



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 08:17 AM UTC

PDB ID : 8YDJ / pdb_00008ydj
EMDB ID : EMD-39173
Title : E.coli transcription translation coupling complex in TTC-P containing mRNA with 39-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-02-20
Resolution : 5.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

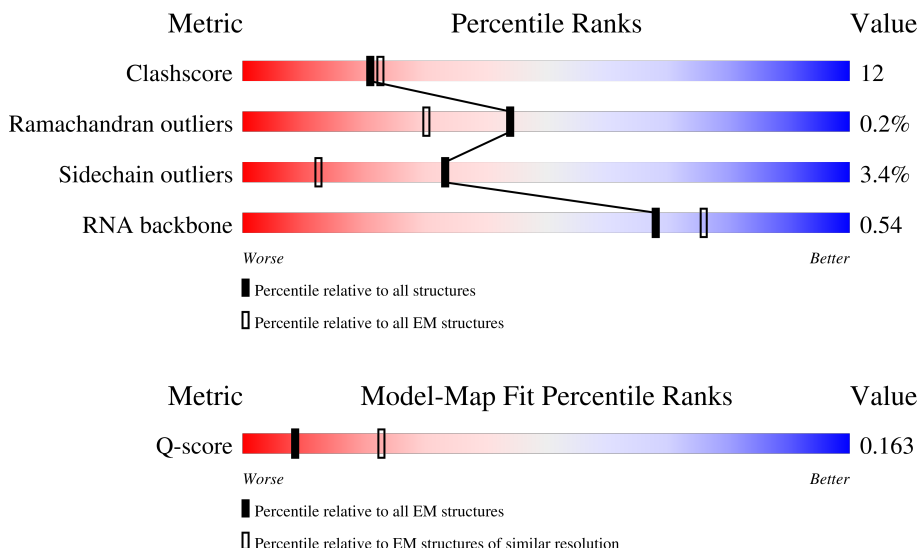
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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.



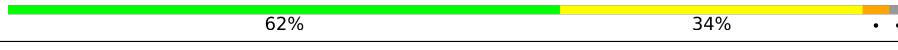
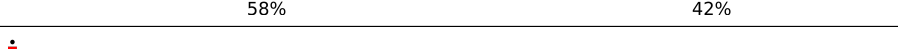
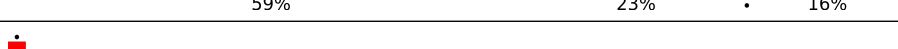
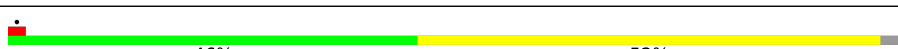
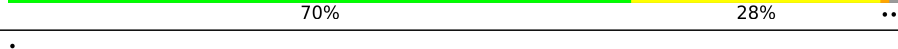
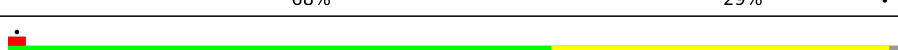
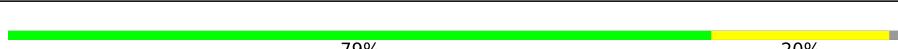
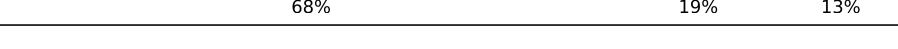
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	844 (4.60 - 5.60)

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	

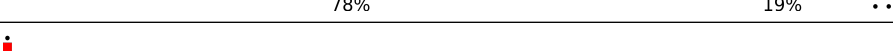
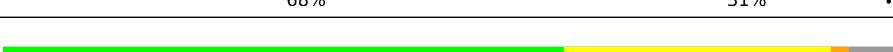
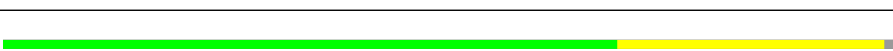
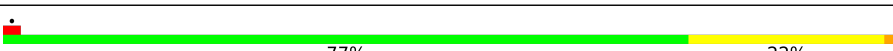
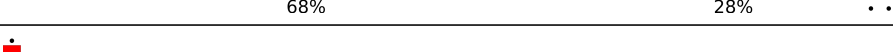
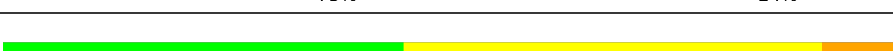
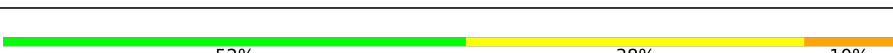
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Mol	Chain	Length	Quality of chain
4	D	46	
5	E	65	
6	F	38	
7	G	241	
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	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

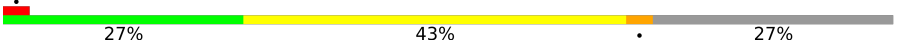
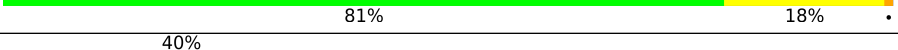
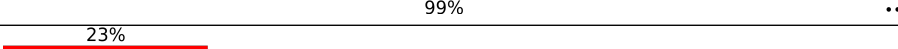
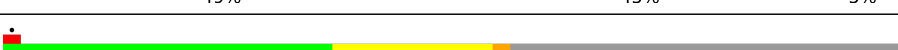
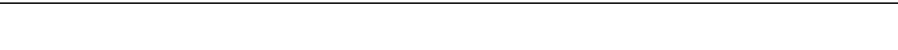
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Mol	Chain	Length	Quality of chain
29	d	201	
30	e	179	
31	f	177	
32	g	149	
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59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

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Mol	Chain	Length	Quality of chain
54	4	56	
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

Continued on next page...

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

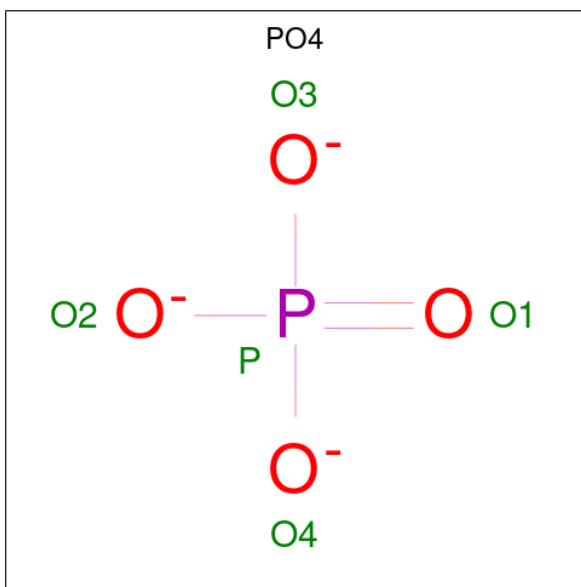
- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 67 | h | 6 | Total | C | N | O | 0 | 0 |
| | | | 48 | 25 | 13 | 10 | | |

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

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being a diphosphate (P₂O₇) moiety. The structure is labeled with various atoms and bonds, including the guanine base (N1, N2, N3, N7, C2, C4, C5, C6, C8), the ribose sugar (C1', C2', C3', C4', C5'), and the phosphate groups (P1, P2, O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B).

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

- WORLDWIDE
PDB
PROTEIN DATA BANK

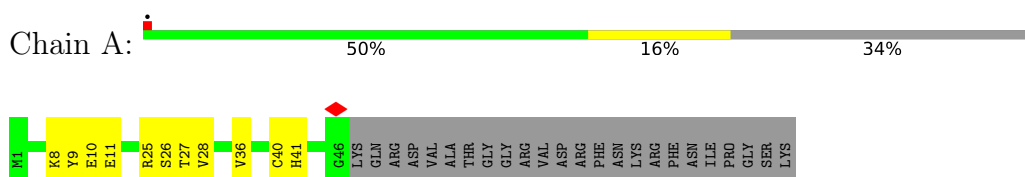


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

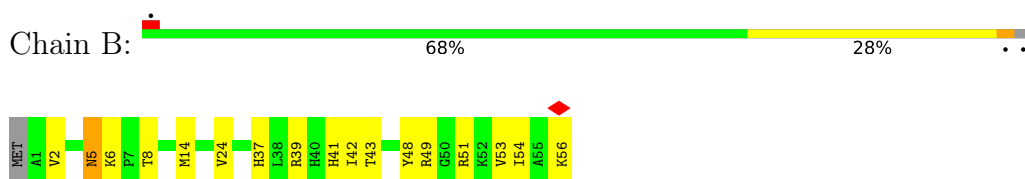
3 Residue-property plots [i](#)

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.

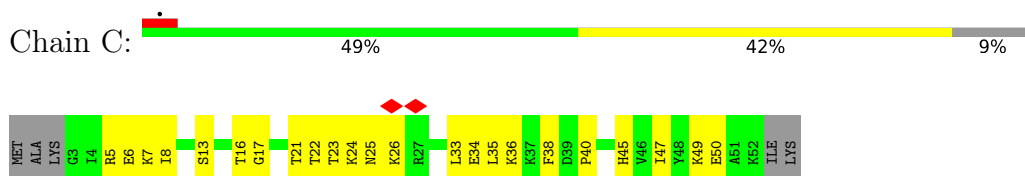
- Molecule 1: 50S ribosomal protein L31



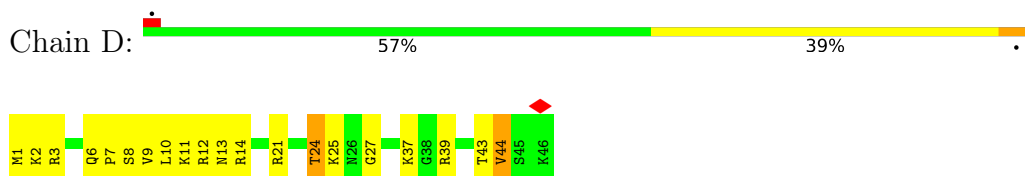
- Molecule 2: 50S ribosomal protein L32



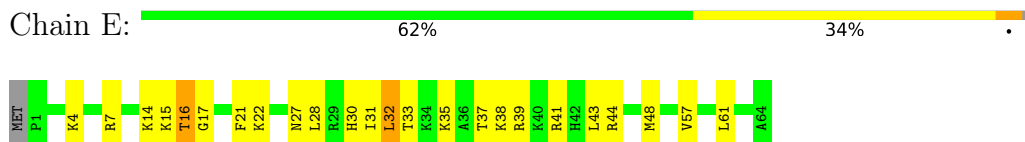
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34

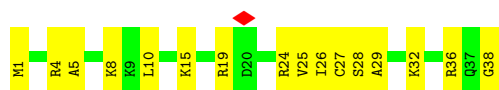


- Molecule 5: 50S ribosomal protein L35



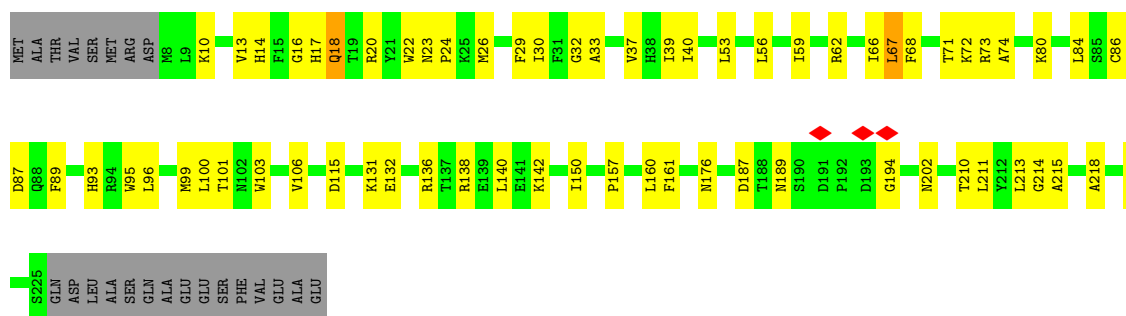
- Molecule 6: 50S ribosomal protein L36

Chain F:  58% 42%



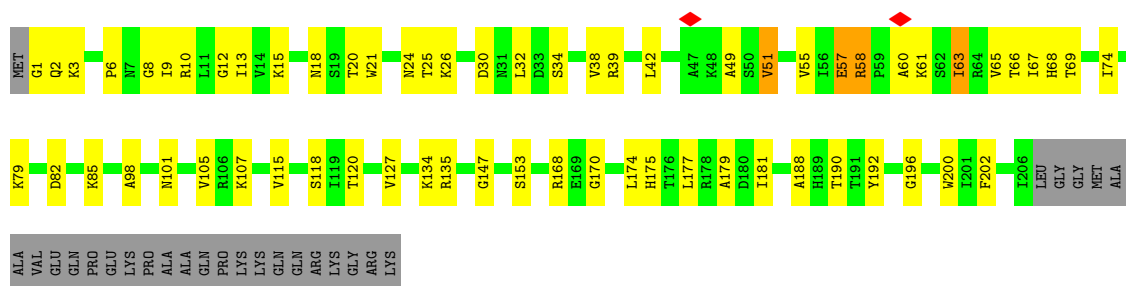
- Molecule 7: 30S ribosomal protein S2

Chain G:  63% 26% 10%



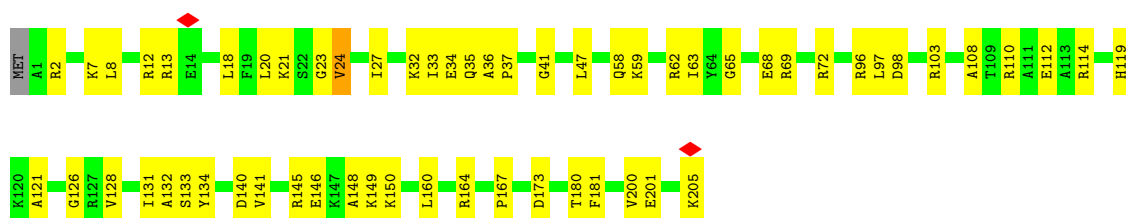
- Molecule 8: 30S ribosomal protein S3

Chain H:  61% 26% 12%



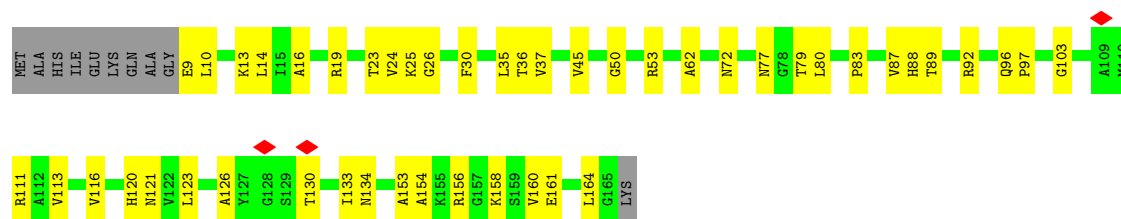
- Molecule 9: 30S ribosomal protein S4

Chain I:  71% 28%

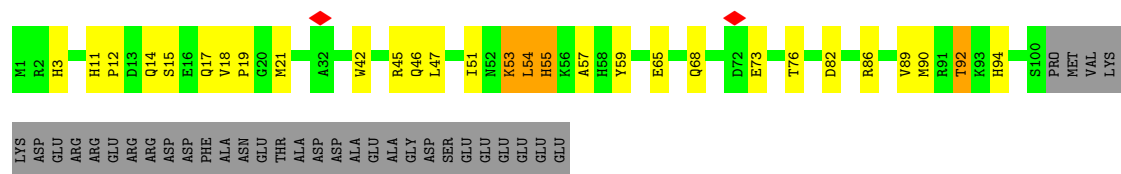


- Molecule 10: 30S ribosomal protein S5

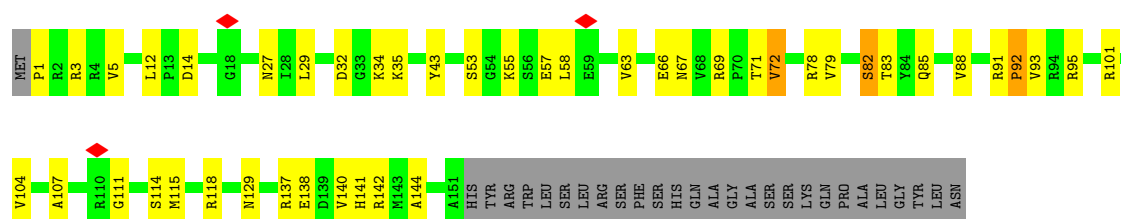
Chain J:  66% 28% 6%



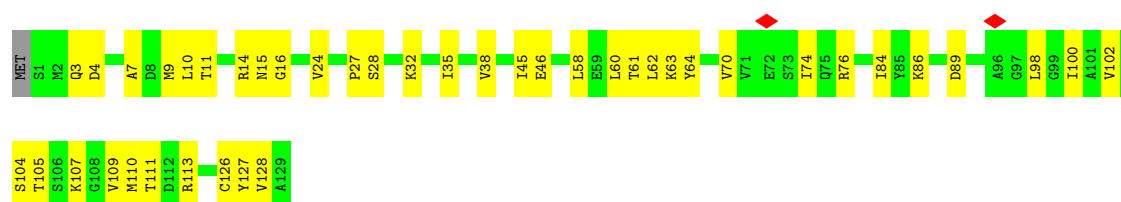
- Molecule 11: 30S ribosomal protein S6, fully modified isoform



