



## wwPDB EM Validation Summary Report ⓘ

Aug 18, 2025 – 02:50 PM JST

PDB ID : 8YDE / pdb\_00008yde  
EMDB ID : EMD-39168  
Title : E.coli transcription translation coupling complex in TTC-B state 1 (subclass 3) containing mRNA with 39-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin  
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.  
Deposited on : 2024-02-20  
Resolution : 5.00 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>.

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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  
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

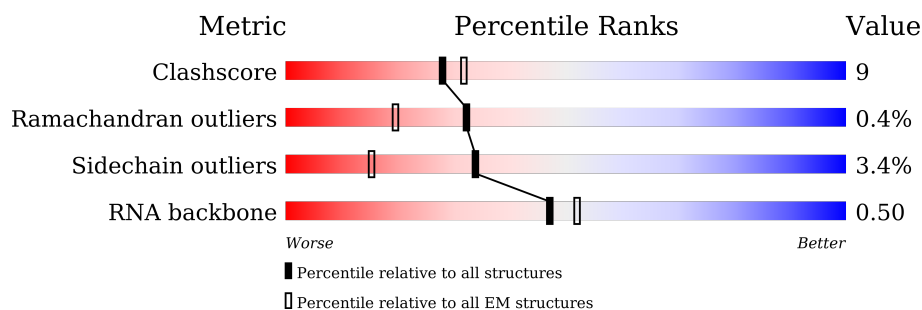
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 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>6%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
2	B	57	<div> <div>79%</div> <div>19%</div> <div>.</div> </div>
3	C	55	<div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
4	D	46	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
5	E	65	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
6	F	38	<div> <div>66%</div> <div>32%</div> <div>.</div> </div>
7	G	241	<div> <div>66%</div> <div>23%</div> <div>.</div> <div>10%</div> </div>

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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	

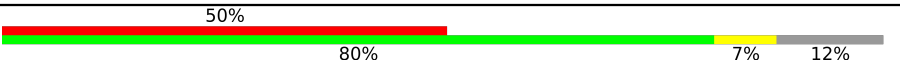

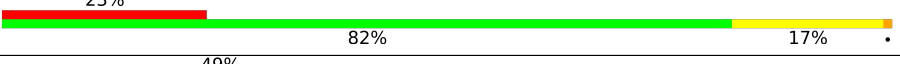
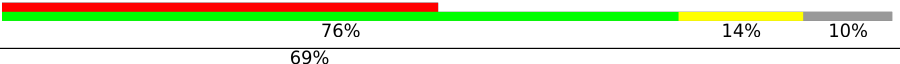
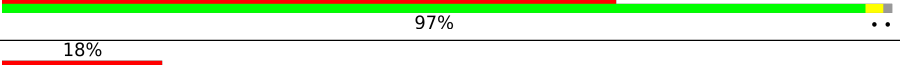
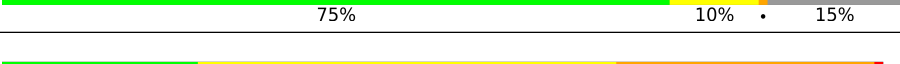
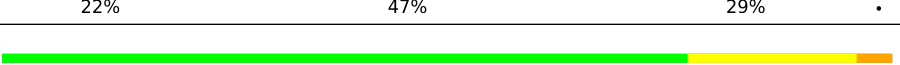
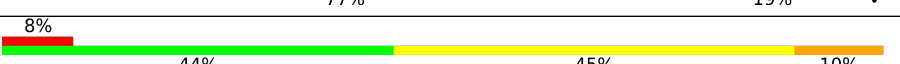


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Mol	Chain	Length	Quality of chain
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	
54	4	56	
55	8	37	
56	9	37	
57	A1	329	

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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	
64	7	77	
65	h	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
65	5OH	h	6	-	-	X	-

## 2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 178130 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
			1624	1028	305	288	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	52	Total	C	N	O	S	0	0
			400	256	73	70	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	35	Total	C	N	O	P	0	0
			729	326	105	263	35		

- 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		
64	7	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 65 is a protein (with D amino acids) called Viomycin.

