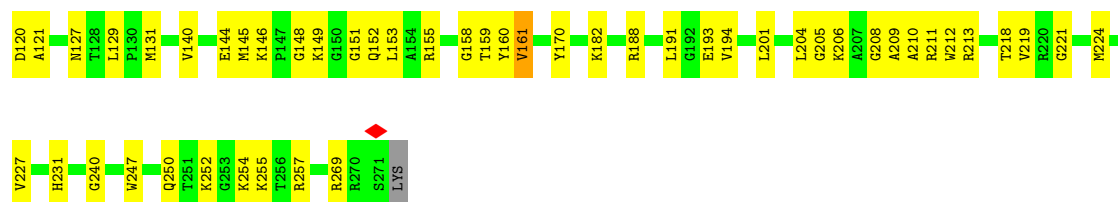
Chain Z:  61% 25% 6% 8%



- Molecule 27: 50S ribosomal protein L2

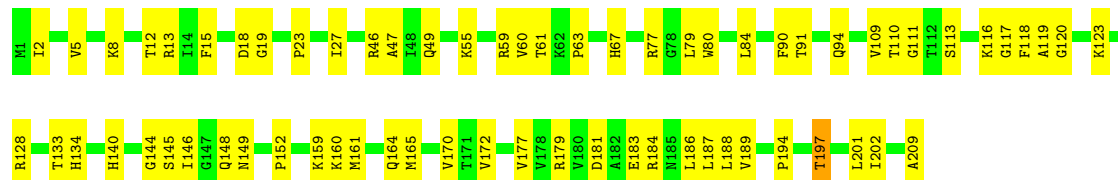
Chain b:  70% 29% 1%





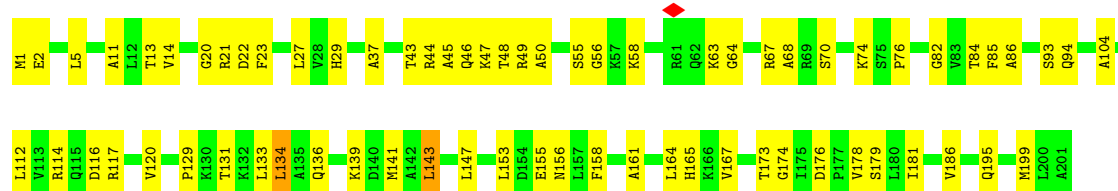
• Molecule 28: 50S ribosomal protein L3

Chain c: 68% 32%



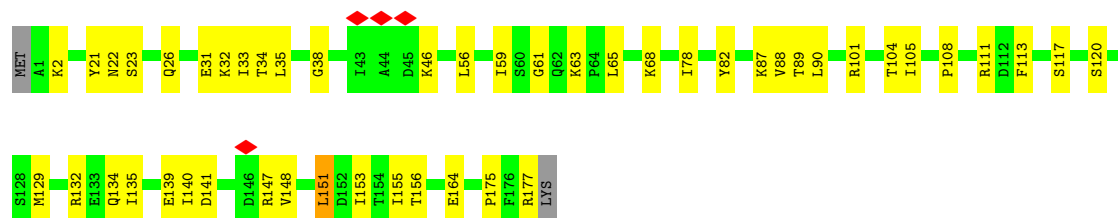
• Molecule 29: 50S ribosomal protein L4

Chain d: 66% 33%



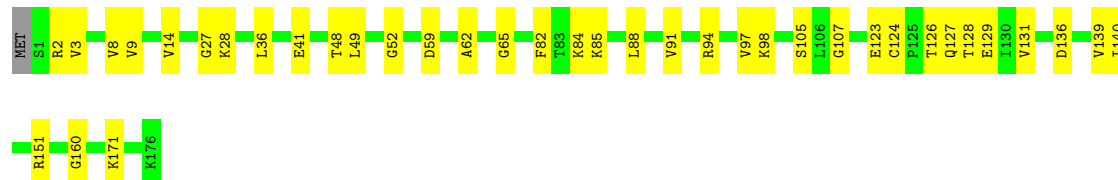
• Molecule 30: 50S ribosomal protein L5

Chain e: 72% 27%

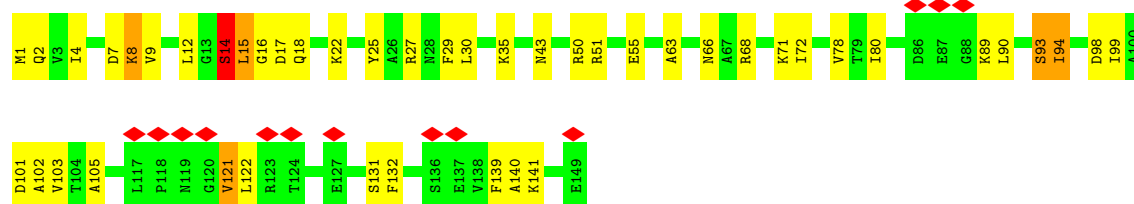


• Molecule 31: 50S ribosomal protein L6

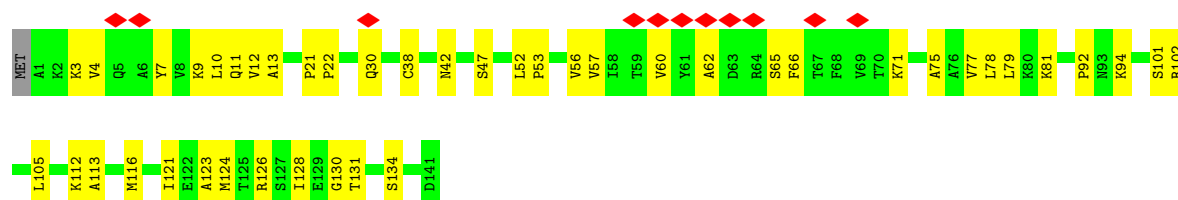
Chain f: 78% 21%



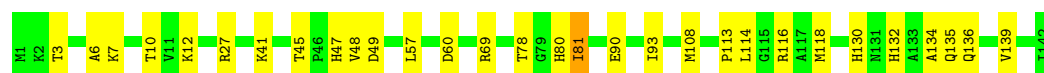
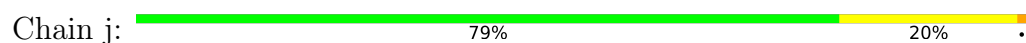
• Molecule 32: 50S ribosomal protein L9



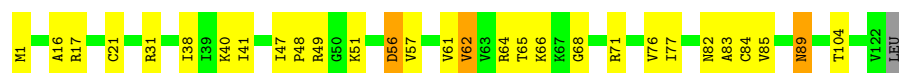
- Molecule 33: 50S ribosomal protein L11



- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



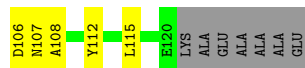
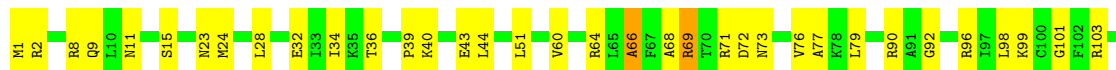
- Molecule 37: 50S ribosomal protein L16





- Molecule 38: 50S ribosomal protein L17

Chain n: 63% 30% 6%



- Molecule 39: 50S ribosomal protein L18

Chain o: 71% 28%



- Molecule 40: 50S ribosomal protein L19

Chain p: 77% 23%



- Molecule 41: 50S ribosomal protein L20

Chain q: 77% 22%



- Molecule 42: 50S ribosomal protein L21

Chain r: 70% 30%

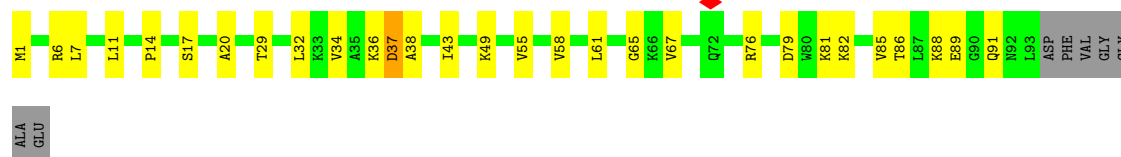


- Molecule 43: 50S ribosomal protein L22

Chain s: 72% 28%



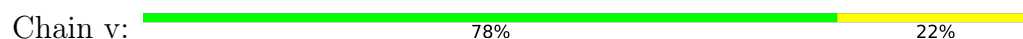
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25



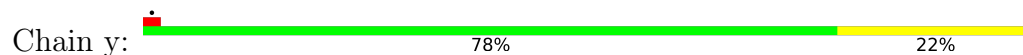
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



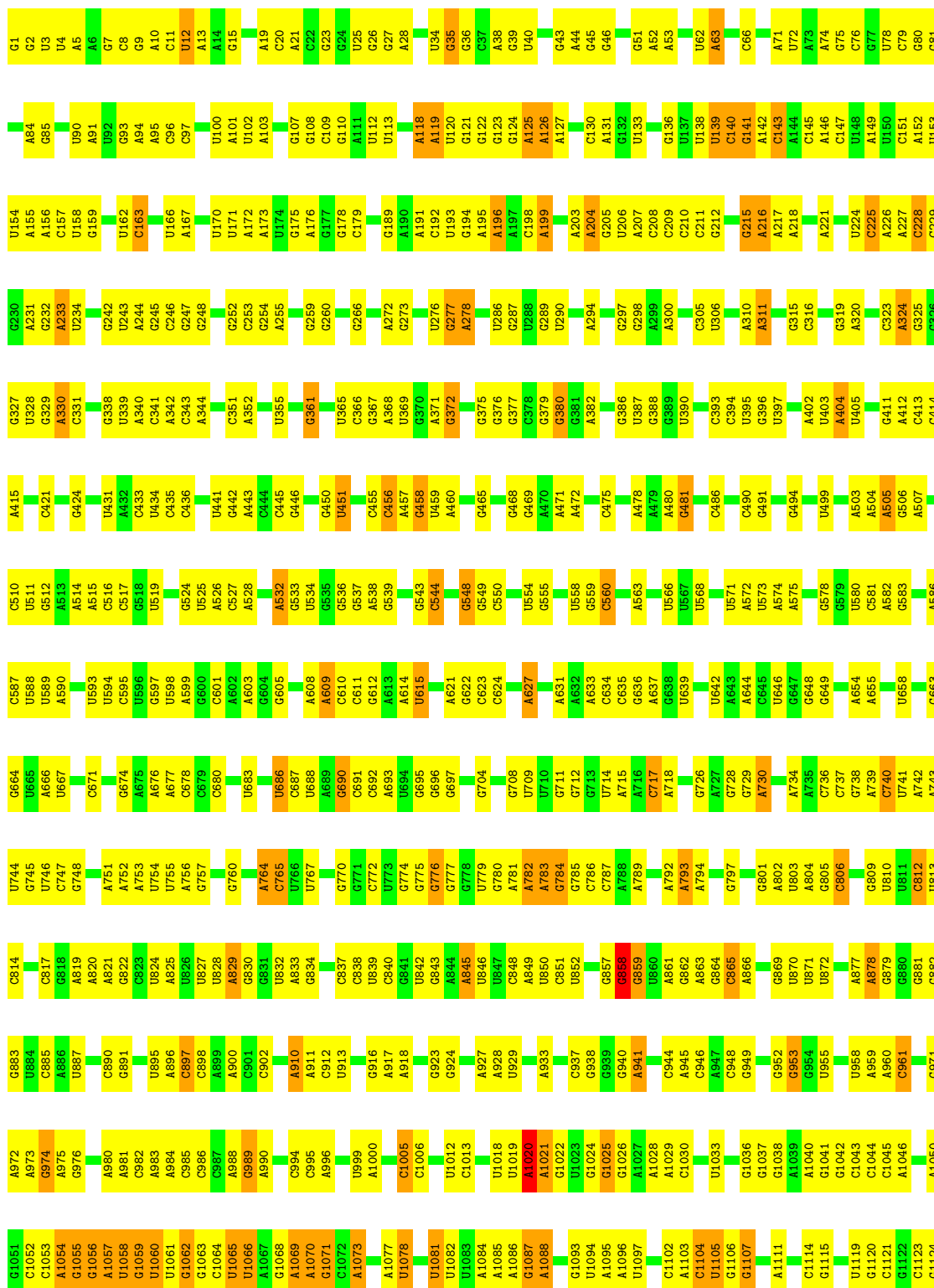
- Molecule 50: 50S ribosomal protein L30



