



## wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 08:53 PM JST

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](mailto: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:

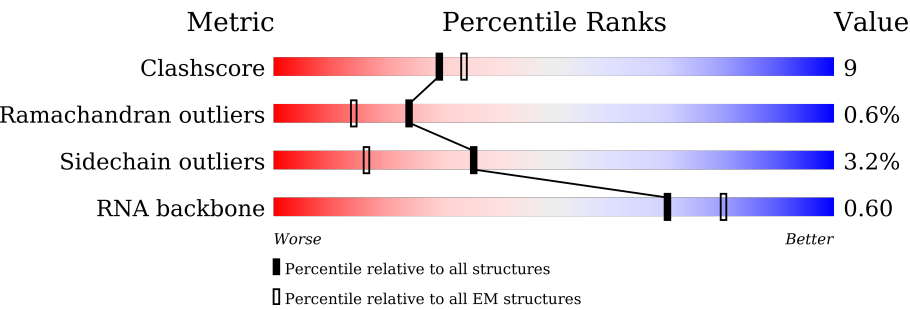
EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	<div><div></div><div>64%29%6%</div></div>
2	B	57	<div><div></div><div>81%18%</div></div>
3	C	55	<div><div></div><div>75%16%9%</div></div>
4	D	46	<div><div></div><div>67%30%</div></div>
5	E	65	<div><div></div><div>80%18%</div></div>
6	F	38	<div><div></div><div>71%29%</div></div>
7	G	241	<div><div></div><div>70%18%10%</div></div>



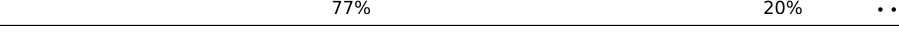
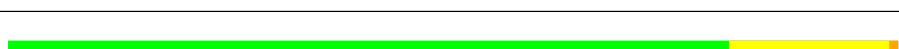



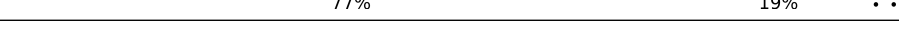



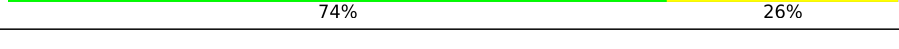

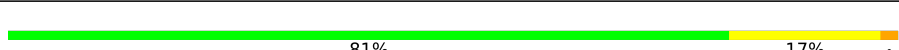


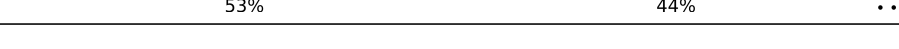
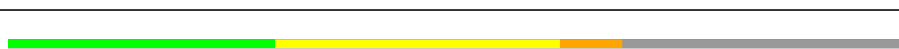
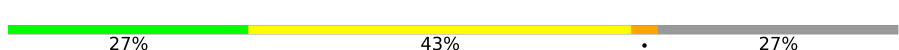





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
29	d	201	
30	e	179	
31	f	177	
32	g	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
54	4	44	
55	8	37	
56	9	37	
57	A1	329	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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

*Continued on next page...*

Continued from previous page...

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

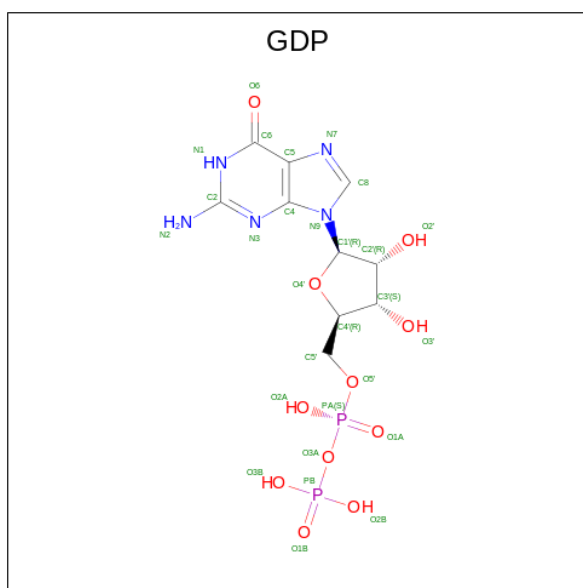
- Molecule 67 is a protein (with D amino acids) called Viomycin.

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

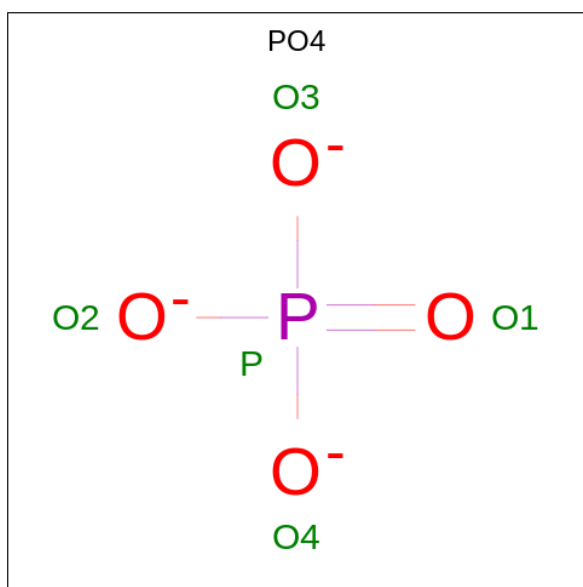
- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





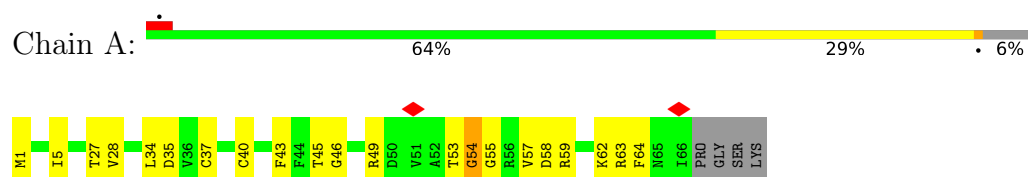


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

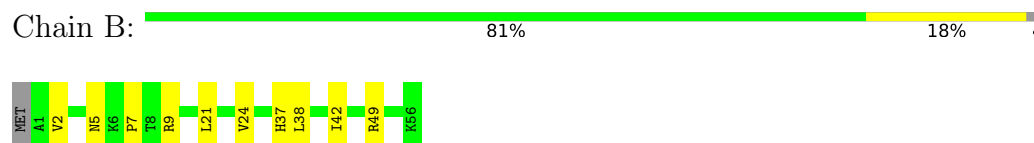
### 3 Residue-property plots [i](#)

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.

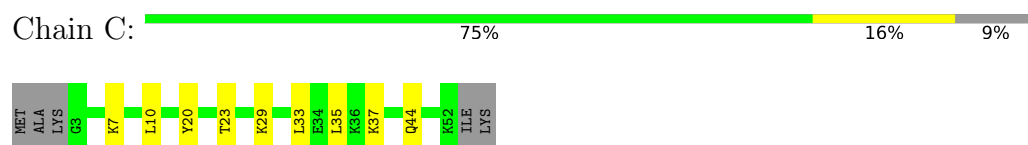
- Molecule 1: 50S ribosomal protein L31



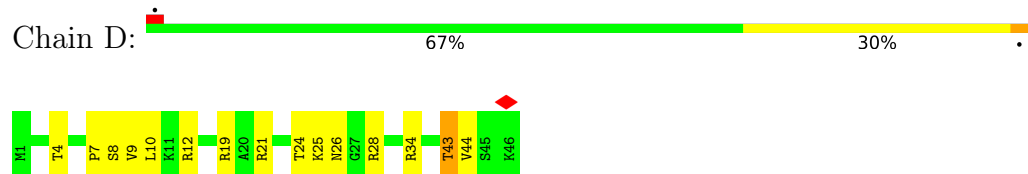
- Molecule 2: 50S ribosomal protein L32



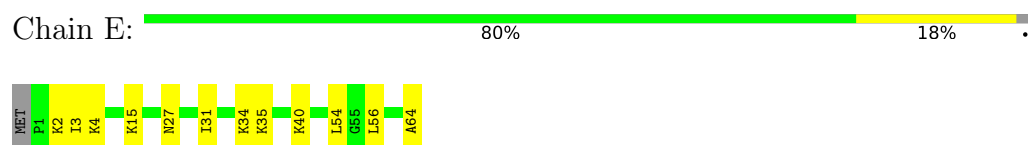
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34



- Molecule 5: 50S ribosomal protein L35



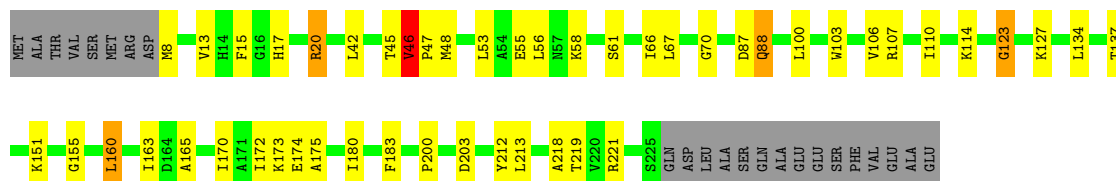
- Molecule 6: 50S ribosomal protein L36

Chain F:  71% 29%



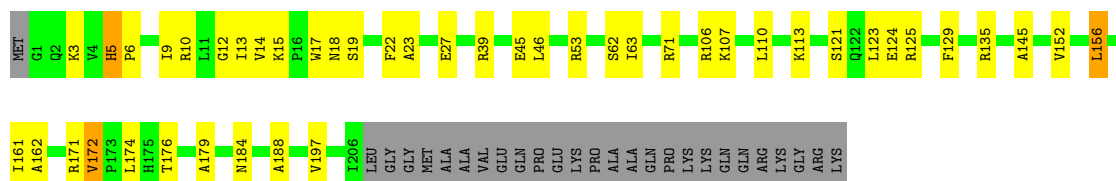
- Molecule 7: 30S ribosomal protein S2

Chain G:  70% 18% 10%



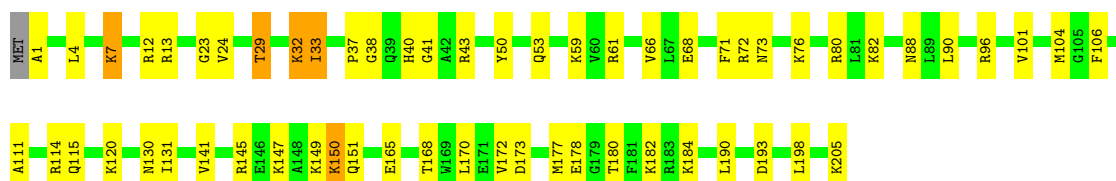
- Molecule 8: 30S ribosomal protein S3

Chain H:  69% 18% 12%



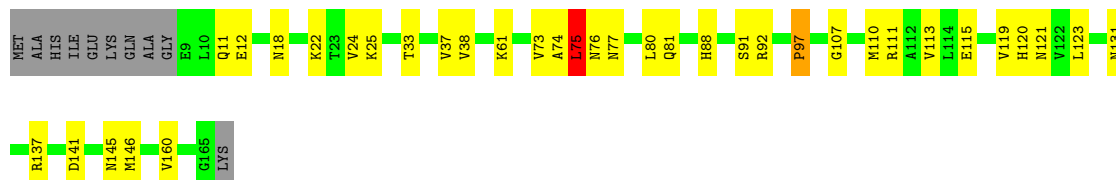
- Molecule 9: 30S ribosomal protein S4

Chain I:  71% 26%



- Molecule 10: 30S ribosomal protein S5

Chain J:  72% 20% 6%



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

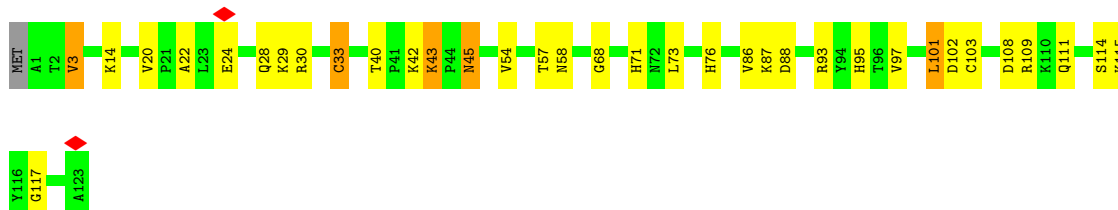
Chain K:  52% 20% 26%





- Molecule 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% .