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

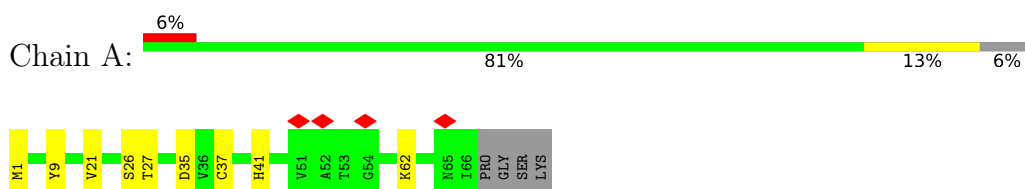
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

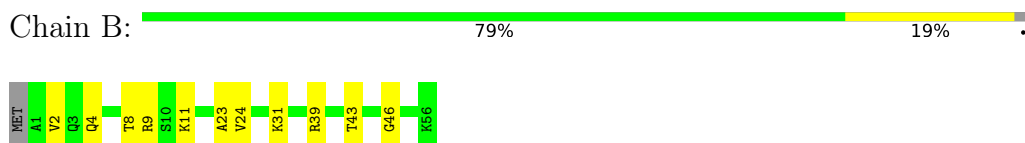
### 3 Residue-property plots [i](#)

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.

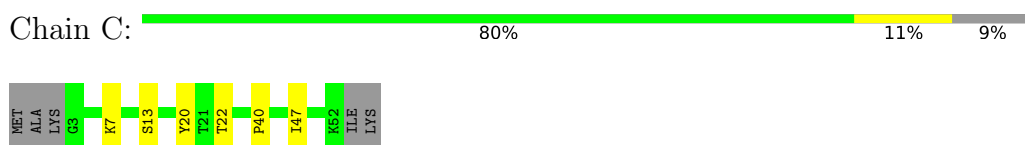
- Molecule 1: 50S ribosomal protein L31



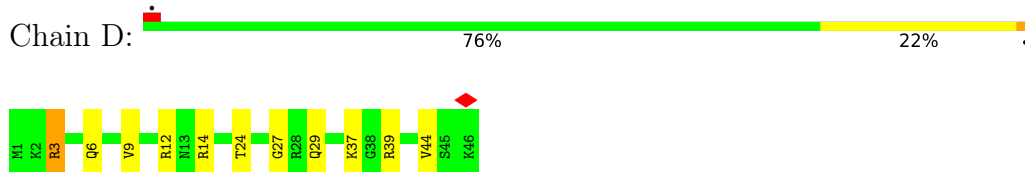
- Molecule 2: 50S ribosomal protein L32



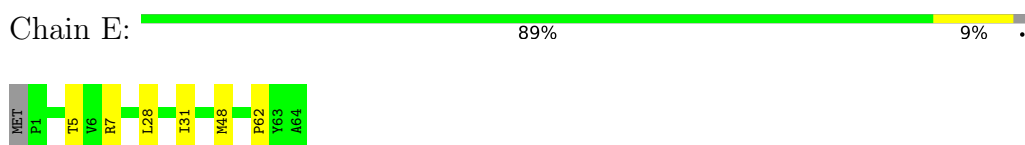
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34



- Molecule 5: 50S ribosomal protein L35



- Molecule 6: 50S ribosomal protein L36

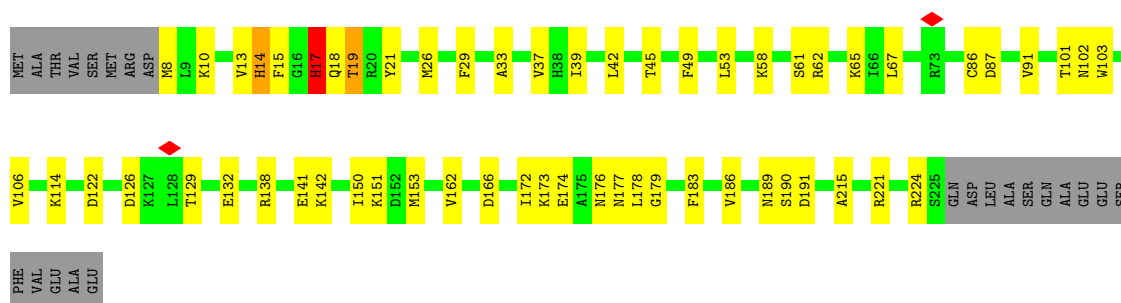


Chain F:  66% 32% .