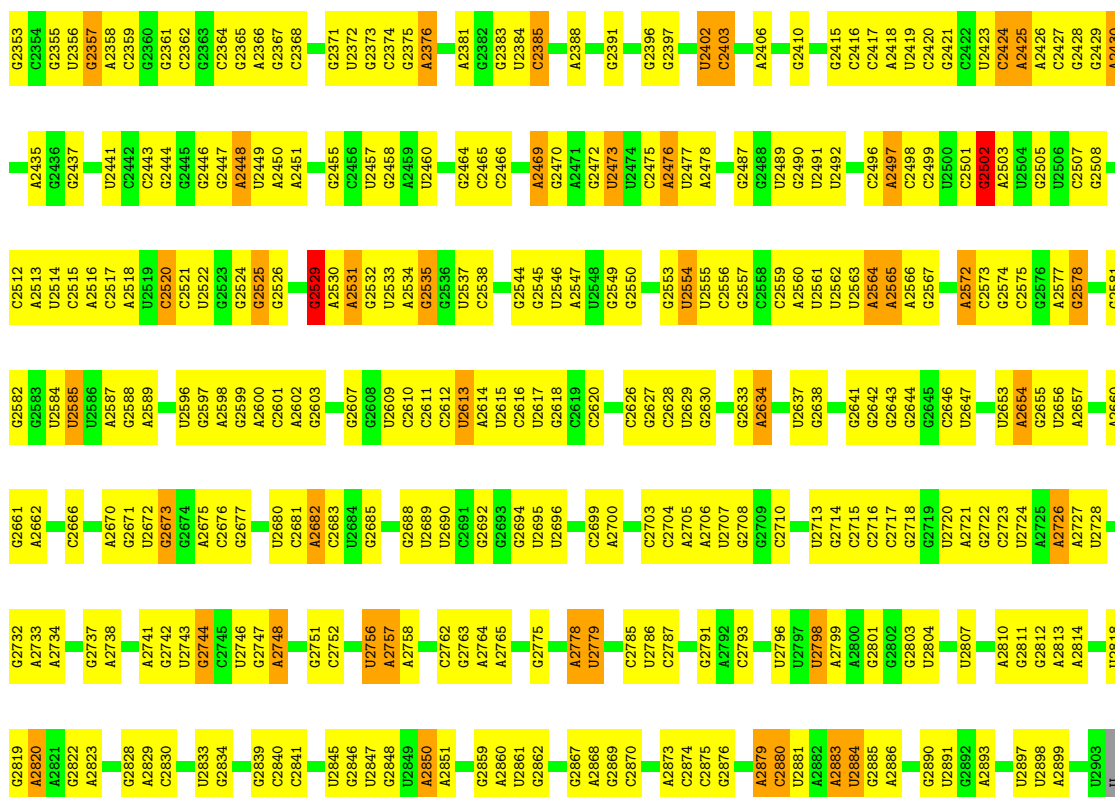


• Molecule 51: 23S rRNA

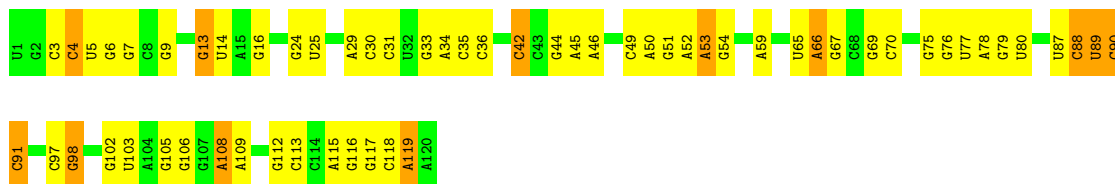
Chain 1: 44% 48% 8%



G2276	G2277	C2283	A2284	C2285	G2286	A2287	G2288	A2297	A2298	U2299	C2300	C2301	C2302	C2303	G2304	U2305	C2306	G2307	G2308	A2309	C2310	A2311	C2312	C2313	A2314	C2315	G2316	A2317	G2318	U2321	U2324	G2325	A2326	A2327	A2328	U2329	G2330	A2333	G2334	A2335	C2338	C2339	C2340	U2344	C2345	U2348	G2349	C2350	A2351	A2352																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C2196	C2197	A2198	A2199	C2200	G2201	U2202	U2203	G2204	A2205	C2206	C2207	C2208	U2209	U2210	A2211	A2212	C2213	C2214	C2215	G2216	G2221	C2222	A2225	C2226	A2227	A2314	C2315	G2230	G2234	G2235	U2236	G2237	G2238	G2239	A2247	C2248	U2249	G2250	G2251	G2255	G2256	U2257	C2258	U2262	C2263	A2267	A2268	G2269	A2270	G2271	U2272	A2273																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G2124	G2125	G2126	G2127	G2128	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	C2146	U2151	G2152	A2154	U2155	C2156	G2157	A2158	G2162	C2165	U2166	G2167	G2168	U2172	C2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	C2183	A2184	U2187	U2188	U2189	A2190	A2191	G2194	A2195																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G2048	G2049	A2050	A2051	A2052	C2055	G2056	A2059	G2060	G2061	A2062	C2063	G2064	C2065	G2066	G2067	U2068	G2069	A2070	A2071	C2072	C2073	U2074	A2080	U2081	A2082	G2083	U2086	G2087	U2092	G2093	A2094	U2099	C2100	A2101	G2102	C2103	U2106	U2107	A2108	U2111	G2112	U2113	A2114	G2115	U2118	U2119	A2120	G2121	U2122	C2123																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C1874	C1875	G1884	G1889	A1890	A1893	C1894	A1899	A1900	A1901	C1902	G1903	G1904	C1905	A1912	A1913	C1914	U1917	U1918	U1919	U1920	A1918	U1923	C1924	C1925	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	C1940	C1941	C1942	U1943	U1951	A1952	A1953	G1954	U1955	U1956	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1803	C1804	A1805	C1806	G1807	A1808	A1809	A1810	G1811	A1815	C1816	U1817	U1818	A1819	U1820	A1821	C1822	G1823	A1824	U1825	G1826	U1827	G1828	C1830	C1832	C1833	C1836	C1837	U1841	G1842	C1843	C1844	A1853	A1854	U1855	U1856	G1857	A1858	G1863	U1864	G1867	C1868	A1869	C1870																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U1716	A1717	G1718	G1719	C1730	U1736	G1737	G1738	A1739	U1740	G1741	U1742	G1743	A1744	A1745	A1746	U1747	C1748	C1752	G1753	A1754	A1755	G1756	A1757	U1758	A1759	G1760	C1761	C1764	G1767	G1770	C1771	A1772	U1773	U1774	U1775	G1776	U1777	A1780	U1781	U1782	A1783	A1784	A1785	A1786	C1787	A1788	A1789	C1790	A1791	G1792	C1793	A1794																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C1635	C1636	C1637	G1638	C1639	A1640	A1641	G1642	G1643	C1644	G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1652	G1653	A1654	A1655	C1656	U1657	C1658	G1659	G1660	G1661	U1662	A1663	A1664	A1665	G1666	C1667	G1674	A1675	A1676	A1677	A1678	A1679	U1680	G1681	C1686	G1687	C1694	G1695	C1696	G1697	A1698	G1699	A1700	A1701	G1707	A1710	A1711	G1715																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1550	A1551	G1555	C1558	U1559	C1564	C1565	A1566	G1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	A1580	G1581	C1582	G1587	G1588	A1591	C1592	A1593	U1594	C1595	A1596	A1597	A1598	U1599	C1600	G1601	U1602	A1603	C1607	A1608	A1609	A1614	C1615	A1616	C1617	A1618	G1619	G1620	U1621	U1622	C1625	A1626	A1630	G1631	A1635	A1640	A1641	A1642	A1643	A1644	A1645	A1646	C1647	A1648	A1649	A1650	A1651	A1652	G1653	A1654	A1655	A1656	A1657	U1658	G1659	G1660	G1661	G1662	G1663	A1664	A1665	A1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	A1674	C1675	A1676	A1677	A1678	A1679	U1680	G1681	C1686	G1687	C1694	G1695	G1696	G1697	A1698	G1699	A1700	A1701	G1707	A1710	A1711	G1715																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1369	C1370	G1371	U1372	A1373	C1374	A1375	A1376	A1377	A1378	U1379	G1380	A1383	A1387	G1388	U1389	G1390	U1391	U1394	A1395	U1396	U1397	A1403	C1404	U1409	G1410	C1507	A1508	U1411	U1412	A1413	G1414	U1415	A1416	C1417	G1418	U1419	A1420	G1424	U1425	C1428	G1429	G1432	A1433	A1434	A1439	U1440	G1444	G1445	C1446	C1447	G1448	A1453																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1197	U1198	U1199	U1203	A1204	A1205	G1206	U1207	U1208	A1209	G1210	A1211	G1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U19

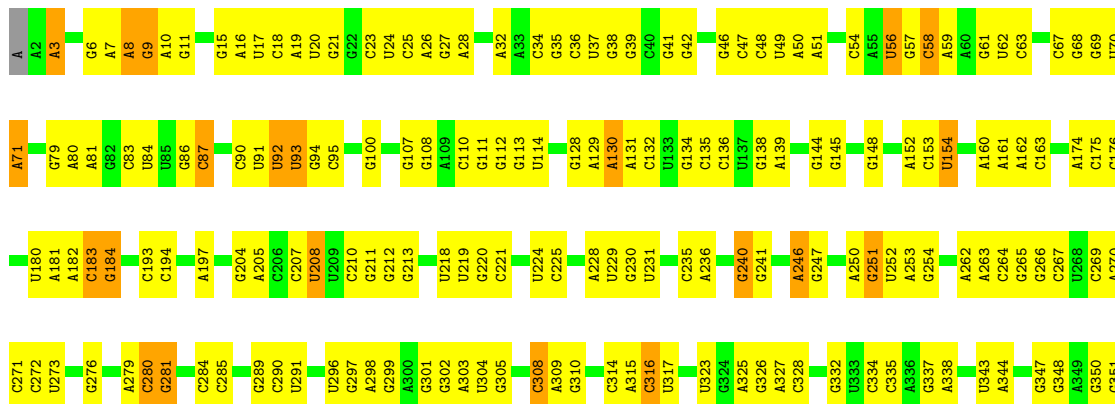


Chain 2: 50% 40% 10%



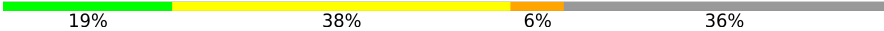
• Molecule 53: 16S rRNA

Chain 3: 45% 48% 6%



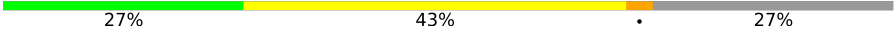
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G1491	G1401	C1327	G1174	C1098	A1019	G945	G859	G769	C679	G597	C513	G425	A353
A1492	C1402	G1253	A1179	G1099	A1022	G946	A860	C770	U684	U598	G514	U426	G354
A1493	C1403	A1254	A1180	C1100	U1023	G947	A861	G771	G685	G599	G515	U427	C355
G1494	C1404	G1255	G1181	A1102	G1024	U950	G862	U772	G690	A600	G516	G428	A356
U1495	G1405	G1331	G1182	C1103	U1025	U951	U863	G773	G691	G601	G517	U429	G357
C1496	U1406	A1257	U1183	C1104	G1026	U952	A864		G692	A602	C518	U358	U358
G1497	G1407	G1184	G1184	A1105	U1027	U953	A865	A777	G693	G607	C519	A431	G359
A1498	A1408	G1185	G1185	C1106	C1028	U954	G866	G778	U701	A608	A520	A432	G362
C1409	C1262	G1186	G1186	C1107	U1029	G954	G867	G779	A702		C528	G433	G363
A1412	C1263	A1188	A1188	G1108	U1030	U955	A872	A782	G703	C613	G529	U434	A363
G1413	U1264	C1109	C1109	C1109	G1031	U956	A873	A782	A706	C620	G530	U437	A366
U1414	G1192	U1193	U1193	A1110	G1032	U957	G874	A792	U793	A621	U531	U438	U867
G1415	U1194	U1194	U1194	A1111	G1033	A958	U875	U793	G710	A622	A532	U439	U867
U1420	C1271	U1195	U1195	A1117	U1034	A959	C876	A794	G711	G623	U533	C440	G369
G1421	A1271	U1196	U1196	A1118	A1035	U960	C877	C795	G713	G624	U534	G445	C372
G1422	A1272	U1197	U1197	U1118	A1042	U961	A878	C796	G714	U625	G535		
G1423	A1273	U1198	U1198	C1119	G1043	G962	G881	G803	A715	G626	A539	A448	G376
G1424	U1275	U1199	U1199	C1120	G1044	A964	G882	U804	G722	G627	G540	G377	G377
U1425	G1278	C1200	C1200	U1121	G1047	U965	C883	C805	A718	G628	G541	G452	G378
G1432	G1279	A1201	A1201	U1122	G1048	G966	U884	C806	C719	C631	C545	G453	G379
U1435	A1280	G1210	G1210	G1124	U1049	C967	G885	A807	C720	U632	A546	G454	G380
G1436	C1281	U1211	U1211	U1125	U1050	A968	G886		G721	G633	A547	G455	
A1437	U1282	U1212	U1212	U1126	G1054	A969		G812	G722	C634			G384
A1441	C1283	C1214	C1214	C1127	C1054	C970	A889	U813	U723	C635	U552	U458	C385
U1446	A1285	G1215	G1215	G1128	G1057	G971	G894	A814	G724	A636	U553	U459	C386
A1447	C1286	U1216	U1216	U1129	G1058	C972	G895	A815	G725	U636	A554	A460	U387
G1448	A1287	G1217	G1217	U1134	C1059	A974	A900	A816	A728	C637	U555	A461	G388
G1452	U1288	C1218	C1218	U1135	C1060	A975	A901	C817		G639	C556	G462	U389
U1453	A1289	U1219	U1219	C1136	U1061	G976	A902	A818	G731	U640	G557	U467	G391
U1454	G1290	G1221	G1221	C1137	G1062	A977	G903	U820	C732	U641	G558	A468	C392
U1457	U1291	G1222	G1222	G1138	U1063	A978	U904	G821	G733	A642	A559	U469	A393
U1458	C1292	C1223	C1223	C1139	C1064	C979	U905	C826	G734	C643	A560	A479	
U1464	C1293	A1225	A1225	C1140	U1065	U981	A906	U827	C735	U644	U561	U480	A397
A1465	G1300	C1226	C1226	C1147	C1069	C990	A907	A831	C737	G650	U562		C400
U1470	U1301	U1301	U1301	U1148	U1070	U991	A908	C738	C738	C651	C564	C483	C401
U1471	C1302	A1229	A1229	C1149	C1071	U992	A909	C739	C739	U652	U565	A493	G402
G1469	G1303	C1230	C1230	A1150	G1072	G993	C923	U835	G742	U653	G566	U485	U405
U1474	G1304	U1232	U1232	A1151	U1073	A994	C924	G836	A743		C569	U486	G406
U1475	G1305	G1233	G1233	A1152	G1074	A1000	A923	U837	A743	C658	G570	U487	G407
U1476	G1306	C1234	C1234	A1153	G1075	A1001	C924	C840	G748	U659	G571	A493	U409
U1477	U1307	A1155	A1155	A1154	U1076	A1004	G925	U841	A749	G661	A572	G410	G410
U1478	U1308	C1156	C1156	G1156	G1077	A1005	C926	U842	C750	A665	A574	G413	G413
U1479	G1309	A1157	A1157	A1157	U1078	A1006	G927	U843	C751	A666	A575	A415	A415
U1485	G1312	C1237	C1237	U1158	G1079	A1007	G928	U844	G752	G667	C578	A502	G416
G1486	U1313	U1189	U1189	C1159	G1084	A1008	G929	U845	G755	G668	A579	G417	G417
G1487	C1314	U1190	U1190	G1160	G1088	U1008	C934	G846	G756	G669	C580	G505	C418
G1488	U1315	C1162	C1162	U1008	U1091	A1012	A935	U850	U757	A673	G581	G506	C419
U1489	G1316	U1091	U1091	A1012	A1092	G1013	C936	G851	C758	G674	G582	A509	U420
U1497	C1317	A1093	A1093	A1013	A1093	A1014	A937	U855	U762	A675	U593	U421	G422
U1498	U1318	U1094	U1094	A1014	U1094	A1015	A938	C856	G763	A676	U594	A510	C422
U1499	C1319	U1095	U1095	A1015	U1095	A1016	A939	U856		U677	A595	G423	G423

