



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 11:42 PM UTC

PDB ID : 8Y5M / pdb_00008y5m
EMDB ID : EMD-38942
Title : E.coli transcription translation coupling complex in TTC-B state 2 containing mRNA with 27-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 : 4.50 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

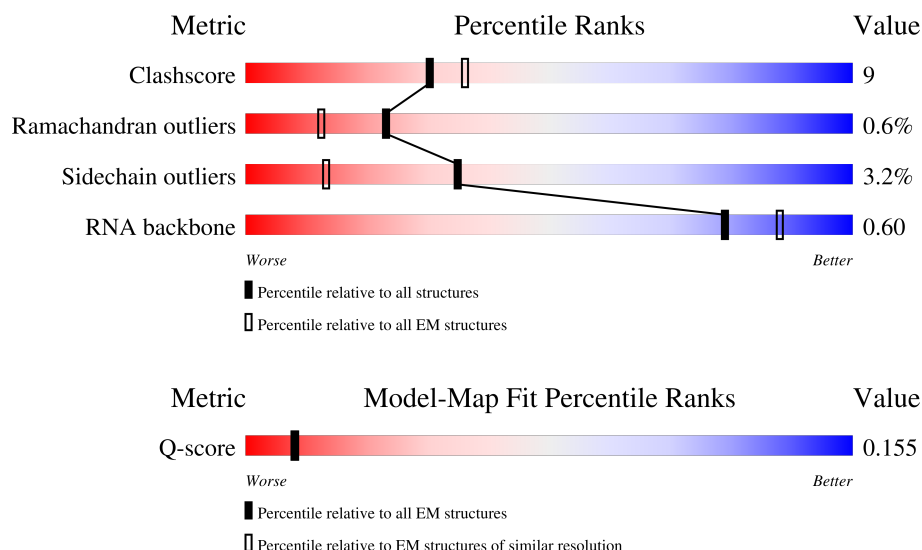
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



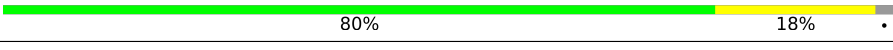
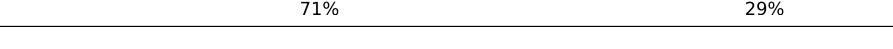
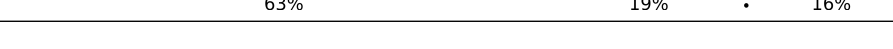
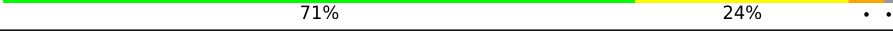
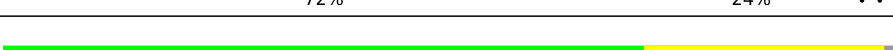
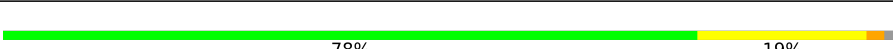
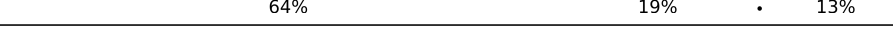
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	

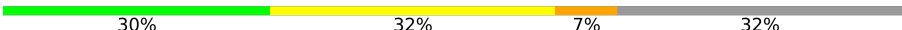
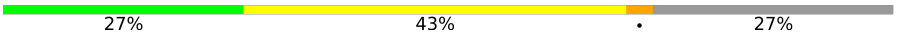
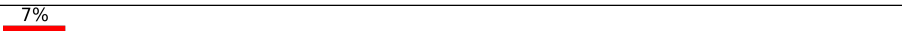
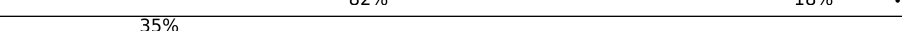
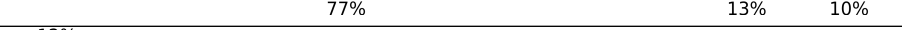
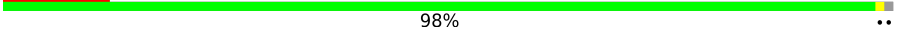
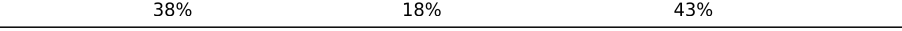
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Mol	Chain	Length	Quality of chain
29	d	201	 83% 17%
30	e	179	 76% 22% ..
31	f	177	 85% 14% ...
32	g	149	 6% 80% 18% .
33	i	142	 54% 38% 6% ..
34	j	142	 84% 15% .
35	k	123	 77% 20% ..
36	l	144	 72% 26% ..
37	m	136	 81% 18% .
38	n	127	 74% 20% . 6%
39	o	117	 75% 22% ..
40	p	115	 78% 21% .
41	q	118	 77% 19% ..
42	r	103	 75% 23% .
43	s	110	 79% 21%
44	t	100	 73% 20% 7%
45	u	104	 84% 13% ..
46	v	94	 74% 26%
47	w	85	 69% 18% . 12%
48	x	78	 79% 17% ..
49	y	63	 81% 17% .
50	z	59	 78% 19% ..
51	1	2904	 56% 38% 7%
52	2	120	 53% 44% ..
53	3	1542	 55% 39% 6%

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Mol	Chain	Length	Quality of chain
54	4	44	
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 183546 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	66	Total	C	N	O	S	0	0
			522	323	99	94	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
			1620	1025	304	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
			1152	717	218	211	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
			776	489	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	134	Total	C	N	O	S	0	0
			1026	645	186	193	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

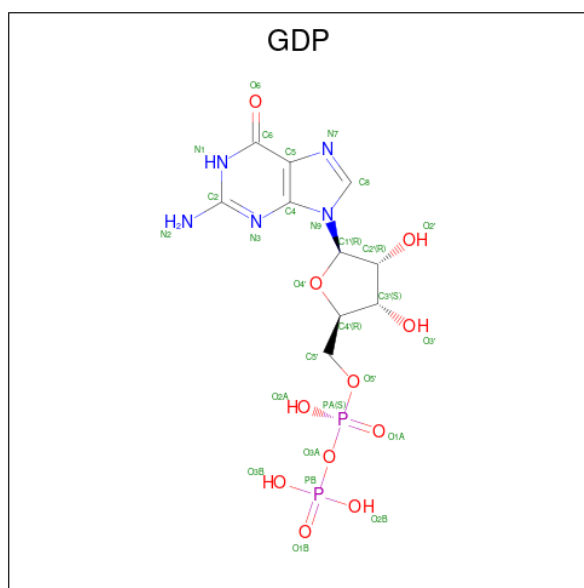
- Molecule 67 is a protein (with D amino acids) called Viomycin.

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).

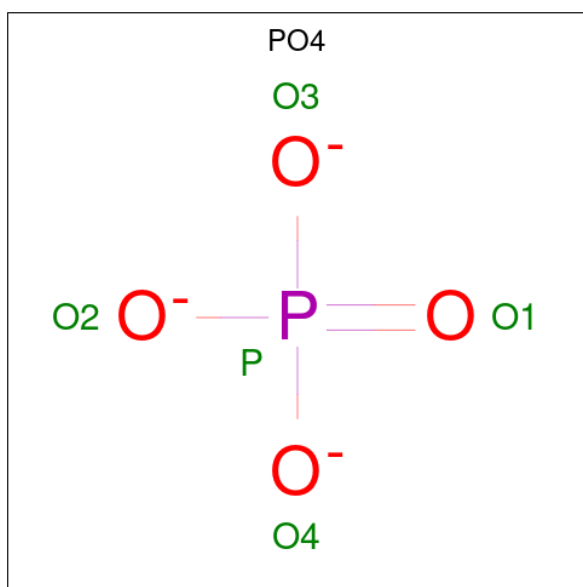
Mol	Chain	Residues	Atoms		AltConf
68	B1	1	Total	Mg	0
			1	1	

- 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).

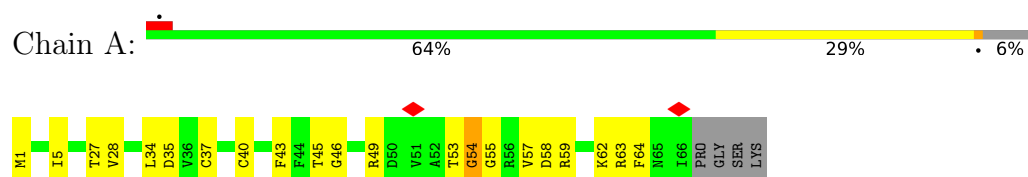


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

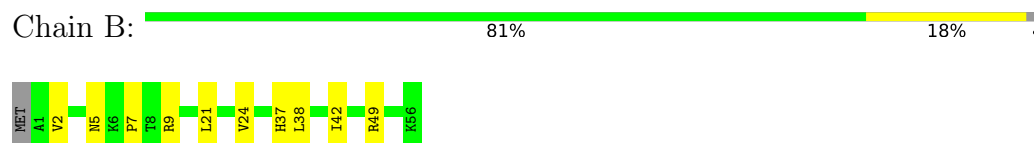
3 Residue-property plots

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.

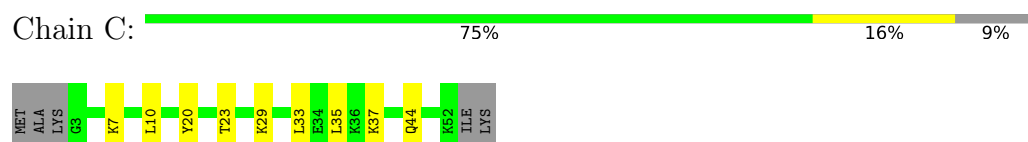
• Molecule 1: 50S ribosomal protein L31



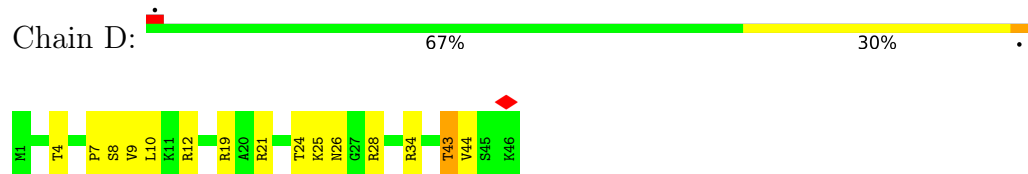
• Molecule 2: 50S ribosomal protein L32



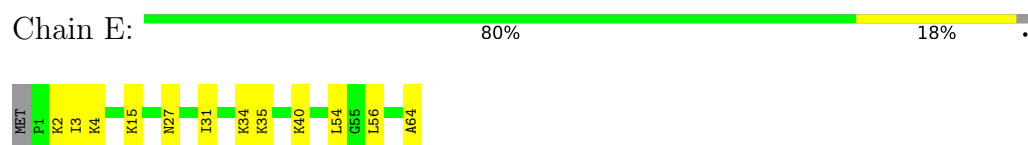
• Molecule 3: 50S ribosomal protein L33



• Molecule 4: 50S ribosomal protein L34



• Molecule 5: 50S ribosomal protein L35



• Molecule 6: 50S ribosomal protein L36

Chain F:  71% 29%



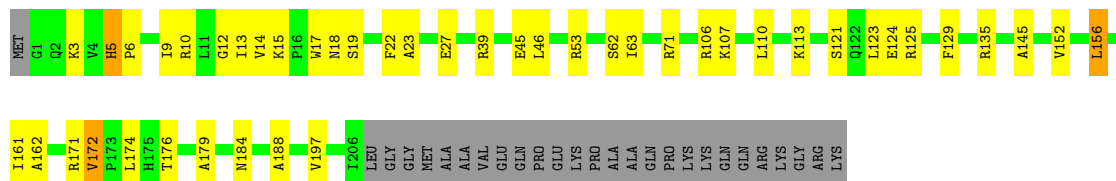
- Molecule 7: 30S ribosomal protein S2

Chain G:  70% 18% 10%



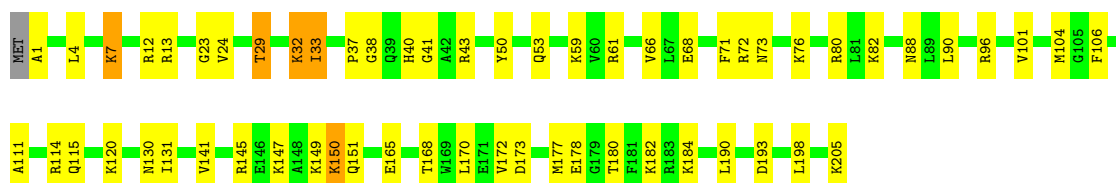
- Molecule 8: 30S ribosomal protein S3

Chain H:  69% 18% 12%



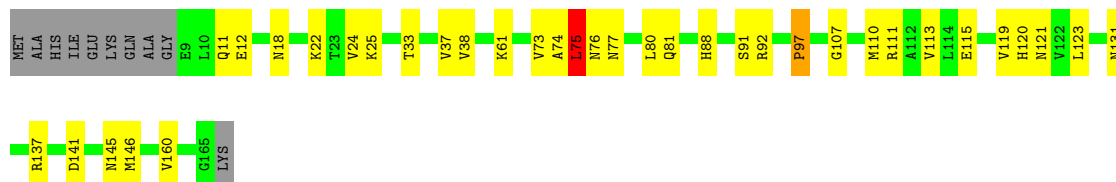
- Molecule 9: 30S ribosomal protein S4

Chain I:  71% 26%



- Molecule 10: 30S ribosomal protein S5

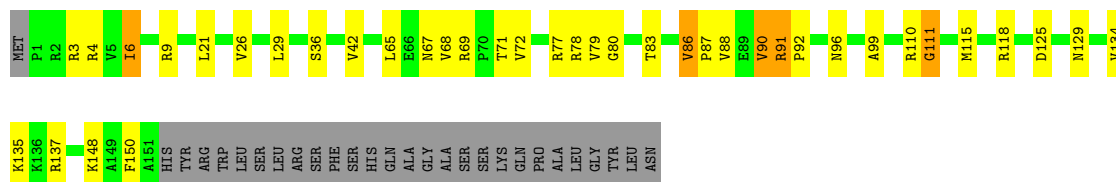
Chain J:  72% 20% 6%



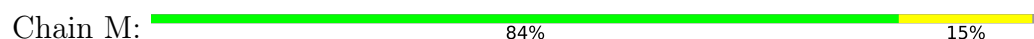
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  52% 20% 26%

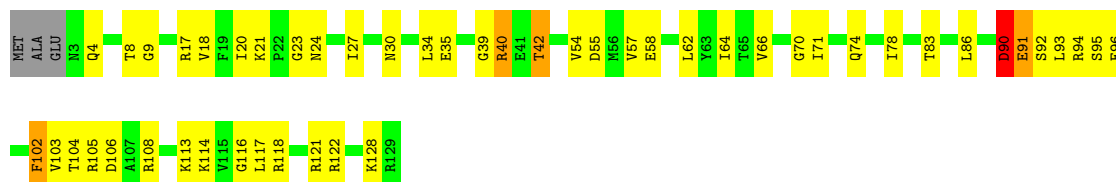
- Molecule 12: 30S ribosomal protein S7



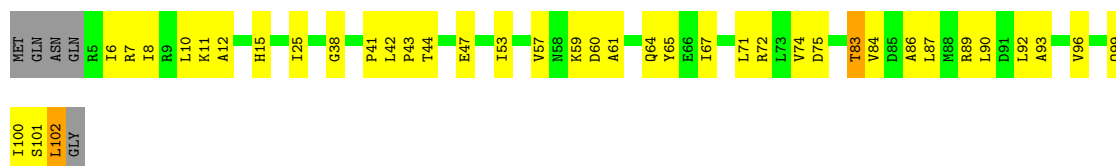
- Molecule 13: 30S ribosomal protein S8



- Molecule 14: 30S ribosomal protein S9



- Molecule 15: 30S ribosomal protein S10



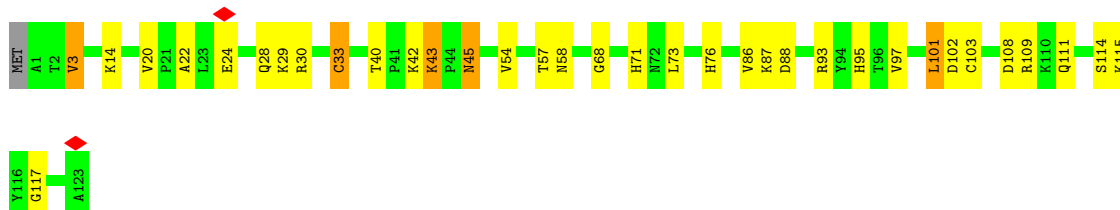
- Molecule 16: 30S ribosomal protein S11





- Molecule 17: 30S ribosomal protein S12

Chain Q: 71% 24% . .