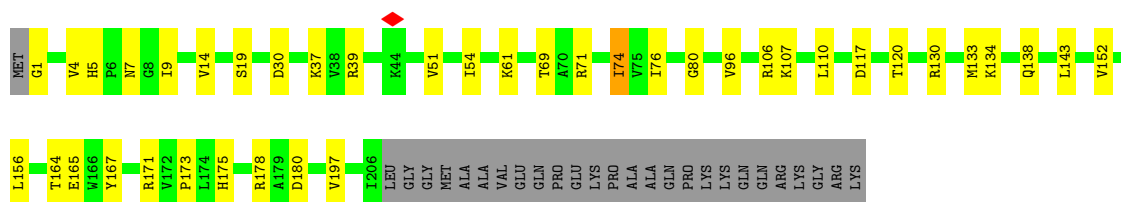
- Molecule 7: 30S ribosomal protein S2

Chain G:  66% 23% . 10%




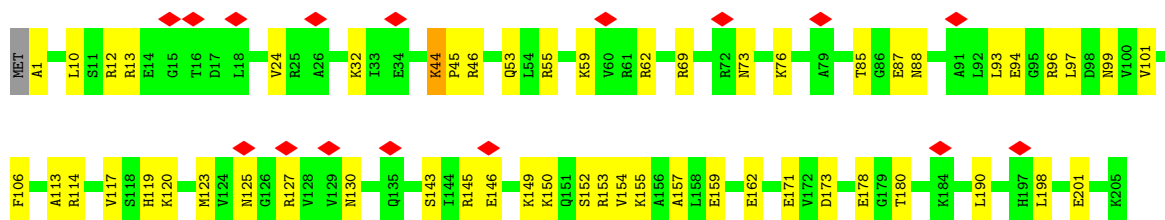
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% 12%



- Molecule 9: 30S ribosomal protein S4

Chain I:  8% 73% 26%

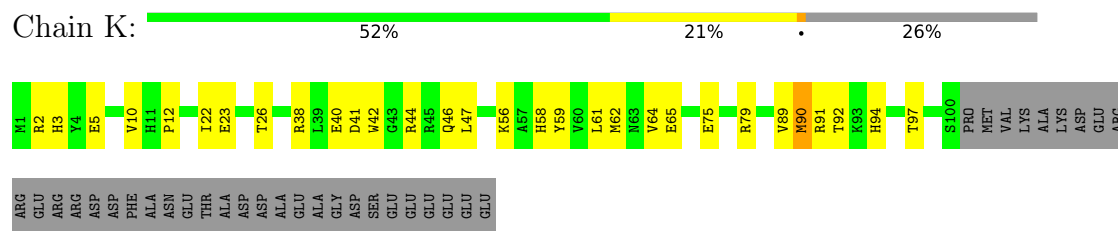


- Molecule 10: 30S ribosomal protein S5

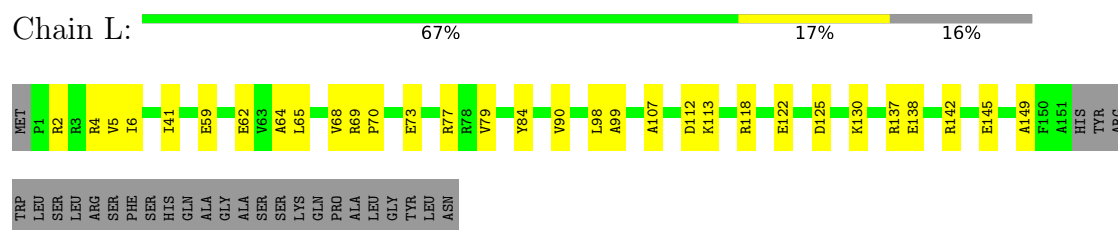
Chain J:  77% 17% 6%



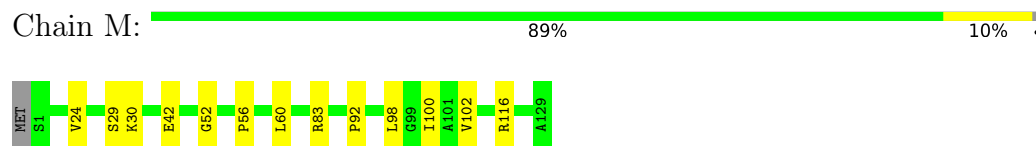
- Molecule 11: 30S ribosomal protein S6, fully modified isoform