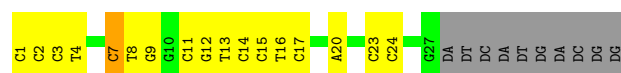
• Molecule 54: mRNA

Chain 4: 



- Molecule 55: template DNA strand

Chain 8: 



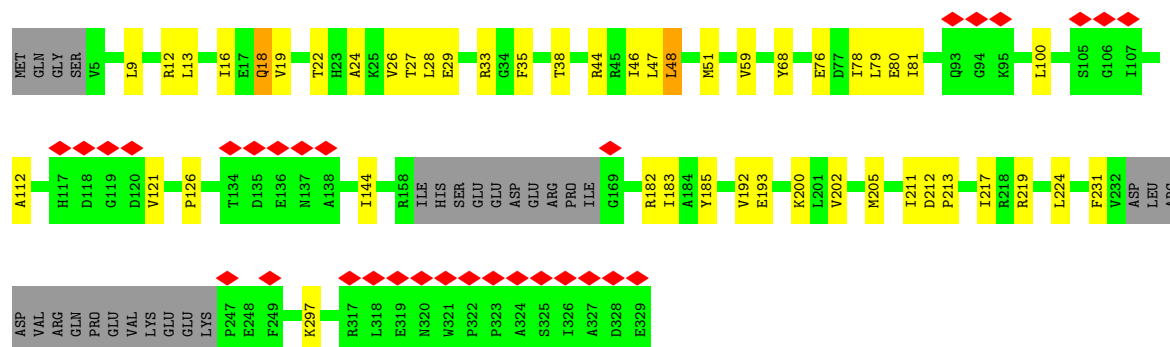
- Molecule 56: non-template DNA strand

Chain 9: 



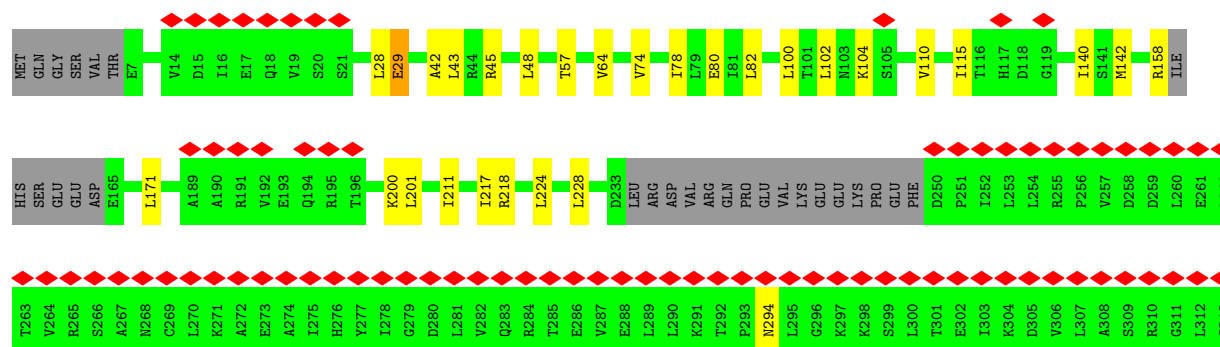
- Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain A1: 

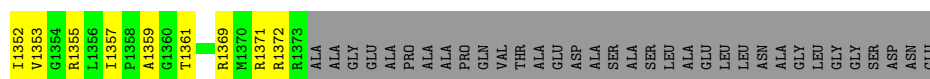


- Molecule 57: DNA-directed RNA polymerase subunit alpha

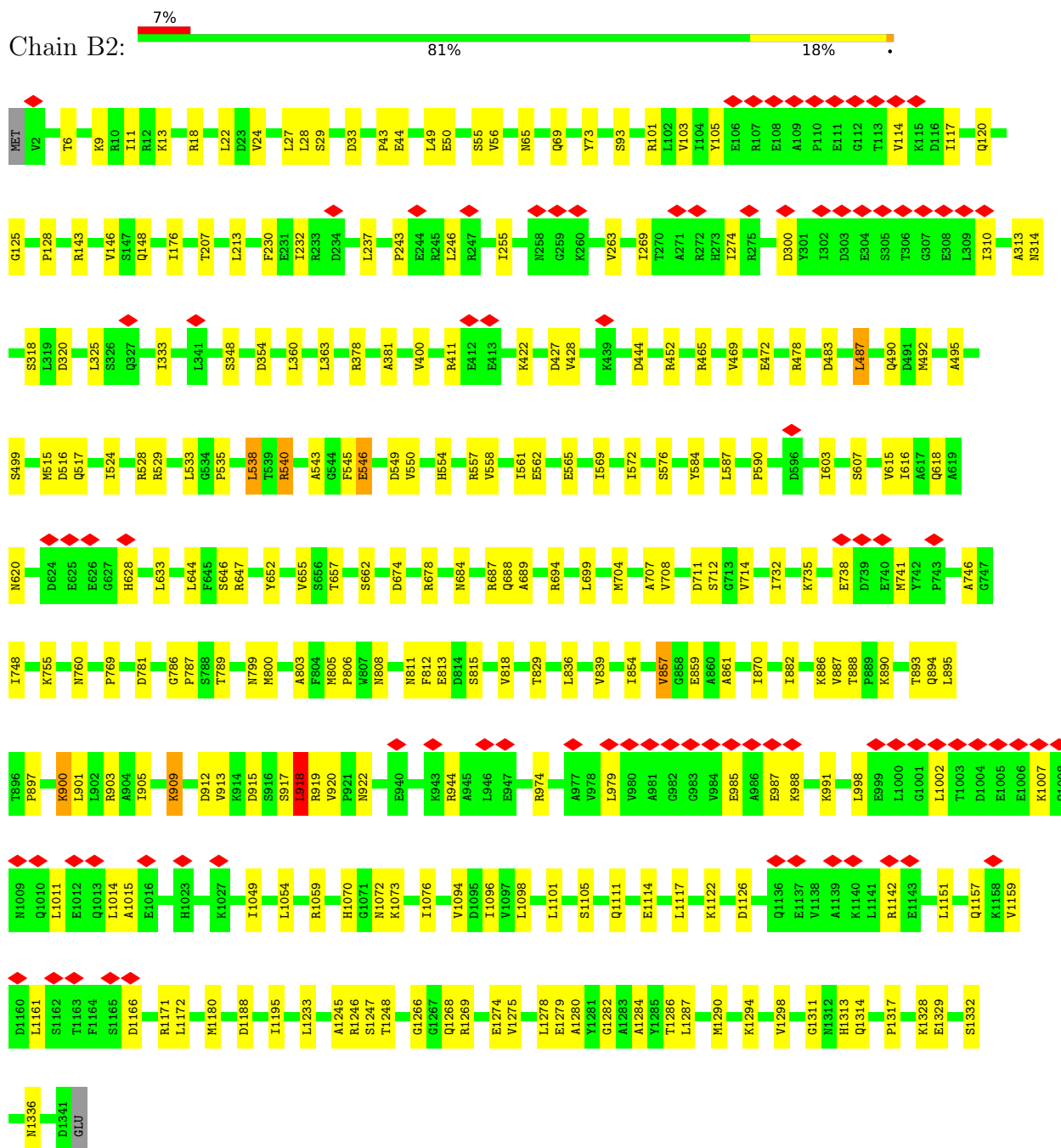
Chain A2: 



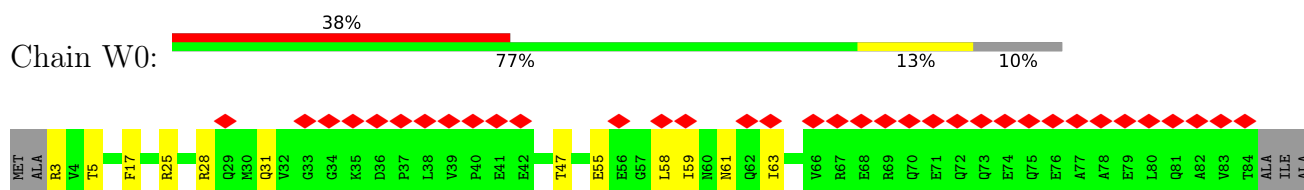




• Molecule 59: DNA-directed RNA polymerase subunit beta

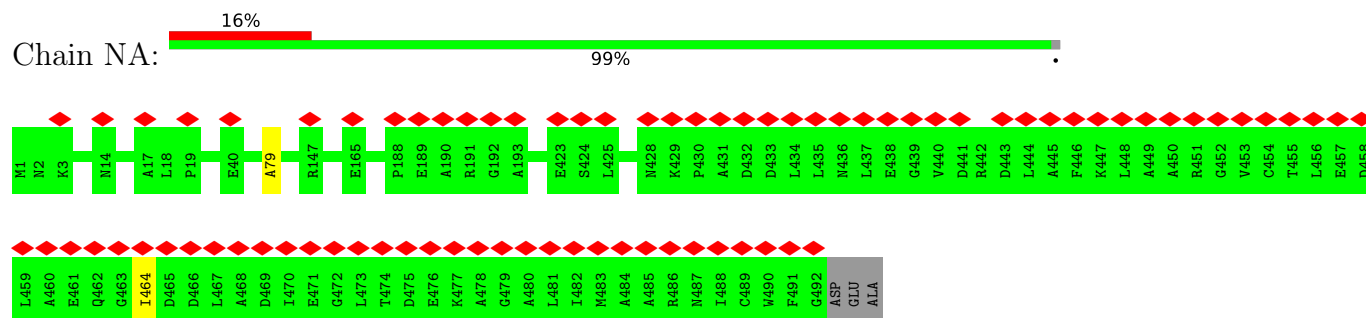


• Molecule 60: DNA-directed RNA polymerase subunit omega

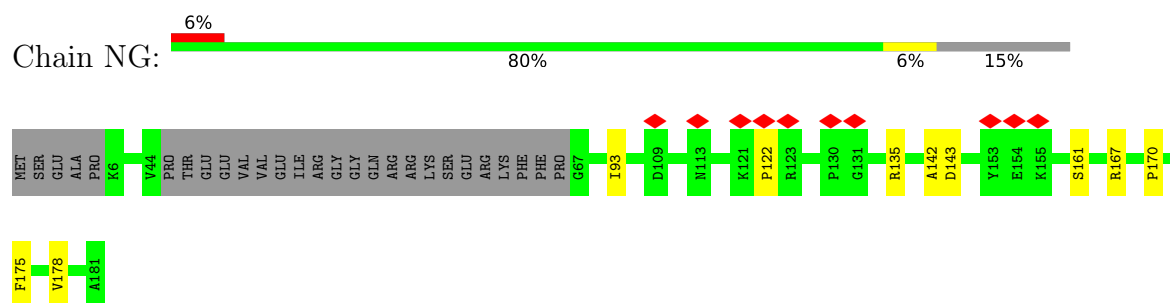


GLU
GLY
ARG
ARG

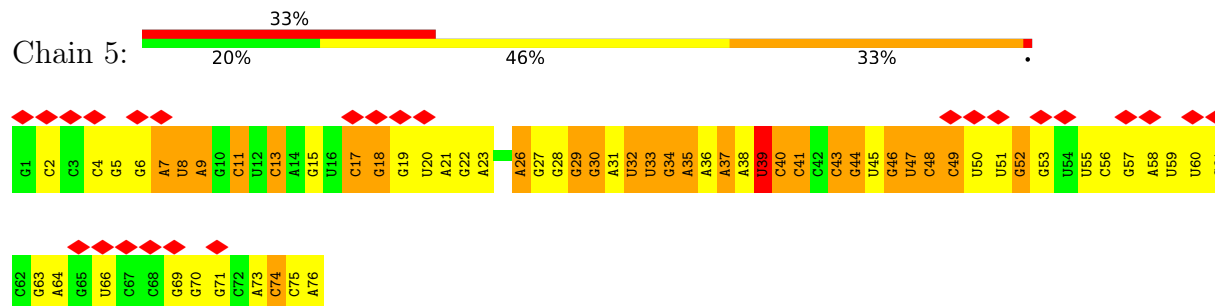
- Molecule 61: Transcription termination/antitermination protein NusA