- Molecule 18: 30S ribosomal protein S13

Chain R: 72% 24% . .



- Molecule 19: 30S ribosomal protein S14

Chain S: 72% 27% .



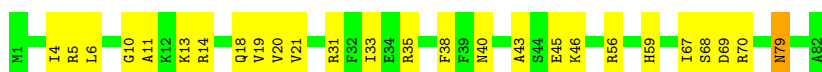
- Molecule 20: 30S ribosomal protein S15

Chain T: 78% 19% . .



- Molecule 21: 30S ribosomal protein S16

Chain U: 68% 30% .



- Molecule 22: 30S ribosomal protein S17

Chain V: 63% 32% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W: 



- Molecule 24: 30S ribosomal protein S19

Chain X: 



- Molecule 25: 30S ribosomal protein S20

Chain Y: 



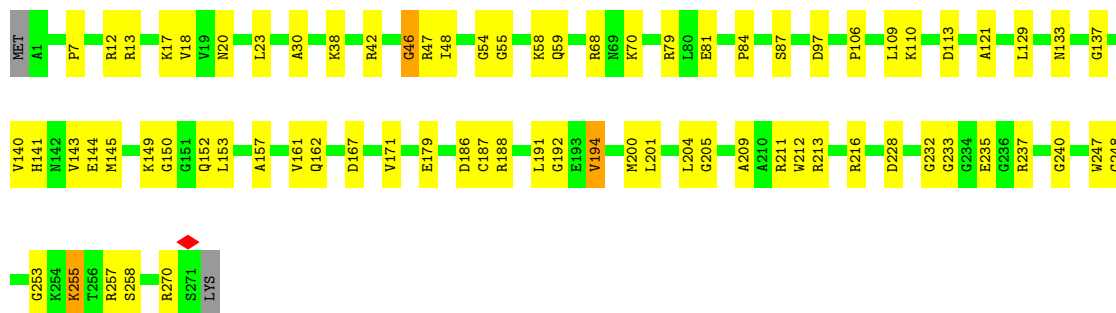
- Molecule 26: 30S ribosomal protein S21

Chain Z: 



- Molecule 27: 50S ribosomal protein L2

Chain b: 



- Molecule 28: 50S ribosomal protein L3

Chain c: 





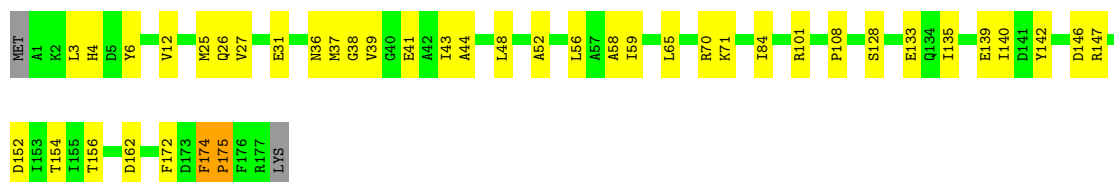
- Molecule 29: 50S ribosomal protein L4

Chain d: 83% 17%



- Molecule 30: 50S ribosomal protein L5

Chain e: 76% 22% ..



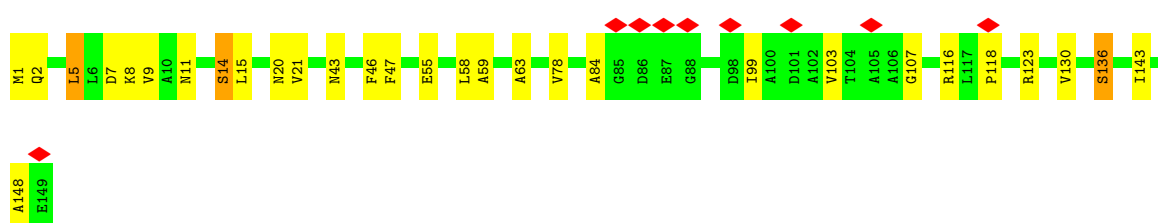
- Molecule 31: 50S ribosomal protein L6

Chain f: 85% 14% ...



- Molecule 32: 50S ribosomal protein L9

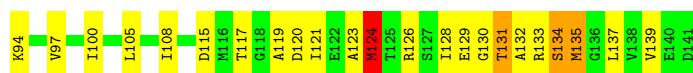
Chain g: 6% 80% 18% .



- Molecule 33: 50S ribosomal protein L11

Chain i: 54% 38% 6% ..





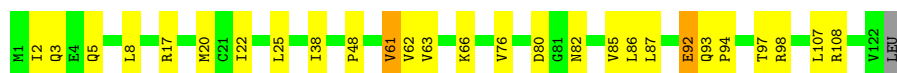
- Molecule 34: 50S ribosomal protein L13

Chain j: 84% 15%



- Molecule 35: 50S ribosomal protein L14

Chain k: 77% 20%



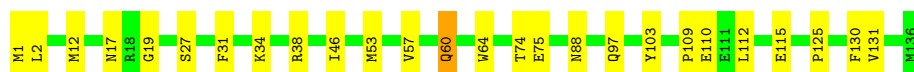
- Molecule 36: 50S ribosomal protein L15

Chain l: 72% 26%



- Molecule 37: 50S ribosomal protein L16

Chain m: 81% 18%



- Molecule 38: 50S ribosomal protein L17

Chain n: 74% 20% 6%



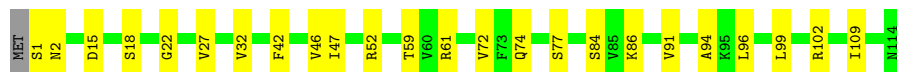
- Molecule 39: 50S ribosomal protein L18

Chain o: 75% 22%



- Molecule 40: 50S ribosomal protein L19

Chain p:  78% 21%



- Molecule 41: 50S ribosomal protein L20

Chain q:  77% 19%



- Molecule 42: 50S ribosomal protein L21

Chain r:  75% 23%



- Molecule 43: 50S ribosomal protein L22

Chain s:  79% 21%



- Molecule 44: 50S ribosomal protein L23

Chain t:  73% 20% 7%



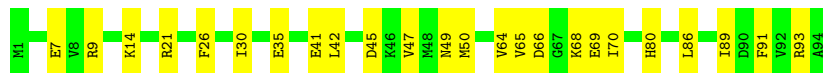
- Molecule 45: 50S ribosomal protein L24

Chain u:  84% 13%



- Molecule 46: 50S ribosomal protein L25

Chain v:  74% 26%



- Molecule 47: 50S ribosomal protein L27

Chain w:  69% 18% 12%

MET ALA HIS LYS LYS ALA GLY GLY SER THR R7 S12 E15 A14 G18 V19 K20 T33 V34 R35 G38 V47 K58 K62 P70 I76 S77 I78 E81

- Molecule 48: 50S ribosomal protein L28

Chain x:  79% 17% ..

MET S1 Q5 V6 I7 G8 K9 M16 R17 S18 N22 K25 P30 N31 L32 R36 T47 V57 K60 R73 Y77

- Molecule 49: 50S ribosomal protein L29

Chain y:  81% 17% .

M1 L19 N20 L21 L22 R23 E24 Q25 R29 N30 Q31 A32 Q36 L37 H41 A63

- Molecule 50: 50S ribosomal protein L30

Chain z:  78% 19% ..

MET A1 R10 S11 A12 I13 G14 R15 L16 P17 K20 G27 R37 T40 P41 A42 I43 M53 E58

- Molecule 51: 23S rRNA

Chain 1:  56% 38% 7%

G1 U4 A5 A6 G7 A10 C11 U12 G17 U18 A19 C20 A21 G26 C32 C33 U34 G35 C41 A42 G48 G51 A63 C69 G70 A71 A74 G75 G76 G77 G85 G89 A94 A95 C96 C97 G98 U99 U100 A101 U102 A103

A118 A119 A120 U121 G122 G123 G124 U133 G134 U135 G136 U139 C140 G141 A142 A149 U150 C151 A152 U153 U154 A155 A156 C157 U158 A161 U162 C163 U174 G175 G178 G179 G180 A181 G182 G186 G187 G188 G189 A195 A196 A197 A198 A199 U200 A207 C208 C209 G214

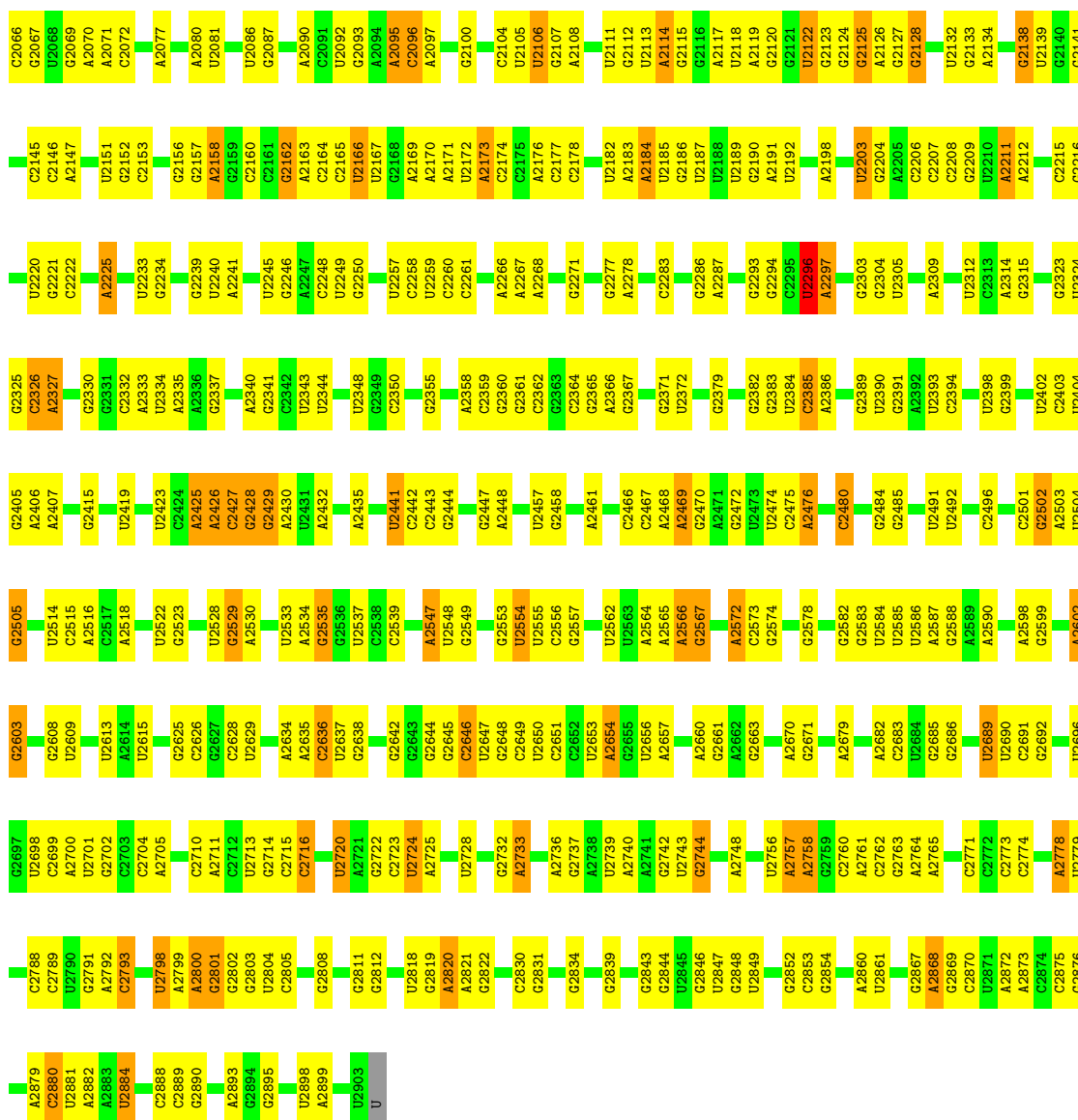
G215 A216 A217 A218 A219 G220 A221 A222 C225 A226 A227 C228 C229 G232 A233 U234 U235 C239 C240 A241 G242 G248 C249 G250 A251 A255 A256 C257 G266 A272 G273 C274 C275 U276 G277 A278 C281 A282 C283 U284 G285 U286 G287 C289 U294 A295 U296 G297 A300

A310 A311 G312 A320 U321 A322 C323 A324 G327 U328 C329 A330 C334 A335 C336 C337 C338 U339 A340 A341 C341 A342 A346 A353 A354 C355 U355 G356 A361 A362 G367 A368 U369 G370 A371 G372 U373 A374 G380 G386 U387 U395 G396 U399 A404 U405 G411 A412

C413 C414 A415 U416 U419 C420 G424 C435 C436 U437 A449 G450 U451 G452 C455 A456 A466 A467 G468 A472 G473 G474 A479 U480 G481 C490 G491 G494 A503 A504 A505 A508 A515 G518 G519 G520 G524 U525 A526 C527 A528 A529 G530 A532