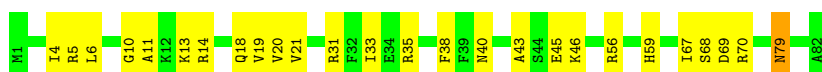
- Molecule 20: 30S ribosomal protein S15

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: 



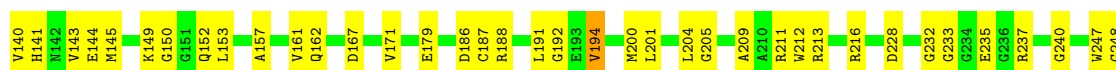
- Molecule 26: 30S ribosomal protein S21

Chain Z: 




- Molecule 27: 50S ribosomal protein L2

Chain b: 



- Molecule 28: 50S ribosomal protein L3

Chain c: 





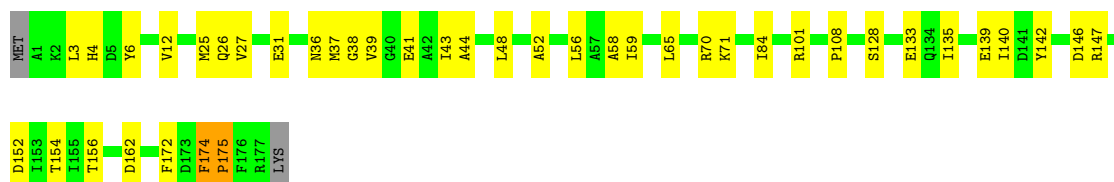
- Molecule 29: 50S ribosomal protein L4

Chain d: 83% 17%



- Molecule 30: 50S ribosomal protein L5

Chain e: 76% 22% ..



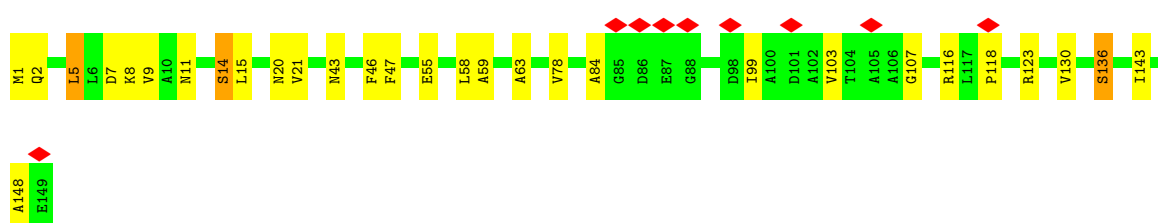
- Molecule 31: 50S ribosomal protein L6

Chain f: 85% 14% ...



- Molecule 32: 50S ribosomal protein L9

Chain g: 6% 80% 18% .



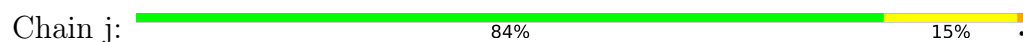
- Molecule 33: 50S ribosomal protein L11

Chain i: 54% 38% 6% ..

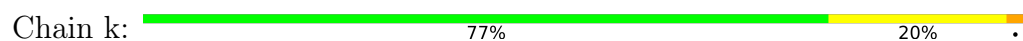




- Molecule 34: 50S ribosomal protein L13



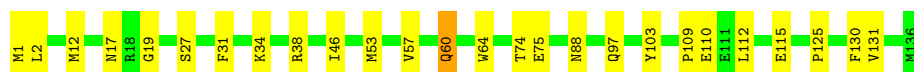
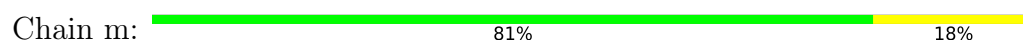
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



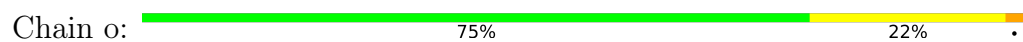
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17




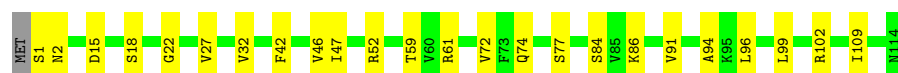
- Molecule 39: 50S ribosomal protein L18




- Molecule 40: 50S ribosomal protein L19



Chain p:  78% 21%



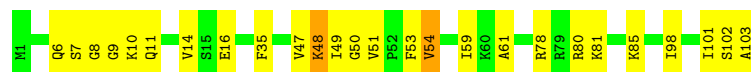
- Molecule 41: 50S ribosomal protein L20

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%



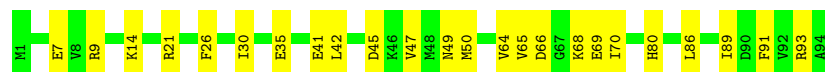
- Molecule 45: 50S ribosomal protein L24

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 A43 G48 G51 A63 C69 G70 A71 A74 G75 G76 G77 G85 A91 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 U182 G186 G187 G188 G189 A195 A196 A197 A198 A199 U200 A207 C208 C209 G214

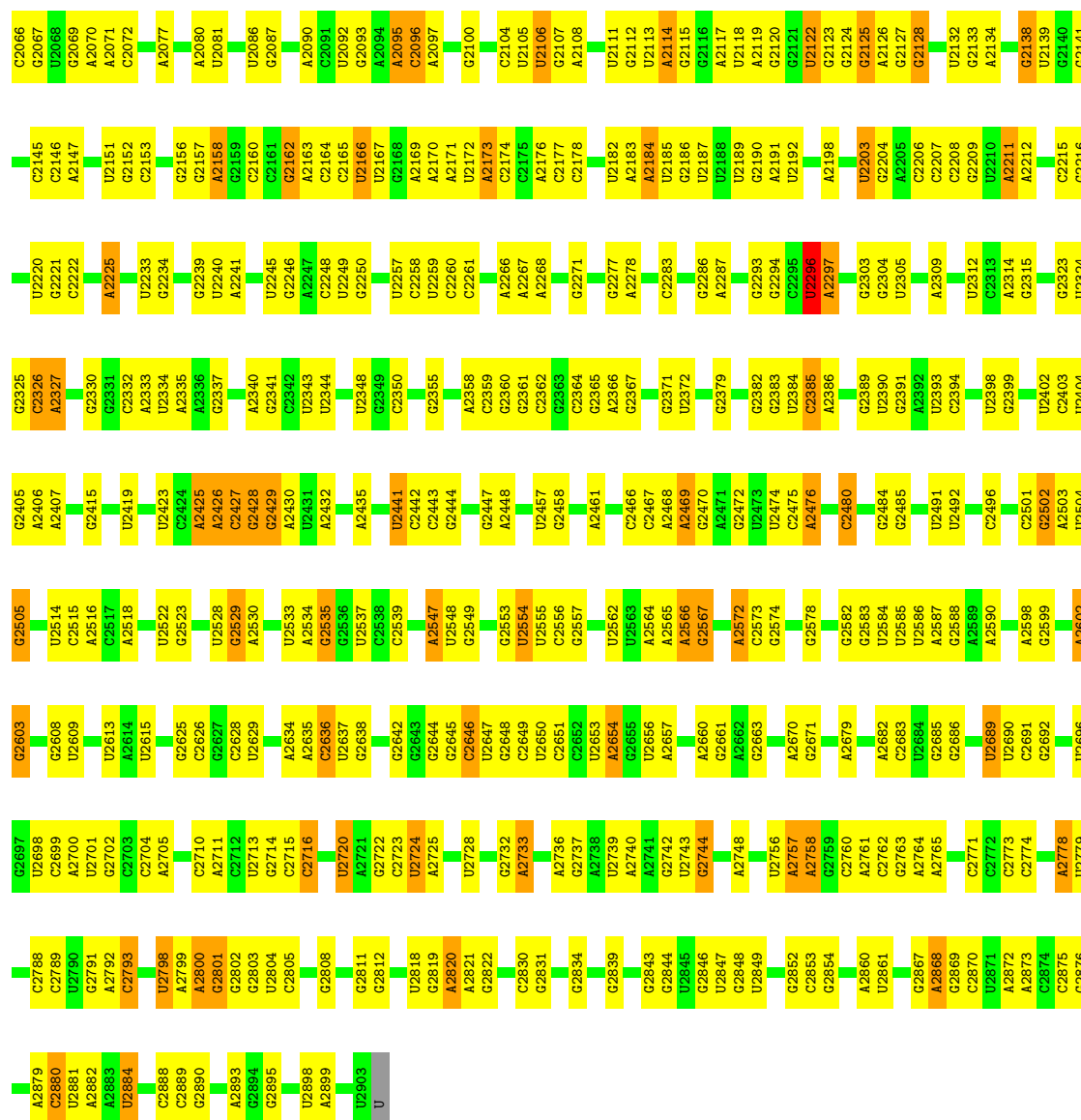
G215 A216 A217 A218 A219 G220 A221 A222 C225 A226 A227 C228 C229 G232 A233 U234 U235 C239 C240 A241 G242 G248 C249 G250 A251 A255 A256 C257 G266 A272 G273 C274 C275 U276 G277 A278 C281 A282 C283 U284 G285 U286 G287 C289 U294 A295 U296 G297 A300

A310 A311 G312 A320 U321 A322 C323 A324 G327 U328 C329 A330 C334 C335 C336 C337 C338 U339 A340 A341 C341 A342 A346 A353 A354 C355 U355 G356 A361 A362 G367 A368 A369 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 U467 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

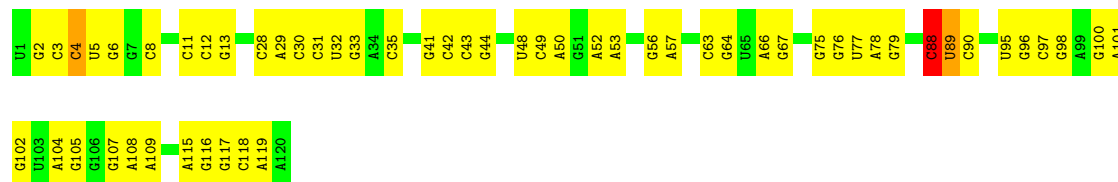
G533 U534 G535 G536 G539 G543 C544 U545 U552 G553 U554 G555 U562 A563 C564 A566 U567 A572 U573 A574 A575 A576 U580 C581 G584 G585 A586 C587 U588 A592 A596 G597 U598 A599 G600 A603 U606 U607 A608 A609 C610 C611 A614 U615