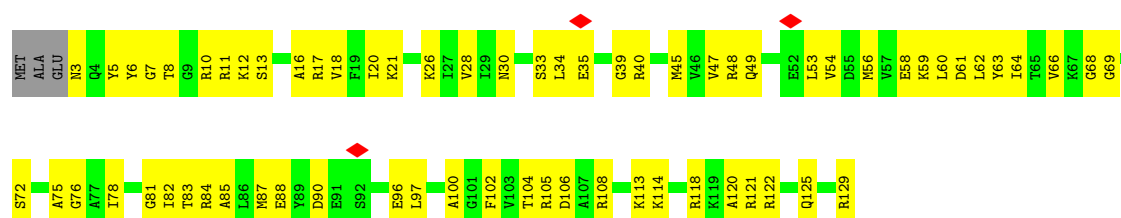
- Molecule 12: 30S ribosomal protein S7



- Molecule 13: 30S ribosomal protein S8

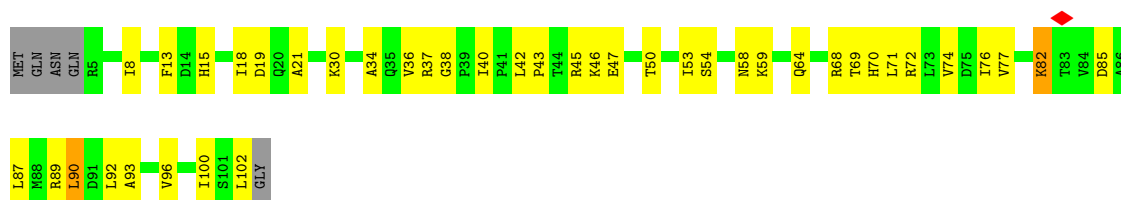


- Molecule 14: 30S ribosomal protein S9



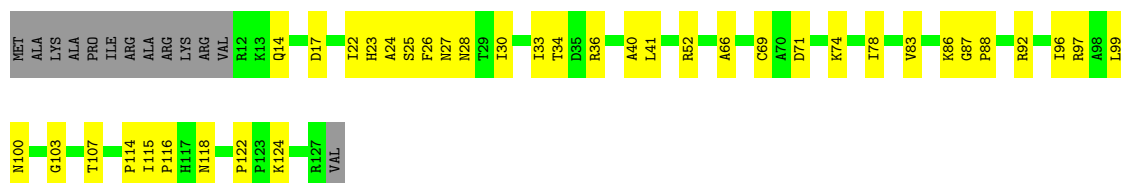
- Molecule 15: 30S ribosomal protein S10

Chain O: 



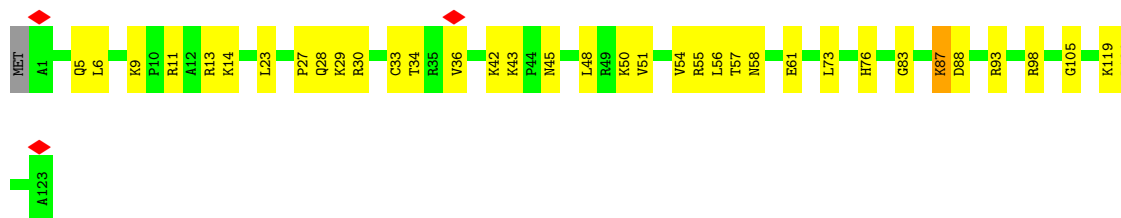
- Molecule 16: 30S ribosomal protein S11

Chain P: 



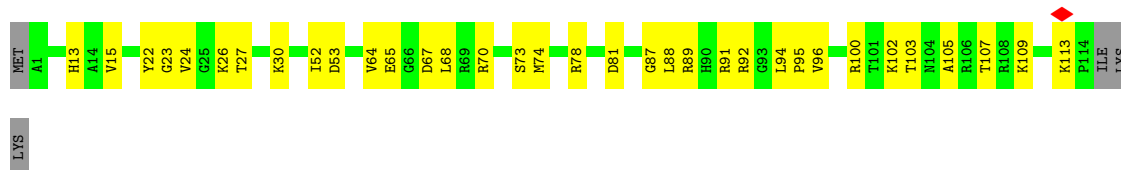
- Molecule 17: 30S ribosomal protein S12

Chain Q: 



- Molecule 18: 30S ribosomal protein S13

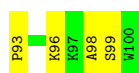
Chain R: 



- Molecule 19: 30S ribosomal protein S14

Chain S: 





- Molecule 20: 30S ribosomal protein S15

Chain T: 79% 20%



- Molecule 21: 30S ribosomal protein S16

Chain U: 72% 28%



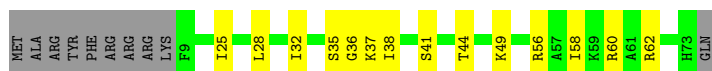
- Molecule 22: 30S ribosomal protein S17

Chain V: 67% 29% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W: 68% 19% 13%



- Molecule 24: 30S ribosomal protein S19

Chain X: 65% 21% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y: 64% 33%

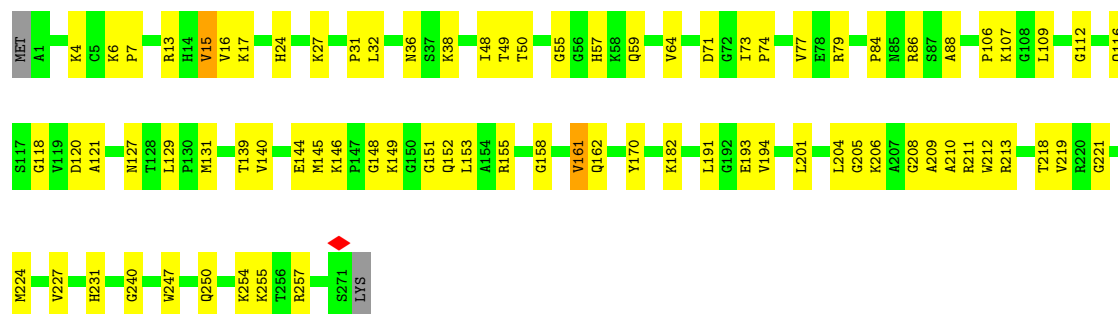


- Molecule 26: 30S ribosomal protein S21

Chain Z: 61% 24% 7% 8%

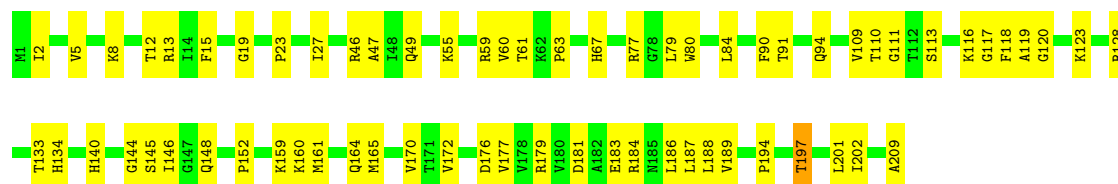
- Molecule 27: 50S ribosomal protein L2

Chain b: 70% 29%



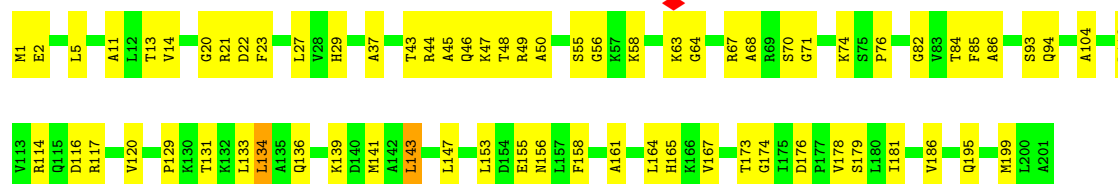
- Molecule 28: 50S ribosomal protein L3

Chain c: 68% 31%

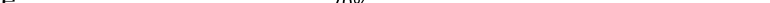


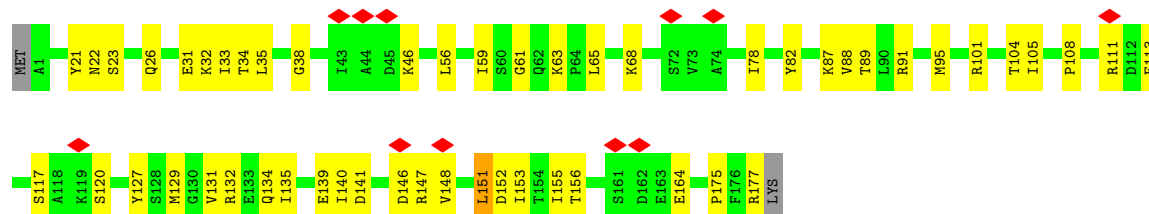
- Molecule 29: 50S ribosomal protein L4

Chain d: 65% 34%



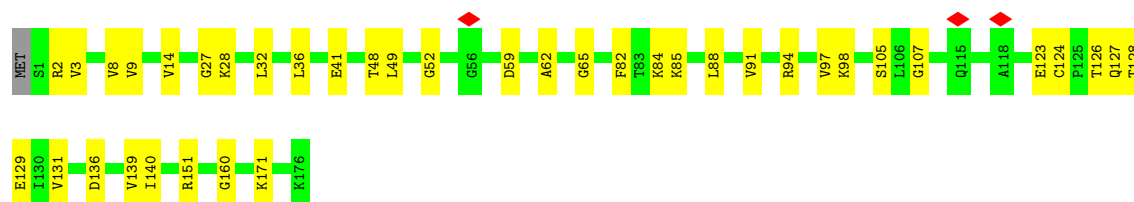
- Molecule 30: 50S ribosomal protein L5

Chain e:  6% 70% 28% ..



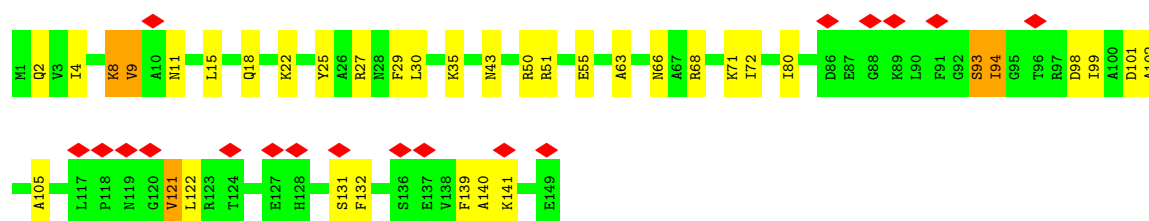
- Molecule 31: 50S ribosomal protein L6

Chain f:  77% 22%



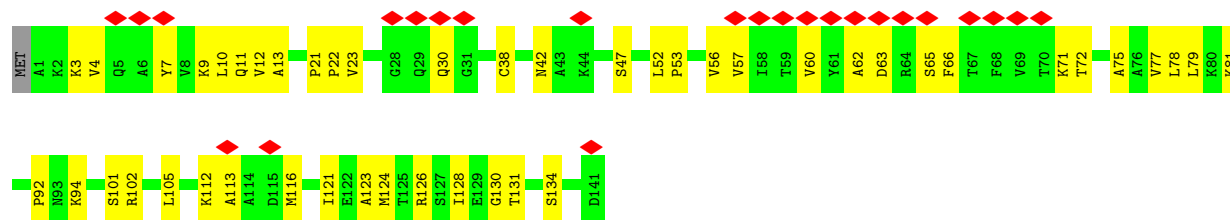
- Molecule 32: 50S ribosomal protein L9

Chain g:  12% 75% 21%



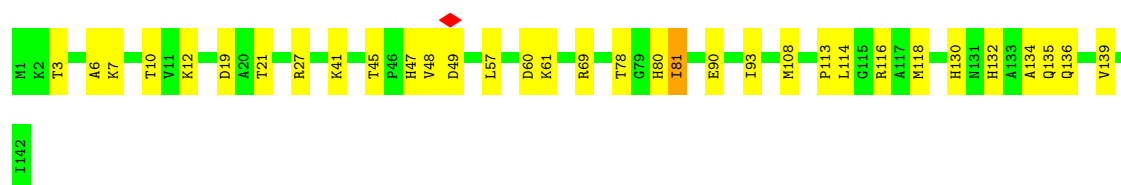
- Molecule 33: 50S ribosomal protein L11

Chain i:  17% 66% 33%



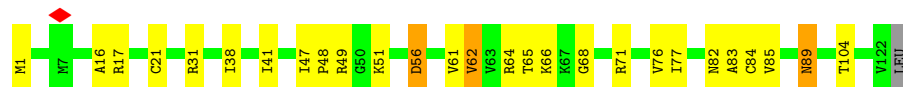
- Molecule 34: 50S ribosomal protein L13

Chain j:  77% 23%

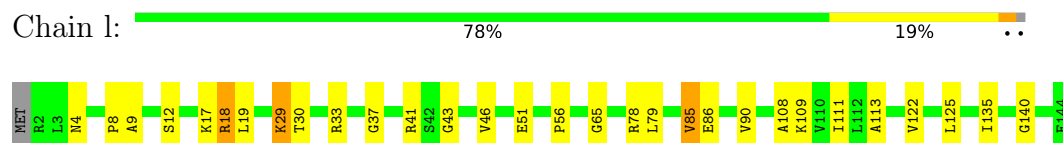


- Molecule 35: 50S ribosomal protein L14

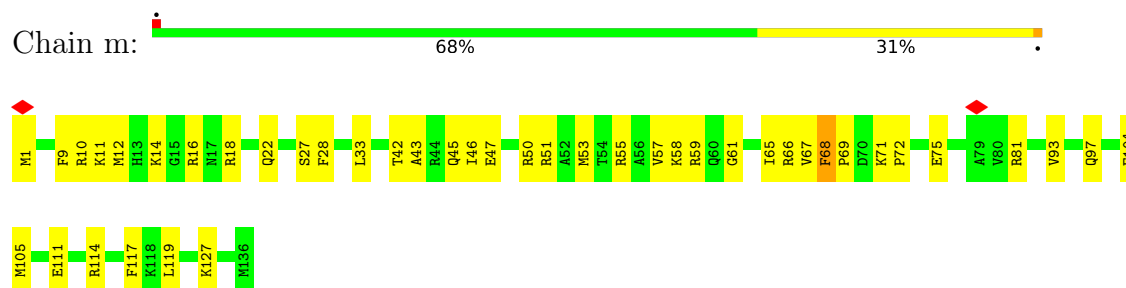
Chain k:  77% 20%



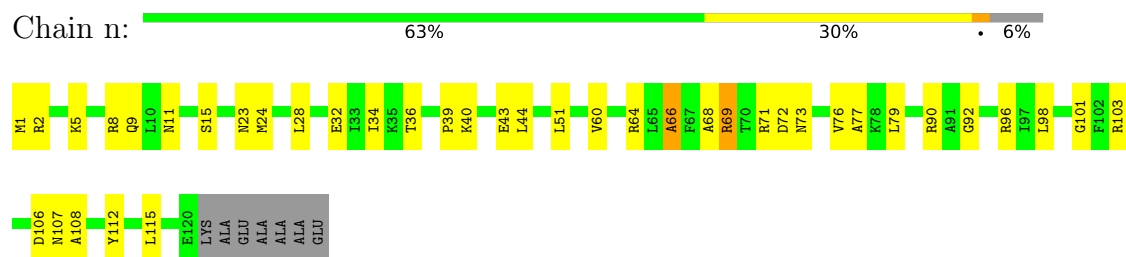
- Molecule 36: 50S ribosomal protein L15



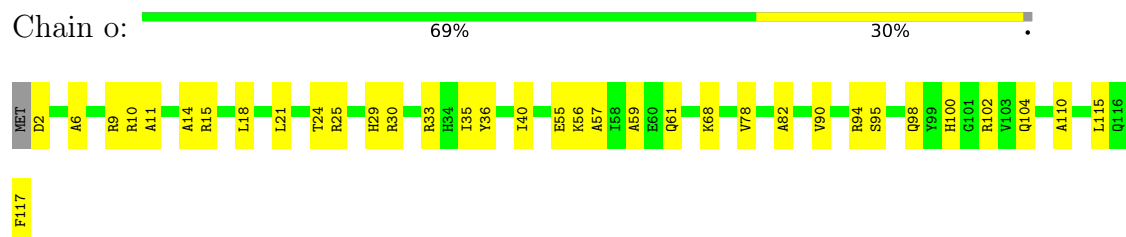
• Molecule 37: 50S ribosomal protein L16



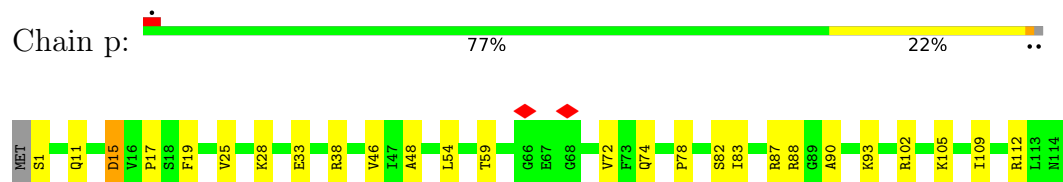
• Molecule 38: 50S ribosomal protein L17



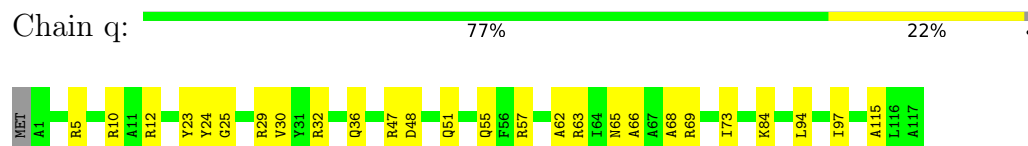
• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

Chain r:  71% 29%



- Molecule 43: 50S ribosomal protein L22

Chain s:  72% 27% .