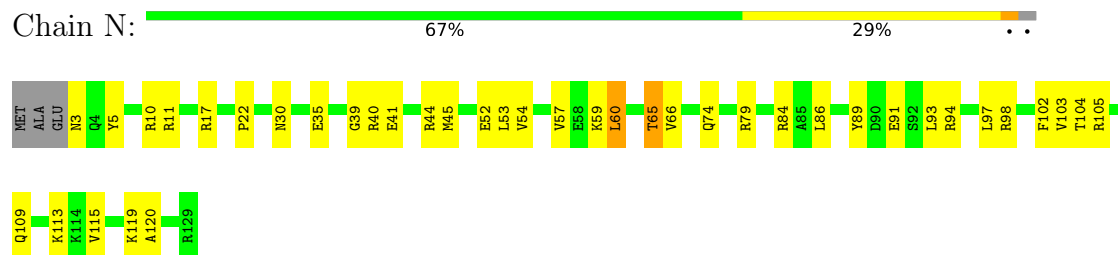
- Molecule 12: 30S ribosomal protein S7



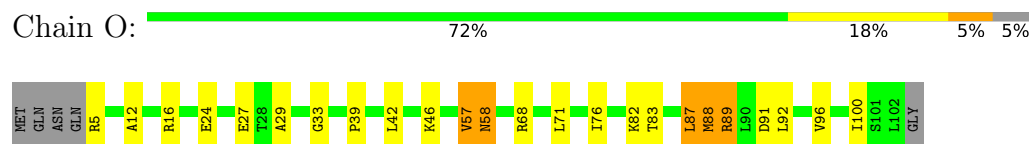
- Molecule 13: 30S ribosomal protein S8



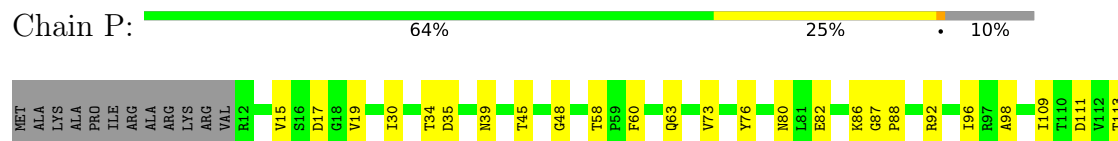
- Molecule 14: 30S ribosomal protein S9

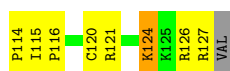


- Molecule 15: 30S ribosomal protein S10



- Molecule 16: 30S ribosomal protein S11





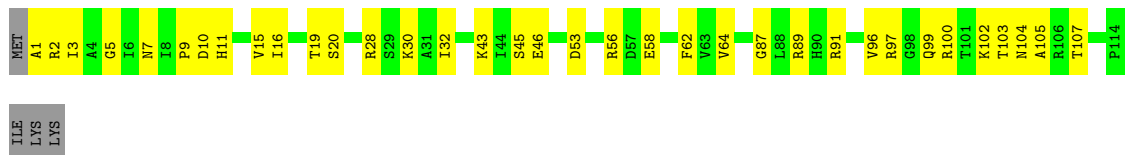
- Molecule 17: 30S ribosomal protein S12

Chain Q: 65% 33%



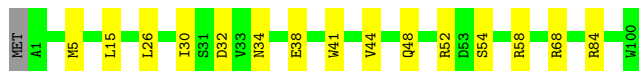
- Molecule 18: 30S ribosomal protein S13

Chain R: 67% 30%



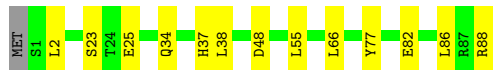
- Molecule 19: 30S ribosomal protein S14

Chain S: 84% 15%



- Molecule 20: 30S ribosomal protein S15

Chain T: 84% 15%



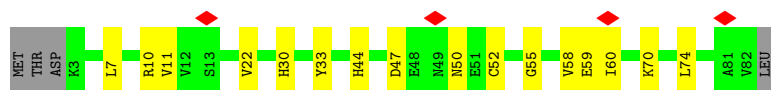
- Molecule 21: 30S ribosomal protein S16

Chain U: 7% 76% 23%



- Molecule 22: 30S ribosomal protein S17

Chain V: 5% 76% 19% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W: 68% 17% 13%



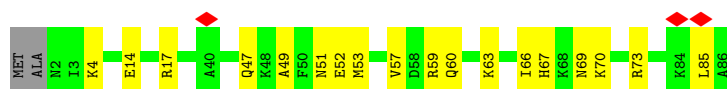
- Molecule 24: 30S ribosomal protein S19