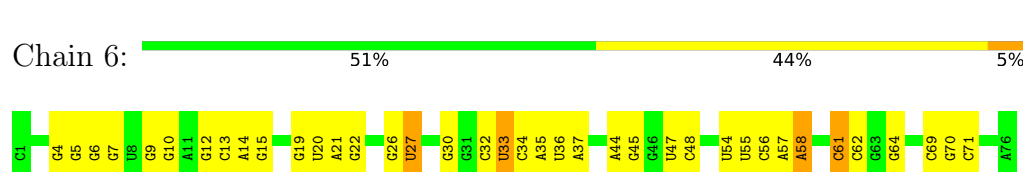
- Molecule 62: Transcription termination/antitermination protein NusG



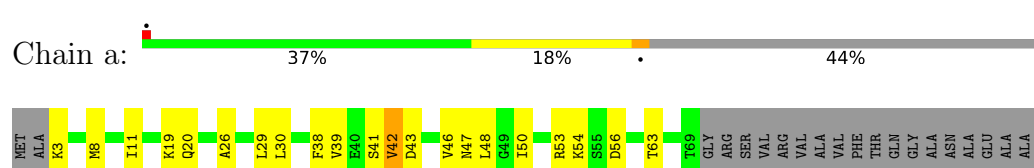
- Molecule 63: tRNA(Phe)

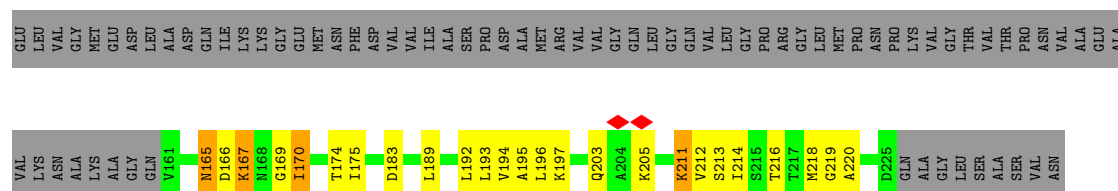


- Molecule 64: tRNA(fMet)



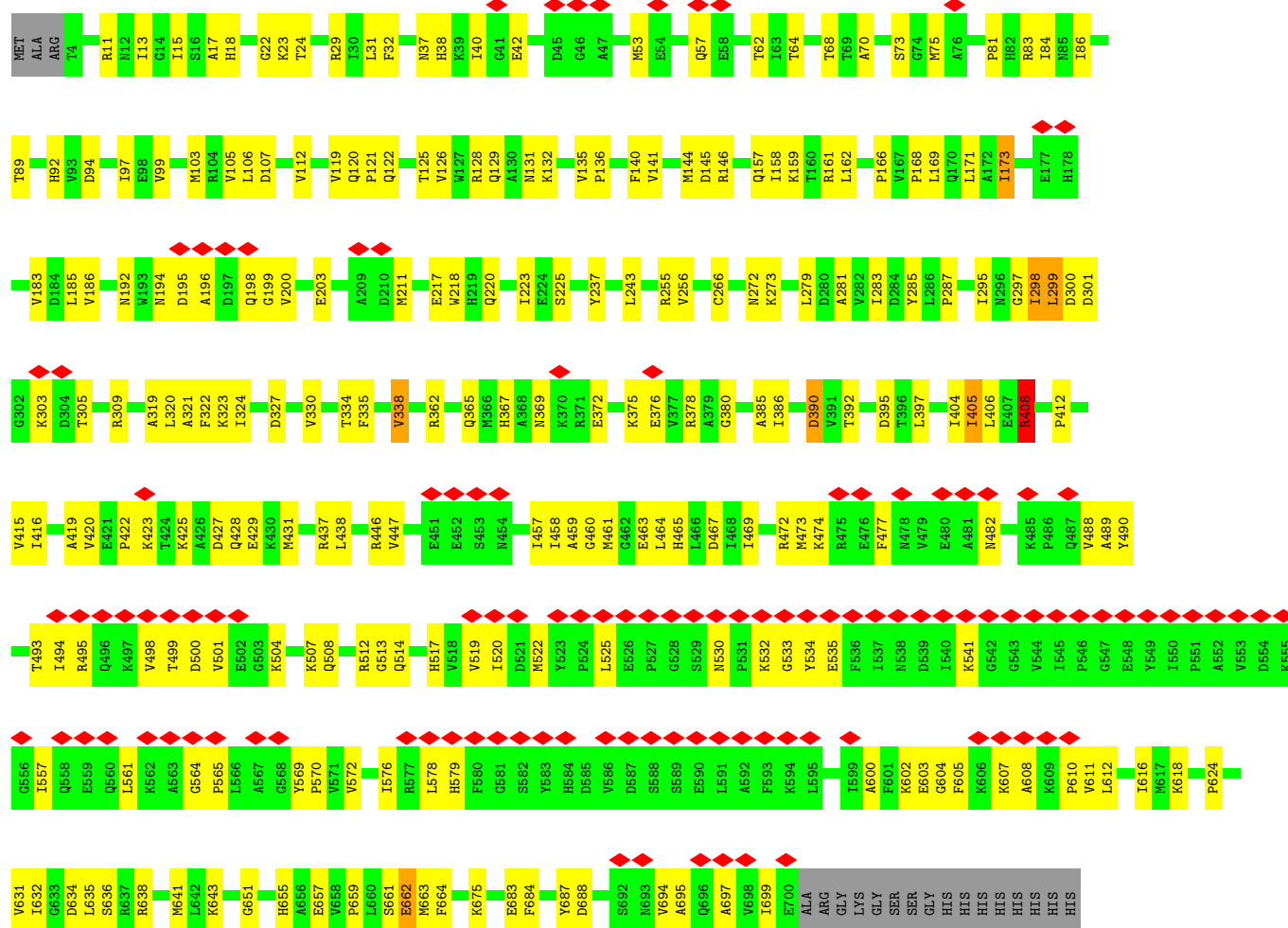
- Molecule 65: Large ribosomal subunit protein uL1





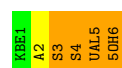
• Molecule 66: Elongation factor G

Chain 0:



• Molecule 67: Viomycin

Chain h:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.57, 1.57, 1.57	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5OH, MG, KBE, GDP, UAL, PO4, DPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/362	0.73	0/485
2	B	0.37	0/450	0.80	2/599 (0.3%)
3	C	0.31	0/416	0.61	0/554
4	D	0.48	0/380	0.95	0/498
5	E	0.46	0/513	0.80	0/676
6	F	0.40	0/303	0.79	0/397
7	G	0.41	0/1735	0.83	0/2338
8	H	0.41	0/1651	0.80	0/2225
9	I	0.31	0/1665	0.77	1/2227 (0.0%)
10	J	0.47	0/1169	0.81	0/1573
11	K	0.44	0/835	0.87	0/1128
12	L	0.41	0/1195	0.82	2/1602 (0.1%)
13	M	0.31	0/989	0.75	0/1326
14	N	0.29	0/1034	0.74	0/1375
15	O	0.56	0/796	0.81	0/1077
16	P	0.47	0/885	0.78	0/1195
17	Q	0.42	0/969	0.80	0/1300
18	R	0.28	0/892	0.68	0/1193
19	S	0.28	0/817	0.68	1/1088 (0.1%)
20	T	0.37	0/722	0.74	0/964
21	U	0.29	0/659	0.63	0/884
22	V	0.33	0/657	0.72	0/881
23	W	0.28	0/544	0.69	0/731
24	X	0.28	0/652	0.65	0/877
25	Y	0.26	0/671	0.64	2/888 (0.2%)
26	Z	0.56	0/550	1.09	1/728 (0.1%)
27	b	0.49	0/2121	0.82	0/2852
28	c	0.45	0/1586	0.77	0/2134
29	d	0.40	0/1571	0.80	3/2113 (0.1%)
30	e	0.32	0/1434	0.66	0/1926
31	f	0.29	0/1343	0.61	0/1816
32	g	0.41	0/1122	0.73	1/1515 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.39	0/1046	0.80	1/1410 (0.1%)
34	j	0.46	0/1152	0.72	0/1551
35	k	0.42	0/947	0.91	1/1268 (0.1%)
36	l	0.41	1/1054 (0.1%)	0.80	2/1403 (0.1%)
37	m	0.39	0/1093	0.81	2/1460 (0.1%)
38	n	0.54	1/973 (0.1%)	0.87	0/1301
39	o	0.32	0/902	0.68	0/1209
40	p	0.39	0/929	0.72	0/1242
41	q	0.43	0/960	0.72	0/1278
42	r	0.42	0/829	0.79	0/1107
43	s	0.52	0/864	0.83	0/1156
44	t	0.48	0/744	0.81	1/994 (0.1%)
45	u	0.38	0/787	0.75	2/1051 (0.2%)
46	v	0.35	0/766	0.66	0/1025
47	w	0.40	0/582	0.80	2/769 (0.3%)
48	x	0.64	0/635	1.13	4/848 (0.5%)
49	y	0.28	0/510	0.71	0/677
50	z	0.36	0/453	0.76	1/605 (0.2%)
51	1	0.59	0/69796	0.60	12/108888 (0.0%)
52	2	0.60	0/2872	0.55	1/4479 (0.0%)
53	3	0.60	0/36963	0.57	4/57662 (0.0%)
54	4	0.61	0/695	0.77	0/1076
55	8	0.56	0/599	0.70	1/919 (0.1%)
56	9	0.49	0/468	0.53	0/719
57	A1	0.56	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.56	4/10510 (0.0%)	0.74	8/14196 (0.1%)
59	B2	0.45	0/10714	0.66	0/14459
60	W0	0.30	0/652	0.61	0/879
61	NA	0.76	0/2431	1.22	0/3385
62	NG	1.16	0/756	1.03	0/1048
63	5	0.59	0/1812	0.90	3/2823 (0.1%)
64	6	0.59	0/1832	0.59	0/2855
65	a	0.49	0/1020	0.81	0/1370
66	0	0.40	0/5501	0.72	3/7446 (0.0%)
67	h	3.21	2/11 (18.2%)	0.75	0/13
All	All	0.54	8/196700 (0.0%)	0.67	61/289390 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
66	0	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	3	SER	CA-C	-6.73	1.38	1.52
67	h	4	SER	CA-C	-6.31	1.39	1.52
38	n	66	ALA	CA-C	-5.95	1.44	1.52
58	B1	1350	ASN	CG-ND2	-5.26	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.16	1.33	1.23

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	PRO	N-CA-C	-10.48	98.48	113.47
51	1	1020	A	C2'-C3'-O3'	7.36	120.54	109.50
48	x	11	PRO	N-CA-C	-7.35	99.50	111.77
12	L	82	SER	N-CA-C	6.91	116.43	108.49
58	B1	450	HIS	CB-CG-CD2	-6.57	122.66	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	0	408	ARG	Sidechain