- Molecule 44: 50S ribosomal protein L23

Chain t:  64% 28% . 7%



- Molecule 45: 50S ribosomal protein L24

Chain u:  74% 23% ..



- Molecule 46: 50S ribosomal protein L25

Chain v:  79% 21%



- Molecule 47: 50S ribosomal protein L27

Chain w:  65% 24% 12%

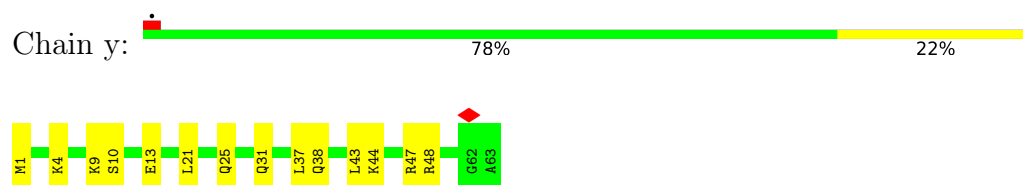


- Molecule 48: 50S ribosomal protein L28

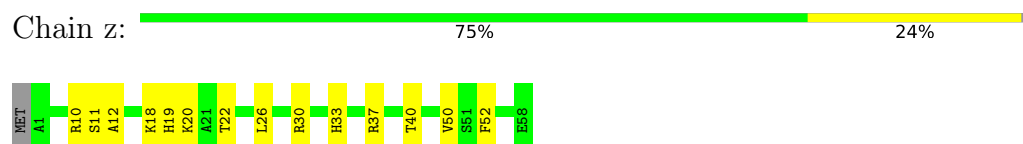
Chain x:  68% 28% ..



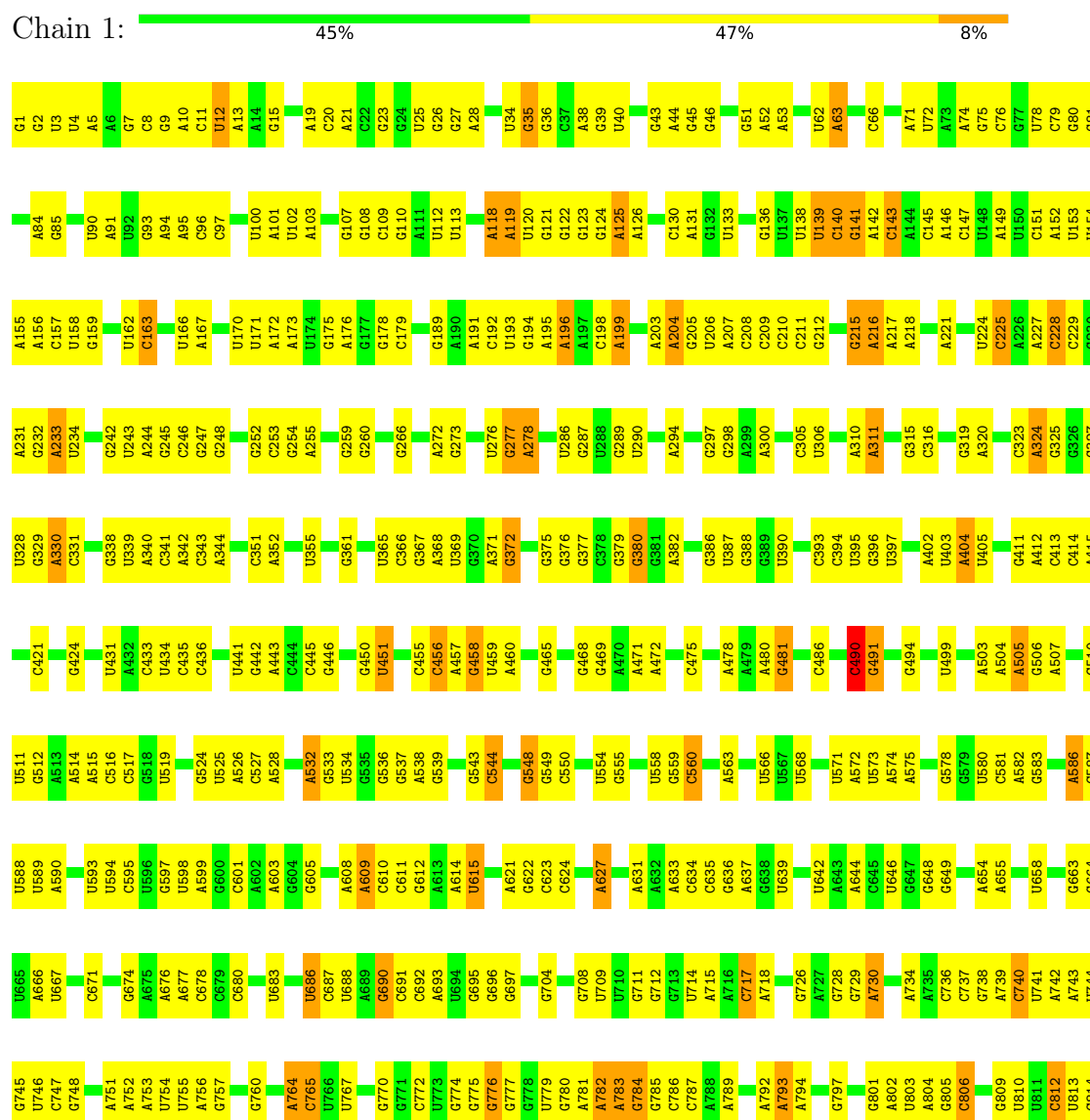
- Molecule 49: 50S ribosomal protein L29



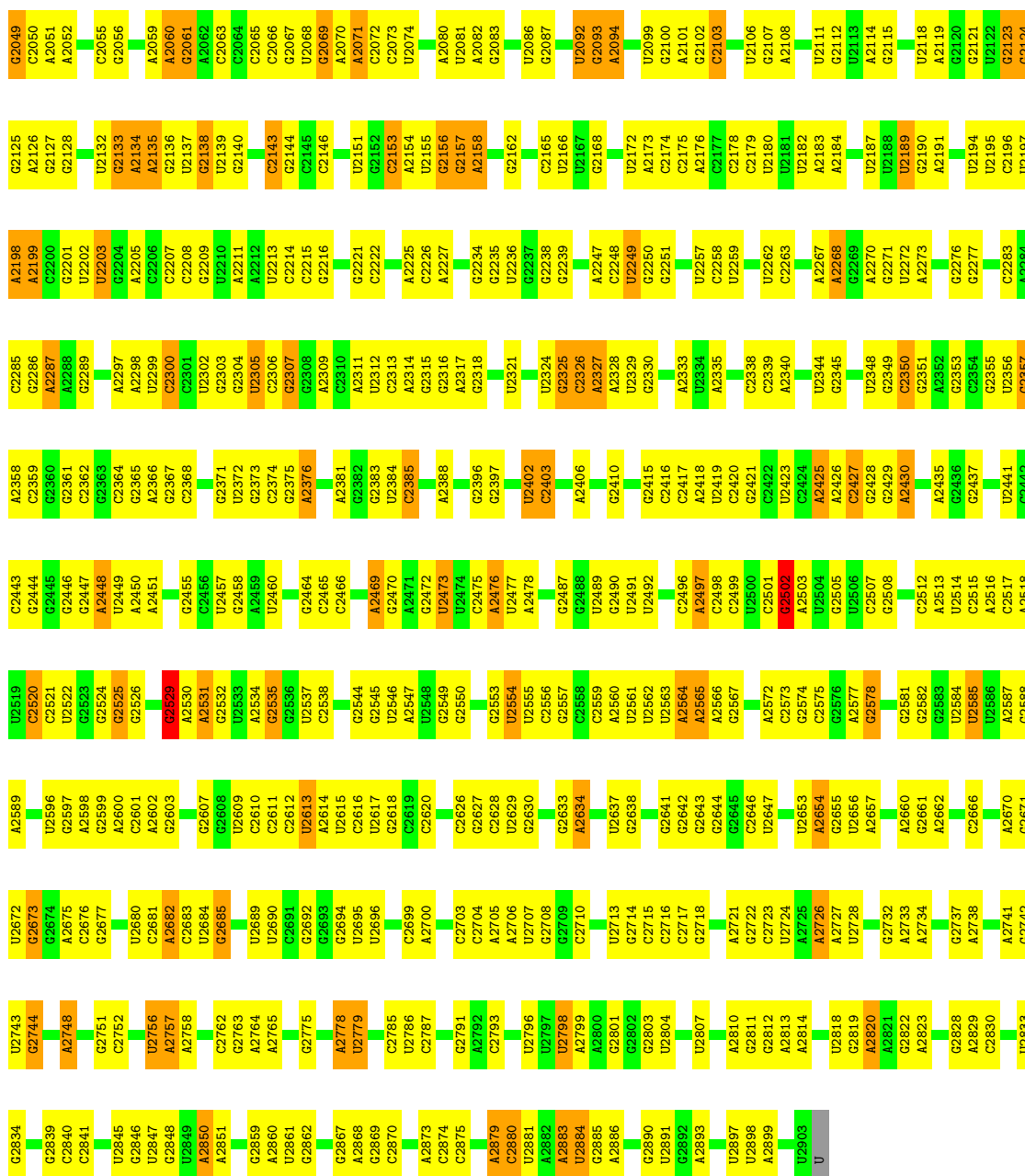
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 23S rRNA

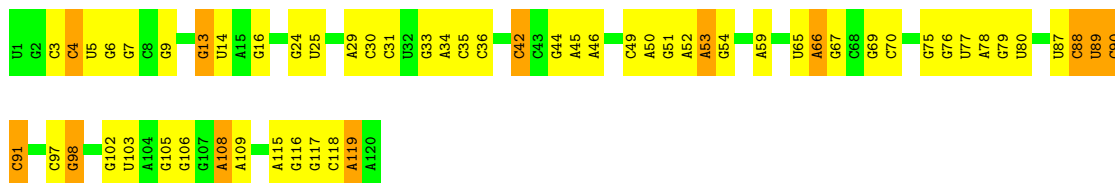


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C1874	C1875	G1884	U1889	A1889	A1890	C1893	C1894	A1900	A1901	G1902	G1903	G1904	C1905	A1912	A1913	A1914	U1917	A1918	U1919	G1991	G1992																																																



• Molecule 52: 5S rRNA

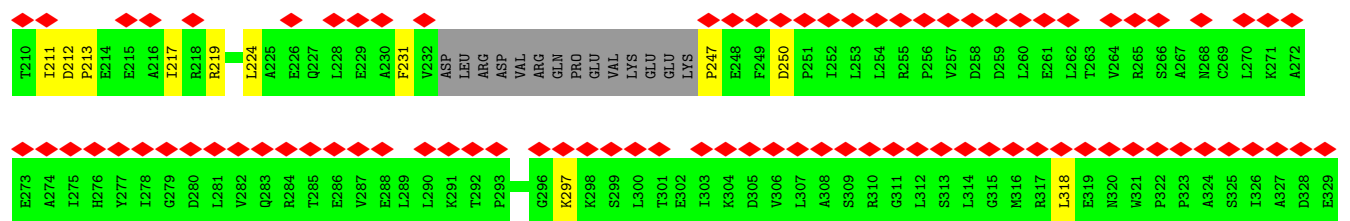
Chain 2: 52% 38% 10%



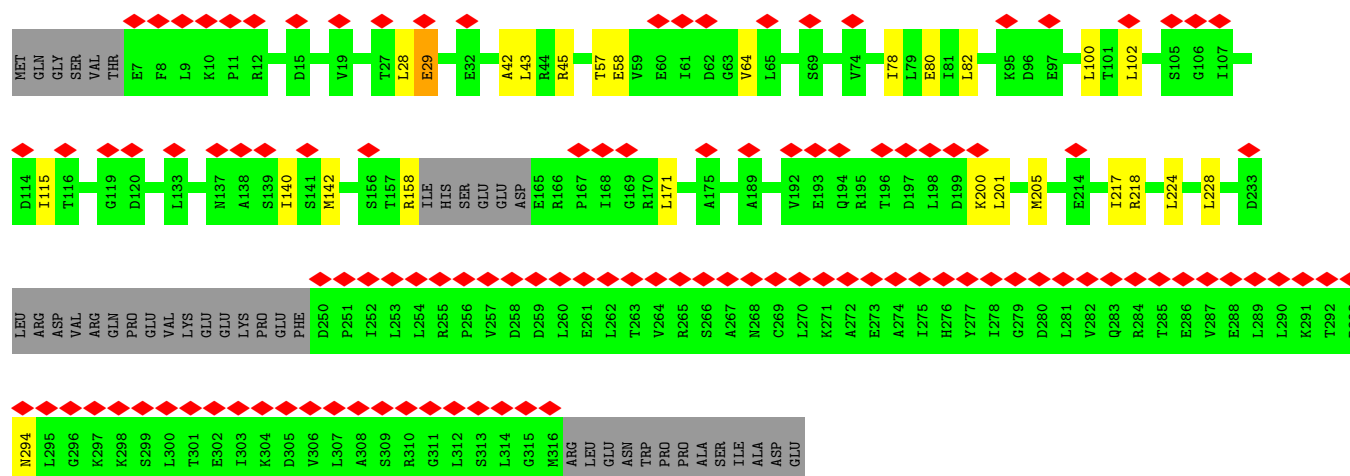
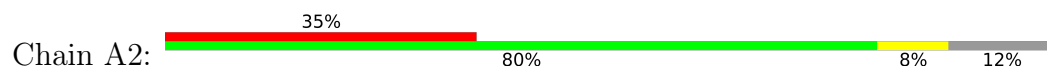
• Molecule 53: 16S rRNA