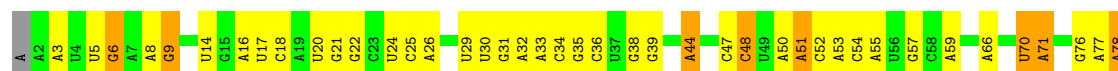
• Molecule 52: 5S rRNA

Chain 2: 53% 44%



• Molecule 53: 16S rRNA

Chain 3: 55% 39% 6%

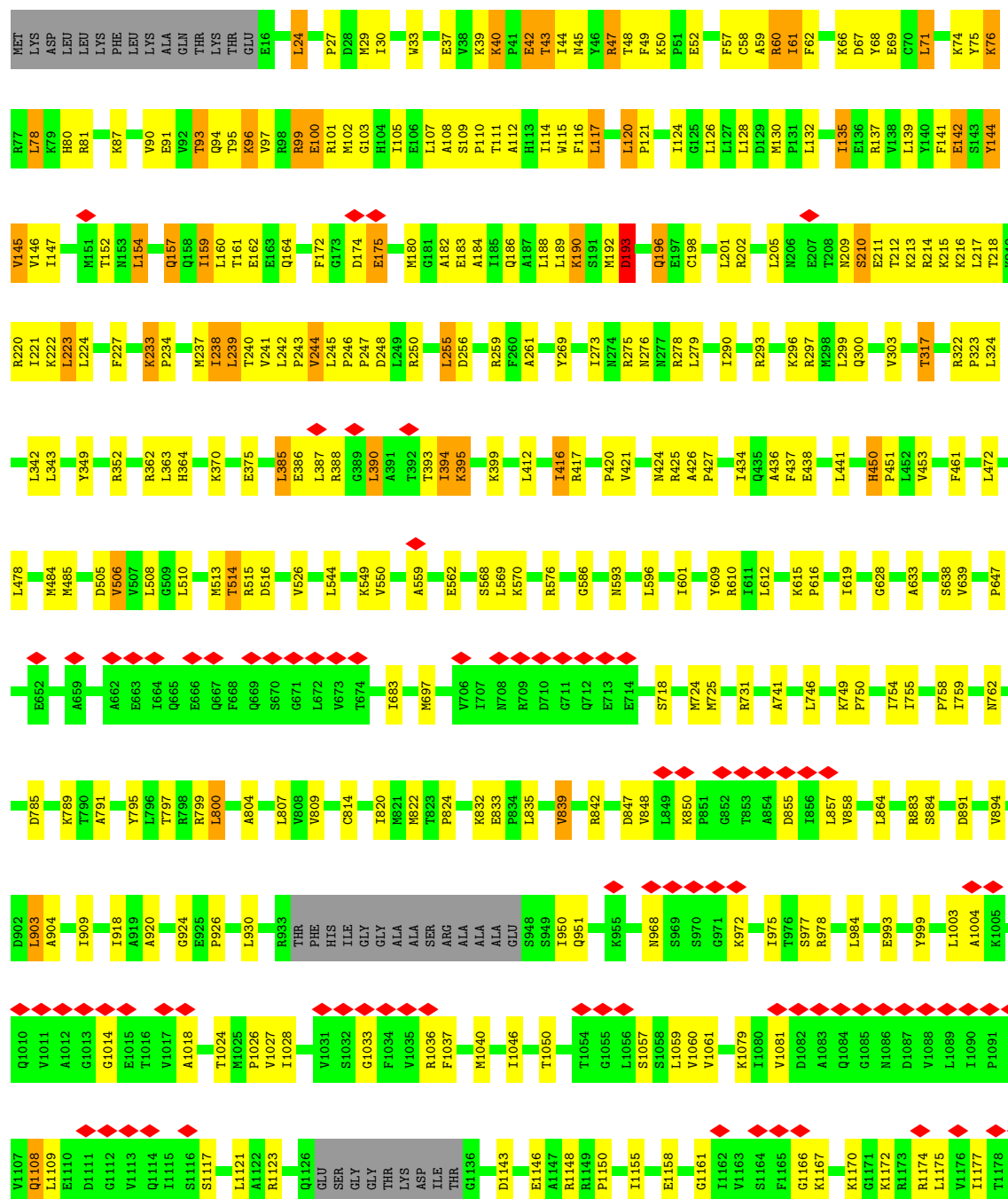


A1413	G1331	A1261		G877	G755	G651	G558	C469	A363	G255	U170	G79
U1414	A1332	CL262	A1176	A878	C756	U652	A559	C470	U367	U256		A80
G1415	A1333	G1268	G1177	C879	C757	U653	A560	U471	U368	G257	U173	A81
	G1334	G1269	G1182	C880	C758	U662	U561	U472	G369		G177	G82
U1419	U1341	A1269	U1078	U884	C764	U663	G566	U473		U261		C83
C1421	C1342	G1270	U1183	G885	A768	G664	G570	U479	C372	A262	A182	U84
G1422	G1343	A1271	U991	G886	G769	A665	U571	U490	G376	C263	C183	U85
G1423	G1343	G1272	U992	G887	G773	U666	A572	U491	U376	G265	G184	G86
	A1346	C1273	A1081	G902	G774	U667	A573	C483	C381	G266		C87
C1427	G1347	A1274	U1086	G903	A777	U668	G574	U484	A382	C267	G187	U88
A1428	U1348	G1276	G1087	G903	G776	U669	G575	U485	U390	U273	C193	U89
	A1349	G1277	G1088	A906	G777	G670	C576	U486	G391	A274	C194	C90
	A1350	G1278	U1095	U911	A778	G671	G577		C392	G275	U195	U92
	U1351	G1279	C779	U916	A780	A675		C490	A196		U93	U93
U1436	C1352	A1280	U917	U918	A781	A676		C491	A393		G94	G94
A1437	G1353	C1281	U918	A918	U793	C680	U589	A495	A397	G281	G198	G97
G1438	U1354	C1282	U919	A919	A794	A681	U590	A496	C401	A288	A199	A98
	C1359	U1283	G1099	A919	C796	G682	G592	A497	G402	G289	G200	C99
		U1284	A1005	C934	U797	U686	A596	A498	G403	U296	G201	G100
		G1207	A1006	C935	A802	C689	C599	A499	G404		G202	A101
		C1208	G1101	A936	G803		A600	A502	U405	A303	G203	
		U1209	C1012	A937	U804		A601	A503	U406	U304		G107
		A1101	A1016	A938	U804		A602	A504	U407		C207	C110
		A1102	A1017	A939	U805		A603	A505	U408	U208	U209	G111
		G1094	G1013	A940	A812		U604	A506	U409	C210	G211	G112
		U1095	G1014	A941	A813		U605	A507	U410	C211	G212	G113
		U1096	G1015	A942	A814		U606	A508	G413	C212	U213	U114
		C1097	G1016	A943	A815		U607	A509	G414	C213		G115
		C1098	G1017	U944	C817		A608	A510	G415	C214		
		C1099	G1018	U945	A818		A609	A511	G416	C215	U216	U121
		G1100	G1019	U946	A819		U610	A512	G417	C216	G217	U123
		C1101	G1100	U947	A820		U611	A513	G418	C217	U218	G128
		A1102	G1101	U948	A821		U612	A514	G419	C218	U219	G129
		G1103	G1102	U949	A822		U613	A515	G420	C219	G220	A130
		U1033	G1032	U950	A823		U614	A516	G421	C220	G221	
		G1034	G1033	U951	A824		C615	A517	G422	C221		
		U1035	G1034	U952	A825		C616	A518	G423	C222		
		G1036	G1035	U953	A826		C617	A519	G424	C223		
		U1037	G1036	U954	A827		C618	A520	G425	C224		
		C1037	G1037	U955	A828		C619	A521	G426	C225		
		U1038	G1038	U956	A829		C620	A522	G427	C226		
		C1038	G1039	U957	A830		C621	A523	G428	C227		
		G1040	G1040	U958	A831		C622	A524	G429	C228		
		U1041	G1041	U959	A832		C623	A525	G430	C229		
		C1041	G1042	U960	A833		C624	A526	G431	C230		
		U1042	G1043	U961	A834		C625	A527	G432	C231		
		G1043	G1044	U962	A835		C626	A528	G433	C232		
		U1044	G1045	U963	A836		C627	A529	G434	C233		
		C1044	G1046	U964	A837		C628	A530	G435	C234		
		G1047	G1047	U965	A838		C629	A531	G436	C235		
		U1048	G1048	U966	A839		C630	A532	G437	C236		
		C1048	G1049	U967	A840		C631	A533	G438	C237		
		U1049	G1050	U968	A841		C632	A534	G439	C238		
		G1050	G1051	U969	A842		C633	A535	G440	C239		
		U1051	G1052	U970	A843		C634	A536	G441	C240		
		C1051	G1053	U971	A844		C635	A537	G442	C241		
		U1052	G1054	U972	A845		C636	A538	G443	C242		
		G1053	G1055	U973	A846		C637	A539	G444	C243		
		U1054	G1056	U974	A847		C638	A540	G445	C244		
		C1054	G1057	U975	A848		C639	A541	G446	C245		
		U1055	G1058	U976	A849		C640	A542	G447	C246		
		G1056	G1059	U977	A850		C641	A543	G448	C247		
		U1057	G1060	U978	A851		C642	A544	G449	C248		
		C1057	G1061	U979	A852		C643	A545	G450	C249		
		U1058	G1062	U980	A853		C644	A546	G451	C250		
		G1059	G1063	U981	A854		C645	A547	G452	C251		
		U1060	G1064	U982	A855		C646	A548	G453	C252		
		C1060	G1065	U983	A856		C647	A549	G454	C253		
		U1061	G1066	U984	A857		C648	A550	G455	C254		
		G1062	G1067	U985	A858		C649	A551	G456	C255		
		C1062	G1068	U986	A859		C650	A552	G457	C256		
		U1063	G1069	U987	A860		C651	A553	G458	C257		
		G1064	G1070	U988	A861		C652	A554	G459	C258		
		U1065	G1071	U989	A862		C653	A555	G460	C259		
		C1065	G1072	U990	A863		C654	A556	G461	C260		
		U1066	G1073	U991	A864		C655	A557	G462	C261		
		G1067	G1074	U992	A865		C656	A558	G463	C262		
		U1068	G1075	U993	A866		C657	A559	G464	C263		
		C1068	G1076	U994	A867		C658	A560	G465	C264		
		G1069	G1077	U995	A868		C659	A561	G466	C265		
		U1070	G1078	U996	A869		C660	A562	G467	C266		
		C1069	G1079	U997	A870		C661	A563	G468	C267		
		U1071	G1080	U998	A871		C662	A564	G469	C268		
		G1072	G1081	U999	A872		C663	A565	G470	C269		
		C1070	G1082	U1000	A873		C664	A566	G471	C270		
		U1072	G1083	U1001	A874		C665	A567	G472	C271		
		G1073	G1084	U1002	A875		C666	A568	G473	C272		
		C1071	G1085	U1003	A876		C667	A569	G474	C273		
		U1073	G1086	U1004	A877		C668	A570	G475	C274		
		G1074	G1087	U1005	A878		C669	A571	G476	C275		
		C1072	G1088	U1006	A879		C670	A572	G477	C276		
		U1074	G1089	U1007	A880		C671	A573	G478	C277		
		G1075	G1090	U1008	A881		C672	A574	G479	C278		
		C1073	G1091	U1009	A882		C673	A575	G480	C279		
		U1075	G1092	U1010	A883		C674	A576	G481	C280		
		G1076	G1093	U1011	A884		C675	A577	G482	C281		
		C1074	G1094	U1012	A885		C676	A578	G483	C282		
		U1076	G1095	U1013	A886		C677	A579	G484	C283		
		G1077	G1096	U1014	A887		C678	A580	G485	C284		
		C1075	G1097	U1015	A888		C679	A581	G486	C285		
		U1077	G1098	U1016	A889		C680	A582	G487	C286		
		G1078	G1099	U1017	A890		C681	A583	G488	C287		
		C1076	G1100	U1018	A891		C682	A584	G489	C288		
		U1078	G1101	U1019	A892		C683	A585	G490	C289		
		G1079	G1102	U1020	A893		C684	A586	G491	C290		
		C1077	G1103	U1021	A894		C685	A587	G492	C291		
		U1079	G1104	U1022	A895		C686	A588	G493	C292		
		G1080	G1105	U1023	A896		C687	A589	G494	C293		
		C1078	G1106	U1024	A897		C688	A590	G495	C294		
		U1080	G1107	U1025	A898		C689	A591	G496	C295		
		G1081	G1108	U1026	A899		C690	A592	G497	C296		
		C1079	G1109	U1027	A900		C691	A593	G498	C297		
		U1081	G1110	U1028	A901		C692	A594	G499	C298		
		G1082	G1111	U1029	A902		C693	A595	G500	C299		
		C1080	G1112	U1030	A903		C694	A596	G501	C300		
		U1082	G1113	U1031	A904		C695	A597	G502	C301		
		G1083	G1114	U1032	A905		C696	A598	G503	C302		
		C1081	G1115	U1033	A906		C697	A599	G504	C303		
		U1083	G1116	U1034	A907		C698	A600	G505	C304		
		G1084	G1117	U1035	A908		C699	A601	G506	C305		
		C1082	G1118	U1036	A909		C700	A602	G507	C306		
		U1084	G1119	U1037	A910		C701	A603	G508	C307		
		G1085	G1120	U1038	A911		C702	A604	G509	C308		
		C1083	G1121	U1039	A912		C703	A605	G510	C309		
		U1085	G1122	U1040	A913		C704	A606	G511	C310		
		G1086	G1123	U1041	A914		C705	A607	G512	C311		
		C1084	G1124	U1042	A915		C706	A608	G513	C312		
		U1086	G1125	U1043	A916		C707	A609	G514	C313		
		G1087	G1126	U1044	A917							