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	A	355	0	353	10	0
2	B	444	0	461	14	0
3	C	409	0	440	17	0
4	D	377	0	418	17	0
5	E	504	0	574	16	0
6	F	302	0	341	14	0
7	G	1704	0	1732	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1624	0	1699	43	0
9	I	1643	0	1710	47	0
10	J	1156	0	1199	38	0
11	K	817	0	808	23	0
12	L	1181	0	1240	44	0
13	M	979	0	1034	32	0
14	N	1022	0	1070	56	0
15	O	786	0	828	32	0
16	P	869	0	878	27	0
17	Q	955	0	1019	34	0
18	R	883	0	944	23	0
19	S	805	0	847	33	0
20	T	714	0	737	18	0
21	U	649	0	666	21	0
22	V	648	0	691	17	0
23	W	535	0	552	15	0
24	X	637	0	665	17	0
25	Y	665	0	714	21	0
26	Z	544	0	579	16	0
27	b	2082	0	2157	73	0
28	c	1565	0	1616	57	0
29	d	1552	0	1619	50	0
30	e	1410	0	1447	40	0
31	f	1323	0	1374	30	0
32	g	1111	0	1148	33	0
33	i	1032	0	1088	34	0
34	j	1129	0	1162	31	0
35	k	938	0	1012	21	0
36	l	1045	0	1117	30	0
37	m	1074	0	1157	29	0
38	n	960	0	1000	34	0
39	o	892	0	923	21	0
40	p	917	0	965	23	0
41	q	947	0	1022	23	0
42	r	816	0	839	24	0
43	s	857	0	922	19	0
44	t	738	0	807	15	0
45	u	779	0	834	23	0
46	v	753	0	780	14	0
47	w	575	0	592	21	0
48	x	625	0	655	23	0
49	y	509	0	543	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	z	449	0	491	10	0
51	1	62317	0	31346	1363	0
52	2	2568	0	1303	59	0
53	3	33012	0	16618	723	0
54	4	627	0	313	8	0
55	8	539	0	305	28	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	27	0
57	A2	2029	0	1864	20	0
58	B1	10353	0	10548	321	0
59	B2	10546	0	10550	171	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	3	0
62	NG	758	0	334	9	0
63	5	1622	0	821	31	0
64	6	1640	0	837	24	0
65	a	1013	0	1081	35	0
66	0	5399	0	5363	154	0
67	h	48	0	40	6	0
68	B1	1	0	0	0	0
69	0	28	0	12	1	0
70	0	5	0	0	0	0
All	All	183377	0	132752	3780	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 3780 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)
12:L:92:PRO:HA	12:L:95:ARG:HE	1.12	1.13
51:1:1060:U:H4'	51:1:1061:U:H5'	1.32	1.10
53:3:112:G:H21	53:3:354:G:H5'	1.16	1.10
51:1:2061:G:H2'	51:1:2501:C:O2'	1.52	1.08
50:z:37:ARG:HH12	51:1:929:U:H5'	1.12	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	44/70 (63%)	38 (86%)	6 (14%)	0	100	100
2	B	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
3	C	48/55 (87%)	37 (77%)	11 (23%)	0	100	100
4	D	44/46 (96%)	35 (80%)	9 (20%)	0	100	100
5	E	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	7	37
6	F	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
7	G	216/241 (90%)	181 (84%)	35 (16%)	0	100	100
8	H	204/233 (88%)	187 (92%)	17 (8%)	0	100	100
9	I	203/206 (98%)	169 (83%)	33 (16%)	1 (0%)	24	62
10	J	155/167 (93%)	129 (83%)	26 (17%)	0	100	100
11	K	98/135 (73%)	79 (81%)	19 (19%)	0	100	100
12	L	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
13	M	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
14	N	125/130 (96%)	110 (88%)	15 (12%)	0	100	100
15	O	96/103 (93%)	82 (85%)	14 (15%)	0	100	100
16	P	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
17	Q	121/124 (98%)	97 (80%)	23 (19%)	1 (1%)	16	52
18	R	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
19	S	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
20	T	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
21	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
22	V	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
23	W	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
24	X	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
25	Y	83/87 (95%)	77 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	63/71 (89%)	47 (75%)	16 (25%)	0	100	100
27	b	269/273 (98%)	227 (84%)	42 (16%)	0	100	100
28	c	207/209 (99%)	177 (86%)	30 (14%)	0	100	100
29	d	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
30	e	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
31	f	174/177 (98%)	157 (90%)	17 (10%)	0	100	100
32	g	147/149 (99%)	125 (85%)	20 (14%)	2 (1%)	9	39
33	i	139/142 (98%)	124 (89%)	15 (11%)	0	100	100
34	j	140/142 (99%)	120 (86%)	20 (14%)	0	100	100
35	k	120/123 (98%)	98 (82%)	22 (18%)	0	100	100
36	l	141/144 (98%)	117 (83%)	24 (17%)	0	100	100
37	m	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
38	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
39	o	114/117 (97%)	103 (90%)	11 (10%)	0	100	100
40	p	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
41	q	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
42	r	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
43	s	108/110 (98%)	92 (85%)	16 (15%)	0	100	100
44	t	91/100 (91%)	77 (85%)	14 (15%)	0	100	100
45	u	100/104 (96%)	82 (82%)	18 (18%)	0	100	100
46	v	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
47	w	73/85 (86%)	63 (86%)	10 (14%)	0	100	100
48	x	75/78 (96%)	65 (87%)	10 (13%)	0	100	100
49	y	61/63 (97%)	61 (100%)	0	0	100	100
50	z	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	22 (8%)	0	100	100
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1207 (91%)	118 (9%)	4 (0%)	36	71
59	B2	1338/1342 (100%)	1205 (90%)	129 (10%)	4 (0%)	36	71
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	476 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	NG	150/181 (83%)	137 (91%)	12 (8%)	1 (1%)	18	54
65	a	128/234 (55%)	105 (82%)	23 (18%)	0	100	100
66	0	695/716 (97%)	617 (89%)	73 (10%)	5 (1%)	18	54
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10486/11185 (94%)	9322 (89%)	1145 (11%)	19 (0%)	44	77

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	15	LEU
58	B1	121	PRO
32	g	14	SER
59	B2	43	PRO
59	B2	918	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	42/62 (68%)	42 (100%)	0	100	100
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	45	64
4	D	38/38 (100%)	35 (92%)	3 (8%)	11	33
5	E	51/52 (98%)	46 (90%)	5 (10%)	7	25
6	F	34/34 (100%)	33 (97%)	1 (3%)	37	58
7	G	180/199 (90%)	172 (96%)	8 (4%)	25	48
8	H	170/190 (90%)	162 (95%)	8 (5%)	23	46
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	64
10	J	119/126 (94%)	113 (95%)	6 (5%)	22	44
11	K	87/116 (75%)	82 (94%)	5 (6%)	18	42
12	L	124/147 (84%)	121 (98%)	3 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	104/105 (99%)	102 (98%)	2 (2%)	50	66
14	N	105/107 (98%)	105 (100%)	0	100	100
15	O	86/90 (96%)	78 (91%)	8 (9%)	8	27
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	55
17	Q	103/104 (99%)	101 (98%)	2 (2%)	50	66
18	R	92/96 (96%)	91 (99%)	1 (1%)	65	73
19	S	83/84 (99%)	82 (99%)	1 (1%)	63	73
20	T	76/77 (99%)	76 (100%)	0	100	100
21	U	65/65 (100%)	65 (100%)	0	100	100
22	V	74/78 (95%)	74 (100%)	0	100	100
23	W	56/65 (86%)	56 (100%)	0	100	100
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	46 (84%)	9 (16%)	2	13
27	b	216/218 (99%)	212 (98%)	4 (2%)	50	66
28	c	164/164 (100%)	163 (99%)	1 (1%)	78	80
29	d	165/165 (100%)	160 (97%)	5 (3%)	36	57
30	e	148/150 (99%)	145 (98%)	3 (2%)	48	65
31	f	137/138 (99%)	136 (99%)	1 (1%)	76	78
32	g	114/114 (100%)	107 (94%)	7 (6%)	17	40
33	i	109/110 (99%)	109 (100%)	0	100	100
34	j	116/116 (100%)	113 (97%)	3 (3%)	40	61
35	k	103/104 (99%)	100 (97%)	3 (3%)	37	58
36	l	102/103 (99%)	100 (98%)	2 (2%)	48	65
37	m	109/109 (100%)	108 (99%)	1 (1%)	70	75
38	n	100/103 (97%)	98 (98%)	2 (2%)	48	65
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	99 (100%)	0	100	100
41	q	89/90 (99%)	89 (100%)	0	100	100
42	r	84/84 (100%)	83 (99%)	1 (1%)	63	73
43	s	93/93 (100%)	87 (94%)	6 (6%)	15	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	t	80/84 (95%)	77 (96%)	3 (4%)	29	51
45	u	83/85 (98%)	80 (96%)	3 (4%)	31	52
46	v	78/78 (100%)	77 (99%)	1 (1%)	61	71
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	65 (97%)	2 (3%)	36	57
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	47 (98%)	1 (2%)	47	65
57	A1	185/286 (65%)	174 (94%)	11 (6%)	18	41
57	A2	186/286 (65%)	184 (99%)	2 (1%)	65	73
58	B1	1110/1168 (95%)	1021 (92%)	89 (8%)	11	32
59	B2	1150/1157 (99%)	1119 (97%)	31 (3%)	39	60
60	W0	70/75 (93%)	69 (99%)	1 (1%)	59	70
65	a	109/181 (60%)	98 (90%)	11 (10%)	7	24
66	0	574/588 (98%)	550 (96%)	24 (4%)	26	49
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8120/8683 (94%)	7832 (96%)	288 (4%)	32	53

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	B2	546	GLU
66	0	662	GLU
59	B2	894	GLN
65	a	211	LYS
36	l	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
58	B1	771	GLN
66	0	276	GLN
58	B1	1238	GLN
59	B2	1237	HIS
21	U	79	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	442 (15%)	8 (0%)
52	2	119/120 (99%)	18 (15%)	0
53	3	1538/1542 (99%)	193 (12%)	1 (0%)
54	4	29/47 (61%)	15 (51%)	5 (17%)
63	5	75/76 (98%)	45 (60%)	11 (14%)
64	6	76/77 (98%)	14 (18%)	0
All	All	4739/4766 (99%)	727 (15%)	25 (0%)

5 of 727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	23	G
51	1	34	U
51	1	35	G

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	7	A
63	5	34	G
63	5	75	C
63	5	32	U
63	5	35	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
67	DPP	h	2	67	4,5,6	0.50	0	1,5,7	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	UAL	h	5	67	6,8,9	2.34	2 (33%)	4,9,11	1.89	1 (25%)
67	5OH	h	6	67	7,12,13	0.77	0	4,16,18	1.32	1 (25%)
67	KBE	h	1	67	8,8,9	0.60	0	6,8,10	1.19	0

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
67	DPP	h	2	67	-	0/2/4/6	-
67	UAL	h	5	67	-	0/3/7/9	-
67	5OH	h	6	67	-	0/2/18/20	0/1/1/1
67	KBE	h	1	67	-	0/7/7/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	5	UAL	C1-N1	-4.87	1.32	1.40
67	h	5	UAL	C-CA	-2.82	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	h	5	UAL	O-C-CA	-3.33	121.21	125.39
67	h	6	5OH	CR-CB-CA	-2.37	110.09	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	h	2	DPP	1	0
67	h	5	UAL	2	0
67	h	6	5OH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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$
69	GDP	0	801	-	29,30,30	1.17	3 (10%)	45,47,47	1.88	8 (17%)
70	PO4	0	802	-	4,4,4	1.00	0	6,6,6	0.50	0

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
69	GDP	0	801	-	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	0	801	GDP	C5-C4	2.79	1.46	1.38
69	0	801	GDP	C6-N1	-2.58	1.34	1.38
69	0	801	GDP	C4-N9	-2.01	1.32	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	0	801	GDP	C5-C4-N3	-6.00	118.84	128.39
69	0	801	GDP	C2-N3-C4	5.07	121.02	112.30
69	0	801	GDP	N9-C4-N3	4.48	134.91	125.95
69	0	801	GDP	C6-C5-N7	3.61	136.85	130.29
69	0	801	GDP	C4-C5-N7	-2.77	106.28	110.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

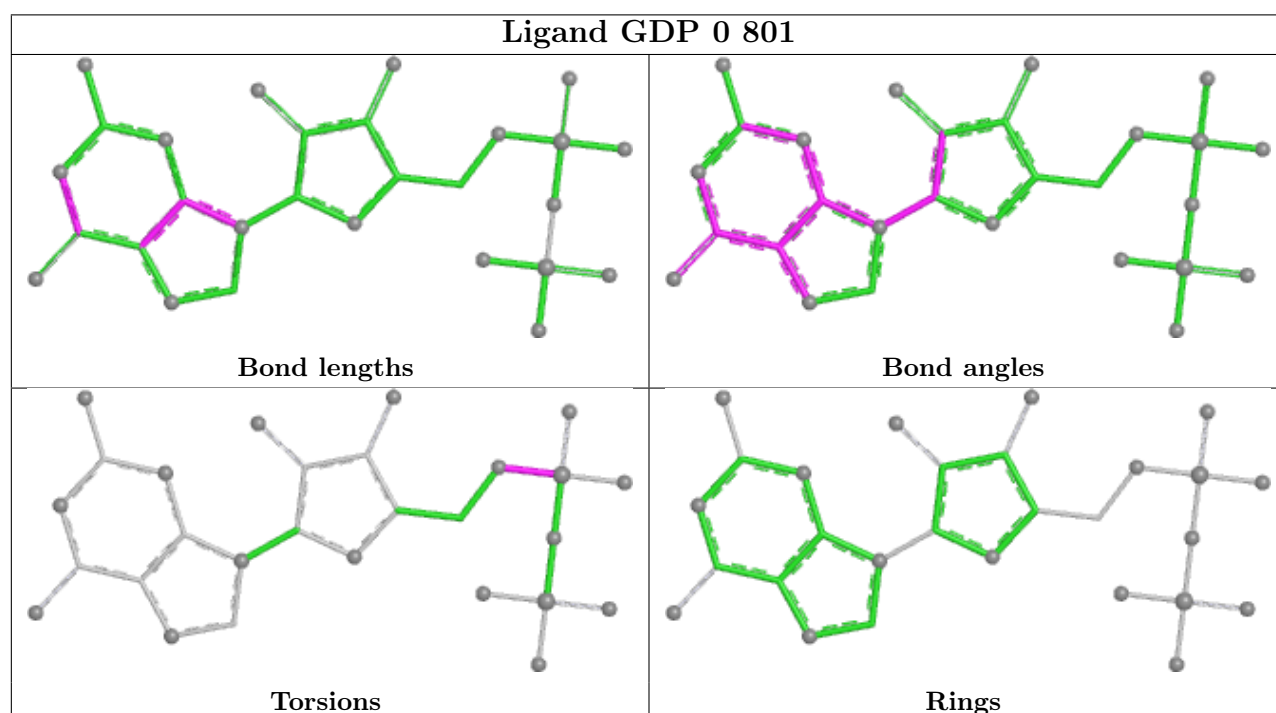
Mol	Chain	Res	Type	Atoms
69	0	801	GDP	C5'-O5'-PA-O3A
69	0	801	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	0	801	GDP	1	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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

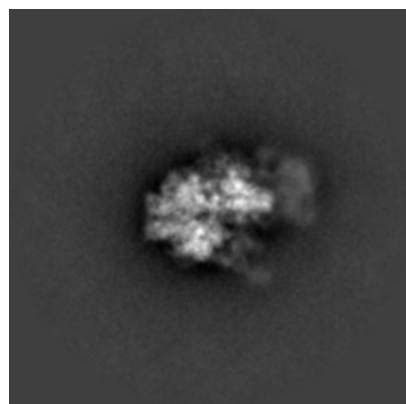
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38944. These allow visual inspection of the internal detail of the map and identification of artifacts.