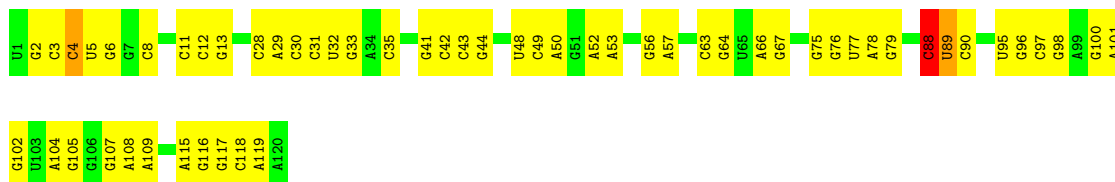
G533 U534 G535 G536 G539 G543 C544 U545 U552 G553 U554 G555 U562 A563 C564 A566 U567 A572 U573 A574 A575 A576 U580 C581 G584 G585 A586 C587 U588 A592 A596 G597 U598 A599 G600 A603 U606 U607 A608 A609 C610 C611 A614 U615

C1967	A1970	A1971	G1972	C1974	U1991	C1893	C1894	U1993	C1986	C1997	A1998	C1999	G2004	A2005	G2010	A2011	G2012	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036	U2039	G2040	U2041	A2042	C2043	G2048	G2049	C2050	A2051	C2055	G2056	A2060	G2061	A2062					
G1873	A1877	A1878	G1879	U1882	U1883	C1893	C1894	A1899	C1900	A1901	G1906	C1907	C1908	C1909	G1910	U1911	A1912	A1913	C1914	U1915	A1916	U1917	C1918	A1919	G1922	U1923	C1924	U1925	U1926	A1927	A1928	G1929	G1930	U1931	A1932	G1933	C1934	A1937	A1938	U1944	G1945	A1952	U1955	A1960	C1961	U1962	U1963	G1964	C1965	A1966			
U1775	G1776	A1780	U1781	U1782	A1783	A1784	A1785	A1786	C1790	A1791	C1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1805	C1806	G1807	A1808	A1809	A1810	G1811	C1816	A1819	U1820	A1821	C1822	G1823	U1827	G1828	A1829	C1837	C1838	G1839	G1842	C1843	C1844	G1845	G1846	A1847	G1857	G1859	C1870	A1871	A1872					
A1669	A1672	G1673	G1674	G1675	A1676	U1680	G1681	G1682	G1687	A1688	G1697	U1698	A1701	G1702	U1709	G1710	G1715	U1716	A1717	G1718	U1725	C1726	C1727	U1728	U1729	C1730	G1731	C1732	G1733	A1735	U1736	G1737	G1738	U1747	C1748	A1749	C1752	G1753	A1754	A1755	G1756	A1757	U1758	A1759	C1760	G1764	A1773	C1774					
G1555	C1556	C1557	C1558	U1559	G1560	C1564	C1565	G1568	A1569	U1578	U1584	U1587	G1597	C1598	A1599	G1601	U1602	A1603	A1608	C1611	A1616	C1617	A1618	G1625	A1626	G1627	G1628	U1636	A1637	C1638	G1645	U1647	U1648	G1649	A1650	G1651	A1654	A1655	C1658	A1665	G1666												
U1458	G1459	U1460	C1461	U1468	A1469	A1470	G1471	C1472	G1473	U1474	G1475	G1478	G1482	A1490	G1491	G1492	C1493	A1494	A1495	A1504	A1505	U1506	C1507	A1508	A1509	C1510	A1515	A1522	U1523	G1524	A1528	G1529	C1533	U1534	A1535	C1536	G1537	G1538	U1539	G1540	G1541	U1542	G1543	A1544	A1545	C1546	C1550	A1551					
C1357	G1358	C1363	G1364	A1365	U1375	G1376	G1377	A1378	U1379	G1380	A1383	A1386	C1387	U1388	G1394	U1397	C1398	U1409	G1410	G1416	C1417	G1418	A1419	A1420	G1424	G1425	G1426	A1427	C1428	G1429	G1430	A1433	A1434	G1435	G1436	C1437	U1438	U1439	U1440	G1441	U1442	U1443	G1444	C1447	G1448	G1449	G1450						
G1252	A1253	U1255	G1256	G1257	U1258	G1259	U1263	G1271	A1272	U1273	A1274	A1275	A1276	G1277	C1278	G1279	A1287	G1288	C1289	G1292	C1293	G1296	C1297	G1300	A1301	G1309	U1318	C1319	G1320	A1321	A1322	U1326	A1327	C1330	C1335	A1336	G1339	U1340	A1341	A1342	G1343	U1344	C1345	U1352									
G1122	C1123	G1124	G1125	U1130	G1131	U1132	A1133	A1134	C1135	G1136	U1137	G1138	C1139	G1140	U1141	A1142	A1143	A1155	A1156	G1157	G1158	U1159	G1160	C1161	G1162	C1172	U1173	U1174	A1175	G1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	G1186	G1187	U1188	A1189	G1190	U1201	G1202	C1211	G1212	C1221	G1225	G1248	U1249			
G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	A1068	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	C1079	A1080	U1081	U1082	U1083	A1084	A1085	G1086	C1087	A1088	G1091	C1092	A1095	A1096	U1097	A1098	G1099	C1102	A1103	C1104	G1106	C1109	G1110	A1111	G1112	U1113	C1117	C1118	U1119	G1120	C1121		
A975	A979	C885	A886	U887	A892	C893	U894	U895	A896	C897	C903	G904	C905	A906	U899	A1000	A1001	C1006	G1011	U1012	C1013	U1015	A1016	G1017	U1018	U992	A993	U994	C935	A936	C937	G938	G940	A941	G942	A943	C946	U947	G948	G949	C961	U967	C968	G969	U970	C971	A972	C876	A973	G974			
A792	A793	G797	G798	G799	A800	A802	U803	A804	C717	A718	C806	U807	G808	G809	U810	C812	U813	C814	C815	C816	C817	A743	U744	U827	U828	A748	A829	G830	C831	U832	A833	U839	A845	U846	G855	G857	G858	C859	U860	A861	G862	A863	G864	C865	G869	U870	A781	U872	A783	U874	G785	A788	
A616	G617	A621	G622	A626	A627	G628	G629	G630	A631	C634	C635	G636	A637	G638	U639	C640	A644	C645	U646	C650	A654	A655	U658	G659	C660	A661	G662	G663	G664	A668	G669	A670	C671	C672	A676	A677	G681	G682	U683	G684	A685	U686	C687	U688	A784	A689	C690	C691	C692	A693			



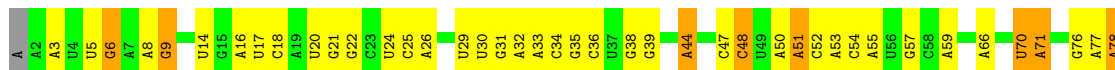
• Molecule 52: 5S rRNA

Chain 2: 53% 44% 3%



• Molecule 53: 16S rRNA

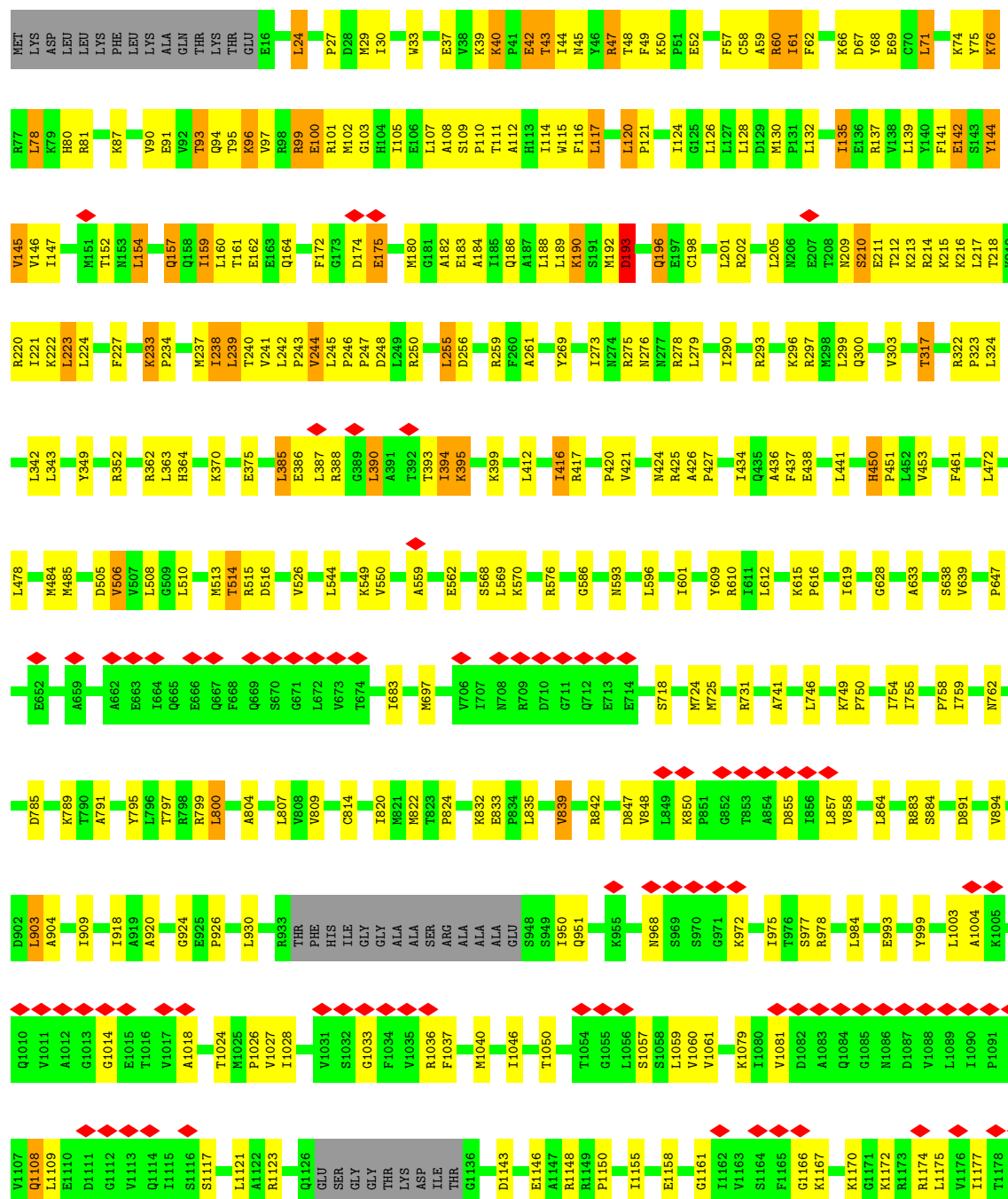
Chain 3: 55% 39% 6%

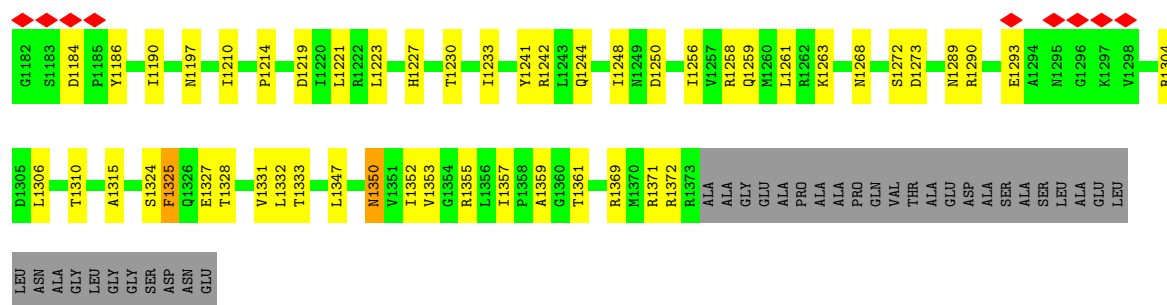




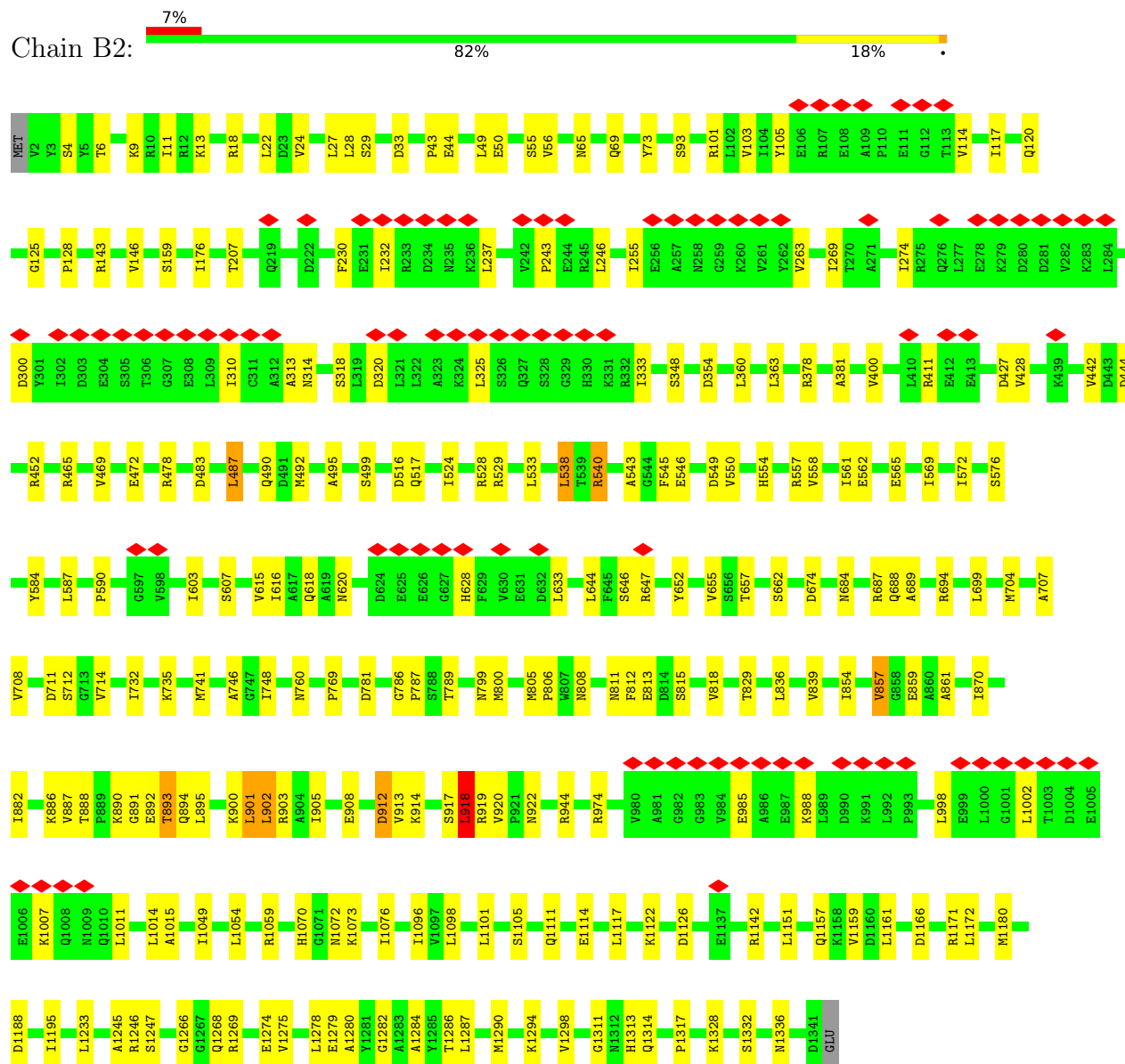


• Molecule 58: DNA-directed RNA polymerase subunit beta'