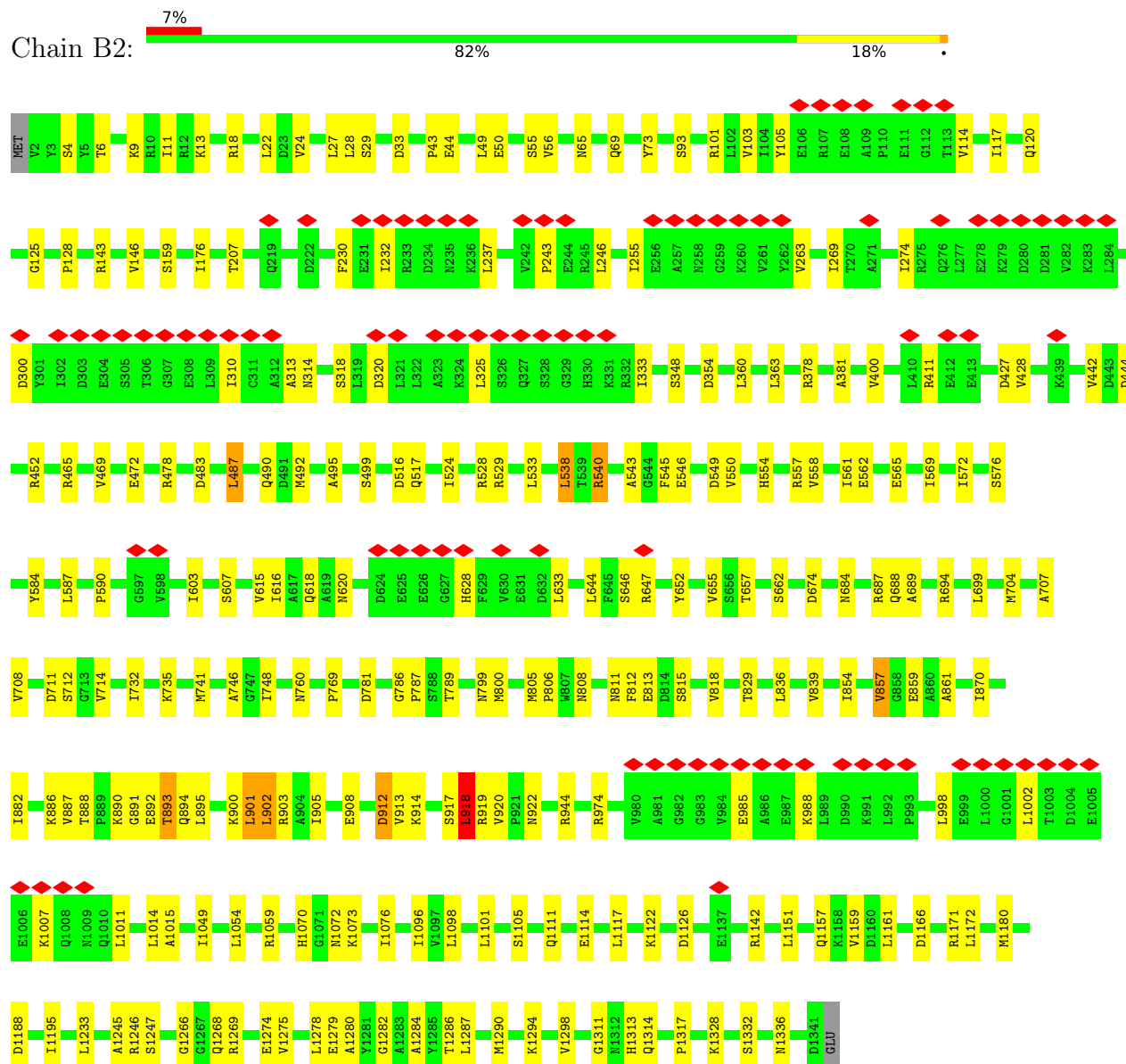




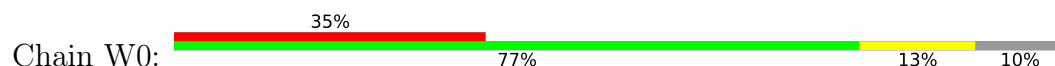
• Molecule 58: DNA-directed RNA polymerase subunit beta'



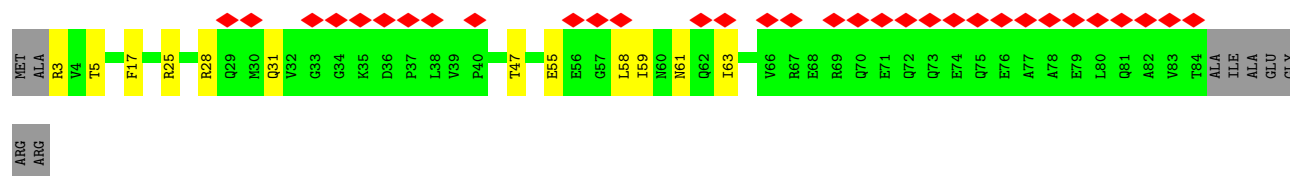
- Molecule 59: DNA-directed RNA polymerase subunit beta



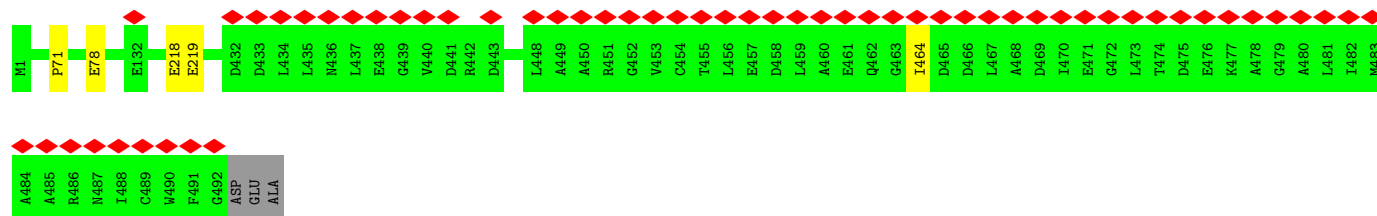
- Molecule 60: DNA-directed RNA polymerase subunit omega



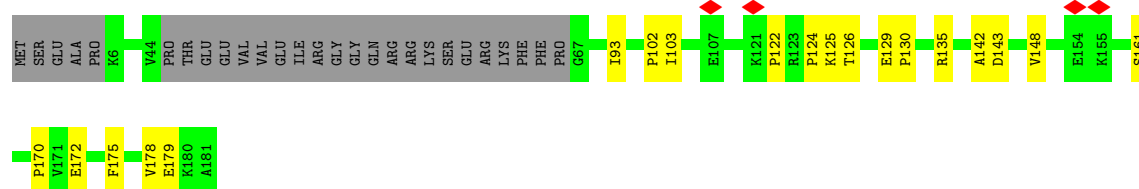
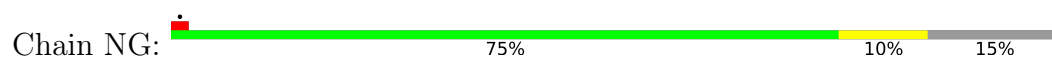




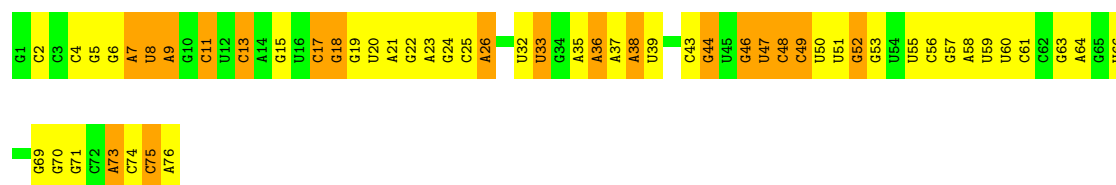
- Molecule 61: Transcription termination/antitermination protein NusA



- Molecule 62: Transcription termination/antitermination protein NusG



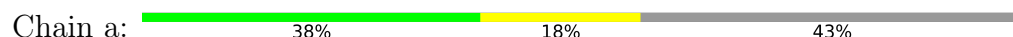
- Molecule 63: tRNA(Phe)

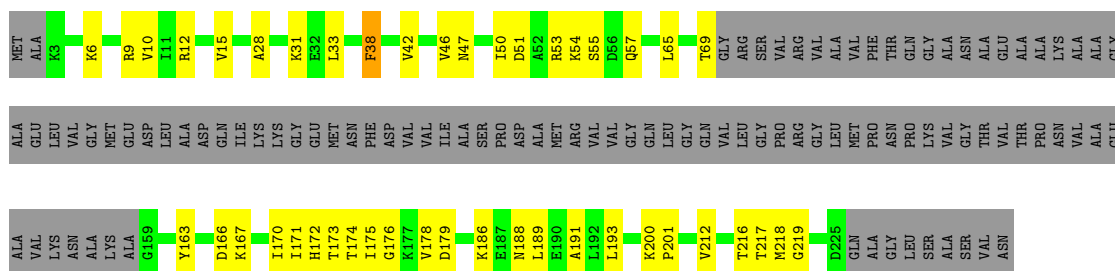


- Molecule 64: tRNA(fMet)



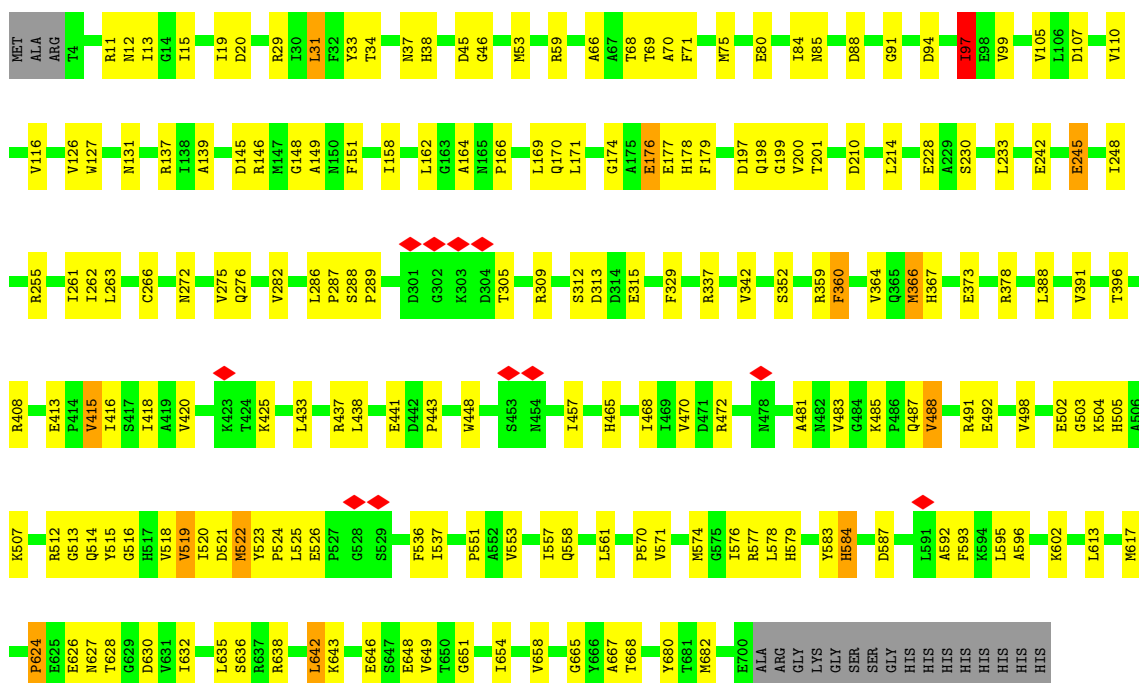
- Molecule 65: Large ribosomal subunit protein uL1





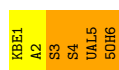
• Molecule 66: Elongation factor G

Chain 0: 71% 25%



• Molecule 67: Viomycin

Chain h: 33% 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: KBE, PO4, UAL, GDP, MG, 5OH, DPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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%)	8	37
6	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	186 (86%)	29 (13%)	1 (0%)	25	64
8	H	204/233 (88%)	184 (90%)	19 (9%)	1 (0%)	25	64
9	I	203/206 (98%)	178 (88%)	24 (12%)	1 (0%)	25	64
10	J	155/167 (93%)	131 (84%)	22 (14%)	2 (1%)	10	42
11	K	98/135 (73%)	83 (85%)	14 (14%)	1 (1%)	13	49
12	L	149/179 (83%)	129 (87%)	18 (12%)	2 (1%)	10	42
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%)	13	49
16	P	114/129 (88%)	90 (79%)	22 (19%)	2 (2%)	7	34
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	51
19	S	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	22
20	T	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	11	44
21	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	42
22	V	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	10	42
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	33
28	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	25	64
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	155 (89%)	18 (10%)	2 (1%)	12	46
31	f	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	7	36
32	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	19	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	i	139/142 (98%)	116 (84%)	22 (16%)	1 (1%)	19	56
34	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	19	56
35	k	120/123 (98%)	99 (82%)	19 (16%)	2 (2%)	7	36
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	51
40	p	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	14	51
42	r	101/103 (98%)	86 (85%)	14 (14%)	1 (1%)	13	49
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%)	13	49
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%)	8	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	68
59	B2	1338/1342 (100%)	1206 (90%)	128 (10%)	4 (0%)	37	72
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	26
65	a	130/234 (56%)	112 (86%)	18 (14%)	0	100	100
66	0	695/716 (97%)	621 (89%)	71 (10%)	3 (0%)	30	68
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10508/11185 (94%)	9407 (90%)	1034 (10%)	67 (1%)	24	60