Chain X: 74% 12% 14%



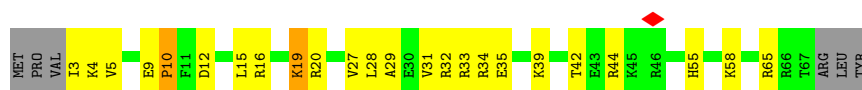
- Molecule 25: 30S ribosomal protein S20

Chain Y: 77% 21% 2%



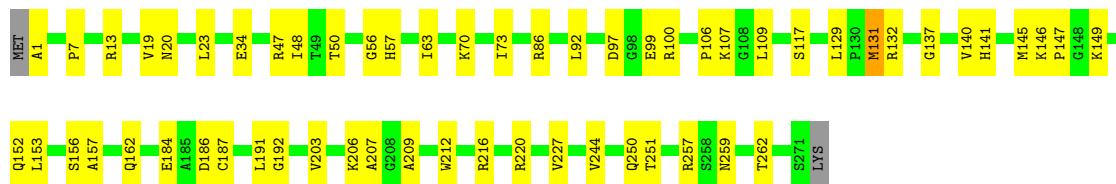
- Molecule 26: 30S ribosomal protein S21

Chain Z: 58% 31% 8%



- Molecule 27: 50S ribosomal protein L2

Chain b: 78% 21% 1%



- Molecule 28: 50S ribosomal protein L3

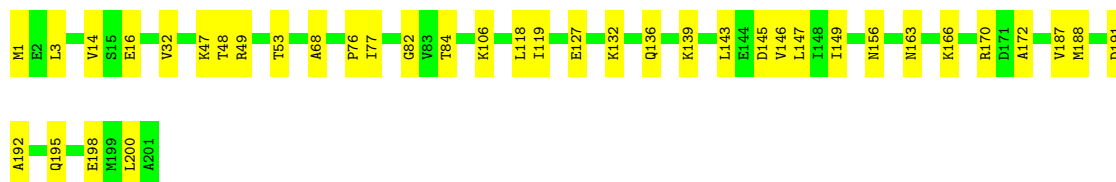
Chain c: 85% 15%





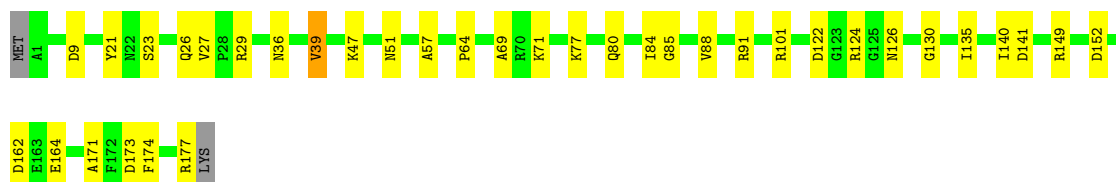
- Molecule 29: 50S ribosomal protein L4

Chain d: 81% 19%



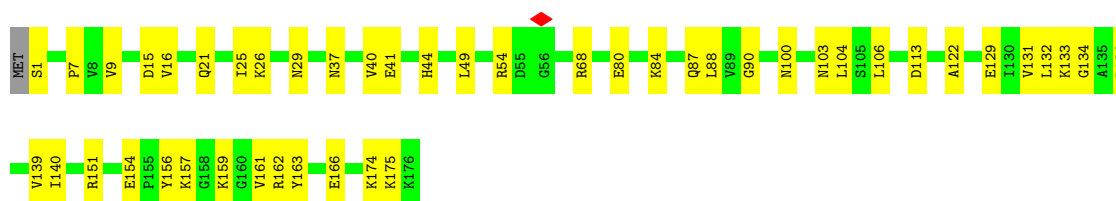
- Molecule 30: 50S ribosomal protein L5

Chain e: 79% 20% ..



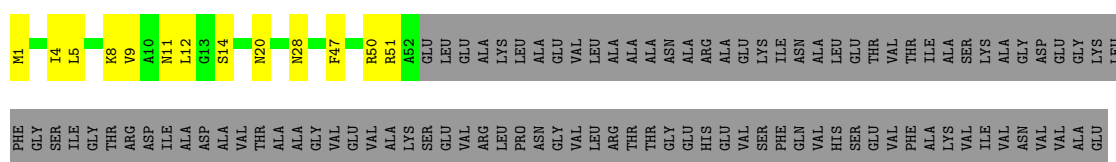
- Molecule 31: 50S ribosomal protein L6

Chain f: 73% 26% .