Chain 3: 45% 48% 6%

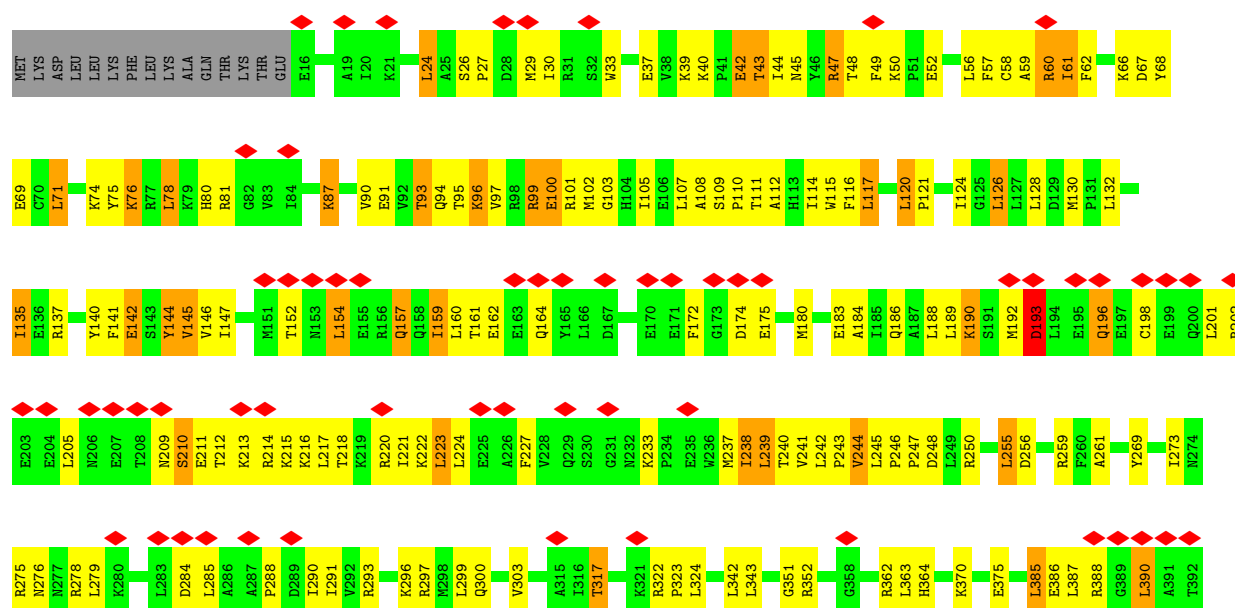
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A1170	G1094	G1015	A935	U850	U757	A674	G581	A510	G423	C352	C271	A181	G79	A2
A1171	U1095	A1016	C936	G851	C768	A675	U593	C511	G424	A353	C272	A182	A80	A3
A1172	C1096	U1017	A937	G851	G761	A676	U594	U512	G425	G354	U273	G183	A81	G6
A1173	C1097	G1018	A938	U855	U762	U677	A595	C513	U426	C355	G276	G184	G82	A7
G1174	C1098	A1019	C939	G856	G763	U678	A596	C514	G428	G357	A279	C193	C83	A8
A1179	G1109	A1022	C940	C857	G763	C679	U597	C515	U429	U388	C280	C194	U84	A9
A1180	A1101	U1023	G945	G858	A768	U684	U598	U516	A430	G359	G281	A197	U85	A10
G1181	A1102	G1024	A946	C859	C769	G685	A600	C517	A431	G362	C284	G204	C90	G15
G1182	C1103	U1025	C947	A860	C770	G685	A601	C518	A432	A363	C285	A205	U91	A16
U1183	G1104	G1026	G950	C861	C771	G690	G602	C519	A434	A363	C285	G204	U92	C18
G1184	A1105	C1027	U950	C862	U772	G691	A602	C520	A435	A366	C289	A206	U93	A19
A1187	C1107	G1028	C951	U863	G773	G691	A607	C521	A436	U367	C290	C206	U94	U20
A1188	A1108	U1029	U952	A864	A777	U701	A608	G529	C436	U368	U291	A197	C87	G11
G1189	C1109	G1030	C953	A865	C778	A702	G703	U531	U437	G369	U291	G207	U85	A10
C1192	A1110	G1032	U955	C866	C779	A703	C613	U532	U438	A363	C284	A197	C87	G11
G1193	A1111	G1033	U956	C867	A782	A706	C620	A532	C440	A363	C284	G204	C90	G15
U1194	A1117	A1035	U957	A872	A782	A707	C621	A533	G445	U367	C289	G204	U91	A16
C1195	U1118	A1035	A958	A873	A782	U707	A621	U534	G445	U367	C289	A205	U92	U17
A1196	C1119	A1042	A959	G874	A792	G710	C622	A535	G445	U368	C290	A206	U93	C18
A1197	U1120	G1043	U960	U875	G710	G710	C623	C536	A448	G369	U291	C207	U94	A19
G1198	C1121	A1043	U961	C876	G713	A714	U625	G537	A452	G377	G302	U208	C95	U20
U1199	U1122	G1047	C962	A877	G714	G715	U626	G538	G453	C379	G303	G220	C110	G22
C1200	U1123	U1048	G963	A878	A715	G715	G627	A539	G454	G390	G305	G221	G111	C23
A1201	G1124	G1049	U965	G881	C803	A718	G628	A540	G455	G384	U224	C225	G112	U24
C1210	U1125	G1050	C966	C882	U804	C719	C631	C545	A456	C385	C308	U229	U114	A32
U1211	C1126	A1051	C967	U876	C805	C720	U632	A546	A457	C386	A309	A228	G128	A33
U1212	G1127	G1053	U968	U884	C806	G721	U633	A547	A458	U387	G310	U229	A129	C34
A1213	C1128	C1054	C969	C885	A807	G722	U634	A548	A459	G388	A460	G230	C36	C35
G1214	U1129	G1057	C970	G886	C812	U723	U635	U552	A461	U389	C314	U231	G38	C36
C1215	A1135	G1058	G971	A889	A814	G724	A636	A553	G462	G391	C316	G232	A131	C40
A1216	U1136	C1059	C972	G894	A815	G725	U637	A554	G462	C392	U317	C235	G134	G41
G1217	C1137	G1060	A974	G895	A816	A728	U638	U555	U467	C393	U317	A236	G135	G42
A1218	U1138	U1061	A975	C895	C817	G731	U640	C557	A478	A397	U323	G236	C136	G46
U1219	C1139	G1063	G976	A900	G818	C732	U641	C558	U479	A397	A325	G240	U137	C47
G1220	U1140	U1064	A977	A901	U820	C733	A642	A559	U490	C401	G326	G241	A139	C48
C1221	C1141	U1065	C980	G903	G821	G734	U644	U561	C492	G402	A327	A246	A144	C49
A1225	U1147	G1069	U981	U904	C826	G735	U657	C562	C493	U405	C328	G246	G145	A51
C1226	C1148	U1070	U982	A907	U827	C736	C650	A563	G484	G406	U332	G247	G145	G46
A1229	A1150	G1071	U992	A908	U837	C737	C651	C564	U485	U407	G332	A250	G148	C47
C1230	C1151	U1072	G993	A909	A831	C738	U652	U565	U486	A408	C334	G251	U56	A55
G1231	G1152	G1073	A994	C910	C832	C739	U653	C566	C492	U409	C335	U252	A152	U56
U1232	C1153	U1074	A994	C910	G832	C739	U653	C566	C492	U409	C335	U252	C153	G57
C1233	G1154	U1075	A1000	A913	U835	G742	U657	C569	A493	G410	C337	G254	U154	C58
G1234	A1155	G1077	C1001	A917	U836	A743	C658	C570	A494	C413	A338	A262	A59	A59
U1235	C1156	U1078	U1005	G917	G836	A743	U659	U571	G497	A414	A338	A262	A60	A60
A1236	A1157	G1079	A1006	G917	U837	A748	C660	A572	G497	A415	U343	A263	G61	G61
C1237	C1158	U1080	A1007	G917	U837	A748	C661	A573	G498	A416	A344	A264	U62	U62
A1238	U1159	G1084	U1008	A923	C840	A749	C661	A574	A498	G417	A344	C265	A162	C63
U1239	G1160	U1085	U1009	A924	C841	C750	A665	A575	C501	G418	G347	G266	C163	G67
G1241	C1161	U1086	U1010	A925	U842	U751	G666	C576	A502	C419	G348	C267	A174	G68
U1242	U1162	U1091	A1012	G927	U843	G752	G667	C577	G505	U420	A349	U268	C175	G69
C1243	A1168	A1092	G1013	A845	A845	G755	C669	A579	G506	U421	G350	C269	C176	U70

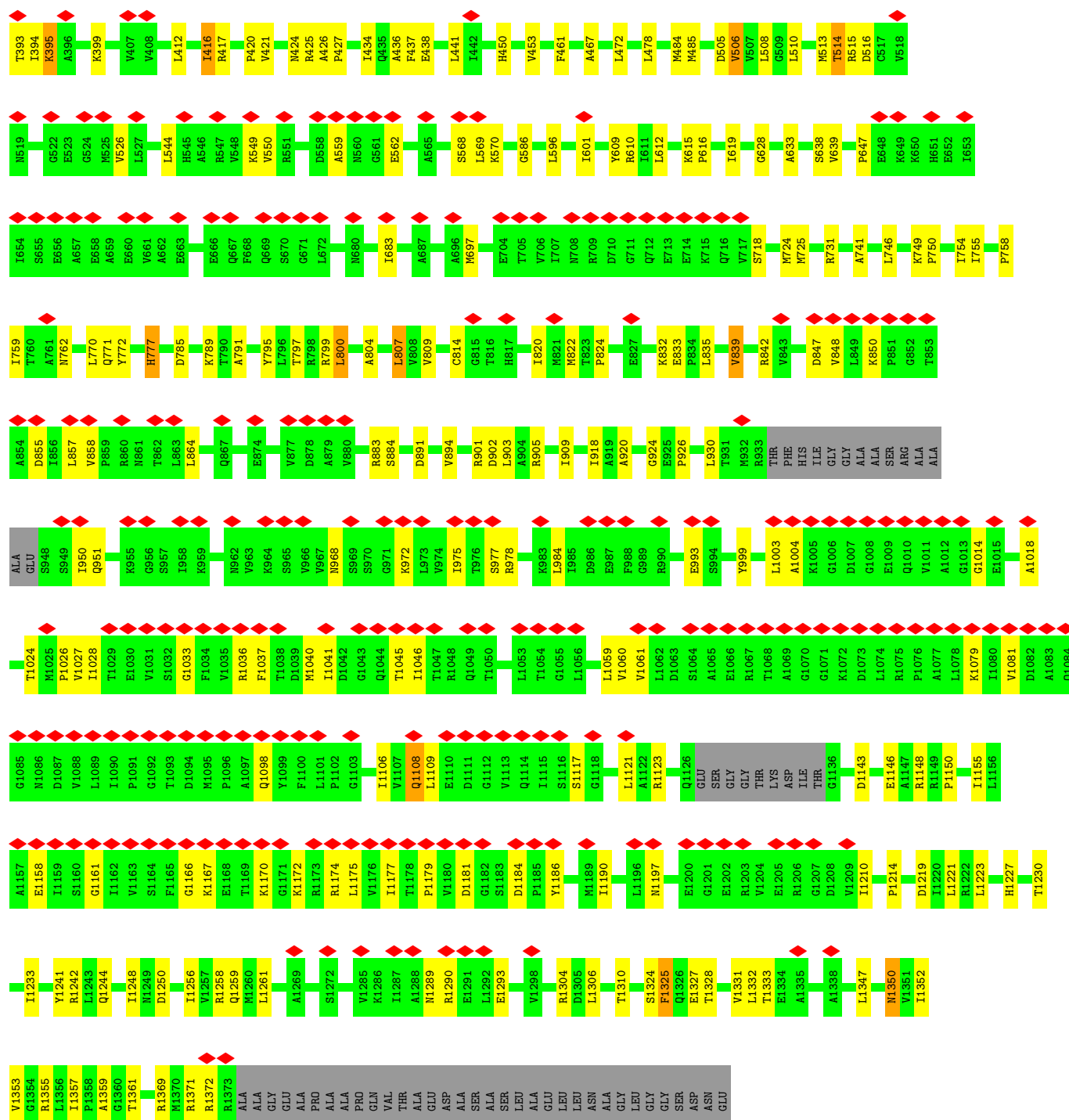


• Molecule 57: DNA-directed RNA polymerase subunit alpha

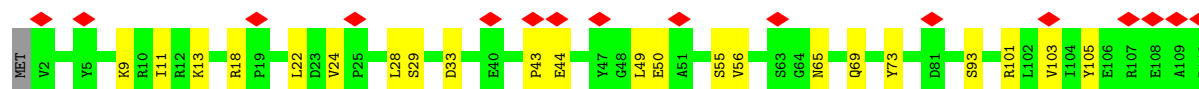
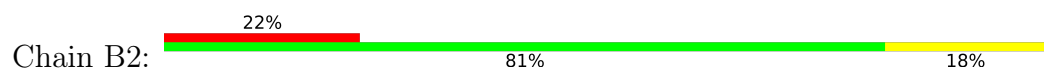


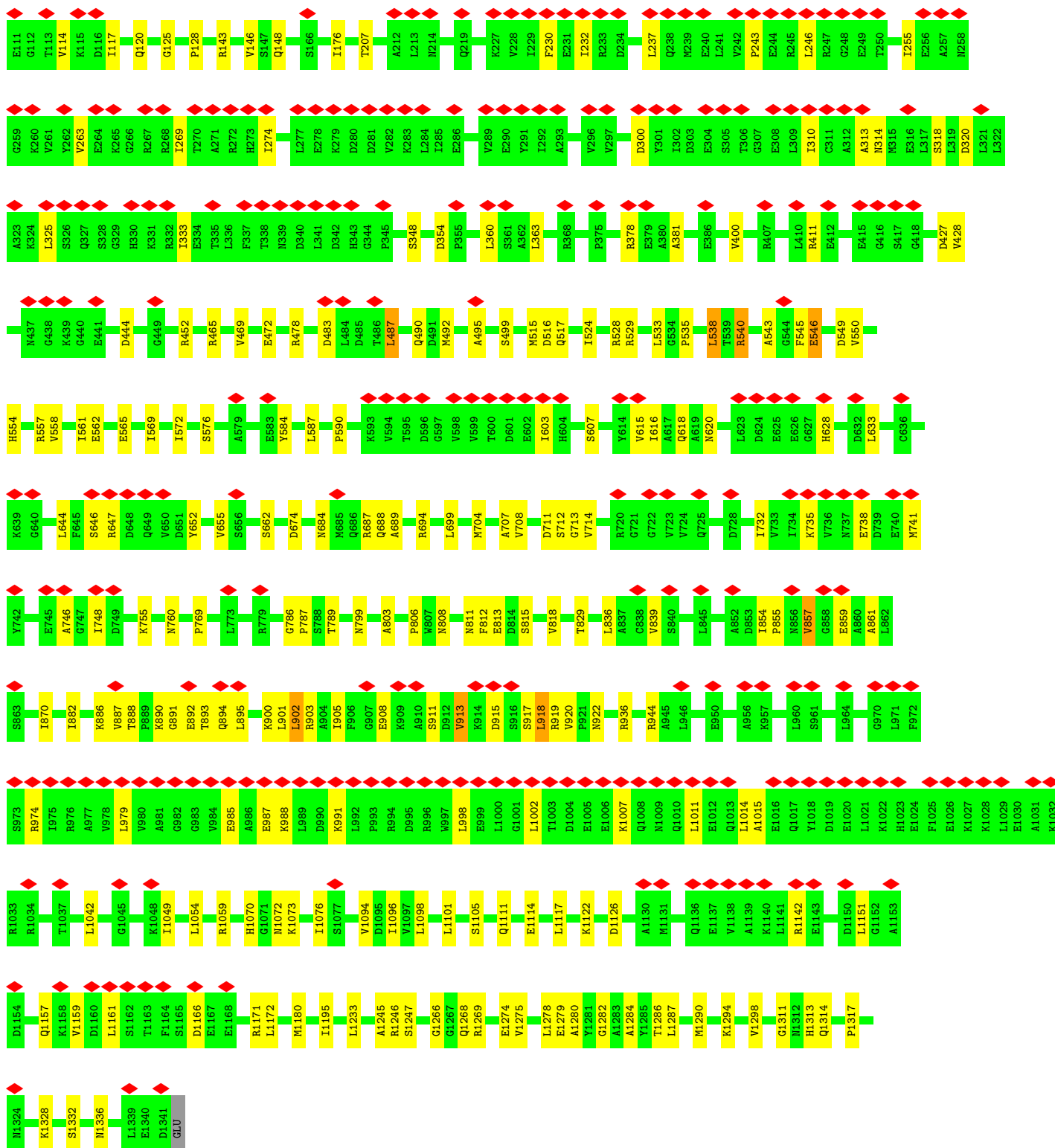
• Molecule 58: DNA-directed RNA polymerase subunit beta'



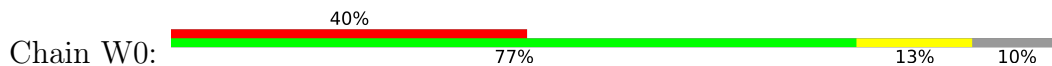


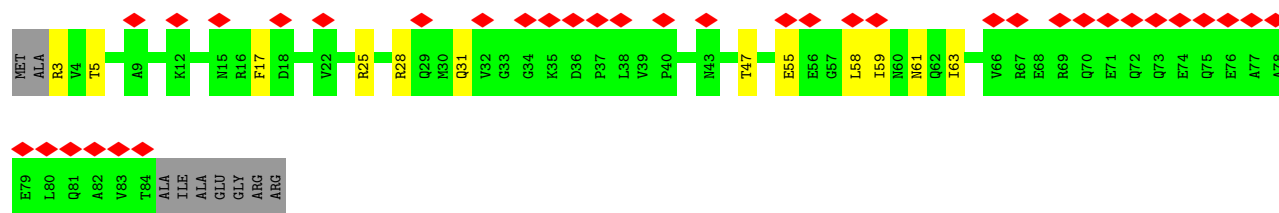
• Molecule 59: DNA-directed RNA polymerase subunit beta