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%)	20	42
2	B	47/48 (98%)	44 (94%)	3 (6%)	14	36
3	C	45/49 (92%)	45 (100%)	0	100	100
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	61
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%)	44	63
9	I	172/173 (99%)	169 (98%)	3 (2%)	56	72
10	J	118/126 (94%)	115 (98%)	3 (2%)	42	62
11	K	87/116 (75%)	83 (95%)	4 (5%)	23	45
12	L	124/147 (84%)	122 (98%)	2 (2%)	58	74
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%)	12	33
16	P	89/99 (90%)	88 (99%)	1 (1%)	70	80
17	Q	103/104 (99%)	98 (95%)	5 (5%)	21	43
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	82 (99%)	1 (1%)	67	79
20	T	76/77 (99%)	75 (99%)	1 (1%)	65	77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	73 (99%)	1 (1%)	62	75
23	W	56/65 (86%)	54 (96%)	2 (4%)	30	52
24	X	70/79 (89%)	69 (99%)	1 (1%)	62	75
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	52 (94%)	3 (6%)	18	40
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	162 (99%)	2 (1%)	67	79
29	d	165/165 (100%)	163 (99%)	2 (1%)	67	79
30	e	148/150 (99%)	147 (99%)	1 (1%)	81	87
31	f	137/138 (99%)	137 (100%)	0	100	100
32	g	114/114 (100%)	112 (98%)	2 (2%)	54	71
33	i	109/110 (99%)	95 (87%)	14 (13%)	3	15
34	j	116/116 (100%)	115 (99%)	1 (1%)	75	83
35	k	103/104 (99%)	100 (97%)	3 (3%)	37	58
36	l	102/103 (99%)	100 (98%)	2 (2%)	50	68
37	m	109/109 (100%)	109 (100%)	0	100	100
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	81
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	97 (98%)	2 (2%)	50	68
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
42	r	84/84 (100%)	81 (96%)	3 (4%)	30	52
43	s	93/93 (100%)	93 (100%)	0	100	100
44	t	80/84 (95%)	79 (99%)	1 (1%)	65	77
45	u	82/85 (96%)	81 (99%)	1 (1%)	67	79
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	56 (98%)	1 (2%)	54	71
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%)	25	47
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	A2	186/286 (65%)	185 (100%)	1 (0%)	86	89
58	B1	1110/1168 (95%)	1021 (92%)	89 (8%)	10	29
59	B2	1150/1157 (99%)	1119 (97%)	31 (3%)	40	60
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	a	110/181 (61%)	110 (100%)	0	100	100
66	0	574/588 (98%)	546 (95%)	28 (5%)	21	43
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8135/8683 (94%)	7874 (97%)	261 (3%)	36	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	7,8,9	2.29	3 (42%)	5,9,11	2.92	2 (40%)
67	5OH	h	6	67	8,12,13	0.79	0	3,16,18	1.51	1 (33%)
67	KBE	h	1	67	8,8,9	0.61	0	7,8,10	1.20	1 (14%)
67	DPP	h	2	67	3,5,6	0.56	0	1,5,7	0.08	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	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	5OH	h	6	67	-	0/2/18/20	0/1/1/1
67	KBE	h	1	67	-	0/7/7/8	-
67	DPP	h	2	67	-	0/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	5	UAL	C1-N1	-4.83	1.32	1.40
67	h	5	UAL	C-CA	-2.88	1.40	1.45
67	h	5	UAL	CA-N	2.02	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	h	5	UAL	CA-CB-N1	-5.30	115.60	125.60
67	h	5	UAL	O-C-CA	-3.26	121.25	125.39
67	h	6	5OH	CR-CB-CA	-2.36	110.06	112.61
67	h	1	KBE	CB-CA-C	-2.05	109.24	112.25

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	6	5OH	4	0
67	h	2	DPP	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	1.11	0	6,6,6	0.69	0
69	GDP	0	801	-	24,30,30	0.93	1 (4%)	30,47,47	1.45	5 (16%)

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	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	0	801	GDP	C6-N1	-2.44	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	0	801	GDP	PA-O3A-PB	-4.36	117.85	132.83
69	0	801	GDP	C3'-C2'-C1'	2.57	104.85	100.98
69	0	801	GDP	C5-C6-N1	2.34	118.09	113.95
69	0	801	GDP	C8-N7-C5	2.22	107.23	102.99
69	0	801	GDP	O6-C6-C5	-2.07	120.33	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

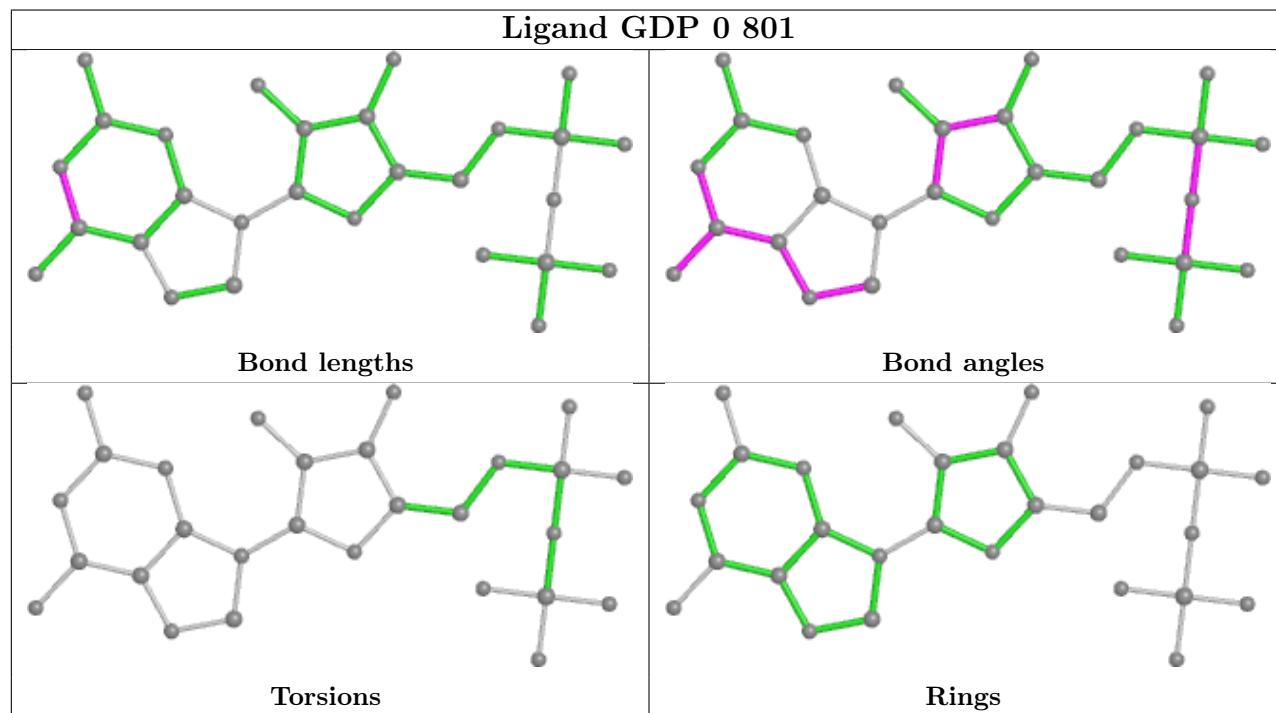
2 monomers are involved in 3 short contacts:

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.

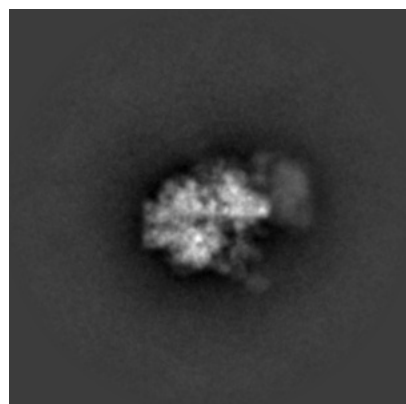
## 6 Map visualisation [i](#)

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.

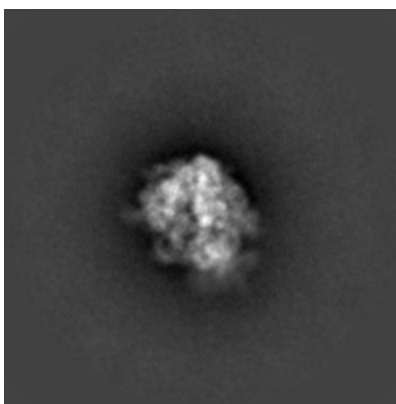
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

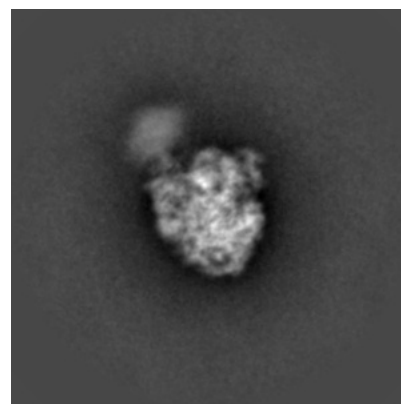
#### 6.1.1 Primary map



X

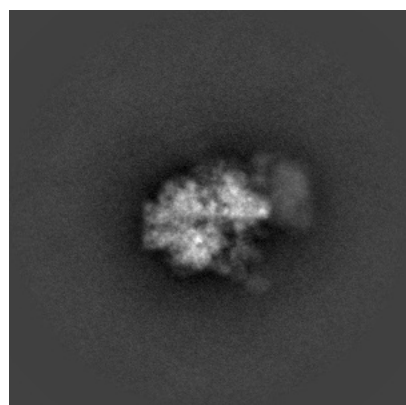


Y

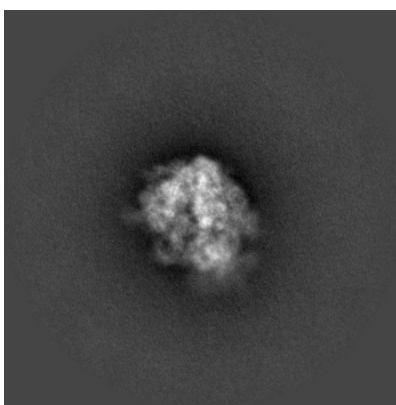


Z

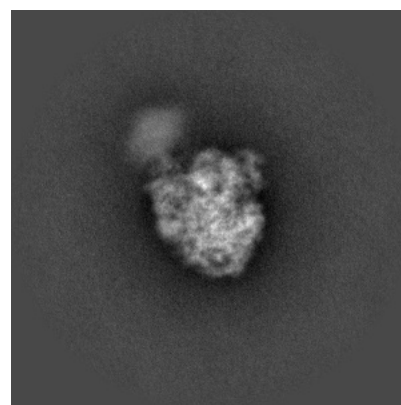
#### 6.1.2 Raw map



X



Y

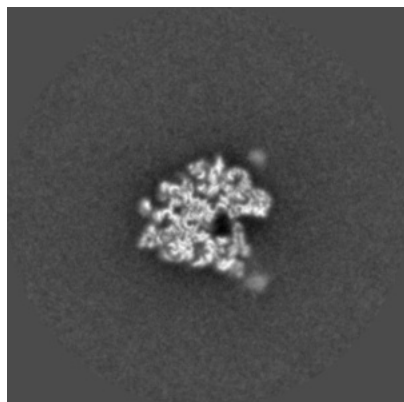


Z

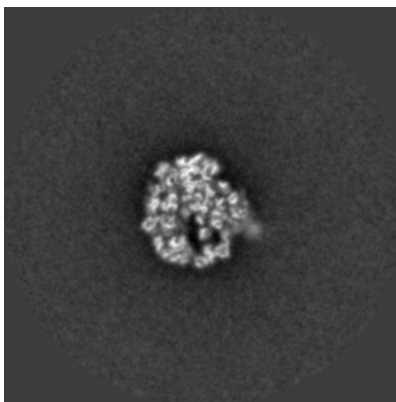
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