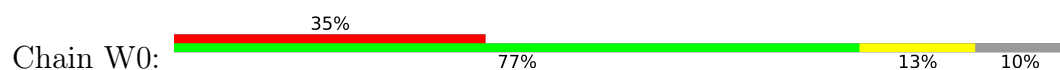


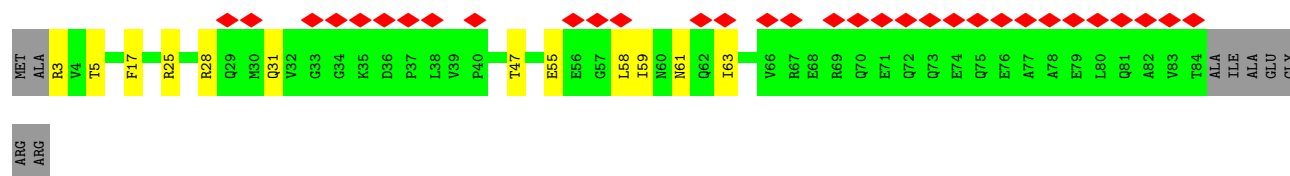


• Molecule 59: DNA-directed RNA polymerase subunit beta

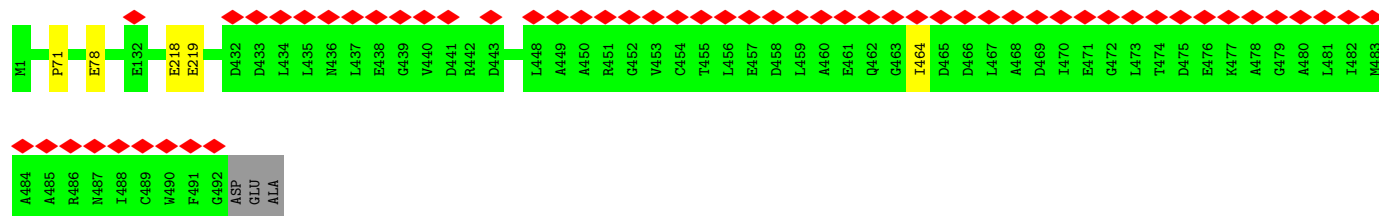


• Molecule 60: DNA-directed RNA polymerase subunit omega

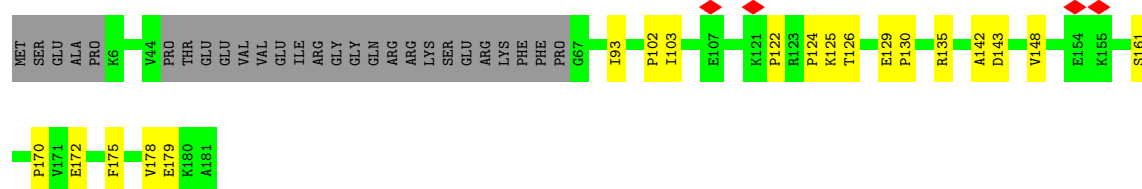
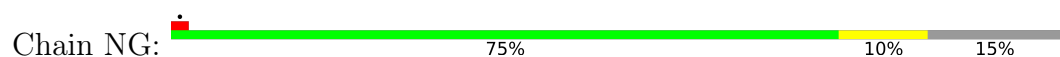




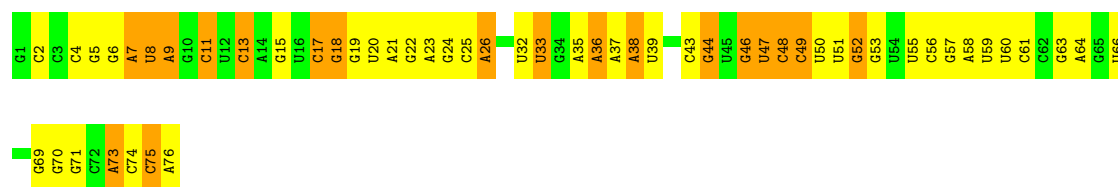
- Molecule 61: Transcription termination/antitermination protein NusA



- Molecule 62: Transcription termination/antitermination protein NusG



- Molecule 63: tRNA(Phe)

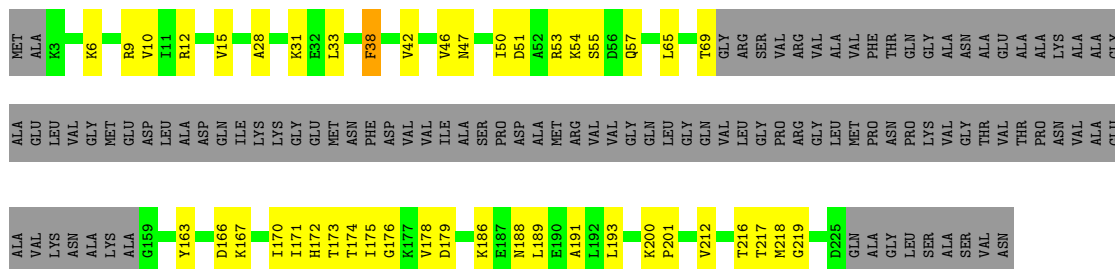


- Molecule 64: tRNA(fMet)



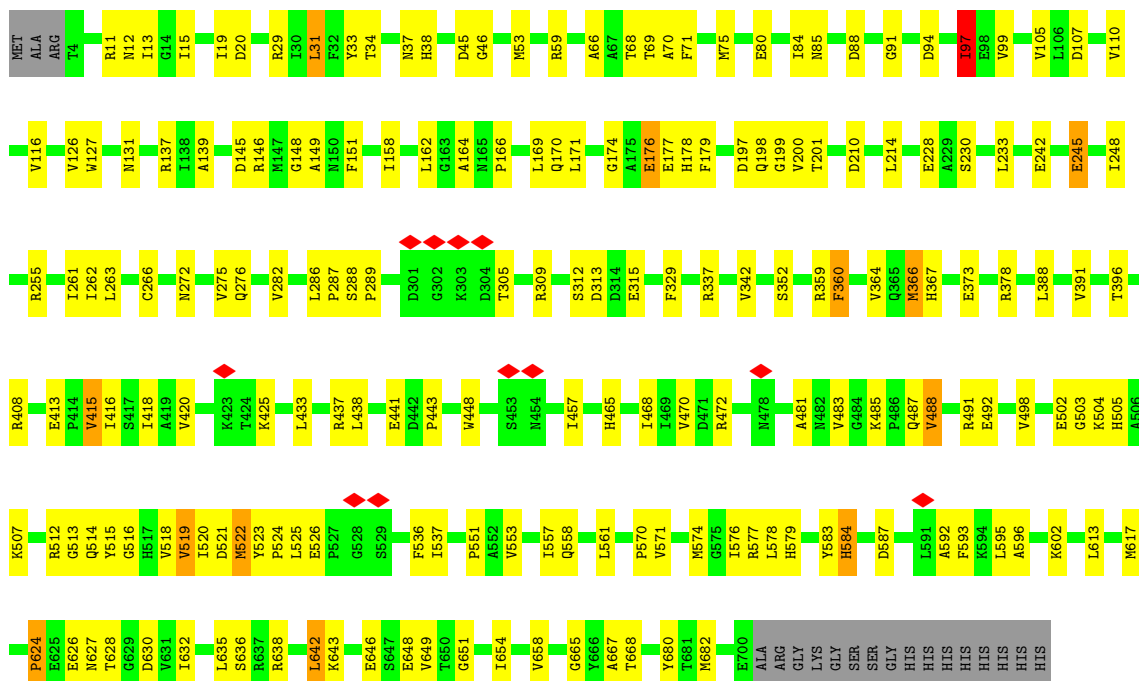
- Molecule 65: Large ribosomal subunit protein uL1





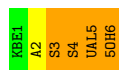
• Molecule 66: Elongation factor G

Chain 0: 71% 25%



• Molecule 67: Viomycin

Chain h: 17% 17% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31000	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	0.091	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0075	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: MG, 5OH, DPP, UAL, KBE, 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	0.47	0/531	0.99	4/709 (0.6%)
2	B	0.50	0/450	0.84	0/599
3	C	0.35	0/416	0.73	0/554
4	D	0.41	0/380	0.89	1/498 (0.2%)
5	E	0.40	0/513	0.86	0/676
6	F	0.35	0/303	0.77	0/397
7	G	0.48	0/1735	0.95	7/2338 (0.3%)
8	H	0.45	0/1647	0.88	3/2221 (0.1%)
9	I	0.45	0/1665	0.98	8/2227 (0.4%)
10	J	0.45	0/1165	0.95	7/1568 (0.4%)
11	K	0.58	0/835	1.02	5/1128 (0.4%)
12	L	0.44	0/1195	1.02	8/1602 (0.5%)
13	M	0.38	0/989	0.80	0/1326
14	N	0.48	0/1034	1.06	6/1375 (0.4%)
15	O	0.54	0/796	1.01	3/1077 (0.3%)
16	P	0.41	0/885	0.98	5/1195 (0.4%)
17	Q	0.51	1/969 (0.1%)	1.06	5/1300 (0.4%)
18	R	0.39	0/892	0.87	1/1193 (0.1%)
19	S	0.39	0/817	0.90	2/1088 (0.2%)
20	T	0.34	0/722	0.85	1/964 (0.1%)
21	U	0.40	0/659	0.91	2/884 (0.2%)
22	V	0.41	0/657	0.85	2/881 (0.2%)
23	W	0.47	0/544	0.95	2/731 (0.3%)
24	X	0.40	0/652	0.95	1/877 (0.1%)
25	Y	0.38	0/671	0.90	2/888 (0.2%)
26	Z	0.59	0/550	1.12	2/728 (0.3%)
27	b	0.45	0/2121	0.93	6/2852 (0.2%)
28	c	0.39	0/1586	0.84	3/2134 (0.1%)
29	d	0.43	0/1571	0.78	0/2113
30	e	0.44	1/1434 (0.1%)	0.91	5/1926 (0.3%)
31	f	0.41	0/1343	0.82	2/1816 (0.1%)
32	g	0.47	0/1122	0.93	3/1515 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.70	1/1046 (0.1%)	1.16	6/1410 (0.4%)
34	j	0.39	0/1152	0.86	4/1551 (0.3%)
35	k	0.49	0/947	0.95	2/1268 (0.2%)
36	l	0.40	0/1054	0.95	5/1403 (0.4%)
37	m	0.39	0/1093	0.85	3/1460 (0.2%)
38	n	0.39	0/973	0.92	3/1301 (0.2%)
39	o	0.39	0/902	0.92	3/1209 (0.2%)
40	p	0.40	0/929	0.85	1/1242 (0.1%)
41	q	0.46	0/960	0.90	3/1278 (0.2%)
42	r	0.45	0/829	0.96	4/1107 (0.4%)
43	s	0.38	0/864	0.84	2/1156 (0.2%)
44	t	0.39	0/744	0.78	0/994
45	u	0.41	0/784	0.92	3/1047 (0.3%)
46	v	0.39	0/766	0.78	0/1025
47	w	0.33	0/582	0.72	0/769
48	x	0.36	0/635	0.85	2/848 (0.2%)
49	y	0.34	0/510	0.87	1/677 (0.1%)
50	z	0.50	0/453	0.75	0/605
51	1	0.44	0/69796	0.54	8/108888 (0.0%)
52	2	0.45	0/2872	0.53	1/4479 (0.0%)
53	3	0.45	0/36963	0.53	3/57662 (0.0%)
54	4	0.56	0/695	0.72	0/1076
55	8	0.56	0/599	0.70	1/919 (0.1%)
56	9	0.48	0/468	0.53	0/719
57	A1	0.55	0/2106	0.82	0/2868
57	A2	0.48	0/2048	0.75	0/2786
58	B1	0.55	5/10510 (0.0%)	0.74	8/14196 (0.1%)
59	B2	0.45	0/10714	0.67	1/14459 (0.0%)
60	W0	0.29	0/652	0.61	0/879
61	NA	0.71	0/2431	1.20	0/3385
62	NG	1.12	0/756	1.03	2/1048 (0.2%)
63	5	0.56	0/1812	0.88	2/2823 (0.1%)
64	6	0.43	0/1832	0.56	0/2855
65	a	0.46	0/1033	0.98	5/1387 (0.4%)
66	0	0.51	0/5501	0.96	19/7446 (0.3%)
67	h	3.18	2/11 (18.2%)	0.75	0/13
All	All	0.46	10/196871 (0.0%)	0.69	188/289618 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	3	SER	CA-C	-6.72	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	4	SER	CA-C	-6.20	1.40	1.52
30	e	174	PHE	N-CA	5.74	1.54	1.46
58	B1	1350	ASN	CG-ND2	-5.27	1.22	1.33
58	B1	424	ASN	CG-ND2	-5.16	1.22	1.33

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	0	174	GLY	N-CA-C	10.08	123.45	111.35
11	K	99	ALA	N-CA-C	9.93	123.44	111.02
65	a	179	ASP	N-CA-C	-9.71	99.88	114.64
16	P	73	VAL	N-CA-C	-9.11	104.46	113.20
66	0	45	ASP	N-CA-C	-8.82	103.64	114.75

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	522	0	524	18	0
2	B	444	0	461	8	0
3	C	409	0	440	7	0
4	D	377	0	418	14	0
5	E	504	0	574	9	0
6	F	302	0	341	10	0
7	G	1704	0	1732	27	0
8	H	1620	0	1688	28	0
9	I	1643	0	1710	43	0
10	J	1152	0	1195	19	0
11	K	817	0	808	15	0
12	L	1181	0	1240	26	0
13	M	979	0	1034	13	0
14	N	1022	0	1070	38	0
15	O	786	0	828	26	0
16	P	869	0	878	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	955	0	1019	20	0
18	R	883	0	944	22	0
19	S	805	0	847	21	0
20	T	714	0	737	13	0
21	U	649	0	666	21	0
22	V	648	0	691	19	0
23	W	535	0	552	14	0
24	X	637	0	665	23	0
25	Y	665	0	714	20	0
26	Z	544	0	579	10	0
27	b	2082	0	2157	51	0
28	c	1565	0	1616	37	0
29	d	1552	0	1619	26	0
30	e	1410	0	1447	26	0
31	f	1323	0	1374	19	0
32	g	1111	0	1148	19	0
33	i	1032	0	1088	61	0
34	j	1129	0	1162	19	0
35	k	938	0	1012	17	0
36	l	1045	0	1117	29	0
37	m	1074	0	1157	17	0
38	n	960	0	1000	21	0
39	o	892	0	923	21	0
40	p	917	0	965	21	0
41	q	947	0	1022	22	0
42	r	816	0	839	16	0
43	s	857	0	922	16	0
44	t	738	0	807	12	0
45	u	776	0	825	7	0
46	v	753	0	780	17	0
47	w	575	0	592	16	0
48	x	625	0	655	15	0
49	y	509	0	543	8	0
50	z	449	0	491	9	0
51	1	62317	0	31346	968	0
52	2	2568	0	1303	58	0
53	3	33012	0	16618	568	0
54	4	627	0	313	8	0
55	8	539	0	305	29	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	26	0
57	A2	2029	0	1864	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B1	10353	0	10548	314	0
59	B2	10546	0	10550	161	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	8	0
62	NG	758	0	334	16	0
63	5	1622	0	821	23	0
64	6	1640	0	837	19	0
65	a	1026	0	1092	32	0
66	0	5399	0	5363	108	0
67	h	48	0	40	7	0
68	B1	1	0	0	0	0
69	0	28	0	12	2	0
70	0	5	0	0	1	0
All	All	183546	0	132910	2831	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 9.