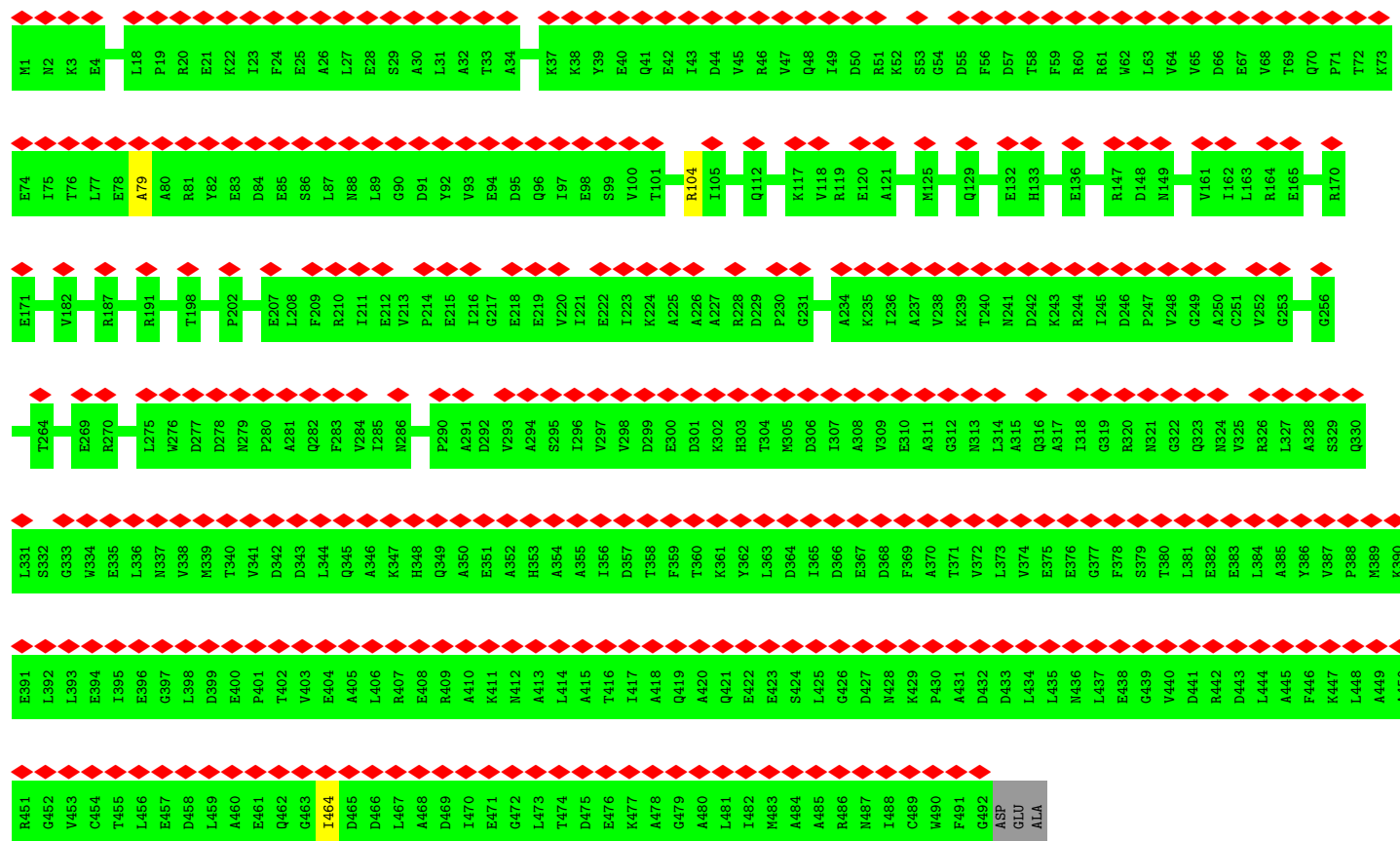
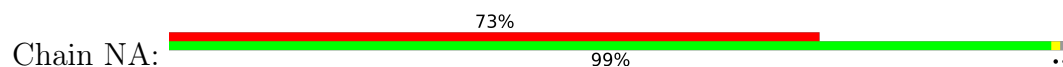


• Molecule 60: DNA-directed RNA polymerase subunit omega

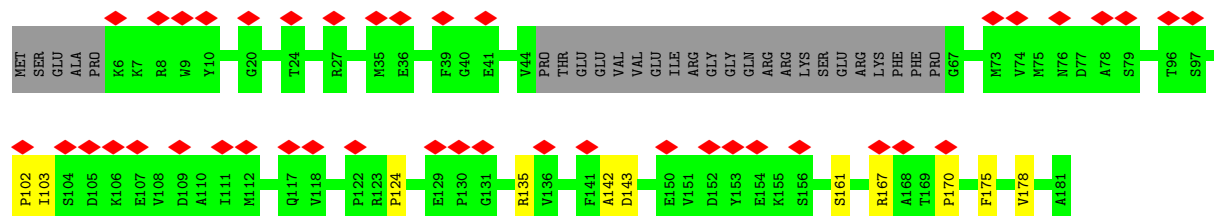
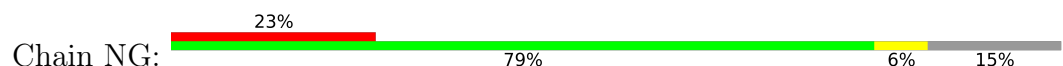




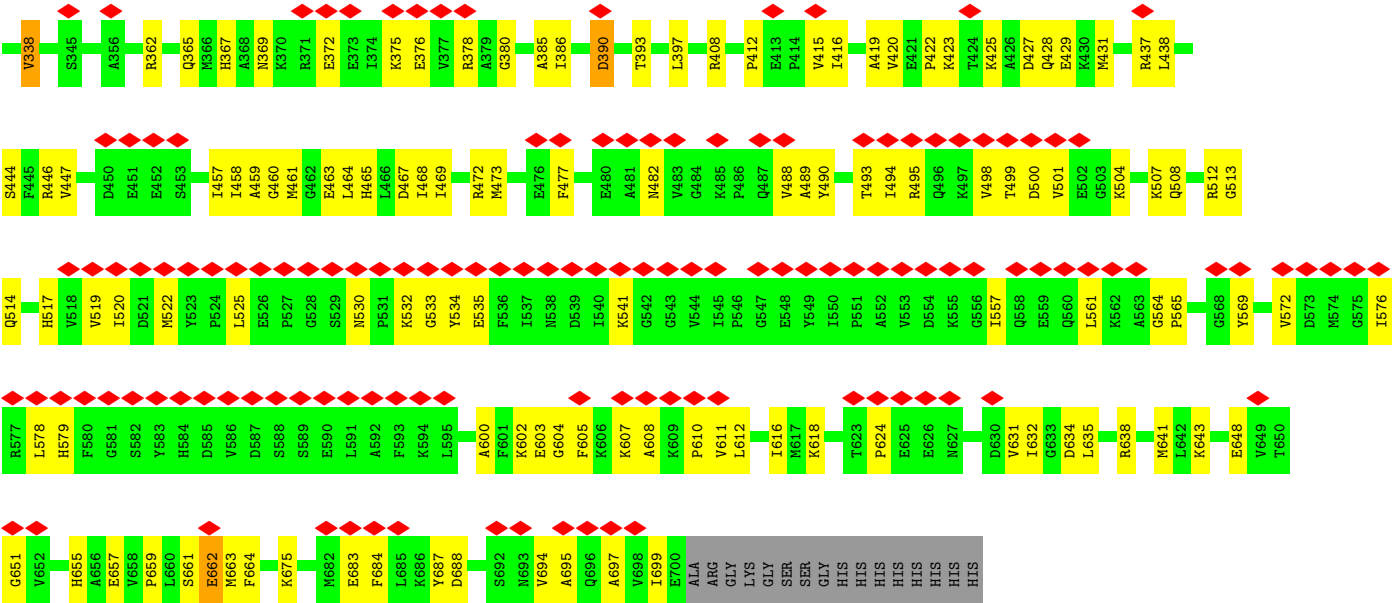
- Molecule 61: Transcription termination/antitermination protein NusA



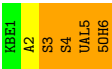
- Molecule 62: Transcription termination/antitermination protein NusG



- Molecule 63: tRNA(Phe)



● Molecule 67: Viomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	513759	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	0.156	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	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, DPP, UAL, PO4, GDP

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	0.32	0/416	0.61	0/554
4	D	0.48	0/380	0.95	0/498
5	E	0.47	0/513	0.80	0/676
6	F	0.41	0/303	0.79	0/397
7	G	0.39	0/1735	0.83	0/2338
8	H	0.41	0/1651	0.80	0/2225
9	I	0.28	0/1665	0.76	1/2227 (0.0%)
10	J	0.46	0/1169	0.80	0/1573
11	K	0.42	0/835	0.86	0/1128
12	L	0.42	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	0.42	0/885	0.76	0/1195
17	Q	0.43	0/969	0.81	0/1300
18	R	0.29	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	0.30	0/659	0.64	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	0.64	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	0.30	0/1434	0.66	0/1926
31	f	0.29	0/1343	0.61	0/1816
32	g	0.34	0/1122	0.77	3/1515 (0.2%)

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	0.40	0/1093	0.81	2/1460 (0.1%)
38	n	0.54	1/973 (0.1%)	0.88	0/1301
39	o	0.32	0/902	0.68	0/1209
40	p	0.39	0/929	0.72	2/1242 (0.2%)
41	q	0.43	0/960	0.72	0/1278
42	r	0.38	0/829	0.79	1/1107 (0.1%)
43	s	0.52	0/864	0.83	0/1156
44	t	0.48	0/744	0.81	1/994 (0.1%)
45	u	0.33	0/787	0.74	2/1051 (0.2%)
46	v	0.36	0/766	0.66	0/1025
47	w	0.40	0/582	0.80	2/769 (0.3%)
48	x	0.62	0/635	1.16	5/848 (0.6%)
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	17/108888 (0.0%)
52	2	0.60	0/2872	0.55	1/4479 (0.0%)
53	3	0.60	0/36963	0.57	5/57662 (0.0%)
54	4	0.60	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	0.55	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.56	4/10510 (0.0%)	0.75	8/14196 (0.1%)
59	B2	0.46	0/10714	0.67	0/14459
60	W0	0.31	0/652	0.63	0/879
61	NA	0.76	0/2431	1.22	0/3385
62	NG	1.15	0/756	1.05	0/1048
63	5	0.59	0/1812	0.90	3/2823 (0.1%)
64	6	0.60	0/1832	0.59	0/2855
65	a	0.50	0/1020	0.81	0/1370
66	0	0.39	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	73/289390 (0.0%)

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	-6.76	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	4	SER	CA-C	-6.29	1.39	1.52
38	n	66	ALA	CA-C	-5.91	1.44	1.52
58	B1	1350	ASN	CG-ND2	-5.26	1.22	1.33
58	B1	777	HIS	ND1-CE1	5.12	1.37	1.32

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	PRO	N-CA-C	-10.52	98.42	113.47
51	1	1020	A	C2'-C3'-O3'	7.36	120.54	109.50
48	x	11	PRO	N-CA-C	-7.32	99.55	111.77
51	1	2425	A	O3'-P-O5'	-6.93	93.61	104.00
12	L	82	SER	N-CA-C	6.88	116.41	108.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	355	0	353	10	0
2	B	444	0	461	14	0
3	C	409	0	440	18	0
4	D	377	0	418	18	0
5	E	504	0	574	18	0
6	F	302	0	341	15	0
7	G	1704	0	1732	45	0
8	H	1624	0	1699	47	0
9	I	1643	0	1710	44	0
10	J	1156	0	1199	39	0
11	K	817	0	808	22	0
12	L	1181	0	1240	47	0
13	M	979	0	1034	30	0
14	N	1022	0	1070	54	0
15	O	786	0	828	34	0
16	P	869	0	878	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	955	0	1019	34	0
18	R	883	0	944	26	0
19	S	805	0	847	33	0
20	T	714	0	737	16	0
21	U	649	0	666	21	0
22	V	648	0	691	17	0
23	W	535	0	552	14	0
24	X	637	0	665	16	0
25	Y	665	0	714	21	0
26	Z	544	0	579	17	0
27	b	2082	0	2157	68	0
28	c	1565	0	1616	53	0
29	d	1552	0	1619	51	0
30	e	1410	0	1447	43	0
31	f	1323	0	1374	31	0
32	g	1111	0	1148	29	0
33	i	1032	0	1088	38	0
34	j	1129	0	1162	34	0
35	k	938	0	1012	21	0
36	l	1045	0	1117	28	0
37	m	1074	0	1157	31	0
38	n	960	0	1000	34	0
39	o	892	0	923	21	0
40	p	917	0	965	22	0
41	q	947	0	1022	22	0
42	r	816	0	839	22	0
43	s	857	0	922	20	0
44	t	738	0	807	15	0
45	u	779	0	834	20	0
46	v	753	0	780	13	0
47	w	575	0	592	19	0
48	x	625	0	655	22	0
49	y	509	0	543	9	0
50	z	449	0	491	10	0
51	1	62317	0	31346	1354	0
52	2	2568	0	1303	56	0
53	3	33012	0	16618	731	0
54	4	627	0	313	6	0
55	8	539	0	305	28	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	26	0
57	A2	2029	0	1864	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B1	10353	0	10548	312	0
59	B2	10546	0	10550	162	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	5	0
62	NG	758	0	334	8	0
63	5	1622	0	821	33	0
64	6	1640	0	837	28	0
65	a	1013	0	1081	33	0
66	0	5399	0	5363	154	0
67	h	48	0	40	5	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	3754	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 3754 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	1.11	1.14
53:3:112:G:H21	53:3:354:G:H5'	1.16	1.11
50:z:37:ARG:HH12	51:1:929:U:H5'	1.12	1.10
51:1:2061:G:H2'	51:1:2501:C:O2'	1.52	1.09
51:1:1060:U:H4'	51:1:1061:U:H5'	1.32	1.06

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	36
6	F	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
7	G	216/241 (90%)	182 (84%)	34 (16%)	0	100	100
8	H	204/233 (88%)	187 (92%)	17 (8%)	0	100	100
9	I	203/206 (98%)	171 (84%)	31 (15%)	1 (0%)	24	63
10	J	155/167 (93%)	129 (83%)	26 (17%)	0	100	100
11	K	98/135 (73%)	81 (83%)	17 (17%)	0	100	100
12	L	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
13	M	127/130 (98%)	110 (87%)	17 (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	53
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
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%)	124 (84%)	23 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	89 (88%)	12 (12%)	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%)	83 (83%)	17 (17%)	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%)	66 (88%)	9 (12%)	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%)	275 (93%)	19 (6%)	1 (0%)	36	72
57	A2	282/329 (86%)	272 (96%)	10 (4%)	0	100	100
58	B1	1329/1407 (94%)	1206 (91%)	119 (9%)	4 (0%)	36	72
59	B2	1338/1342 (100%)	1208 (90%)	126 (9%)	4 (0%)	36	72
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	475 (97%)	15 (3%)	0	100	100
62	NG	150/181 (83%)	136 (91%)	11 (7%)	3 (2%)	6	30
65	a	128/234 (55%)	107 (84%)	21 (16%)	0	100	100
66	0	695/716 (97%)	618 (89%)	72 (10%)	5 (1%)	18	55
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10486/11185 (94%)	9335 (89%)	1131 (11%)	20 (0%)	44	78

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	B1	121	PRO
62	NG	124	PRO
59	B2	43	PRO
59	B2	911	SER
62	NG	102	PRO

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	32
5	E	51/52 (98%)	46 (90%)	5 (10%)	7	24
6	F	34/34 (100%)	33 (97%)	1 (3%)	37	58
7	G	180/199 (90%)	172 (96%)	8 (4%)	25	46
8	H	170/190 (90%)	162 (95%)	8 (5%)	23	45
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	74
10	J	119/126 (94%)	112 (94%)	7 (6%)	18	39
11	K	87/116 (75%)	82 (94%)	5 (6%)	18	40
12	L	124/147 (84%)	121 (98%)	3 (2%)	43	63
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	26
16	P	89/99 (90%)	87 (98%)	2 (2%)	45	64
17	Q	103/104 (99%)	101 (98%)	2 (2%)	50	66
18	R	92/96 (96%)	91 (99%)	1 (1%)	65	74
19	S	83/84 (99%)	82 (99%)	1 (1%)	63	74
20	T	76/77 (99%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	11
27	b	216/218 (99%)	212 (98%)	4 (2%)	50	66
28	c	164/164 (100%)	163 (99%)	1 (1%)	78	82
29	d	165/165 (100%)	160 (97%)	5 (3%)	36	57
30	e	148/150 (99%)	146 (99%)	2 (1%)	59	72
31	f	137/138 (99%)	136 (99%)	1 (1%)	76	80
32	g	114/114 (100%)	111 (97%)	3 (3%)	40	61
33	i	109/110 (99%)	108 (99%)	1 (1%)	70	77
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	66
37	m	109/109 (100%)	108 (99%)	1 (1%)	70	77
38	n	100/103 (97%)	98 (98%)	2 (2%)	48	66
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%)	84 (100%)	0	100	100
43	s	93/93 (100%)	86 (92%)	7 (8%)	12	32
44	t	80/84 (95%)	77 (96%)	3 (4%)	29	50
45	u	83/85 (98%)	82 (99%)	1 (1%)	63	74
46	v	78/78 (100%)	77 (99%)	1 (1%)	61	73
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	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	A2	186/286 (65%)	185 (100%)	1 (0%)	81	82
58	B1	1110/1168 (95%)	1018 (92%)	92 (8%)	10	30
59	B2	1150/1157 (99%)	1118 (97%)	32 (3%)	38	59
60	W0	70/75 (93%)	69 (99%)	1 (1%)	59	72
65	a	109/181 (60%)	98 (90%)	11 (10%)	7	23
66	0	574/588 (98%)	554 (96%)	20 (4%)	32	53
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8120/8683 (94%)	7841 (97%)	279 (3%)	33	54