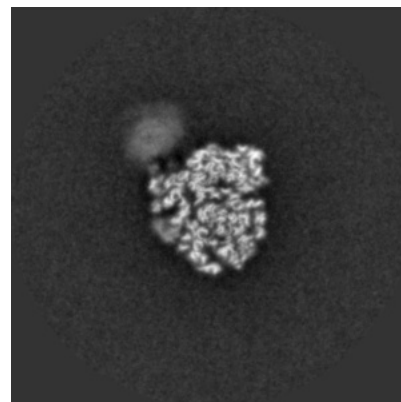
### 6.2.1 Primary map



X Index: 240

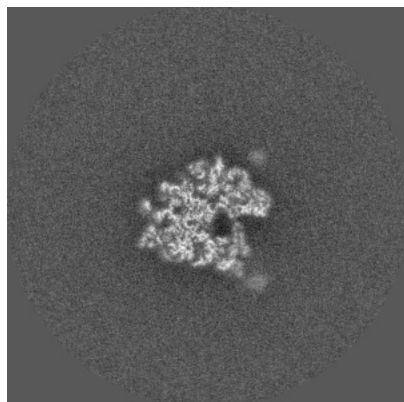


Y Index: 240

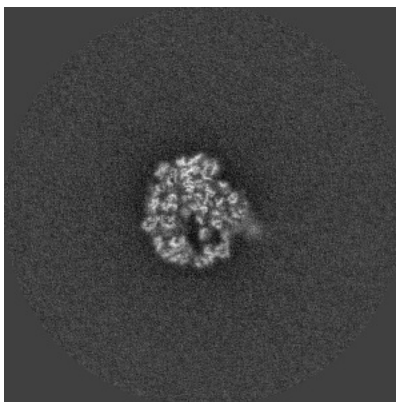


Z Index: 240

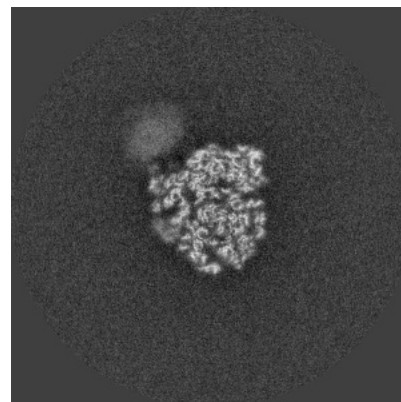
### 6.2.2 Raw map



X Index: 240



Y Index: 240

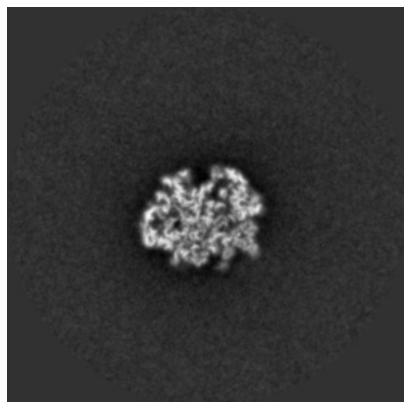


Z Index: 240

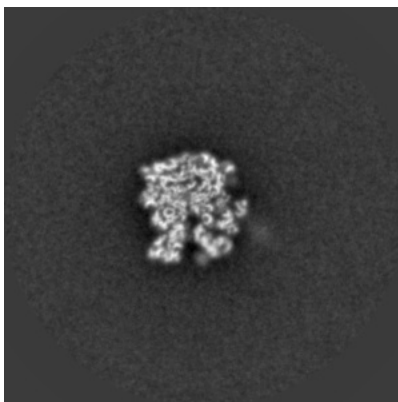
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

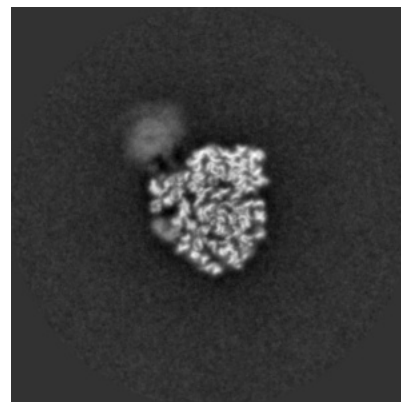
### 6.3.1 Primary map



X Index: 264

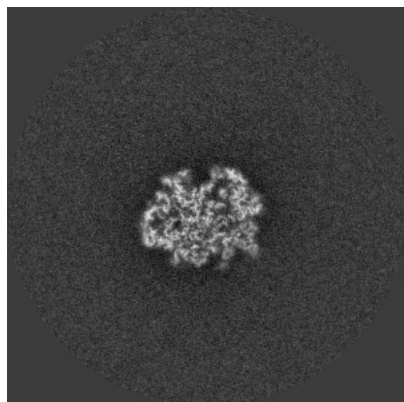


Y Index: 223

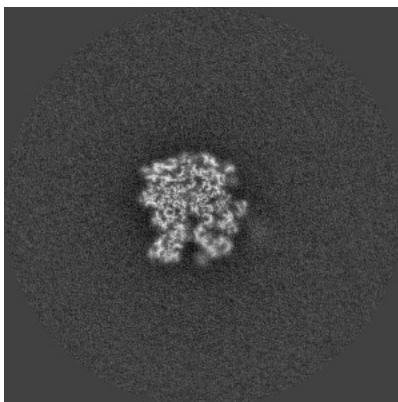


Z Index: 238

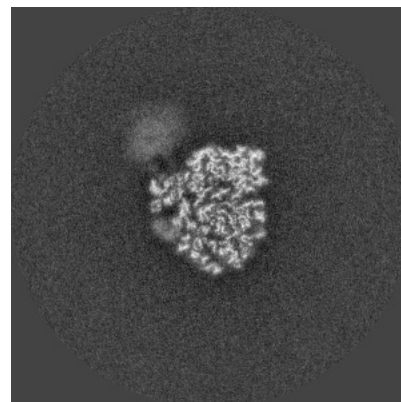
### 6.3.2 Raw map



X Index: 264



Y Index: 222

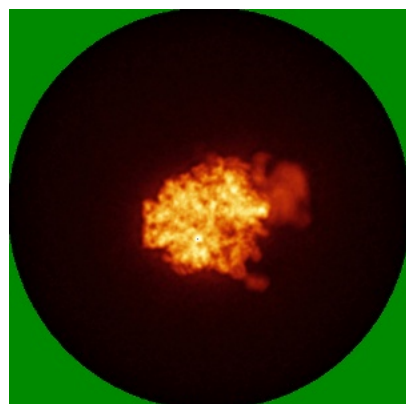


Z Index: 238

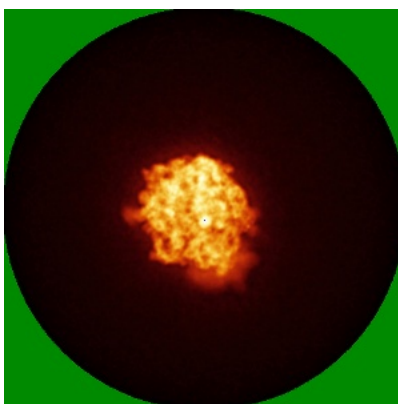
The images above show the largest variance slices of the map in three orthogonal directions.

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

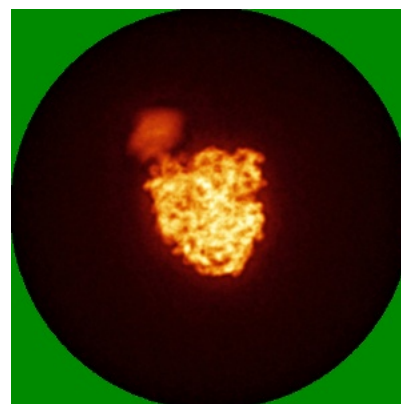
### 6.4.1 Primary map



X

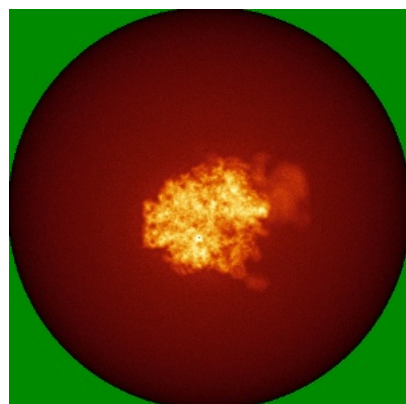


Y

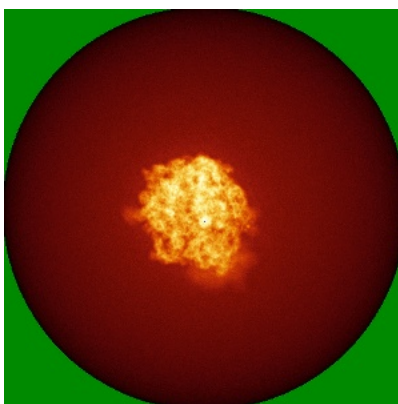


Z

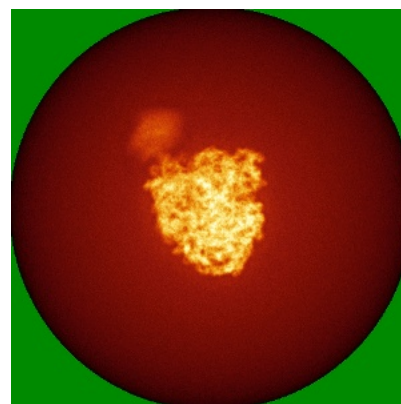
### 6.4.2 Raw map



X



Y



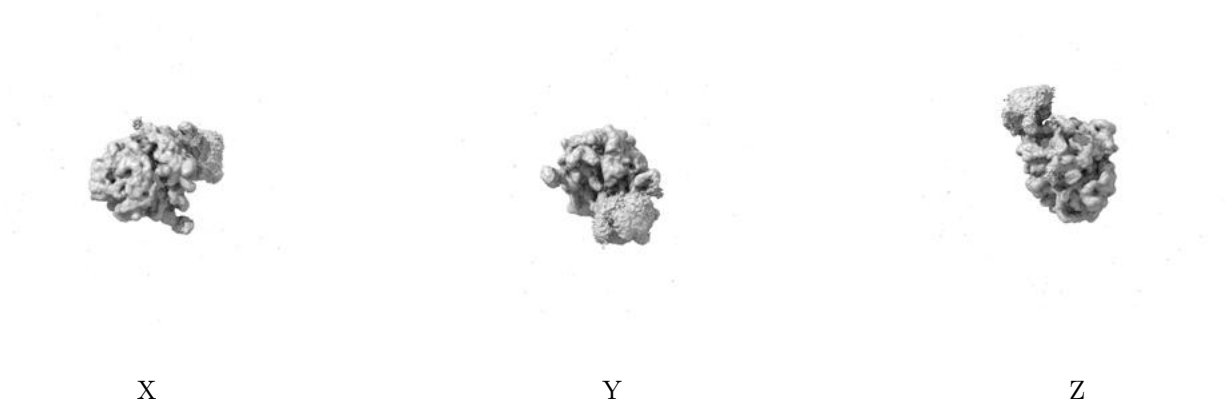
Z

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.



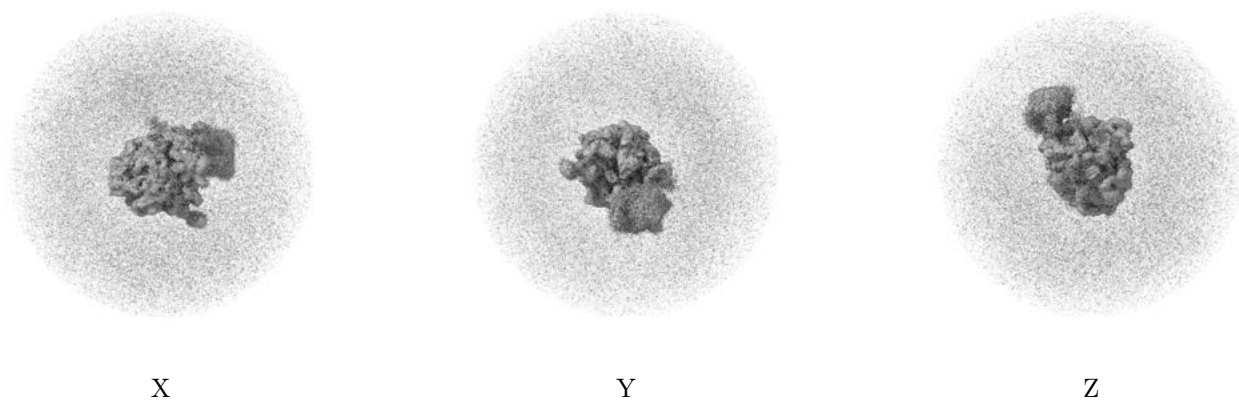
## 6.5 Orthogonal surface views [i](#)

### 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.

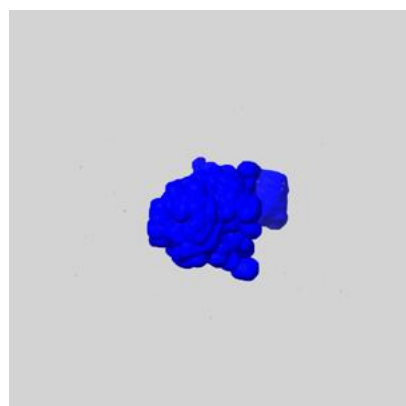
## 6.6 Mask visualisation [i](#)

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

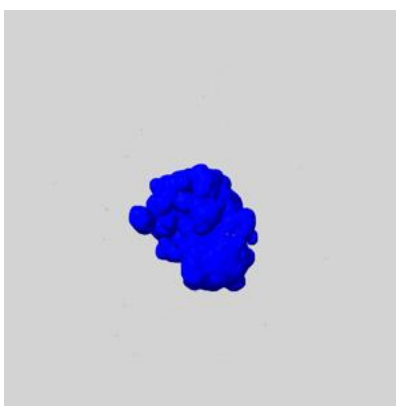
A mask typically either:

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

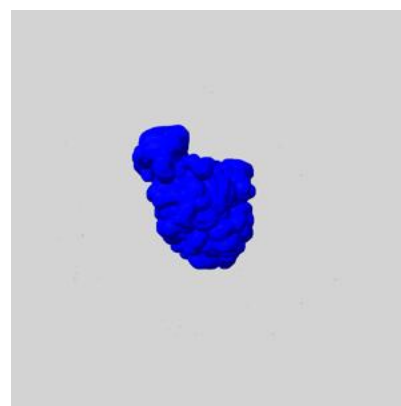
### 6.6.1 emd\_38942\_msk\_1.map [i](#)



X



Y

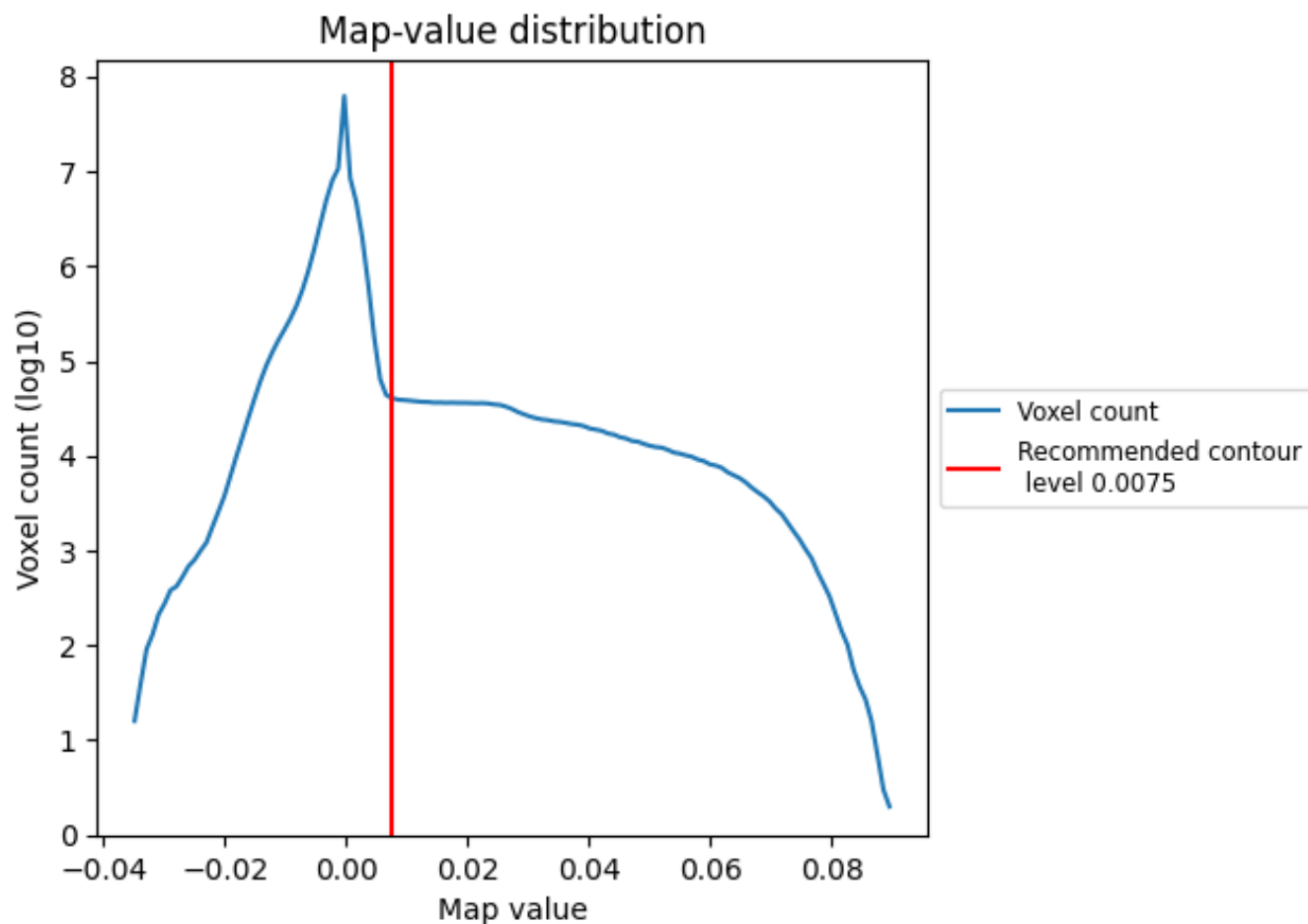


Z

## 7 Map analysis [i](#)

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

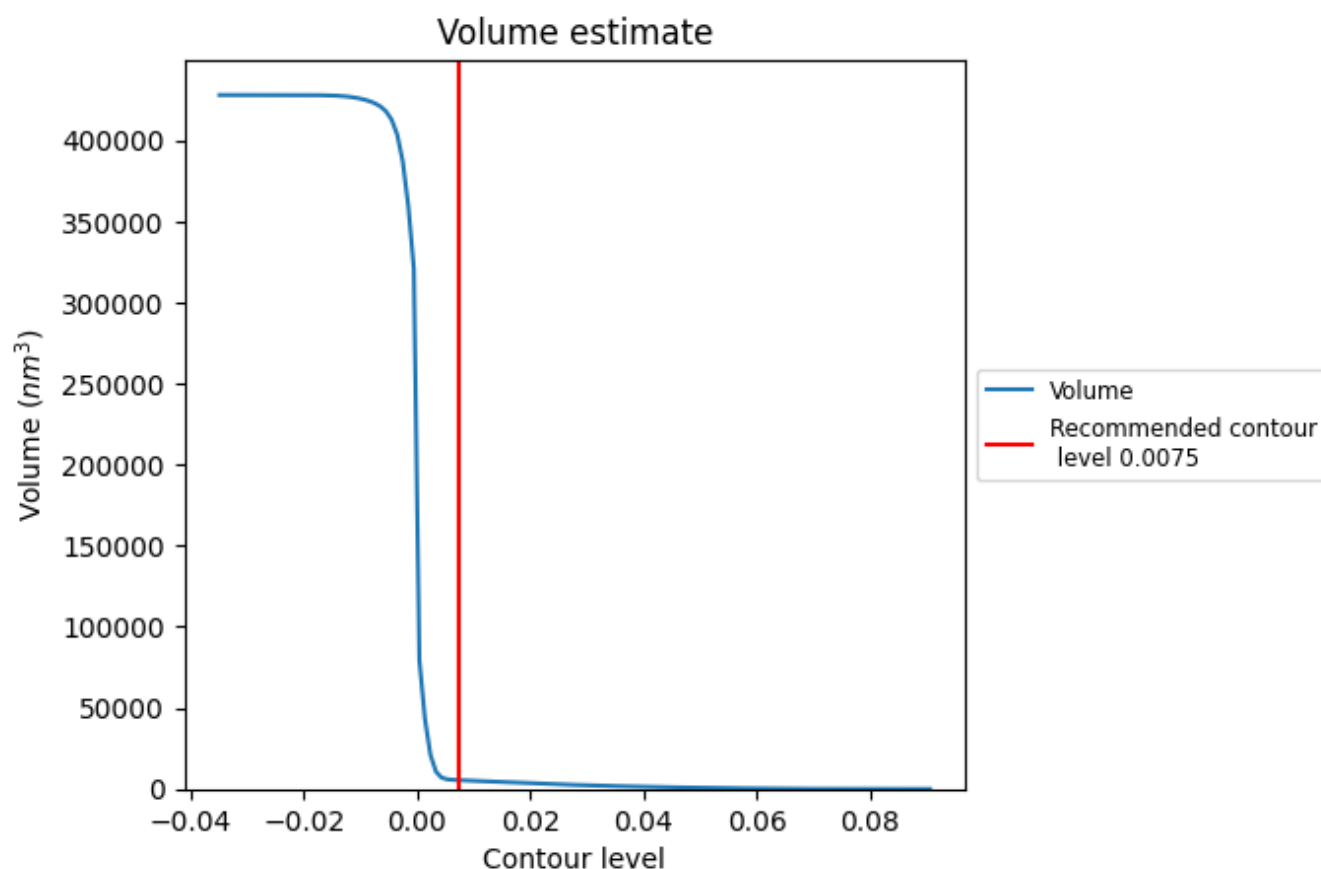
### 7.1 Map-value distribution [i](#)



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.



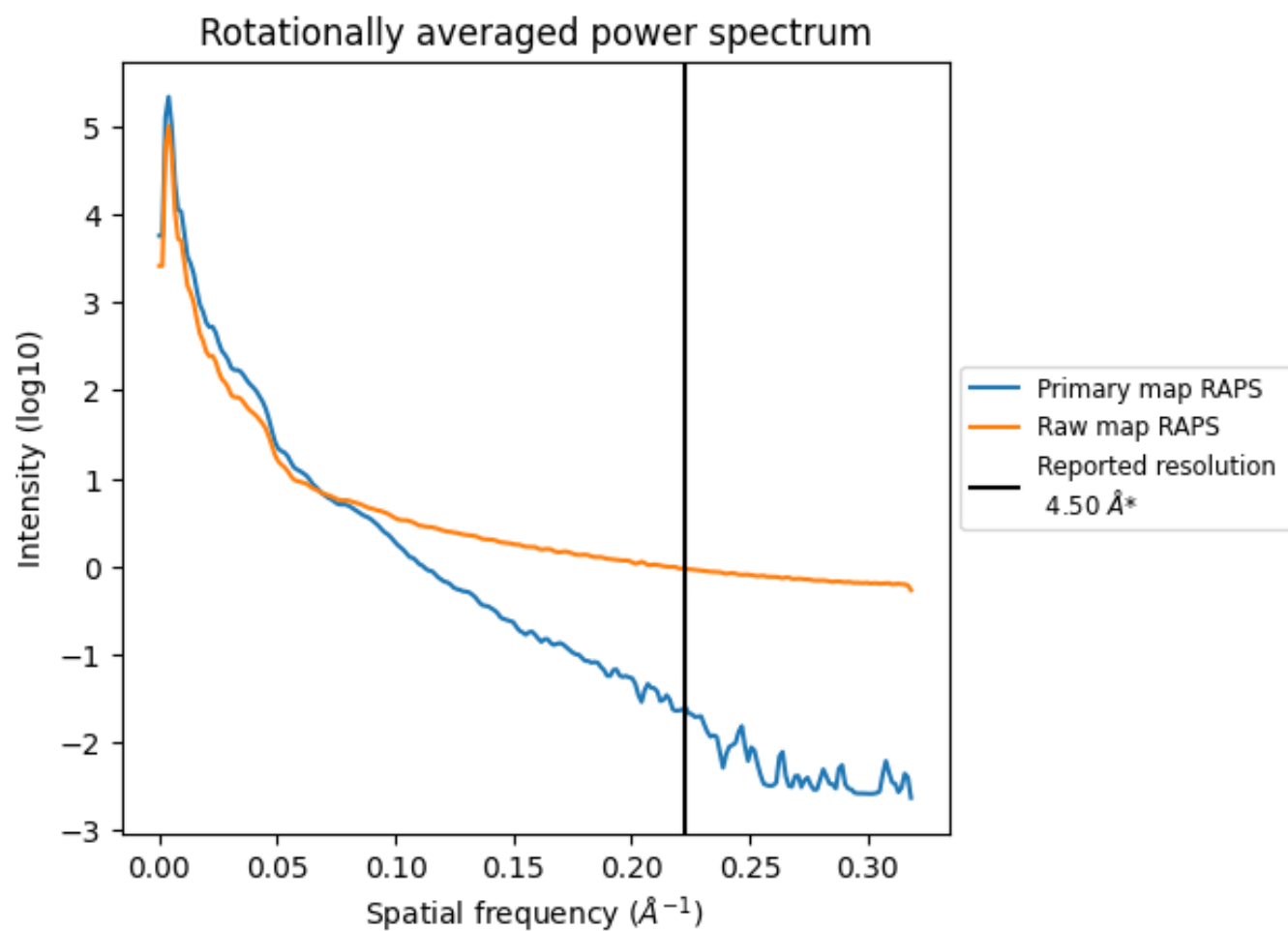
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5419  $\text{nm}^3$ ; 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 ⓘ