The worst 5 of 2831 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)
23:W:42:ARG:NH2	53:3:721:G:H5''	1.59	1.18
35:k:48:PRO:HB3	53:3:1423:G:H5''	1.23	1.14
51:1:2682:A:H61	51:1:2728:U:H1'	1.18	1.08
23:W:42:ARG:HH21	53:3:721:G:H5''	0.97	1.08
33:i:93:ASN:HB2	51:1:1077:A:H5'	1.12	1.08

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	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
2	B	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	C	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
4	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
5	E	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7	37
6	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	186 (86%)	29 (13%)	1 (0%)	24	63
8	H	204/233 (88%)	184 (90%)	19 (9%)	1 (0%)	24	63
9	I	203/206 (98%)	178 (88%)	24 (12%)	1 (0%)	24	63
10	J	155/167 (93%)	131 (84%)	22 (14%)	2 (1%)	9	41
11	K	98/135 (73%)	83 (85%)	14 (14%)	1 (1%)	12	47
12	L	149/179 (83%)	129 (87%)	18 (12%)	2 (1%)	9	41
13	M	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	N	125/130 (96%)	95 (76%)	25 (20%)	5 (4%)	2	18
15	O	96/103 (93%)	77 (80%)	18 (19%)	1 (1%)	12	47
16	P	114/129 (88%)	90 (79%)	22 (19%)	2 (2%)	6	33
17	Q	121/124 (98%)	97 (80%)	18 (15%)	6 (5%)	1	16
18	R	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	49
19	S	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	22
20	T	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	43
21	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	41
22	V	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	9	41
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%)	80 (96%)	3 (4%)	0	100	100
26	Z	63/71 (89%)	45 (71%)	18 (29%)	0	100	100
27	b	269/273 (98%)	233 (87%)	31 (12%)	5 (2%)	6	32
28	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	24	63
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	155 (89%)	18 (10%)	2 (1%)	11	45
31	f	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	7	35
32	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	i	139/142 (98%)	116 (84%)	22 (16%)	1 (1%)	18	55
34	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	18	55
35	k	120/123 (98%)	99 (82%)	19 (16%)	2 (2%)	7	35
36	l	141/144 (98%)	121 (86%)	20 (14%)	0	100	100
37	m	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
38	n	118/127 (93%)	101 (86%)	17 (14%)	0	100	100
39	o	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	14	49
40	p	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	14	49
42	r	101/103 (98%)	86 (85%)	14 (14%)	1 (1%)	12	47
43	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
44	t	91/100 (91%)	78 (86%)	13 (14%)	0	100	100
45	u	100/104 (96%)	81 (81%)	18 (18%)	1 (1%)	12	47
46	v	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
47	w	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
48	x	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
49	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	7	37
50	z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
57	A1	295/329 (90%)	276 (94%)	19 (6%)	0	100	100
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1205 (91%)	119 (9%)	5 (0%)	30	67
59	B2	1338/1342 (100%)	1206 (90%)	128 (10%)	4 (0%)	36	71
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	482 (98%)	8 (2%)	0	100	100
62	NG	150/181 (83%)	135 (90%)	11 (7%)	4 (3%)	4	25
65	a	130/234 (56%)	112 (86%)	18 (14%)	0	100	100
66	0	695/716 (97%)	621 (89%)	71 (10%)	3 (0%)	30	67
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10508/11185 (94%)	9407 (90%)	1034 (10%)	67 (1%)	23	58

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	ILE
9	I	29	THR
14	N	57	VAL
14	N	90	ASP
14	N	91	GLU

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	59/62 (95%)	56 (95%)	3 (5%)	21	43
2	B	47/48 (98%)	44 (94%)	3 (6%)	16	38
3	C	45/49 (92%)	45 (100%)	0	100	100
4	D	38/38 (100%)	37 (97%)	1 (3%)	40	60
5	E	51/52 (98%)	51 (100%)	0	100	100
6	F	34/34 (100%)	34 (100%)	0	100	100
7	G	180/199 (90%)	175 (97%)	5 (3%)	38	59
8	H	169/190 (89%)	165 (98%)	4 (2%)	43	63
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	67
10	J	118/126 (94%)	115 (98%)	3 (2%)	42	62
11	K	87/116 (75%)	83 (95%)	4 (5%)	24	46
12	L	124/147 (84%)	122 (98%)	2 (2%)	55	69
13	M	104/105 (99%)	104 (100%)	0	100	100
14	N	105/107 (98%)	102 (97%)	3 (3%)	37	58
15	O	86/90 (96%)	80 (93%)	6 (7%)	14	36
16	P	89/99 (90%)	88 (99%)	1 (1%)	65	74
17	Q	103/104 (99%)	98 (95%)	5 (5%)	22	44
18	R	92/96 (96%)	91 (99%)	1 (1%)	65	74
19	S	83/84 (99%)	82 (99%)	1 (1%)	63	73
20	T	76/77 (99%)	75 (99%)	1 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	65/65 (100%)	64 (98%)	1 (2%)	57	70
22	V	74/78 (95%)	73 (99%)	1 (1%)	59	71
23	W	56/65 (86%)	54 (96%)	2 (4%)	31	52
24	X	70/79 (89%)	69 (99%)	1 (1%)	59	71
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	52 (94%)	3 (6%)	19	42
27	b	216/218 (99%)	212 (98%)	4 (2%)	50	66
28	c	164/164 (100%)	162 (99%)	2 (1%)	63	73
29	d	165/165 (100%)	163 (99%)	2 (1%)	63	73
30	e	148/150 (99%)	147 (99%)	1 (1%)	76	79
31	f	137/138 (99%)	137 (100%)	0	100	100
32	g	114/114 (100%)	112 (98%)	2 (2%)	51	67
33	i	109/110 (99%)	95 (87%)	14 (13%)	4	17
34	j	116/116 (100%)	115 (99%)	1 (1%)	70	76
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%)	109 (100%)	0	100	100
38	n	100/103 (97%)	99 (99%)	1 (1%)	68	76
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	97 (98%)	2 (2%)	48	65
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	54
42	r	84/84 (100%)	81 (96%)	3 (4%)	31	52
43	s	93/93 (100%)	93 (100%)	0	100	100
44	t	80/84 (95%)	79 (99%)	1 (1%)	61	72
45	u	82/85 (96%)	81 (99%)	1 (1%)	63	73
46	v	78/78 (100%)	77 (99%)	1 (1%)	61	72
47	w	57/63 (90%)	56 (98%)	1 (2%)	51	67
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	26	48
57	A1	185/286 (65%)	174 (94%)	11 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	A2	186/286 (65%)	185 (100%)	1 (0%)	81	81
58	B1	1110/1168 (95%)	1021 (92%)	89 (8%)	11	32
59	B2	1150/1157 (99%)	1119 (97%)	31 (3%)	39	59
60	W0	70/75 (93%)	69 (99%)	1 (1%)	59	71
65	a	110/181 (61%)	110 (100%)	0	100	100
66	0	574/588 (98%)	546 (95%)	28 (5%)	22	44
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8135/8683 (94%)	7874 (97%)	261 (3%)	35	55

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	B2	1151	LEU
66	0	418	ILE
66	0	649	VAL
47	w	19	VAL
44	t	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
58	B1	865	HIS
66	0	344	ASN
59	B2	69	GLN
59	B2	1237	HIS
66	0	579	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	420 (14%)	10 (0%)
52	2	119/120 (99%)	12 (10%)	1 (0%)
53	3	1538/1542 (99%)	181 (11%)	6 (0%)
54	4	28/44 (63%)	13 (46%)	3 (10%)
63	5	75/76 (98%)	38 (50%)	7 (9%)
64	6	76/77 (98%)	18 (23%)	0
All	All	4738/4763 (99%)	682 (14%)	27 (0%)

5 of 682 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	35	G
51	1	42	A
51	1	46	G

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	3	1054	C
54	4	13	U
63	5	60	U
53	3	1395	C
54	4	18	U

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	UAL	h	5	67	6,8,9	2.36	2 (33%)	4,9,11	1.89	1 (25%)
67	DPP	h	2	67	4,5,6	0.50	0	1,5,7	0.07	0
67	KBE	h	1	67	8,8,9	0.58	0	6,8,10	1.18	0
67	5OH	h	6	67	7,12,13	0.72	0	4,16,18	1.33	1 (25%)

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	UAL	h	5	67	-	0/3/7/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	DPP	h	2	67	-	0/2/4/6	-
67	KBE	h	1	67	-	0/7/7/8	-
67	5OH	h	6	67	-	0/2/18/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	5	UAL	C1-N1	-4.95	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	-3.31	121.25	125.39
67	h	6	5OH	CR-CB-CA	-2.40	110.06	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	5	UAL	1	0
67	h	2	DPP	1	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	$\# Z > 2$
70	PO4	0	802	-	4,4,4	1.15	0	6,6,6	0.73	0
69	GDP	0	801	-	29,30,30	1.13	4 (13%)	45,47,47	1.76	6 (13%)

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	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	0	801	GDP	C5-C4	2.84	1.46	1.38
69	0	801	GDP	C6-N1	-2.47	1.34	1.38
69	0	801	GDP	C5-N7	-2.25	1.34	1.39
69	0	801	GDP	C4-N9	-2.18	1.32	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	0	801	GDP	C5-C4-N3	-5.58	119.52	128.39
69	0	801	GDP	C2-N3-C4	4.88	120.71	112.30
69	0	801	GDP	N9-C4-N3	3.93	133.80	125.95
69	0	801	GDP	C6-C5-N7	3.51	136.69	130.29
69	0	801	GDP	C4-C5-N7	-2.55	106.63	110.67

There are no chirality outliers.

There are no torsion outliers.

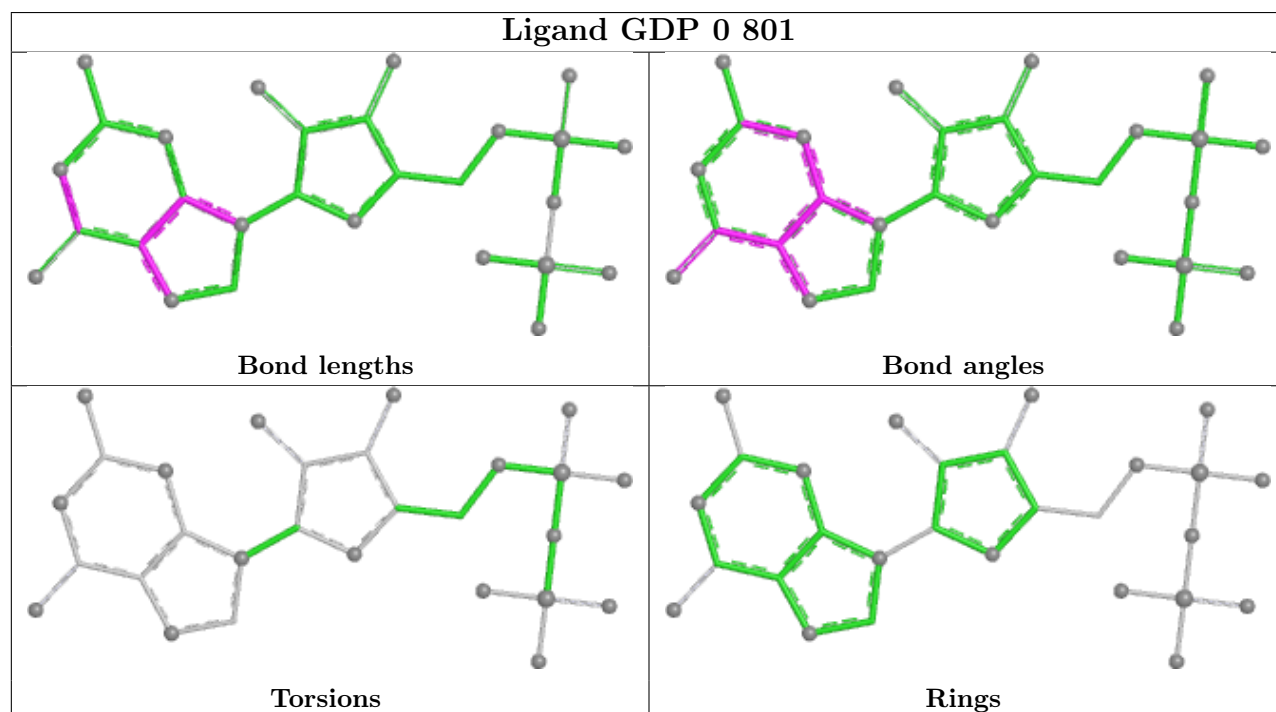
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	0	802	PO4	1	0
69	0	801	GDP	2	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.

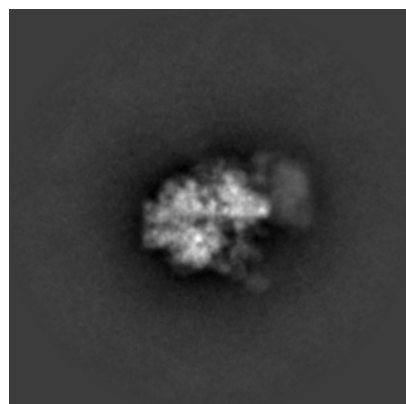
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38942. These allow visual inspection of the internal detail of the map and identification of artifacts.