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	B2	892	GLU
59	B2	903	ARG
66	0	173	ILE
43	s	65	ASP
38	n	15	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
58	B1	865	HIS
66	0	514	GLN
59	B2	314	ASN
60	W0	31	GLN
21	U	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	440 (15%)	6 (0%)
52	2	119/120 (99%)	18 (15%)	0
53	3	1538/1542 (99%)	193 (12%)	1 (0%)
54	4	28/56 (50%)	17 (60%)	4 (14%)
63	5	75/76 (98%)	45 (60%)	10 (13%)
64	6	76/77 (98%)	14 (18%)	0
All	All	4738/4775 (99%)	727 (15%)	21 (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 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	35	A
63	5	57	G
63	5	75	C
63	5	60	U
63	5	48	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	0.52	0	1,5,7	0.06	0
67	5OH	h	6	67	7,12,13	0.75	0	4,16,18	1.34	1 (25%)
67	UAL	h	5	67	6,8,9	2.34	2 (33%)	4,9,11	1.86	1 (25%)
67	KBE	h	1	67	8,8,9	0.59	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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	5OH	h	6	67	-	0/2/18/20	0/1/1/1
67	UAL	h	5	67	-	0/3/7/9	-
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	-4.88	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	-3.28	121.28	125.39
67	h	6	5OH	CR-CB-CA	-2.39	110.07	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	h	2	DPP	1	0
67	h	6	5OH	3	0
67	h	5	UAL	1	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	$\# Z > 2$
70	PO4	0	802	-	4,4,4	1.01	0	6,6,6	0.51	0
69	GDP	0	801	-	29,30,30	1.17	3 (10%)	45,47,47	1.88	8 (17%)

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	2.81	1.46	1.38
69	0	801	GDP	C6-N1	-2.65	1.33	1.38
69	0	801	GDP	C4-N9	-2.03	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	-5.99	118.85	128.39
69	0	801	GDP	C2-N3-C4	5.05	120.99	112.30
69	0	801	GDP	N9-C4-N3	4.48	134.90	125.95
69	0	801	GDP	C6-C5-N7	3.62	136.88	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:

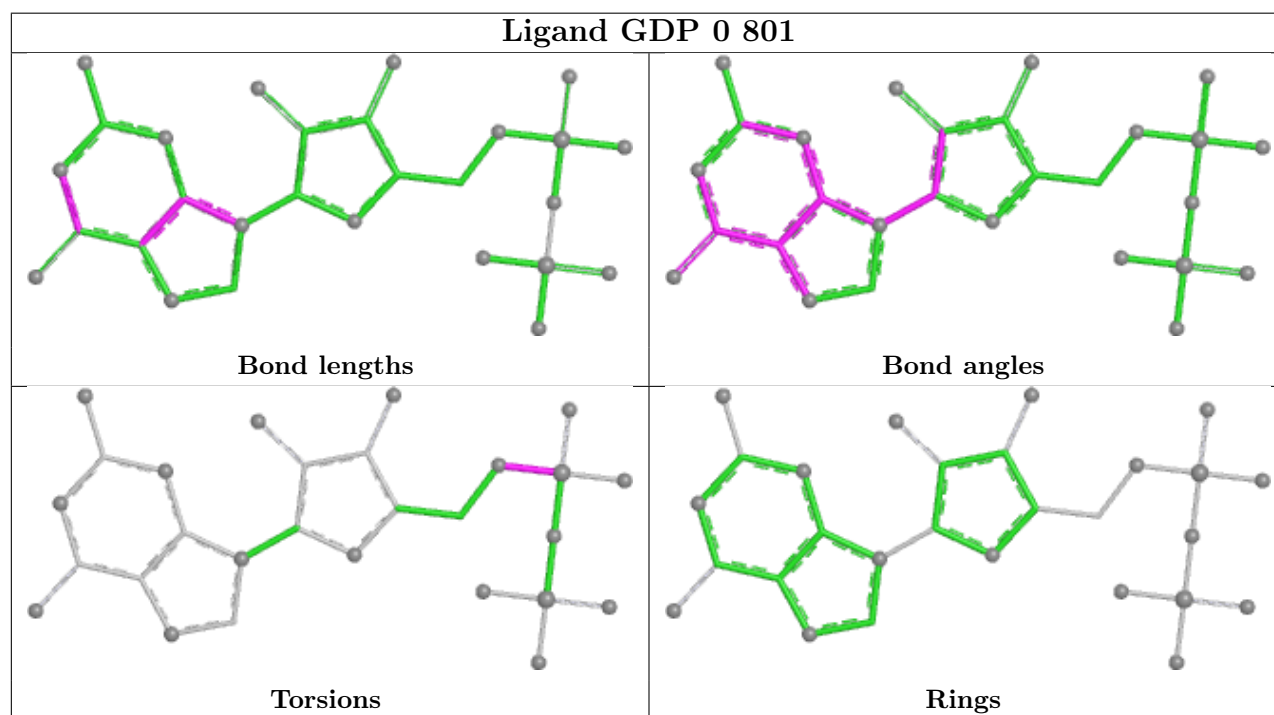
Mol	Chain	Res	Type	Atoms
69	0	801	GDP	C5'-O5'-PA-O3A
69	0	801	GDP	C5'-O5'-PA-O1A

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

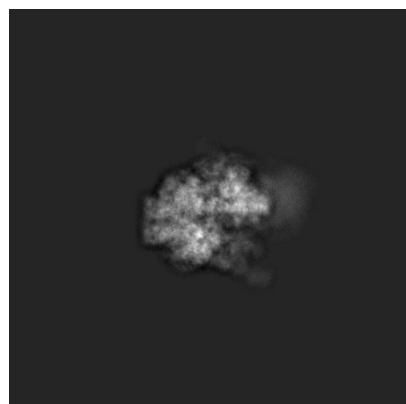
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39173. These allow visual inspection of the internal detail of the map and identification of artifacts.

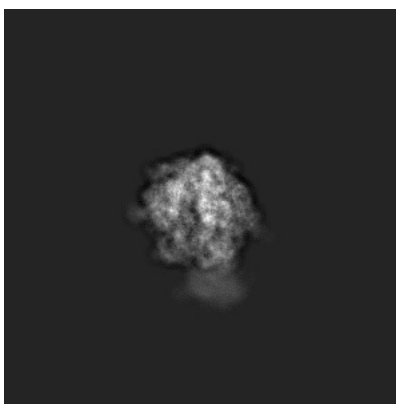
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

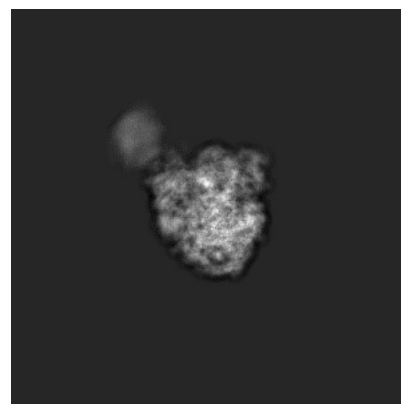
6.1.1 Primary map



X

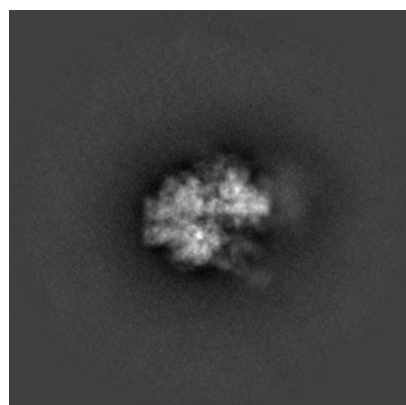


Y

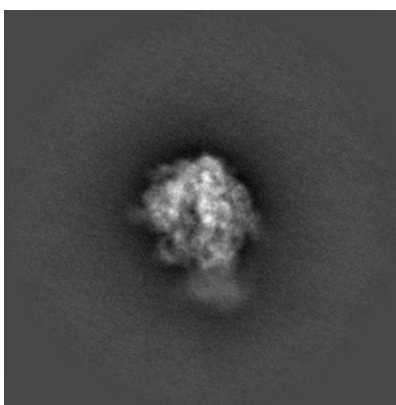


Z

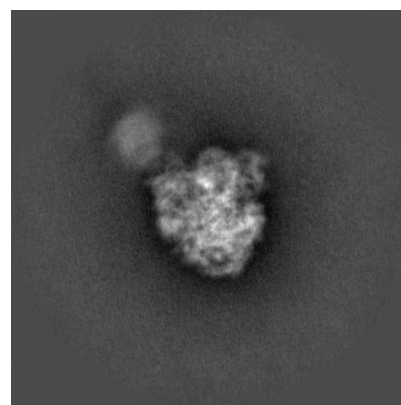
6.1.2 Raw map



X



Y

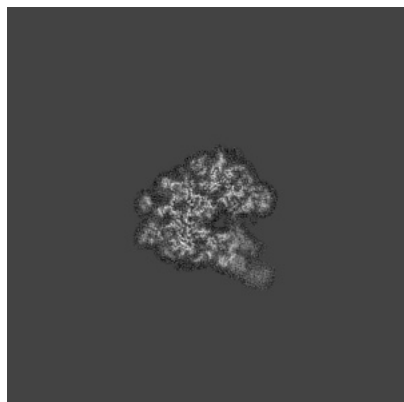


Z

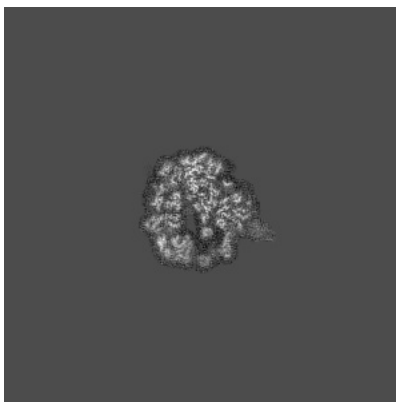
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

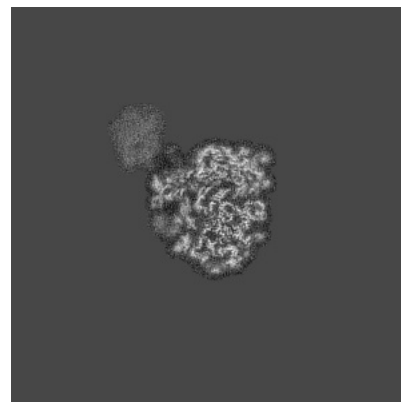
6.2.1 Primary map



X Index: 240

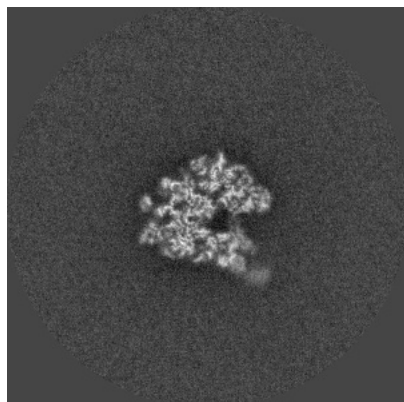


Y Index: 240

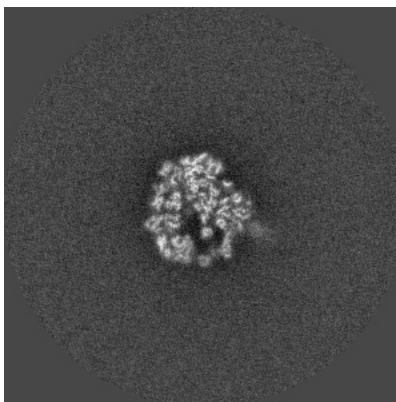


Z Index: 240

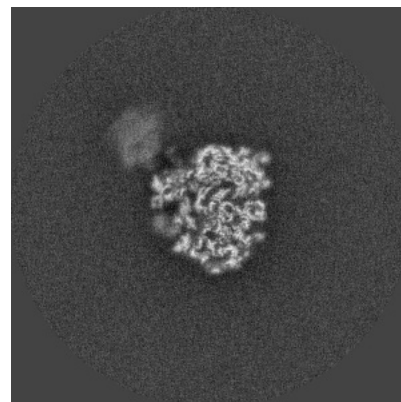
6.2.2 Raw map



X Index: 240



Y Index: 240

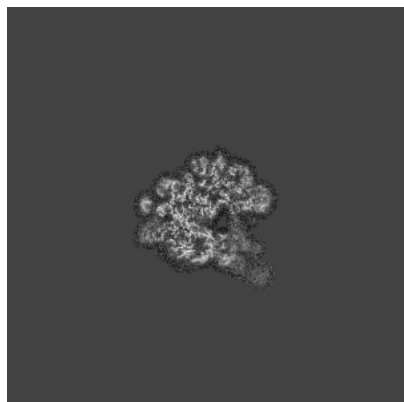


Z Index: 240

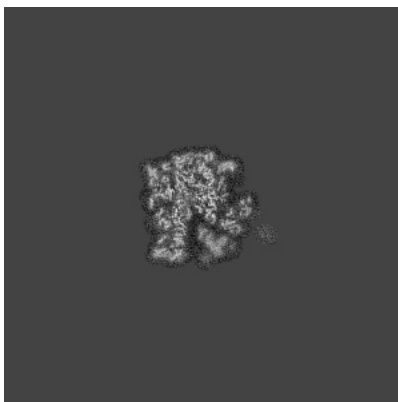
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

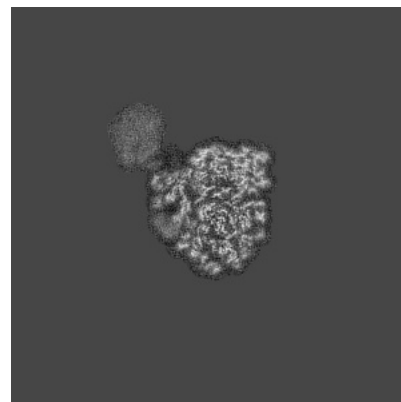
6.3.1 Primary map



X Index: 243

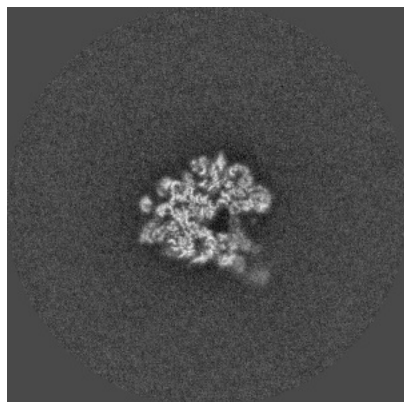


Y Index: 228

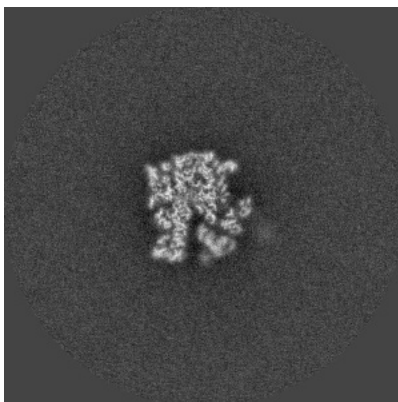


Z Index: 243

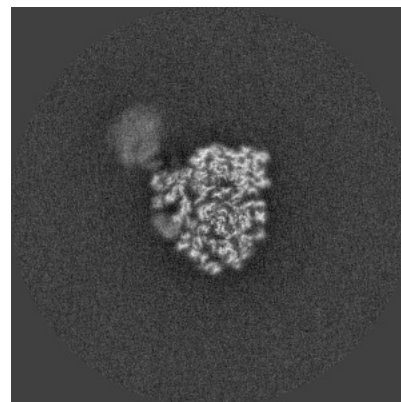
6.3.2 Raw map



X Index: 242



Y Index: 227

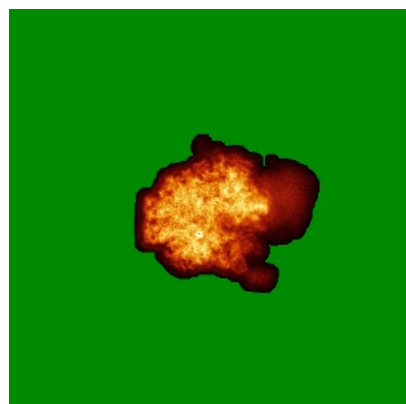


Z Index: 243

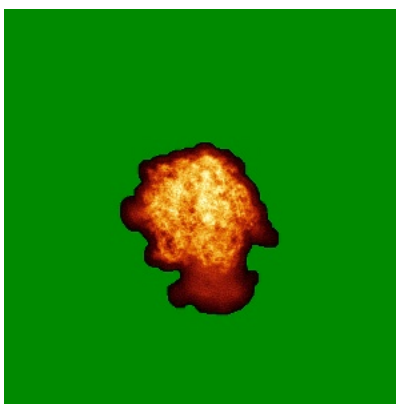
The images above show the largest variance slices of the map in three orthogonal directions.