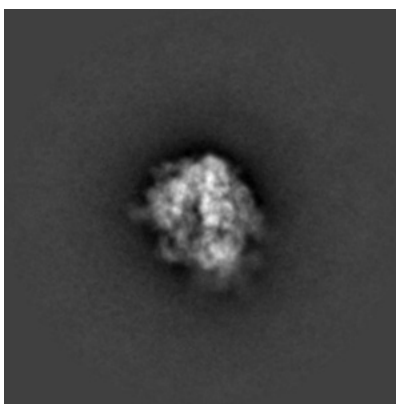
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

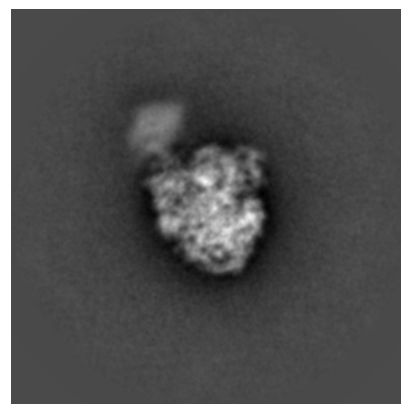
6.1.1 Primary map



X

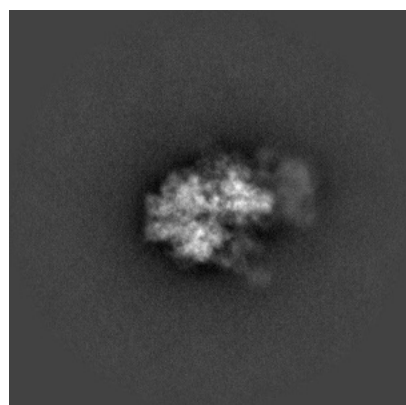


Y

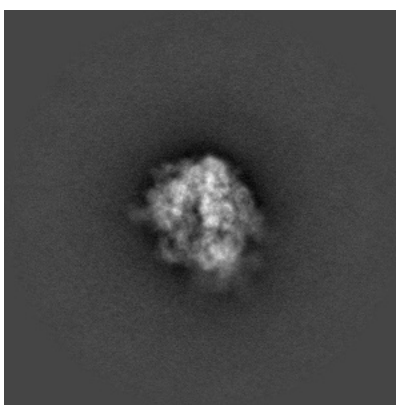


Z

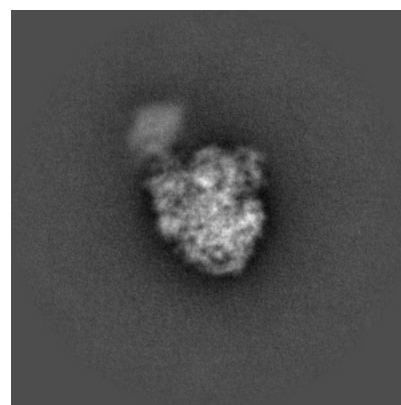
6.1.2 Raw map



X



Y

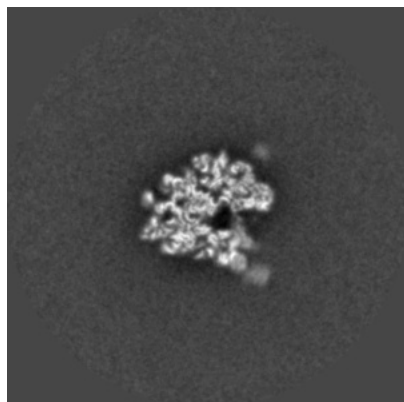


Z

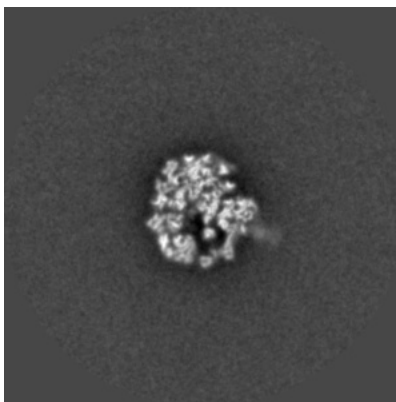
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

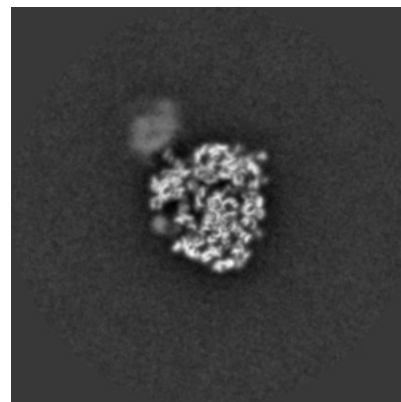
6.2.1 Primary map



X Index: 240

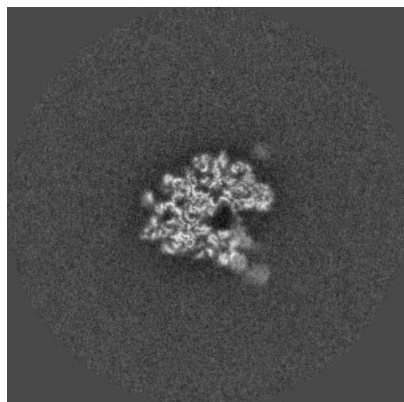


Y Index: 240

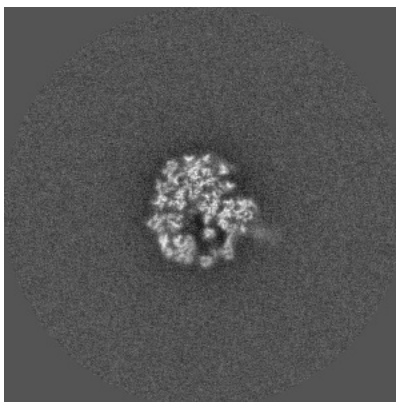


Z Index: 240

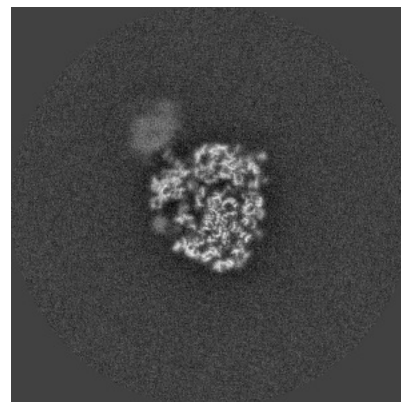
6.2.2 Raw map



X Index: 240



Y Index: 240

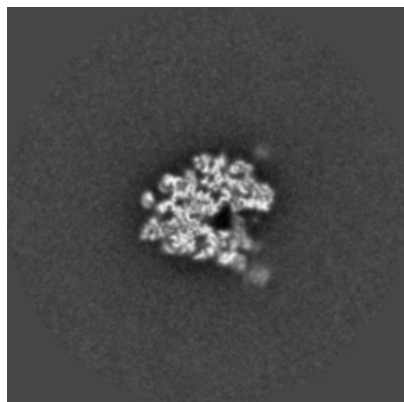


Z Index: 240

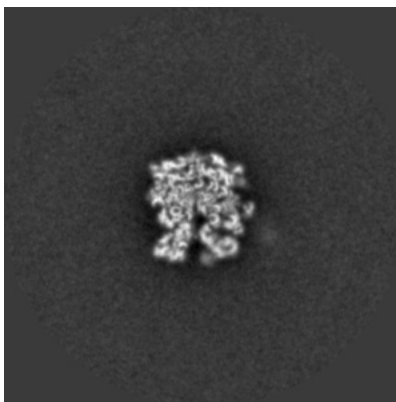
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

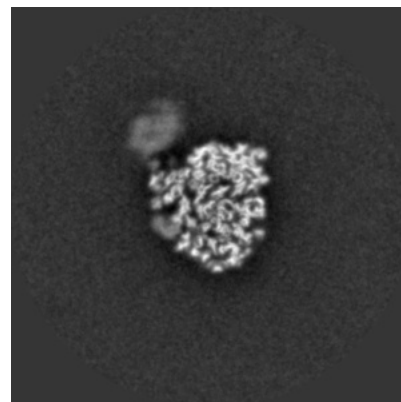
6.3.1 Primary map



X Index: 242

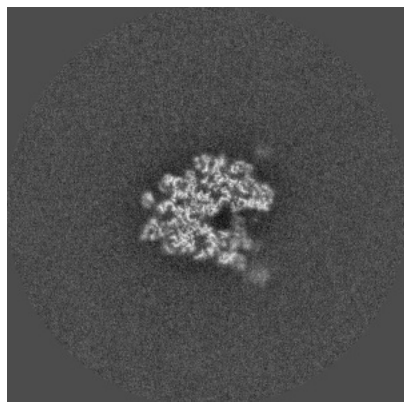


Y Index: 225

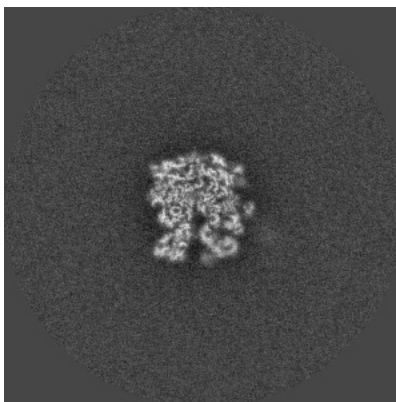


Z Index: 245

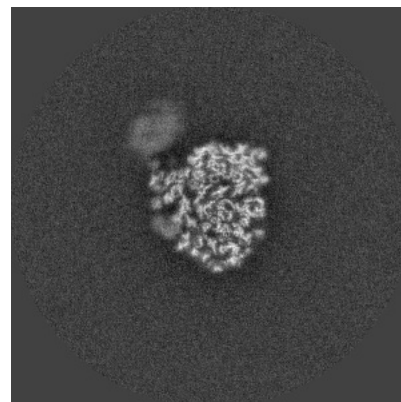
6.3.2 Raw map



X Index: 242



Y Index: 225



Z Index: 245

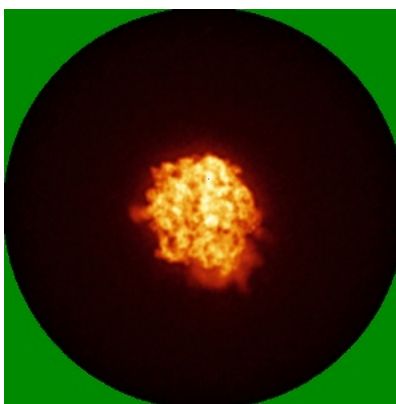
The images above show the largest variance slices of the map in three orthogonal directions.

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

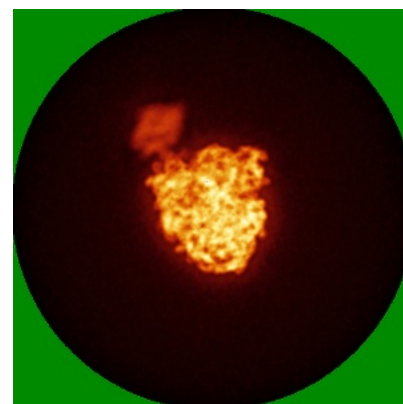
6.4.1 Primary map



X

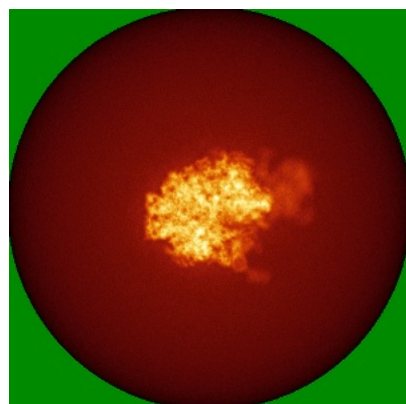


Y

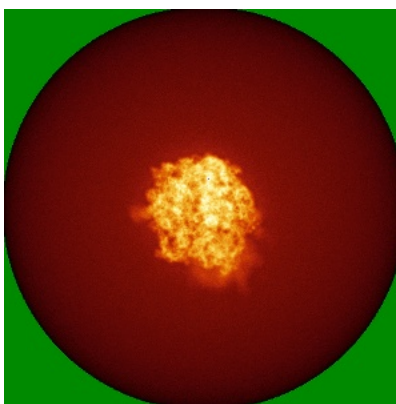


Z

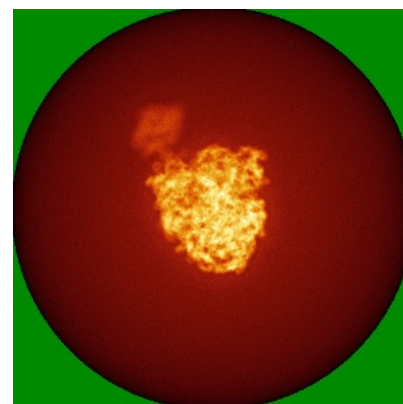
6.4.2 Raw map



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.

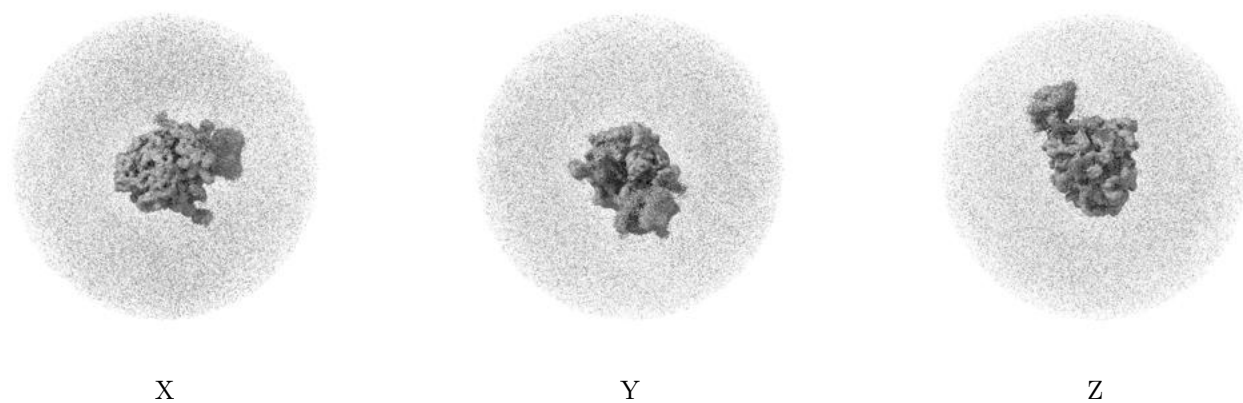
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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



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.