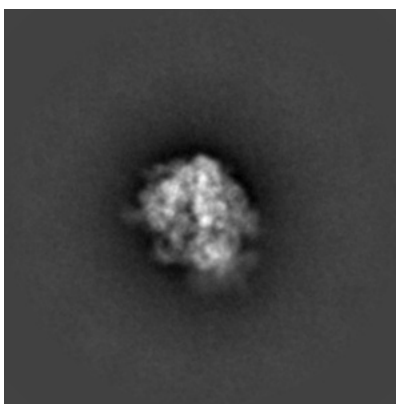
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

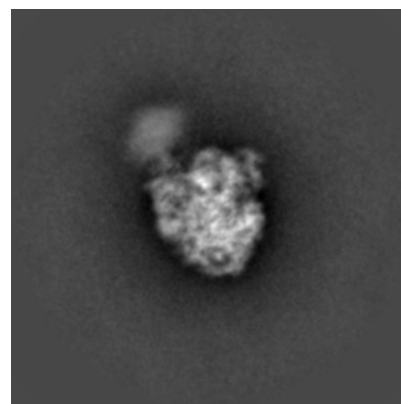
6.1.1 Primary map



X

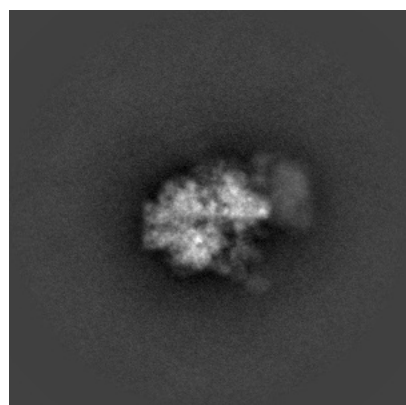


Y

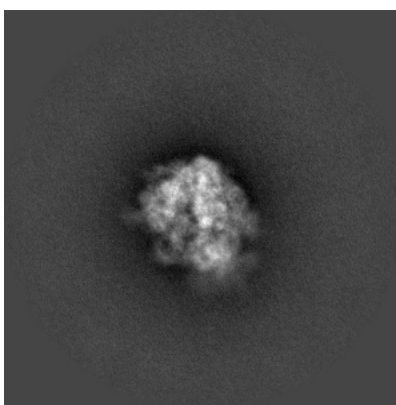


Z

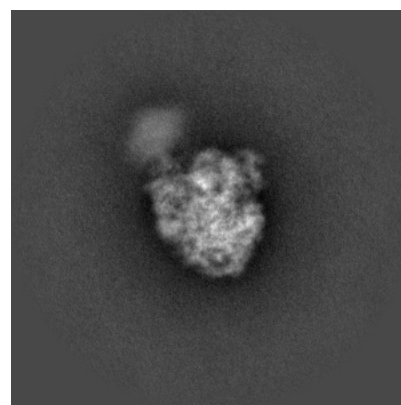
6.1.2 Raw map



X



Y

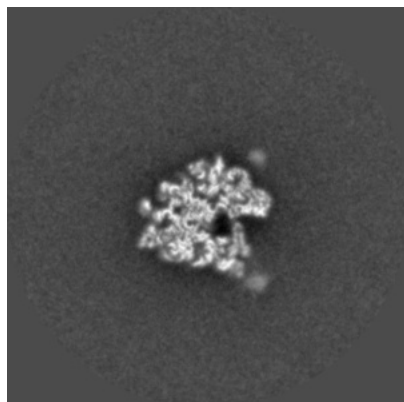


Z

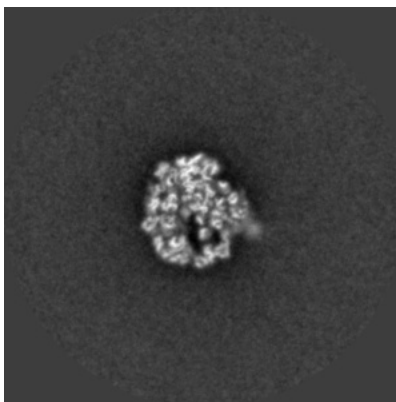
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

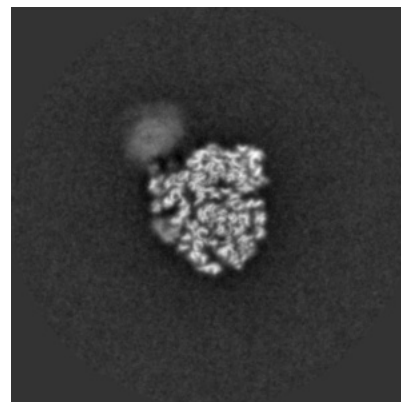
6.2.1 Primary map



X Index: 240

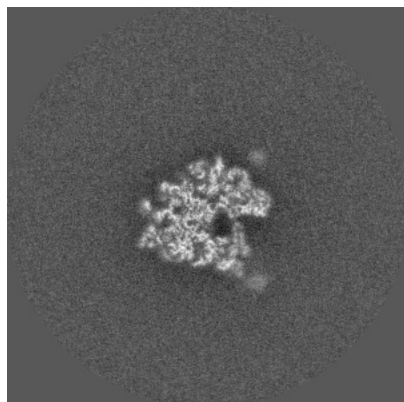


Y Index: 240

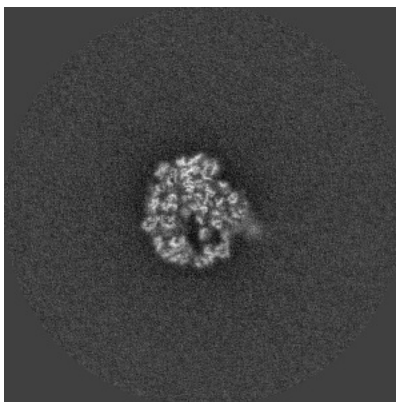


Z Index: 240

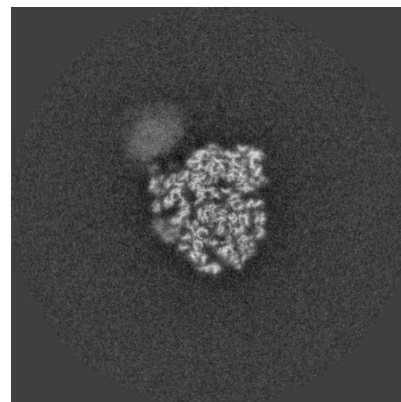
6.2.2 Raw map



X Index: 240



Y Index: 240

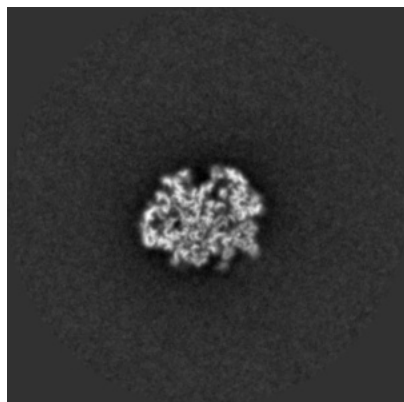


Z Index: 240

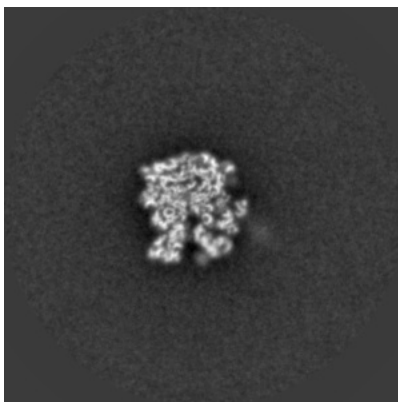
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

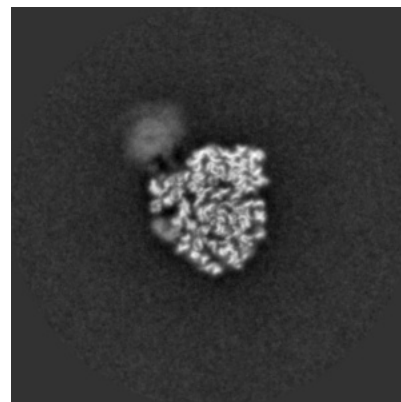
6.3.1 Primary map



X Index: 264

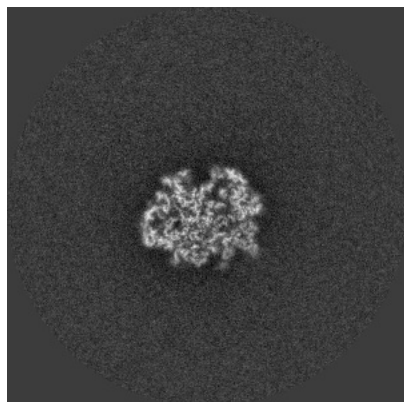


Y Index: 223

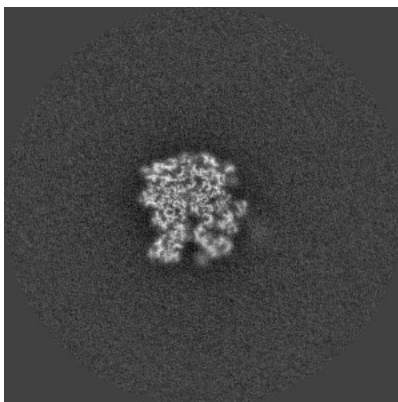


Z Index: 238

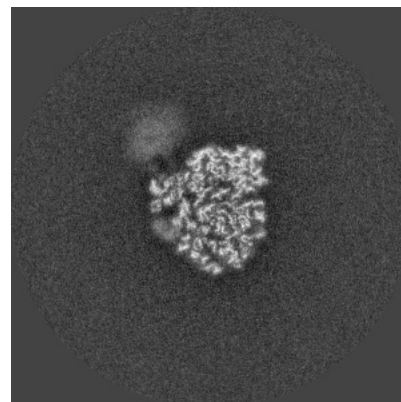
6.3.2 Raw map



X Index: 264



Y Index: 222



Z Index: 238

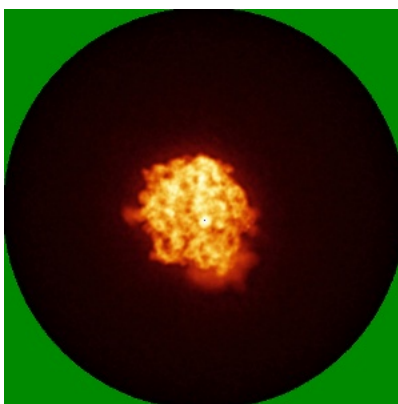
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

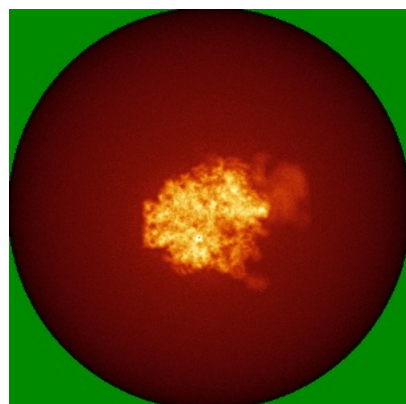


Y

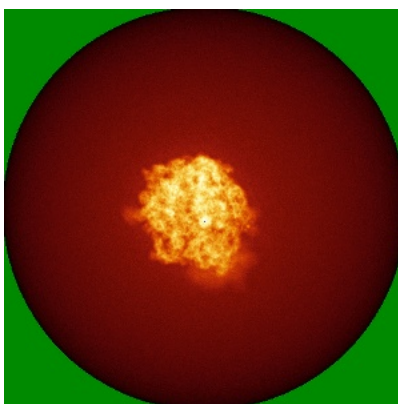


Z

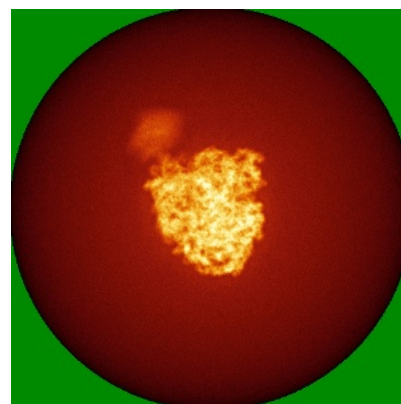
6.4.2 Raw map



X



Y

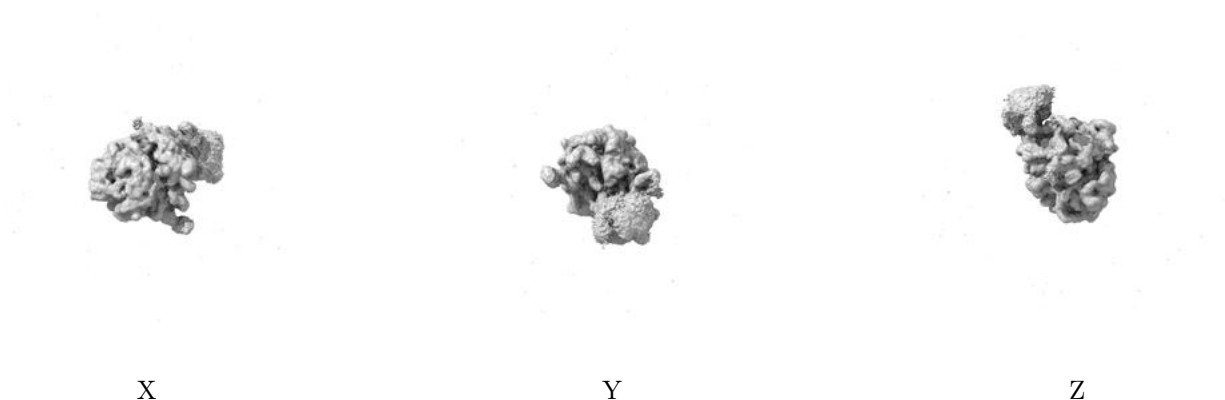


Z

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.

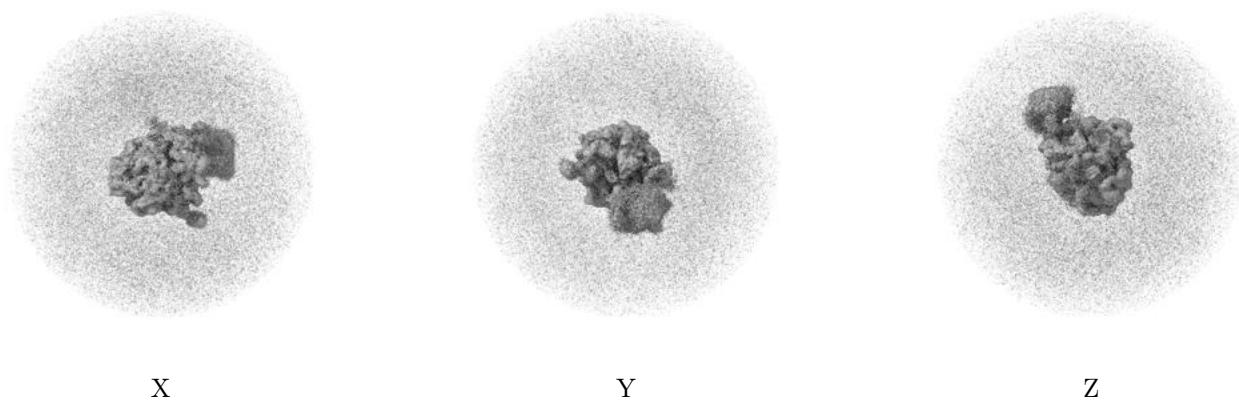
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. 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.