- Molecule 32: 50S ribosomal protein L9

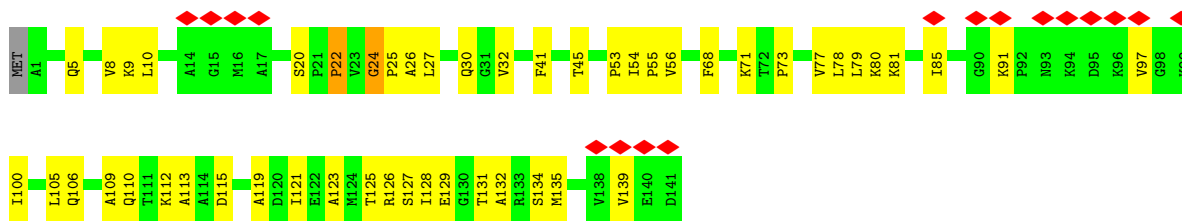
Chain g: 26% 9% 65%



- Molecule 33: 50S ribosomal protein L11

Chain i: 12% 64% 34% ..





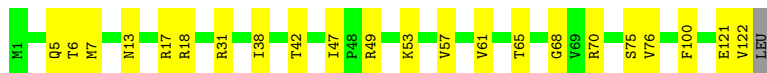
- Molecule 34: 50S ribosomal protein L13

Chain j:   82% 18%



- Molecule 35: 50S ribosomal protein L14

Chain k:   81% 18%



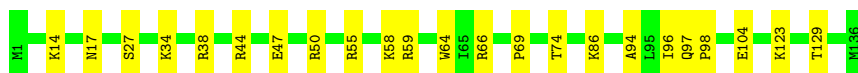
- Molecule 36: 50S ribosomal protein L15

Chain l:   86% 13%



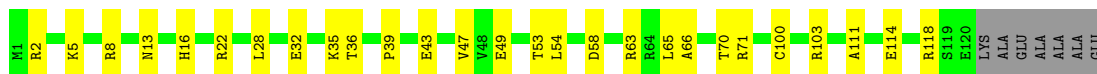
- Molecule 37: 50S ribosomal protein L16

Chain m:   83% 17%



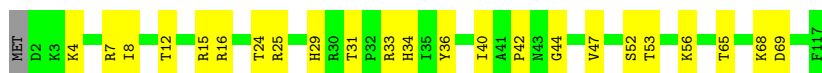
- Molecule 38: 50S ribosomal protein L17

Chain n:    73% 21% 6%




- Molecule 39: 50S ribosomal protein L18

Chain o:    79% 20%




- Molecule 40: 50S ribosomal protein L19

Chain p:  84% 15%



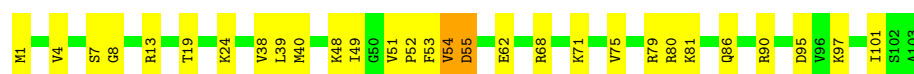
- Molecule 41: 50S ribosomal protein L20

Chain q:  84% 14%




- Molecule 42: 50S ribosomal protein L21

Chain r:  72% 26%



- Molecule 43: 50S ribosomal protein L22

Chain s:  85% 15%



- Molecule 44: 50S ribosomal protein L23

Chain t:  74% 19% 7%




- Molecule 45: 50S ribosomal protein L24

Chain u:  72% 26%



- Molecule 46: 50S ribosomal protein L25

Chain v:  85% 15%



- Molecule 47: 50S ribosomal protein L27

Chain w:  74% 14% 12%




- Molecule 48: 50S ribosomal protein L28

Chain x:  74% 23% ..