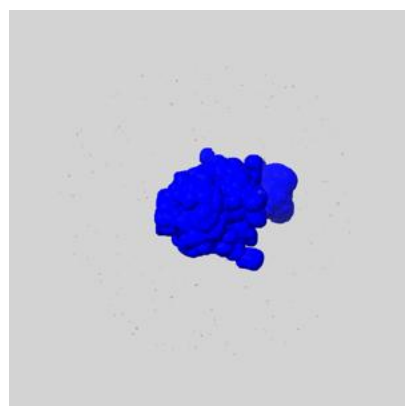
6.6 Mask visualisation [i](#)

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

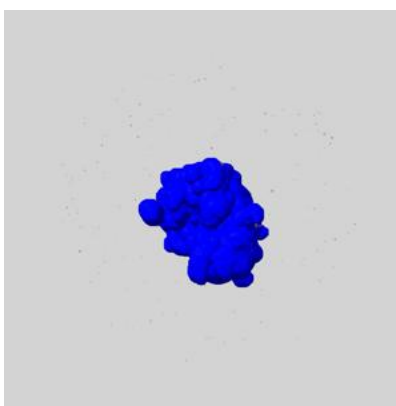
A mask typically either:

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

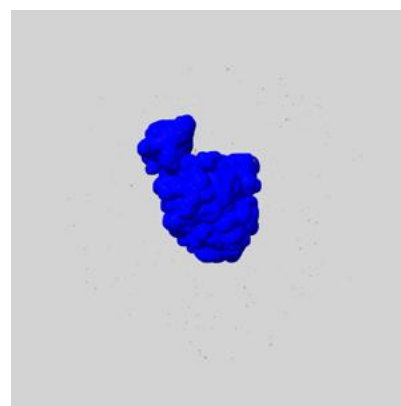
6.6.1 emd_38944_msk_1.map [i](#)



X



Y

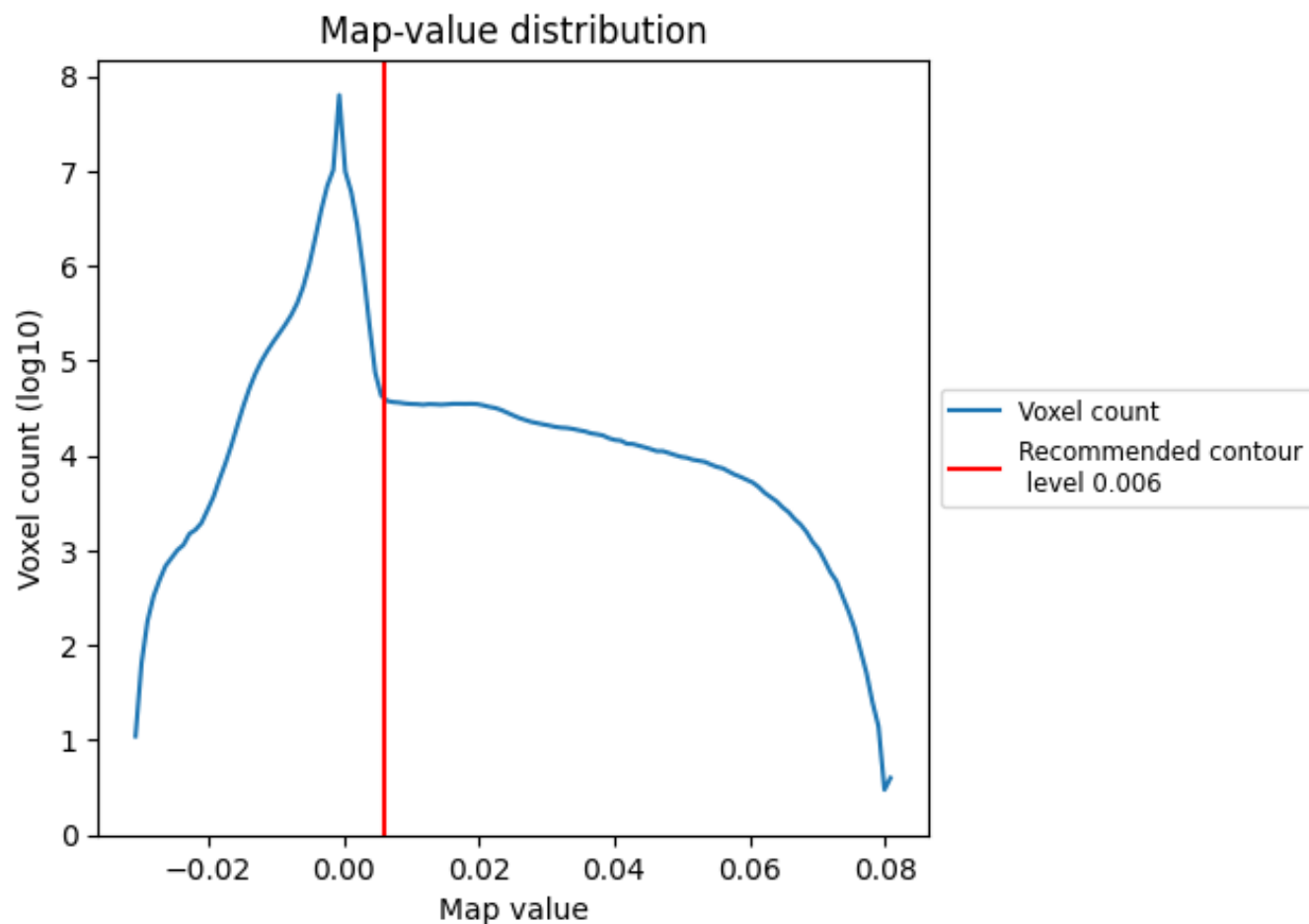


Z

7 Map analysis [i](#)

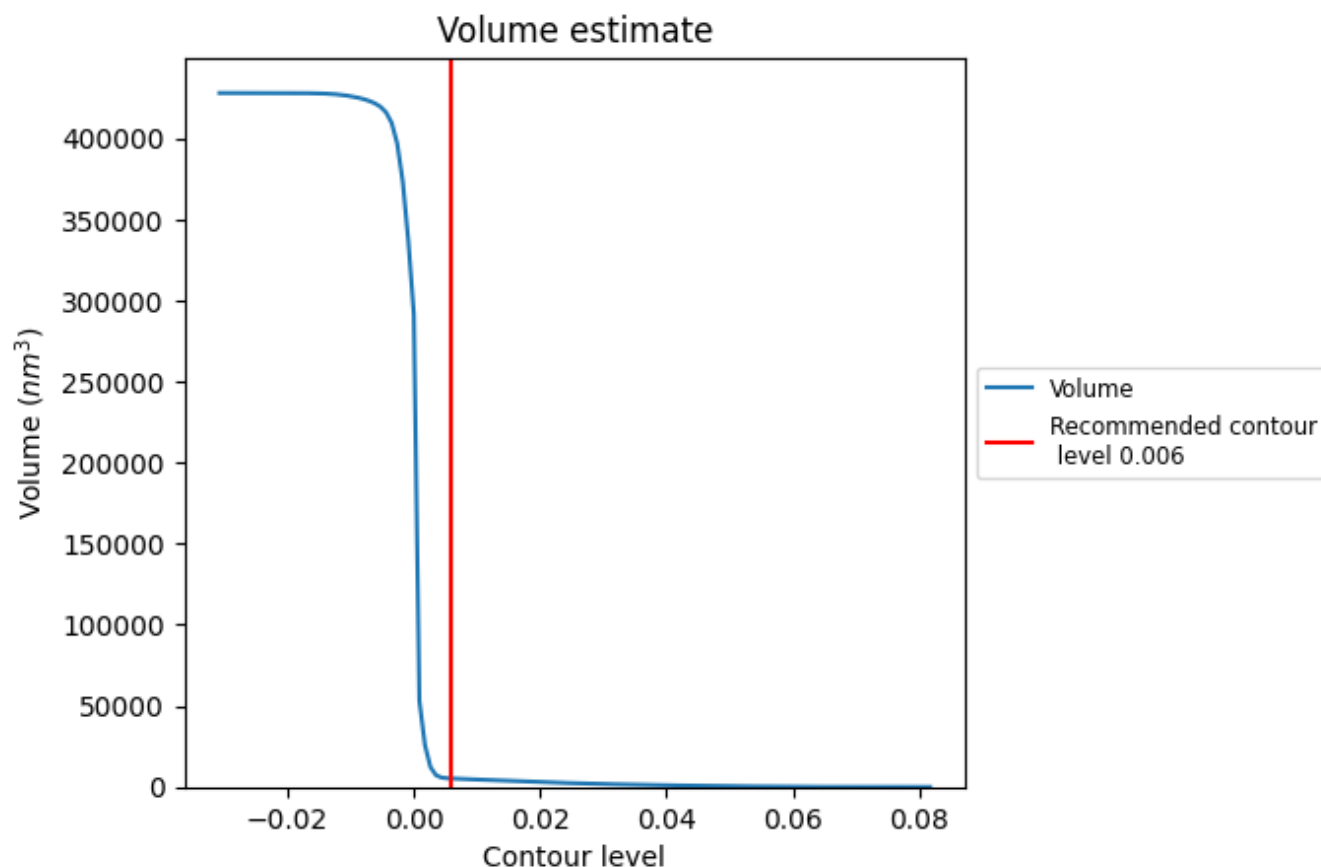
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

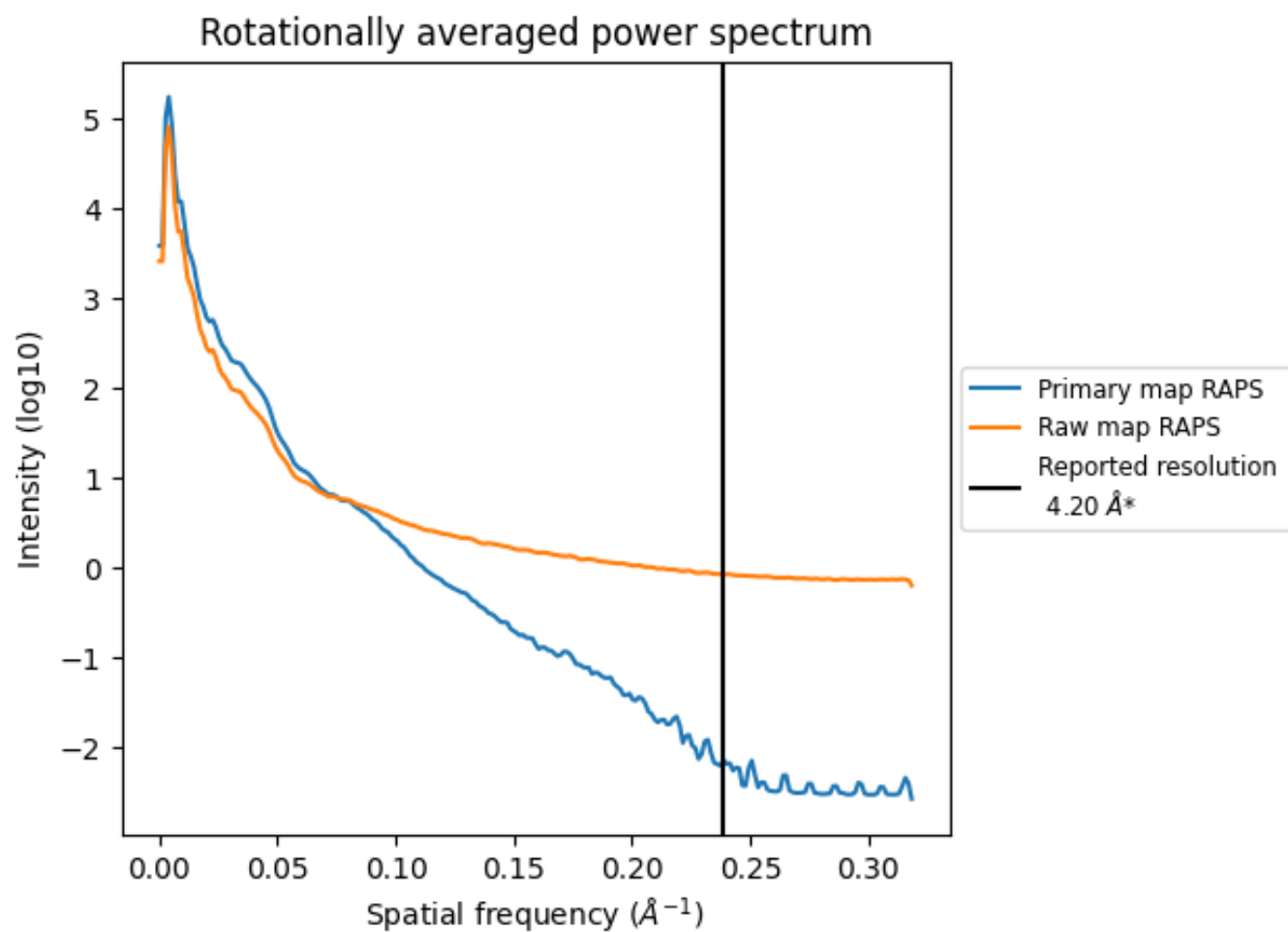
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5225 nm³; this corresponds to an approximate mass of 4720 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](#)