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

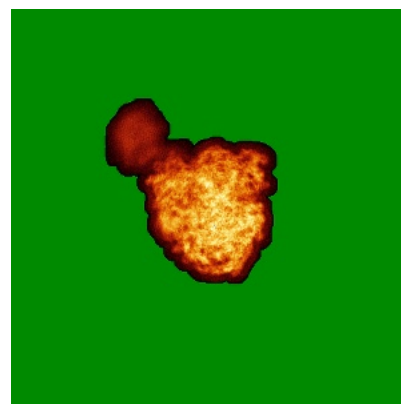
6.4.1 Primary map



X

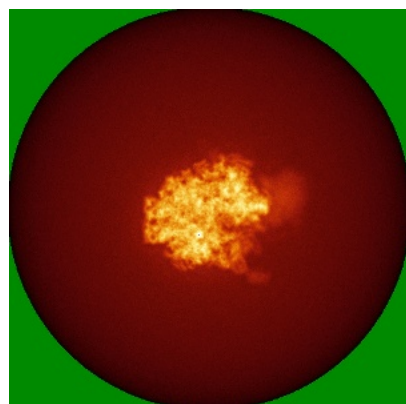


Y

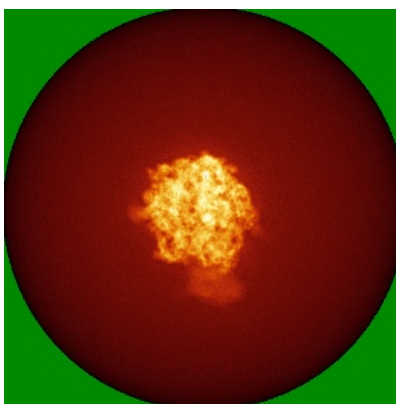


Z

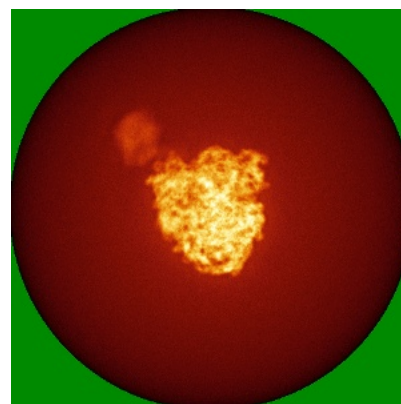
6.4.2 Raw map



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.

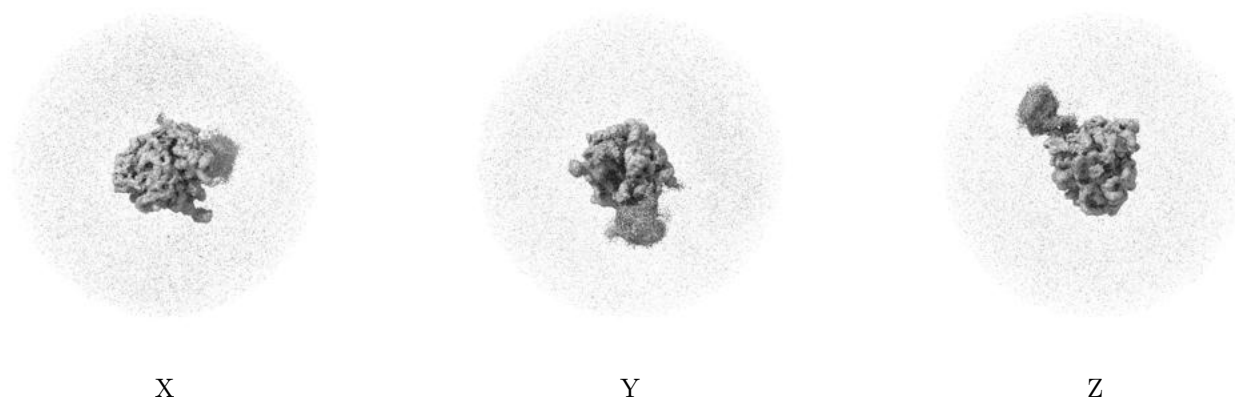
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

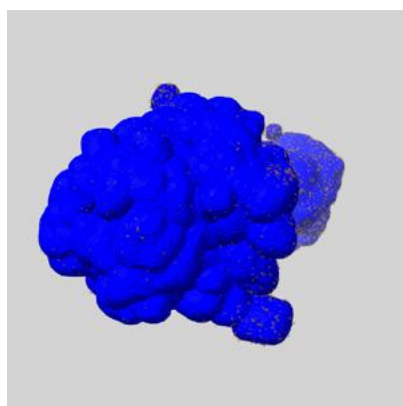
6.6 Mask visualisation [i](#)

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

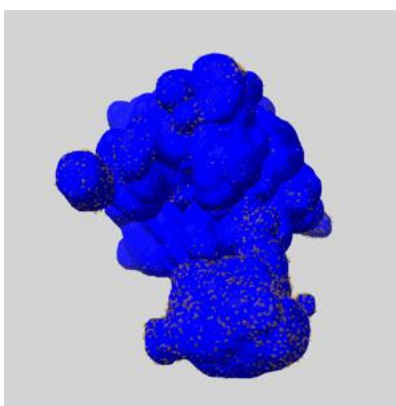
A mask typically either:

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

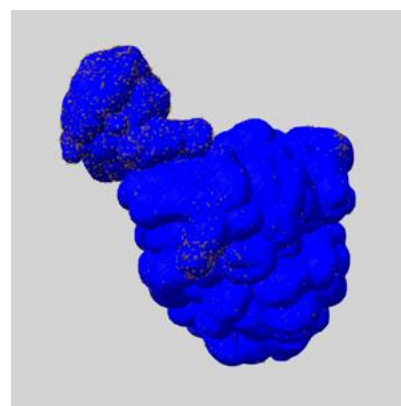
6.6.1 emd_39173_msk_1.map [i](#)



X



Y

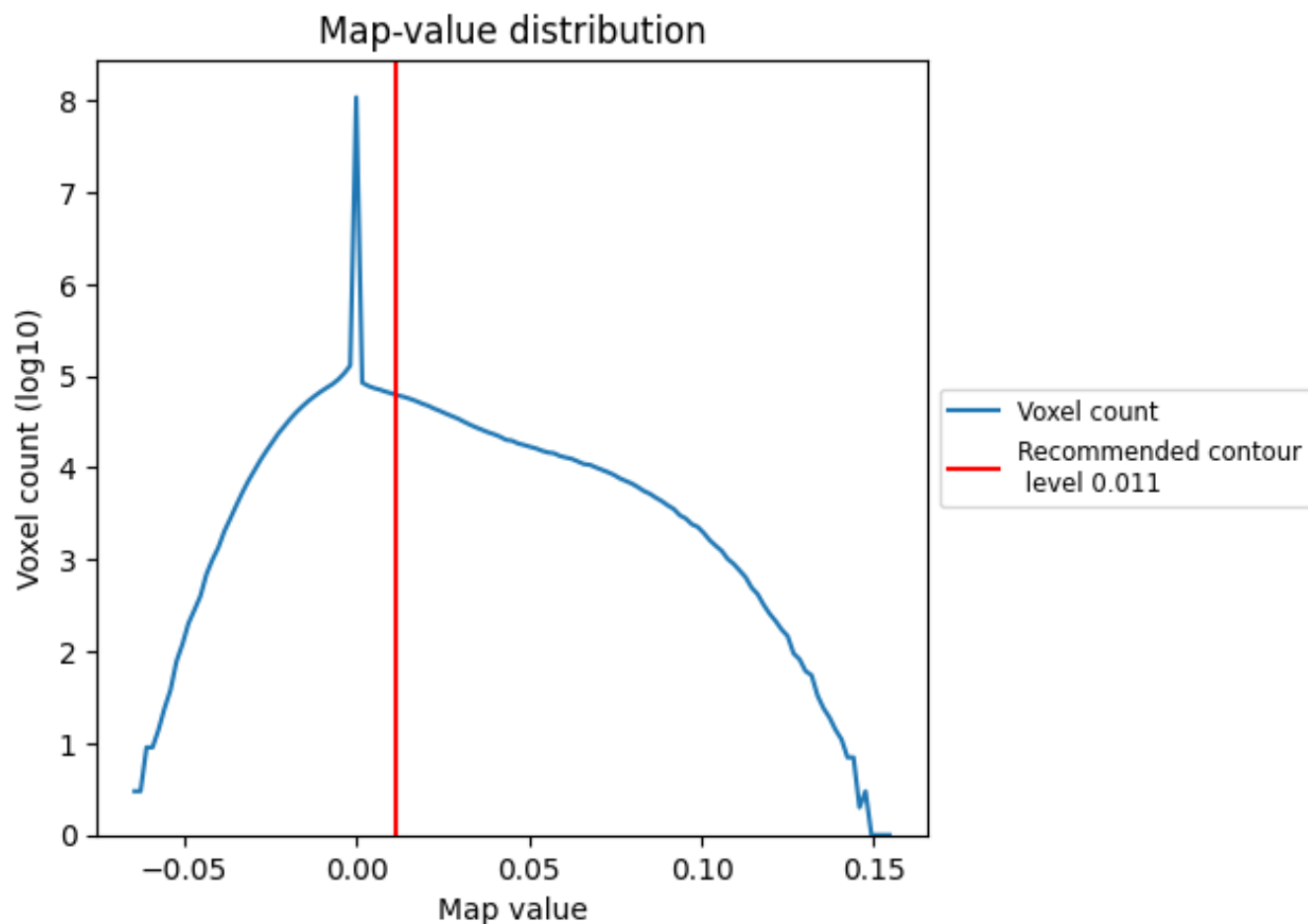


Z

7 Map analysis [i](#)

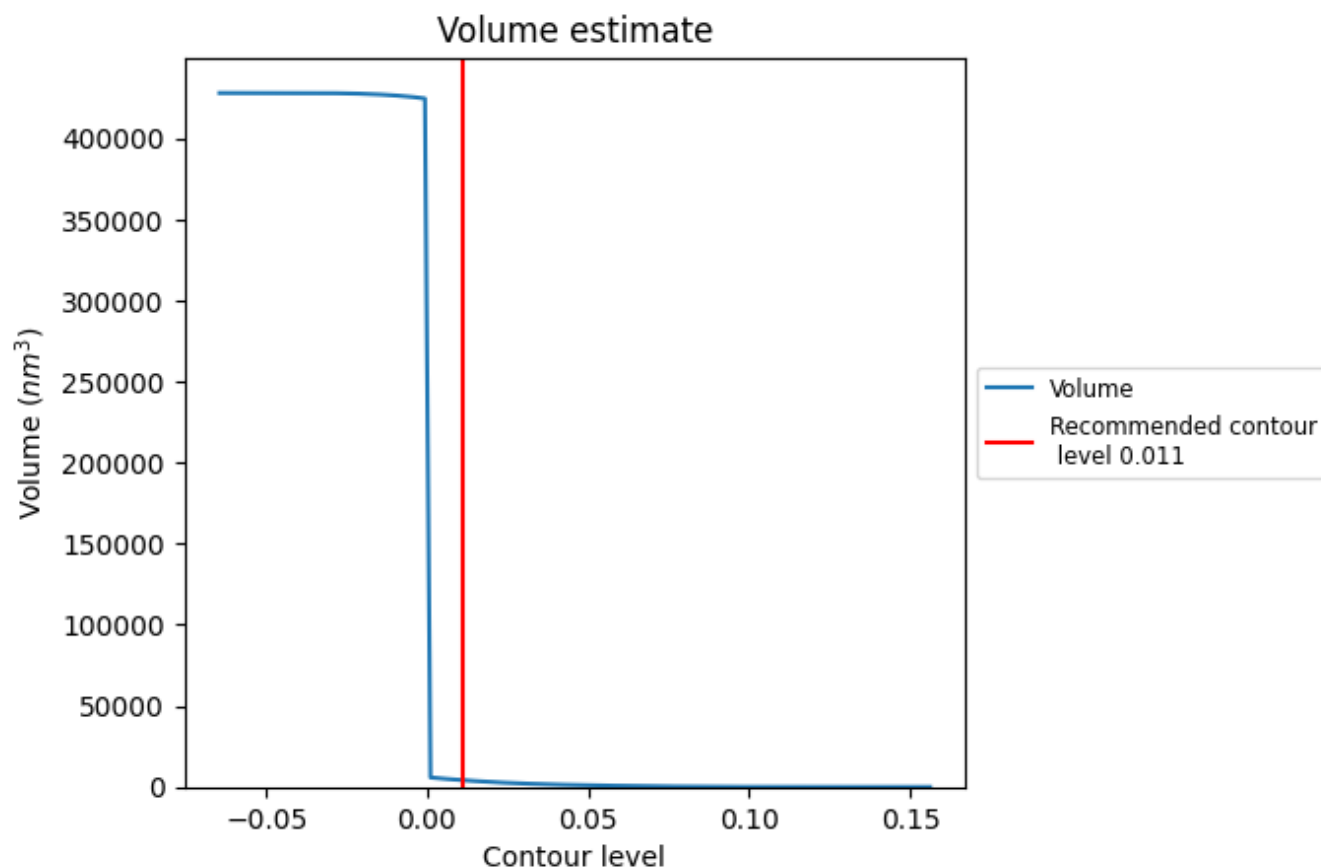
This section contains the results of statistical analysis of the map.

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.

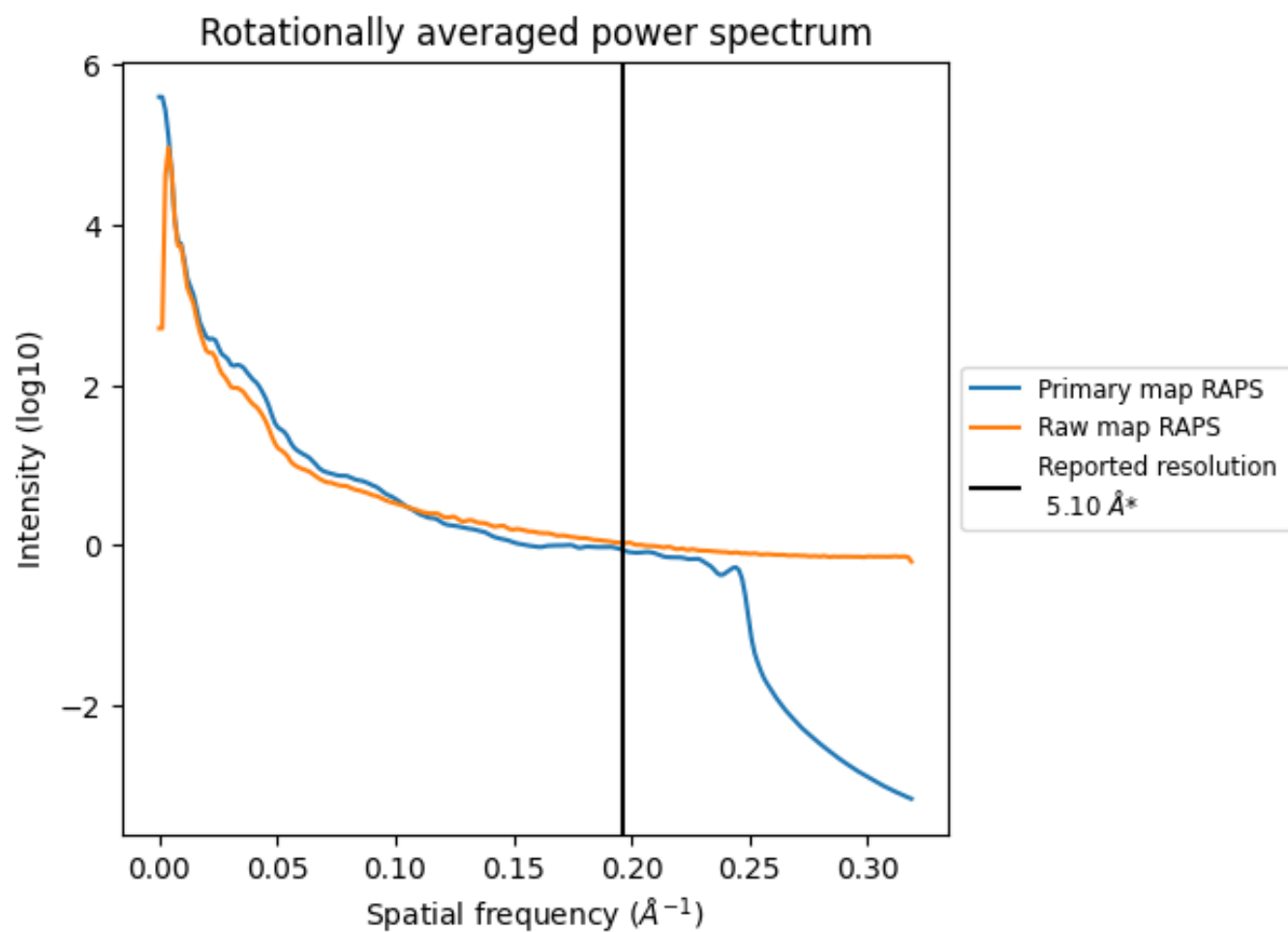
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4189 nm^3 ; this corresponds to an approximate mass of 3784 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