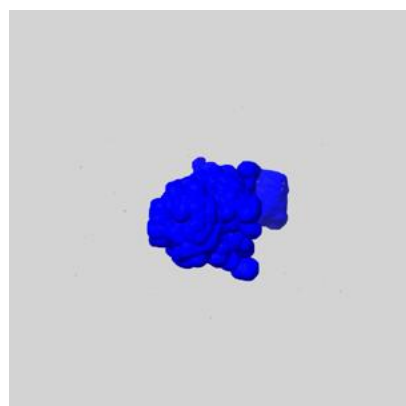
6.6 Mask visualisation [i](#)

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

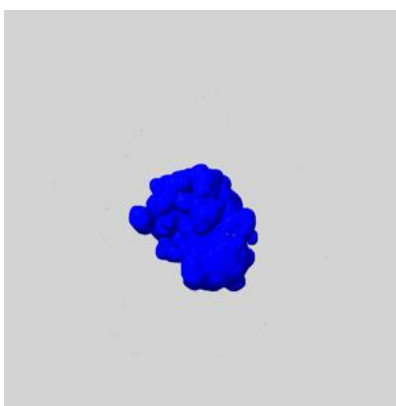
A mask typically either:

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

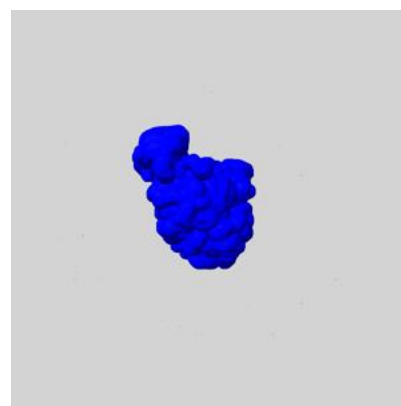
6.6.1 emd_38942_msk_1.map [i](#)



X



Y

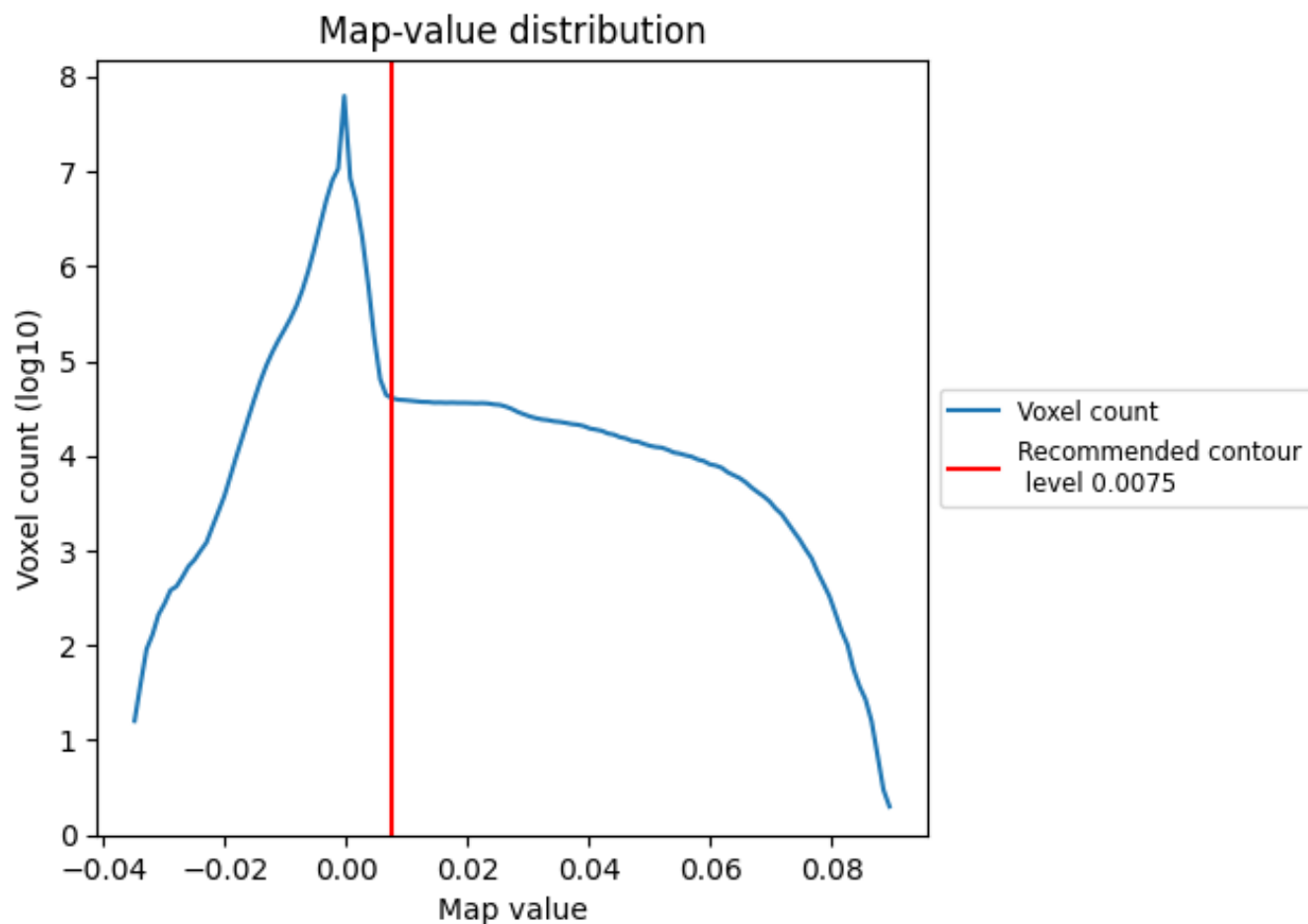


Z

7 Map analysis [i](#)

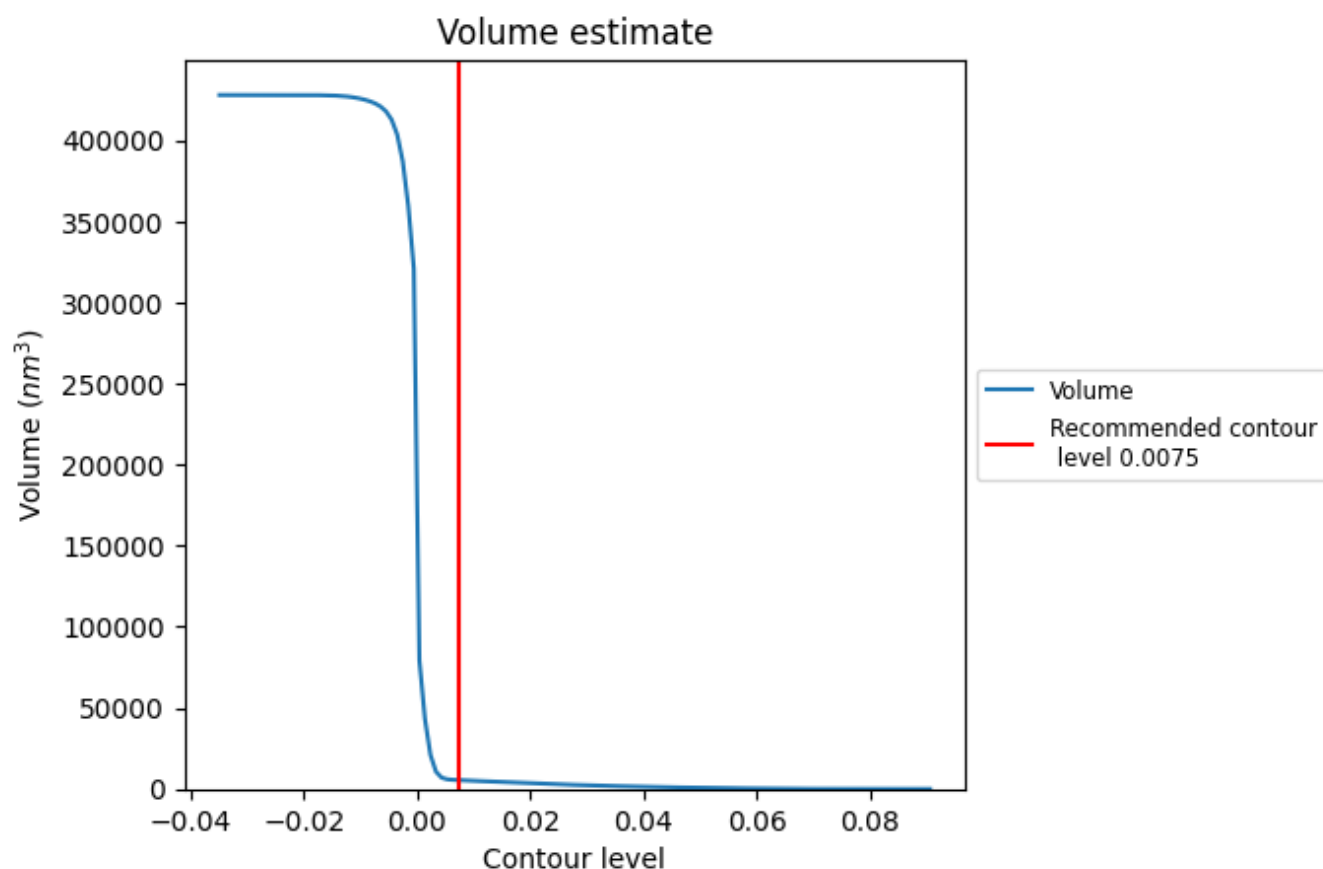
This section contains the results of statistical analysis of the map.

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.

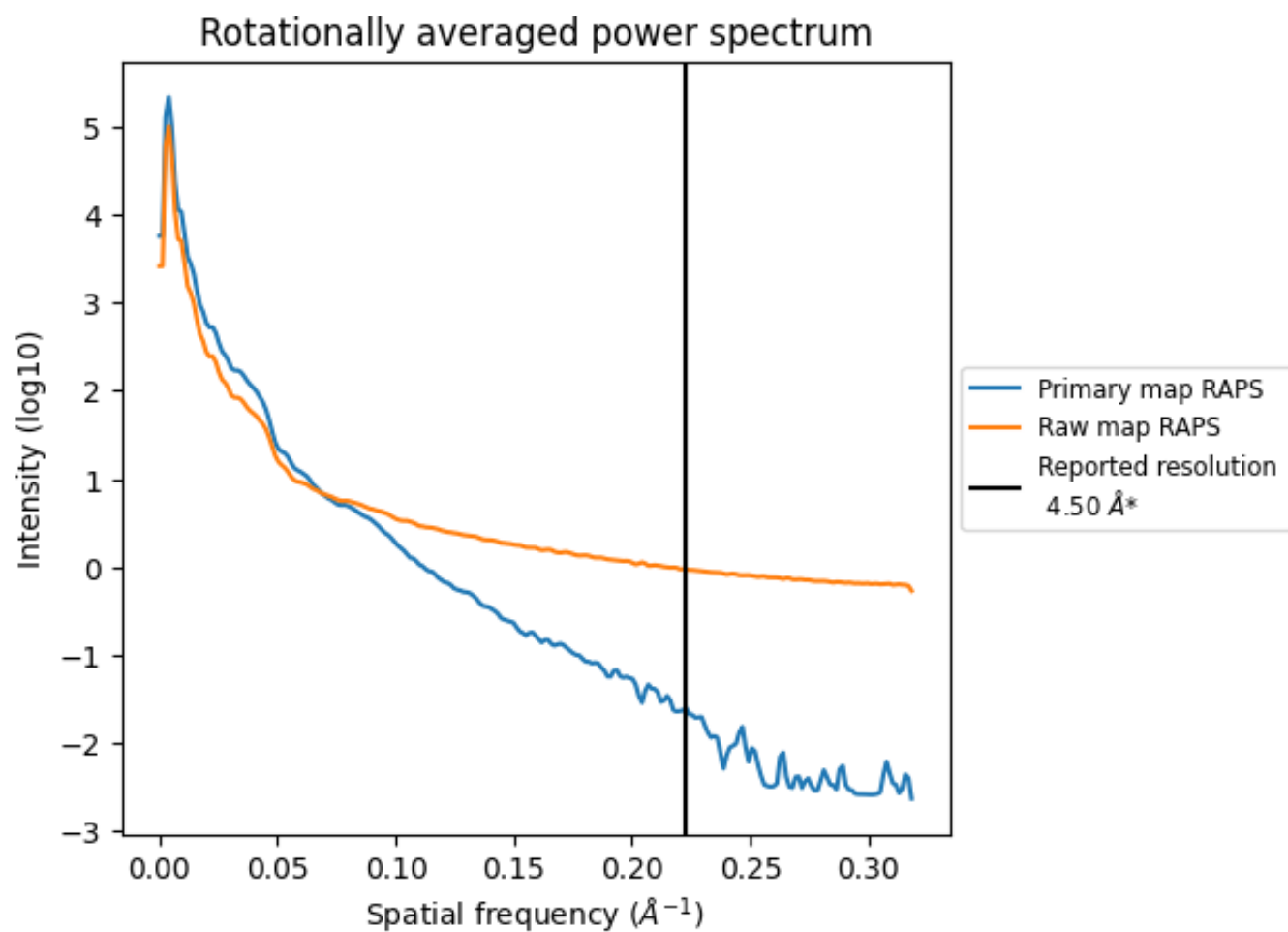
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5419 nm^3 ; this corresponds to an approximate mass of 4895 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 ⓘ