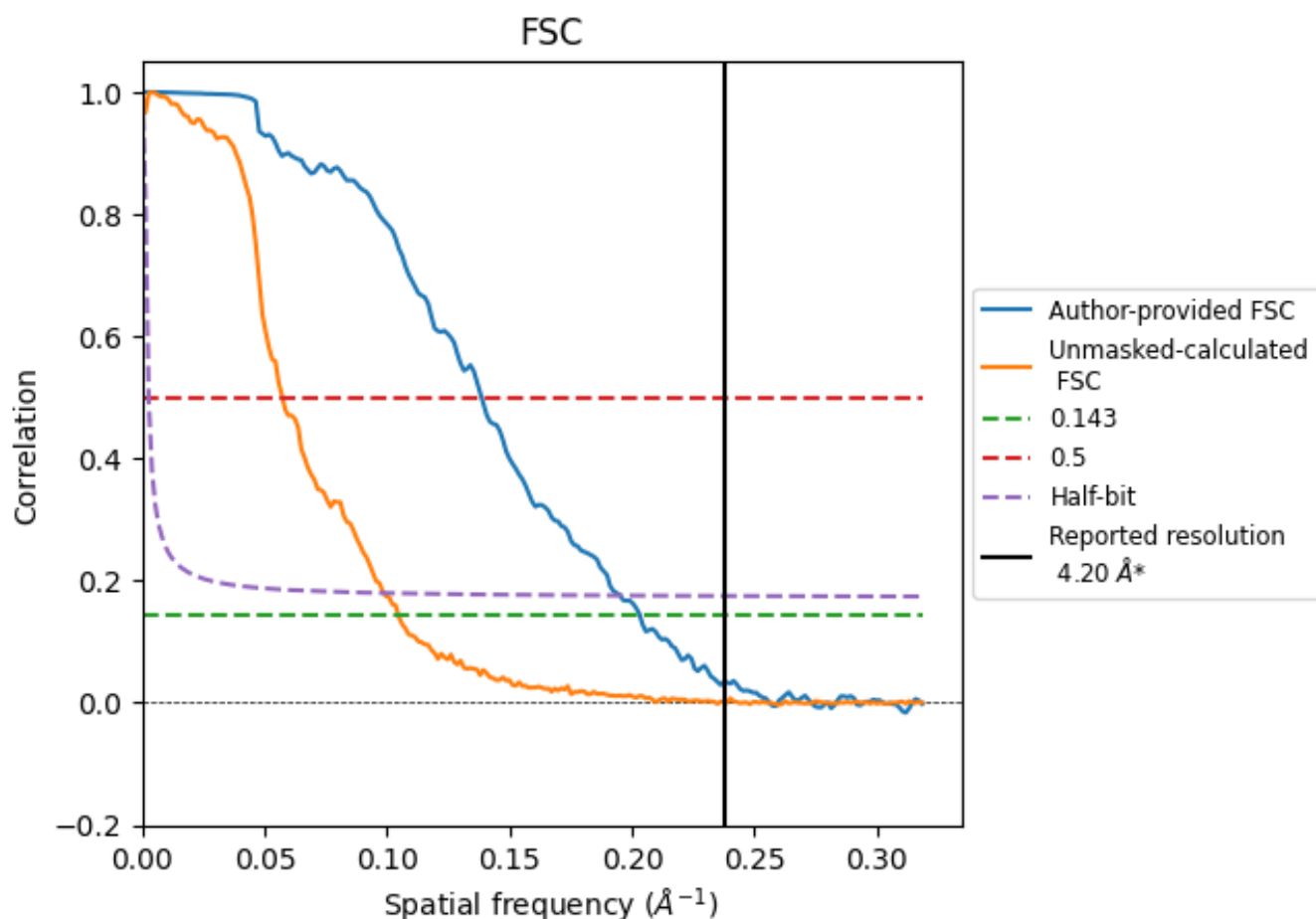


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.92	7.22	5.12
Unmasked-calculated*	9.56	17.48	10.13

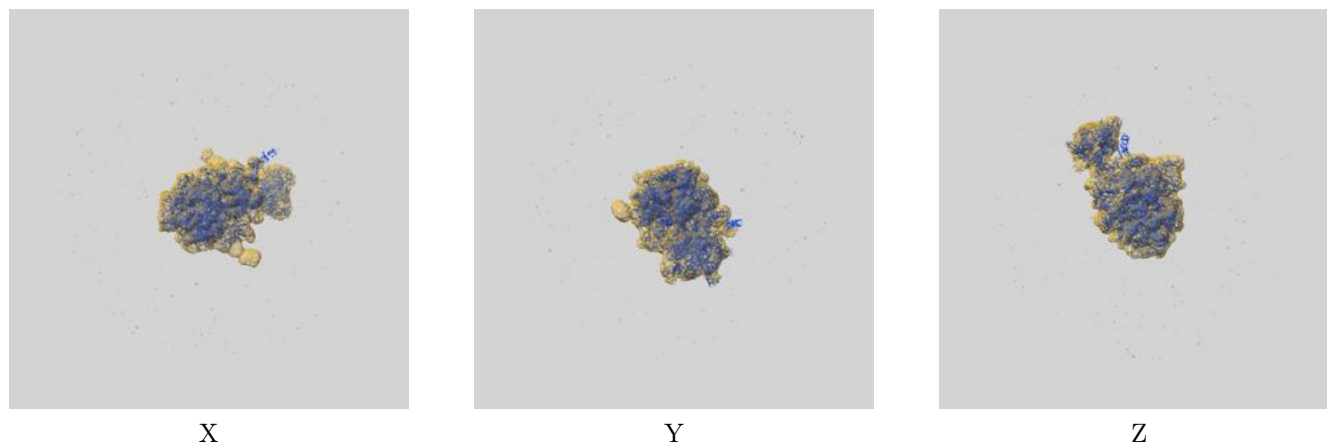
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.92 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.56 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38944 and PDB model 8Y5O. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



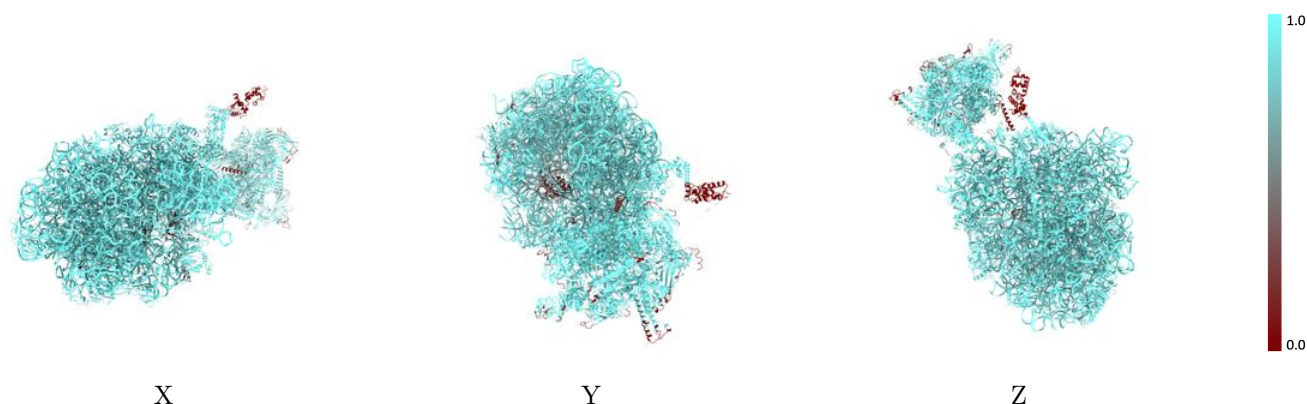
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



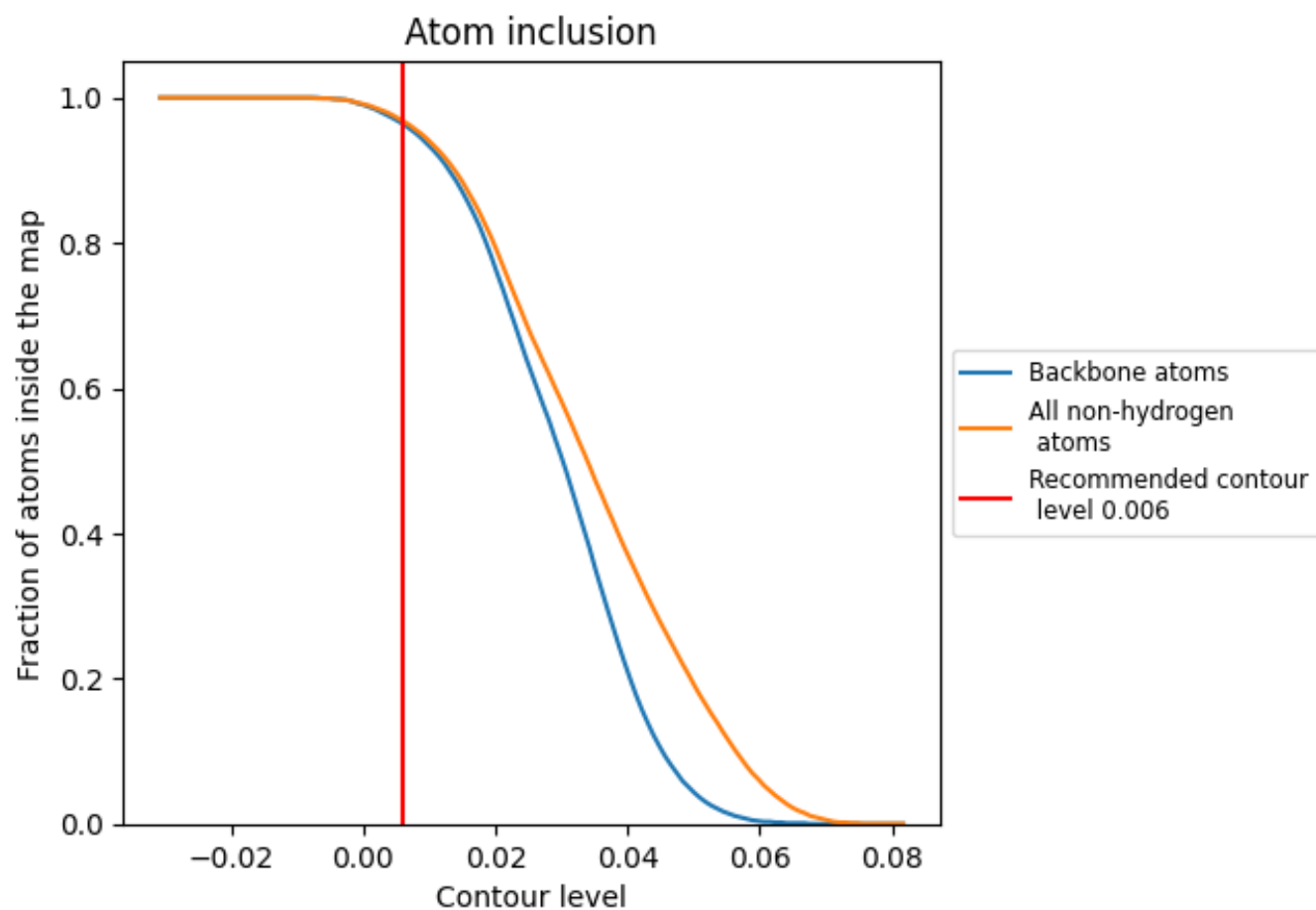
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.1480
0	 0.7960	 0.0940
1	 0.9980	 0.1980
2	 1.0000	 0.1570
3	 0.9990	 0.1790
4	 0.9680	 0.1100
5	 0.6240	 0.0980
6	 0.9930	 0.1720
8	 1.0000	 0.0200
9	 1.0000	 0.0670
A	 0.9970	 0.1130
A1	 0.8930	 0.0340
A2	 0.7520	 0.0430
B	 0.9860	 0.1430
B1	 0.9350	 0.0230
B2	 0.9170	 0.0360
C	 0.9550	 0.1350
D	 0.9750	 0.1360
E	 0.9980	 0.1230
F	 0.9930	 0.1030
G	 0.9800	 0.1360
H	 0.9880	 0.1440
I	 0.9920	 0.1270
J	 0.9900	 0.1410
K	 0.9850	 0.1510
L	 0.9730	 0.1380
M	 0.9760	 0.1110
N	 0.9810	 0.1040
NA	 0.8340	 0.1340
NG	 0.9350	 0.0530
O	 0.9950	 0.1140
P	 0.9870	 0.1500
Q	 0.9450	 0.1460
R	 0.9740	 0.1410
S	 0.9970	 0.1150



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.9960	 0.1360
U	 1.0000	 0.1100
V	 0.9890	 0.1100
W	 0.9980	 0.1440
W0	 0.5380	 0.0170
X	 1.0000	 0.1160
Y	 0.9790	 0.1170
Z	 0.9340	 0.1470
a	 0.9770	 0.0990
b	 0.9810	 0.1670
c	 0.9940	 0.1550
d	 0.9890	 0.1430
e	 0.9500	 0.1060
f	 0.9880	 0.1370
g	 0.8680	 0.1230
h	 1.0000	 0.1790
i	 0.8950	 0.0460
j	 0.9940	 0.1560
k	 0.9580	 0.1810
l	 0.9940	 0.1200
m	 0.9630	 0.1320
n	 0.9990	 0.1550
o	 1.0000	 0.0960
p	 0.9930	 0.1790
q	 0.9970	 0.1290
r	 0.9940	 0.1370
s	 0.9880	 0.1620
t	 0.9850	 0.1470
u	 0.9840	 0.1410
v	 0.9920	 0.1410
w	 0.9890	 0.1050
x	 0.9970	 0.1580
y	 0.9900	 0.1450
z	 0.9820	 0.1480