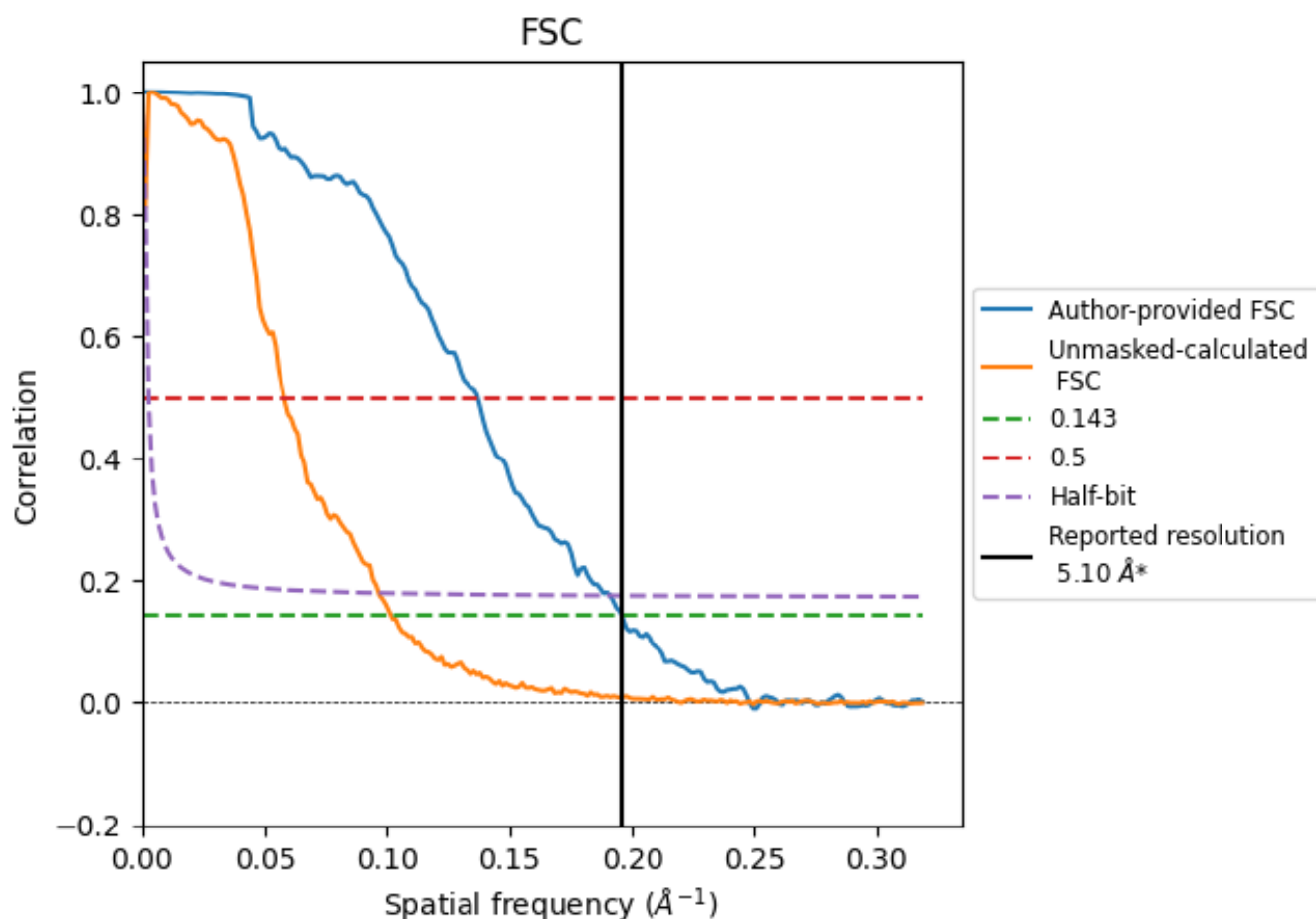


*Reported resolution corresponds to spatial frequency of 0.196 Å⁻¹

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 0.196 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

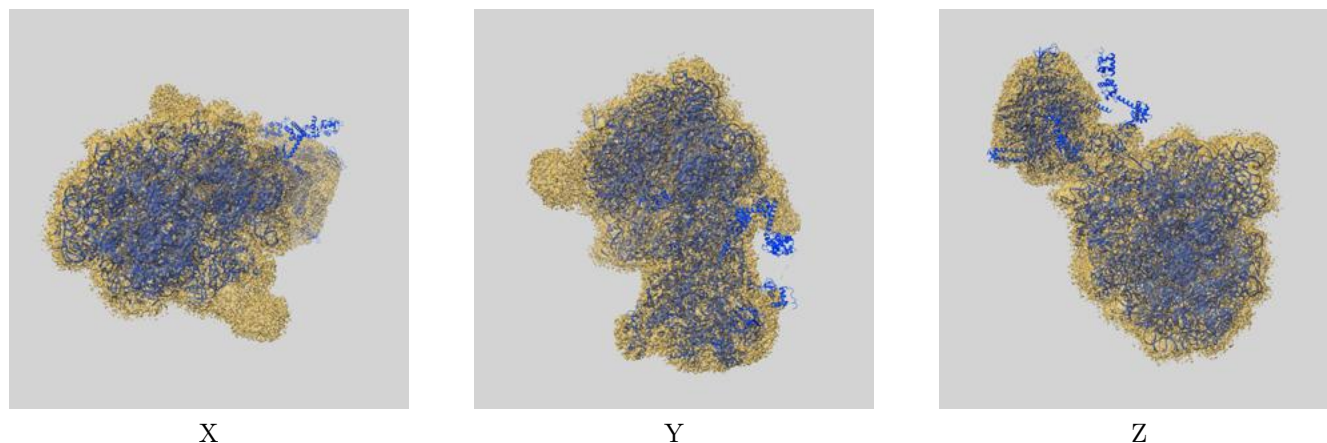
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	5.11	7.30	5.23
Unmasked-calculated*	9.84	17.27	714.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.84 differs from the reported value 5.1 by more than 10 %

9 Map-model fit [i](#)

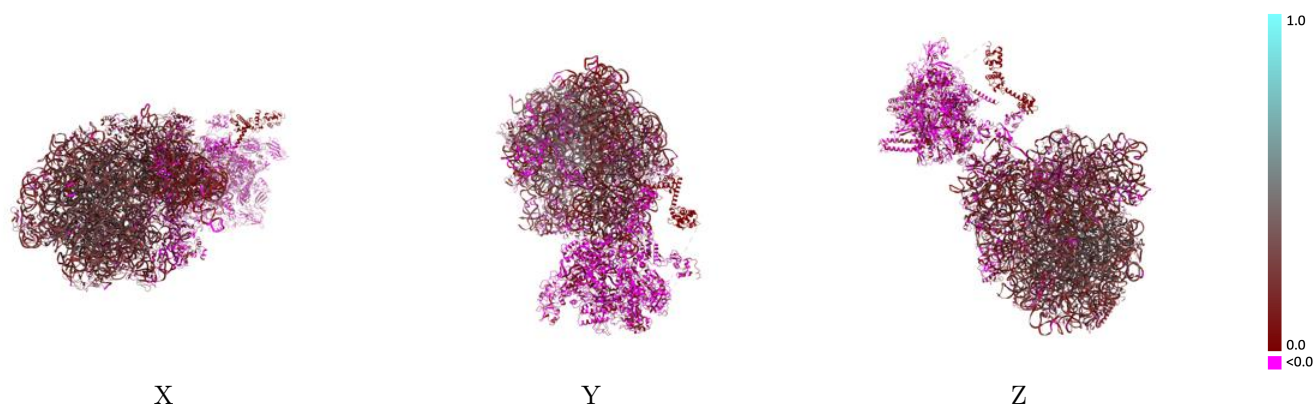
This section contains information regarding the fit between EMDB map EMD-39173 and PDB model 8YDJ. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



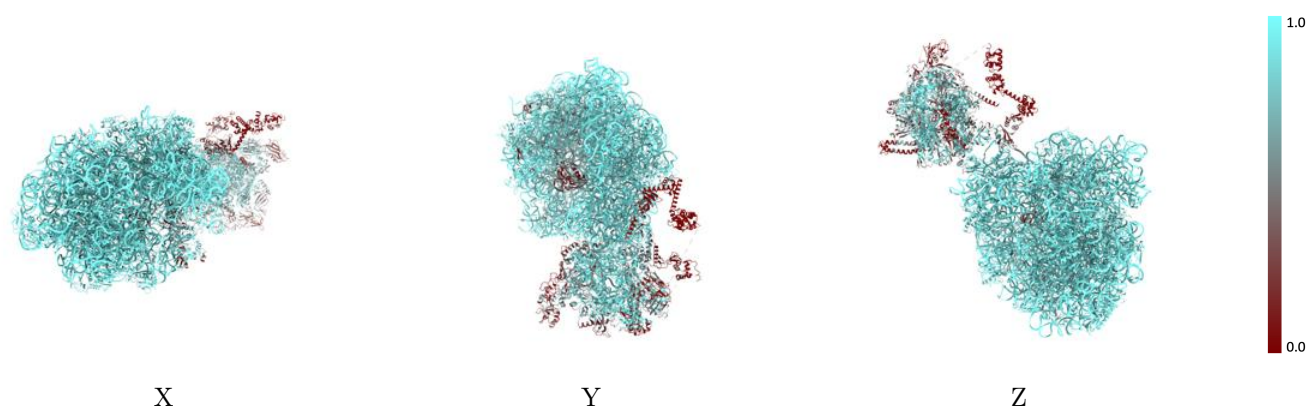
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



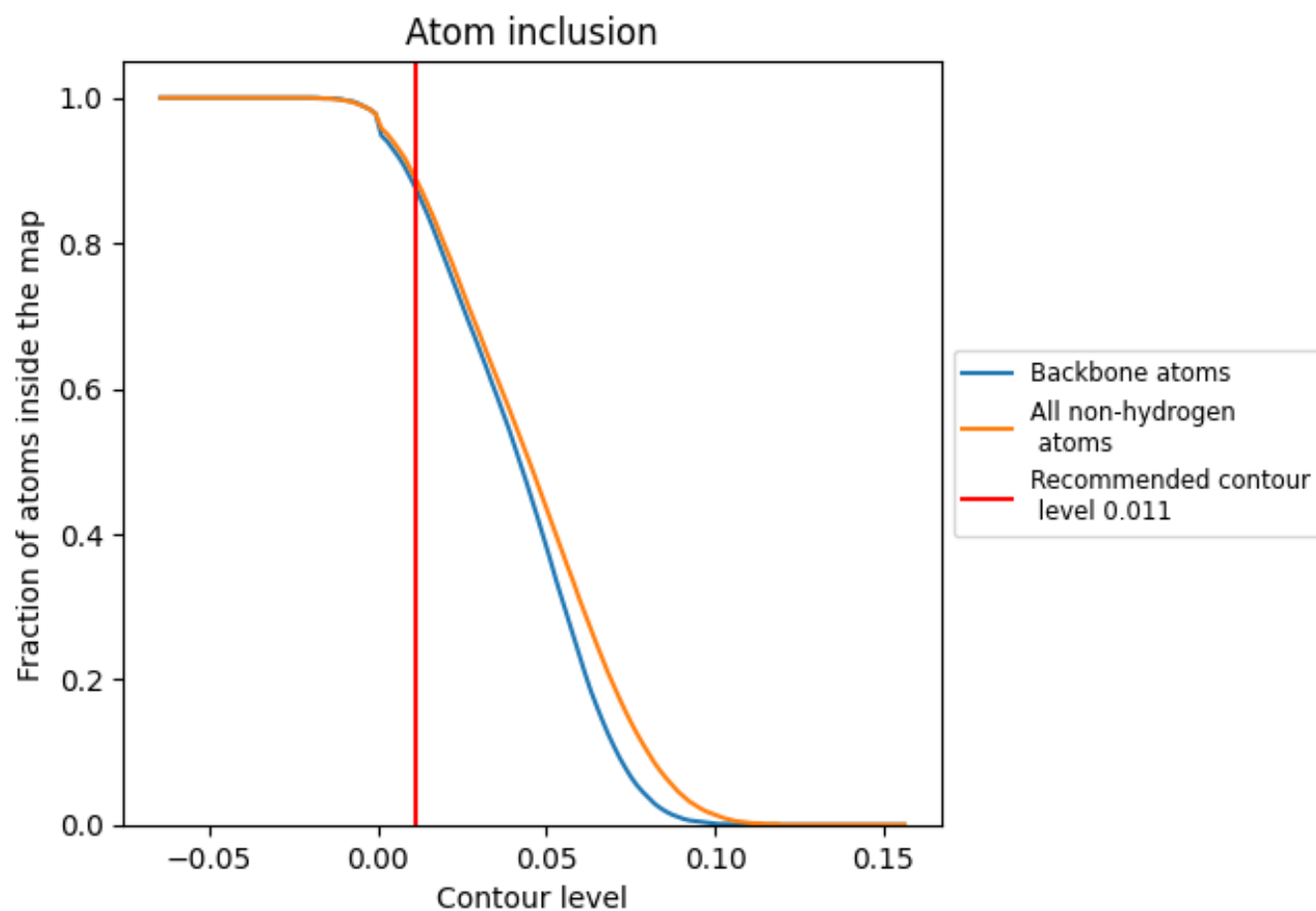
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.1630
0	 0.6170	 0.0440
1	 0.9880	 0.2460
2	 0.9790	 0.1390
3	 0.9820	 0.1930
4	 0.8500	 0.0680
5	 0.4280	 0.0410
6	 0.9630	 0.1960
8	 0.8200	 0.0220
9	 0.9040	 0.0500
A	 0.9090	 0.0620
A1	 0.3200	 -0.0120
A2	 0.5590	 -0.0060
B	 0.9390	 0.2500
B1	 0.6730	 -0.0000
B2	 0.6840	 0.0120
C	 0.8780	 0.1010
D	 0.9320	 0.2970
E	 0.9180	 0.1920
F	 0.9310	 0.1730
G	 0.9120	 0.1110
H	 0.9000	 0.1300
I	 0.9330	 0.1280
J	 0.8870	 0.1270
K	 0.9260	 0.1350
L	 0.8950	 0.1080
M	 0.9040	 0.1100
N	 0.9070	 0.1000
NA	 0.2630	 0.0010
NG	 0.6940	 0.0110
O	 0.9030	 0.0950
P	 0.9420	 0.1640
Q	 0.8600	 0.1700
R	 0.9110	 0.1240
S	 0.9130	 0.1000



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.9330	 0.1470
U	 0.9390	 0.1010
V	 0.9110	 0.0880
W	 0.9300	 0.1570
W0	 0.4950	 0.0110
X	 0.9400	 0.1370
Y	 0.9260	 0.1060
Z	 0.8320	 0.1120
a	 0.9280	 0.0560
b	 0.9220	 0.2740
c	 0.9500	 0.2320
d	 0.9390	 0.1670
e	 0.8860	 0.0790
f	 0.9180	 0.1040
g	 0.7470	 0.0830
h	 1.0000	 0.2940
i	 0.7790	 0.0160
j	 0.9410	 0.2390
k	 0.8860	 0.2540
l	 0.9250	 0.1730
m	 0.8740	 0.1600
n	 0.9610	 0.2530
o	 0.9550	 0.0450
p	 0.9210	 0.2120
q	 0.9580	 0.2380
r	 0.9520	 0.1800
s	 0.9270	 0.2590
t	 0.9210	 0.1640
u	 0.9530	 0.1540
v	 0.9390	 0.1100
w	 0.9270	 0.1120
x	 0.9370	 0.2230
y	 0.9360	 0.1350
z	 0.9200	 0.1250