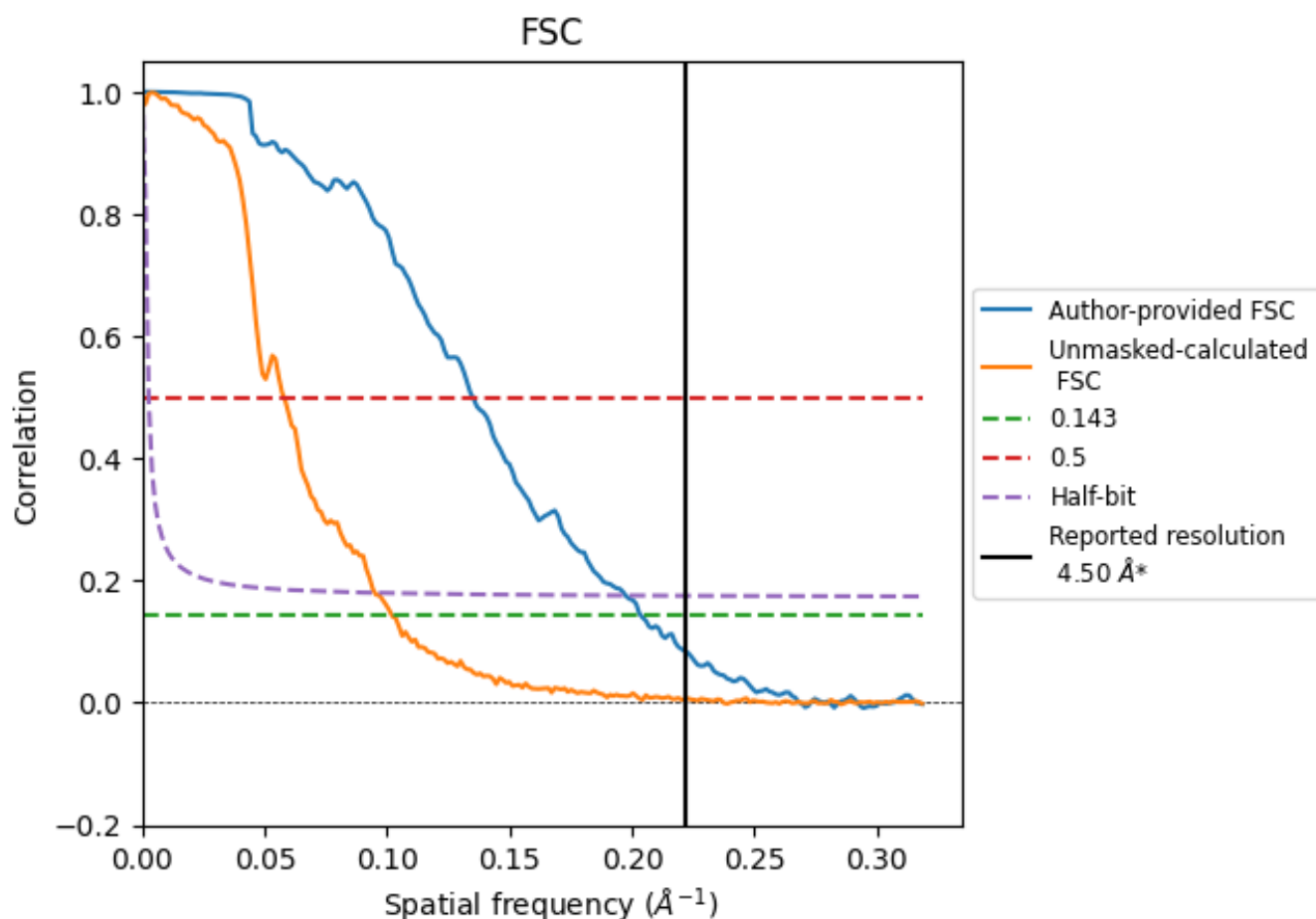


\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

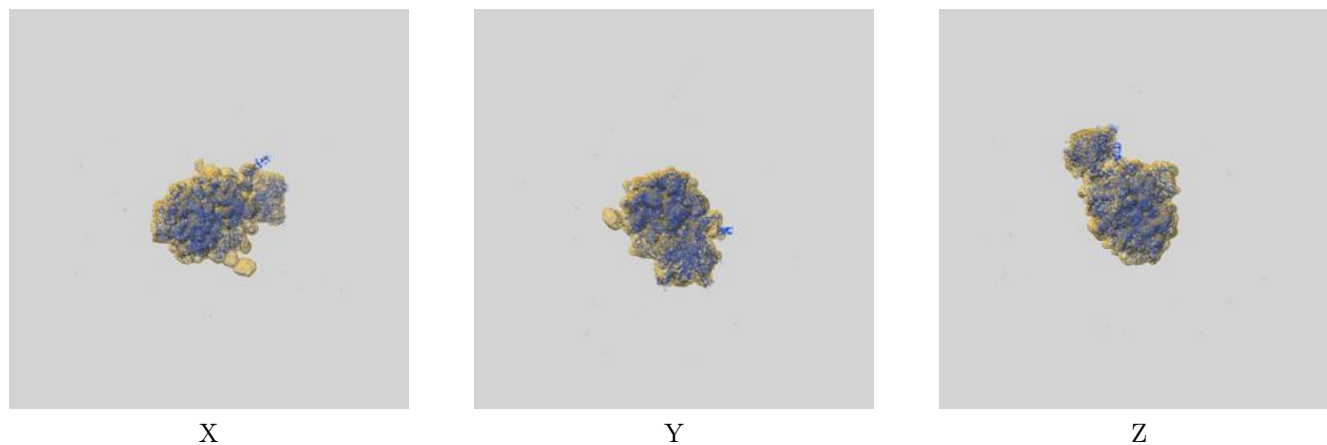
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.91	7.41	5.07
Unmasked-calculated*	9.81	17.30	10.52

\*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](#)

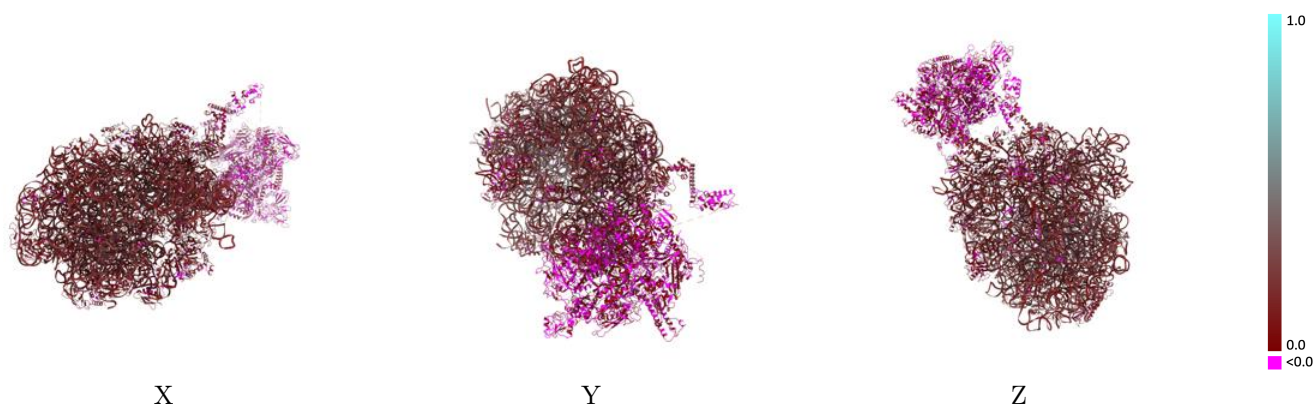
This section contains information regarding the fit between EMDB map EMD-38942 and PDB model 8Y5M. Per-residue inclusion information can be found in section [3](#) on page [18](#).

### 9.1 Map-model overlay [i](#)



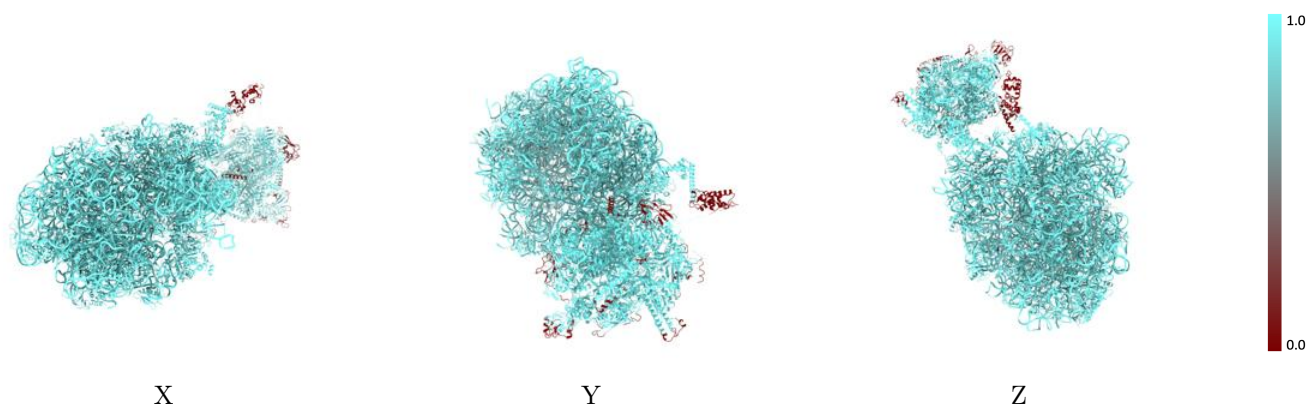
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



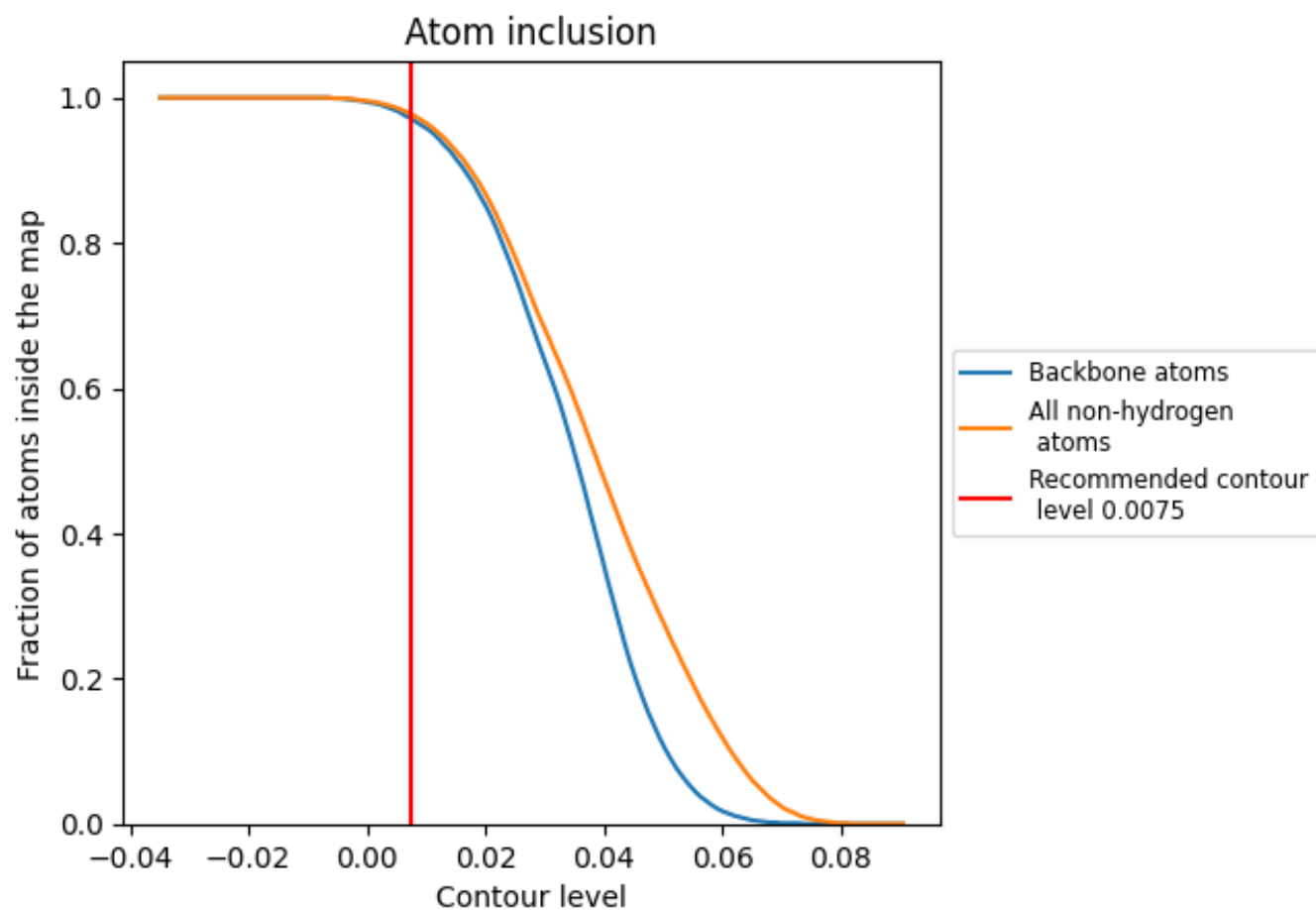
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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...*



*Continued from previous page...*

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