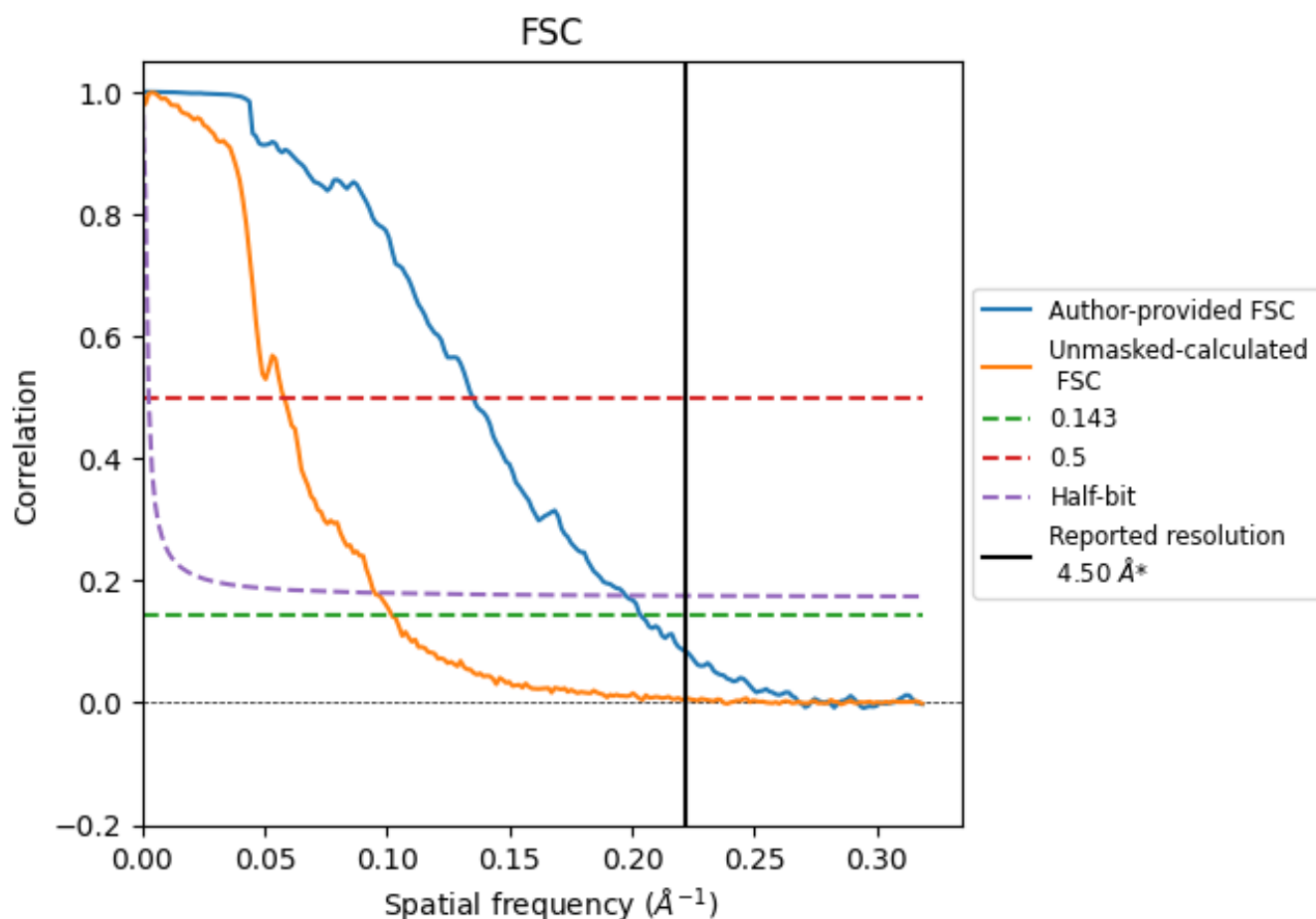


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

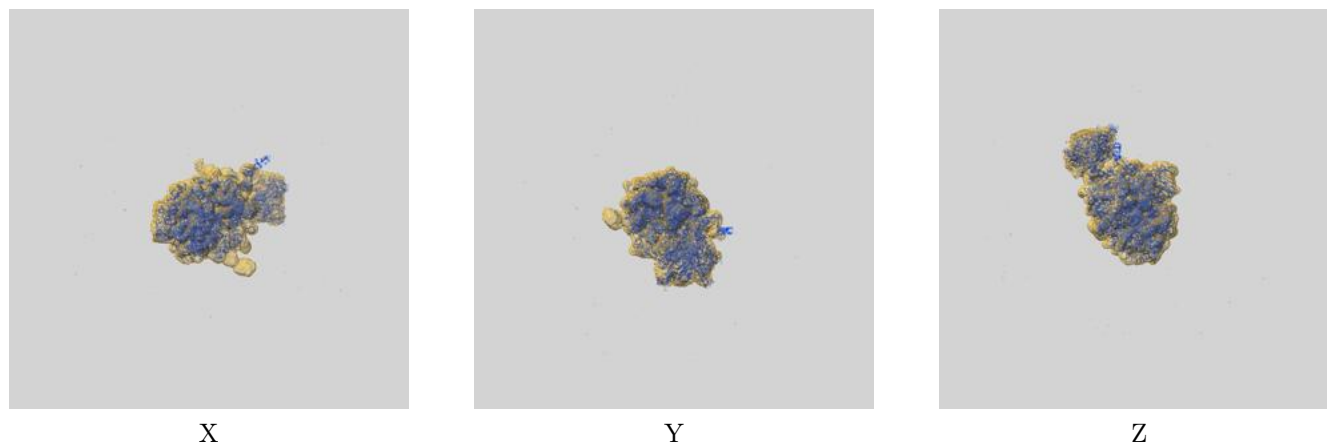
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.91	7.41	5.07
Unmasked-calculated*	9.81	17.30	10.52

*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 9.81 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

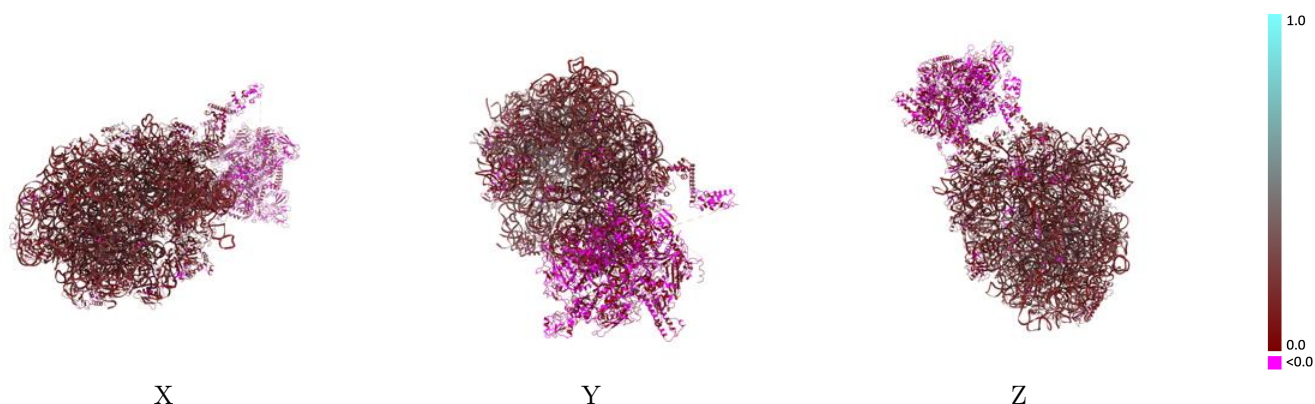
This section contains information regarding the fit between EMDB map EMD-38942 and PDB model 8Y5M. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



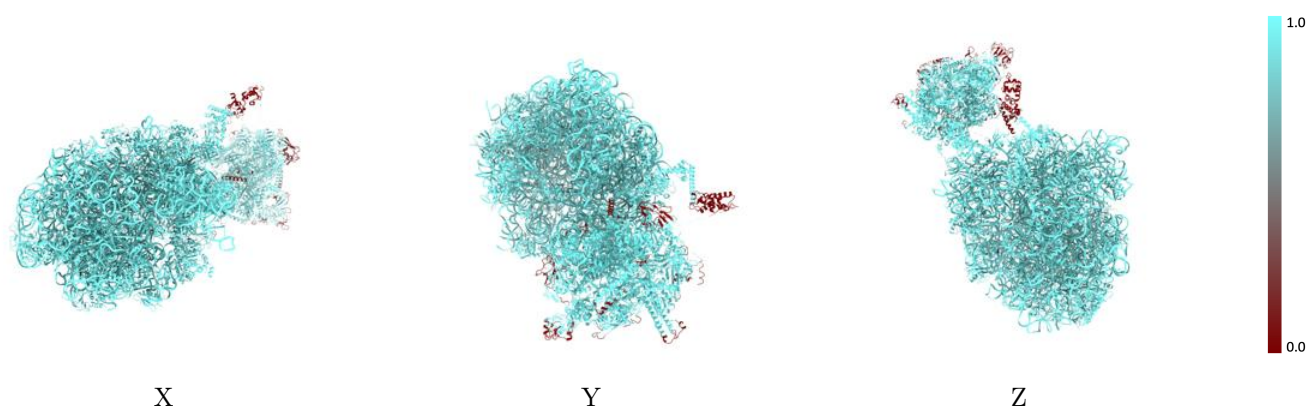
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



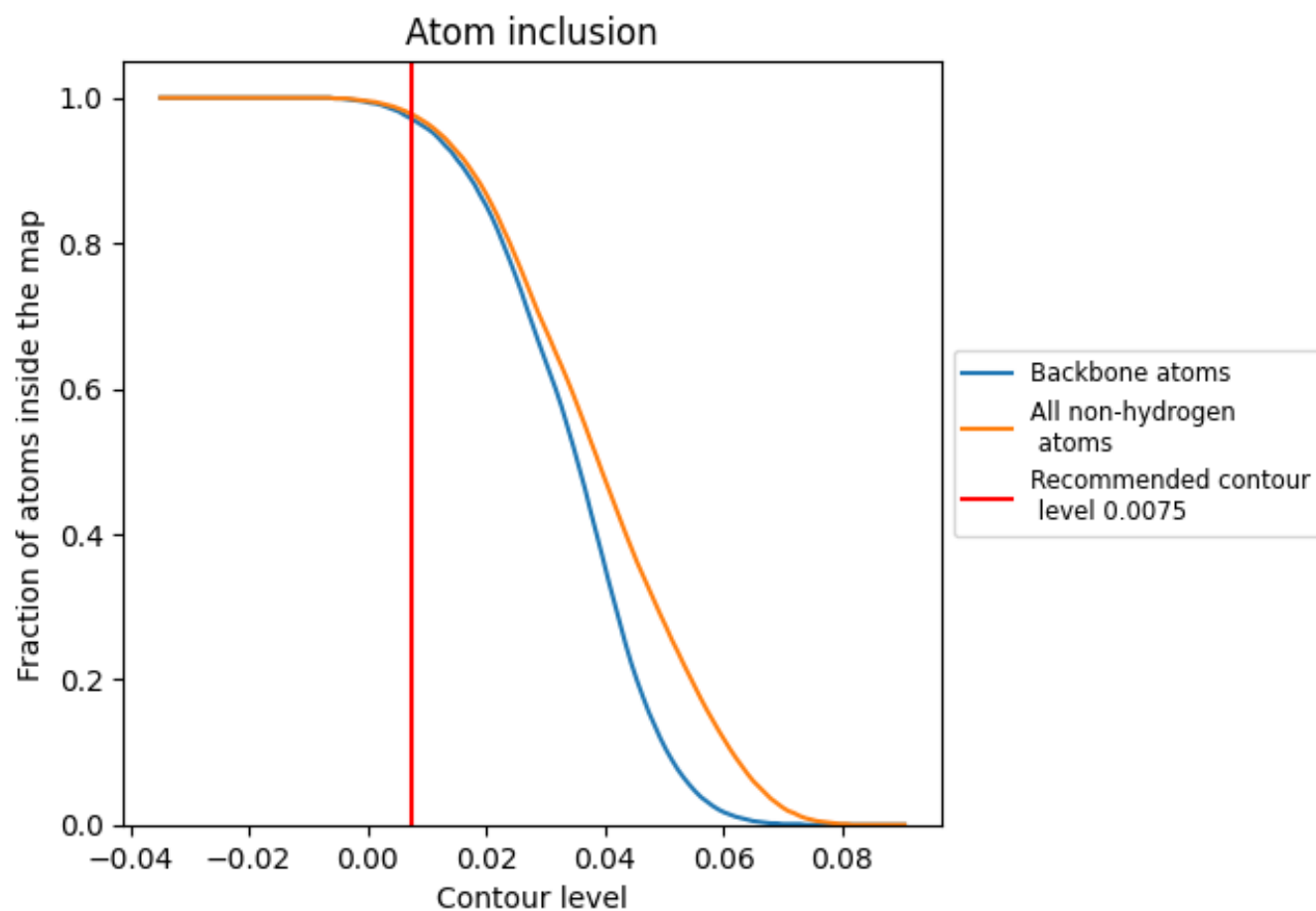
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.1550
0	 0.9680	 0.1420
1	 1.0000	 0.2040
2	 1.0000	 0.1720
3	 1.0000	 0.1910
4	 0.9750	 0.0940
5	 0.9950	 0.1250
6	 0.9950	 0.1820
8	 1.0000	 0.0050
9	 1.0000	 0.0520
A	 0.9260	 0.0890
A1	 0.6540	 0.0140
A2	 0.8070	 0.0190
B	 0.9980	 0.1500
B1	 0.9130	 0.0230
B2	 0.9190	 0.0300
C	 0.9880	 0.1570
D	 0.9750	 0.1320
E	 1.0000	 0.1560
F	 1.0000	 0.0960
G	 0.9920	 0.1230
H	 0.9890	 0.1510
I	 0.9990	 0.1330
J	 0.9930	 0.1430
K	 0.9840	 0.1350
L	 0.9780	 0.1450
M	 0.9740	 0.1270
N	 0.9990	 0.1190
NA	 0.8830	 0.1380
NG	 0.9660	 0.0530
O	 0.9960	 0.1270
P	 0.9960	 0.1510
Q	 0.9570	 0.1600
R	 0.9910	 0.1590
S	 0.9990	 0.1480



Continued on next page...

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Chain	Atom inclusion	Q-score
T	 0.9930	 0.1370
U	 0.9970	 0.1330
V	 0.9910	 0.1450
W	 1.0000	 0.1240
W0	 0.5980	 -0.0110
X	 1.0000	 0.1500
Y	 0.9890	 0.1540
Z	 0.9790	 0.1320
a	 0.9950	 0.0760
b	 0.9920	 0.1670
c	 0.9940	 0.1590
d	 0.9950	 0.1600
e	 0.9800	 0.1280
f	 0.9920	 0.1440
g	 0.9090	 0.1210
h	 1.0000	 0.1620
i	 0.9800	 0.0990
j	 0.9960	 0.1460
k	 0.9810	 0.2100
l	 0.9970	 0.1540
m	 0.9920	 0.1580
n	 0.9980	 0.1480
o	 1.0000	 0.1230
p	 0.9930	 0.1850
q	 0.9990	 0.1340
r	 0.9990	 0.1460
s	 0.9920	 0.1640
t	 0.9900	 0.1180
u	 0.9950	 0.1290
v	 0.9960	 0.1260
w	 1.0000	 0.1280
x	 0.9970	 0.1560
y	 0.9960	 0.1260
z	 0.9950	 0.1560