- Molecule 49: 50S ribosomal protein L29

Chain y:  76% 24%



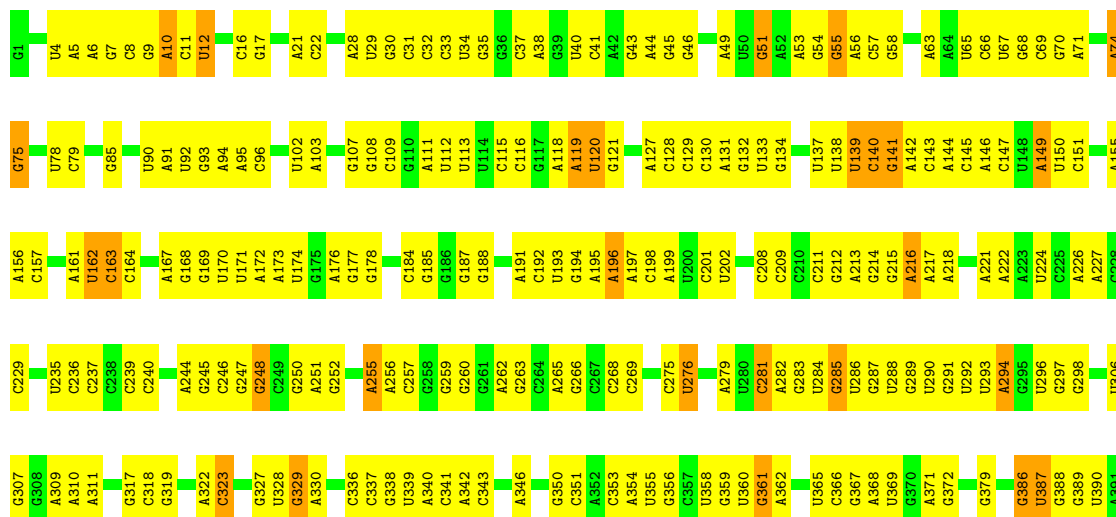
- Molecule 50: 50S ribosomal protein L30

Chain z:  76% 22% .



- Molecule 51: 23S rRNA

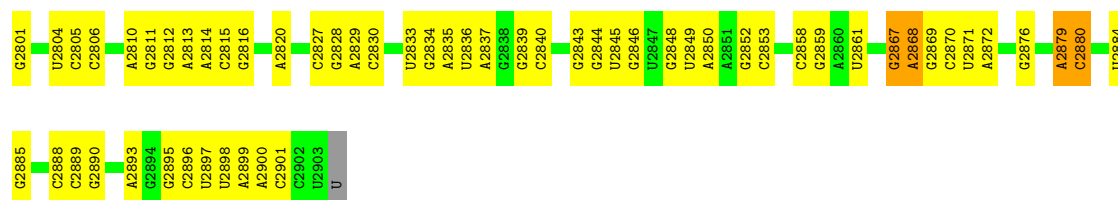
Chain 1:  42% 51% 7%





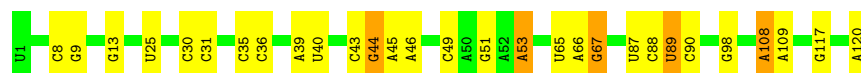
C1507	G1436	G1334	G1266	U1173	G1106	G1044	U958	A877	A800	G707	C624	U546	A472	U392
A1508	A1427	C1335	U1267	U1174	G1107	C1045	A959	A878	G801	G708	C627	A547	G473	C393
A1509	C1428	A1336	G1287	A1175	U1108	A1046	A960	G879	G805	U709	A627	G548	G474	C394
G1510	G1429	G1337	G1270	U1176	C1109	G1047	C961	G885	G809	G712	G628	G550	G475	U395
G1511	G1430	G1338	C1271	G1177	G1110	A1048	C968	C886	U810	G713	G629	G551	G476	G396
C1512	A1431	G1339	A1272	C1178	A1111	A1049	C969	U887	G815	G714	G630	U552		U397
	G1432		U1273	G1179	G1112	A1050	A972	C888	U811	A718	A633	U553	G481	
A1515	A1433	G1343	A1274	U1180	C1113		A973	C889	G812	C719	C634	U554	A482	A402
G1516	A1434	U1344	U1275	U1181	G1115	A1054	A974	C890	G813	U720	C635	U555	C485	A403
G1517	G1435	C1345	A1276	U1182	G1116	G1055	A975	C891	U814	U721	C636	A556	C486	A404
C1518	G1436	G1346	G1278	U1183	G1117	G1056	A976	C892	C814	A722	C637	C557	G487	U405
G1519	C1437	A1347	C1279	U1184	C1118	A1057	A977	C893	G815	C723	G638	U558	G488	G406
U1520	G1438	C1348	G1279	U1185	C1119	U1058	A979	C894	A819	C724	U639		G489	G409
G1521	A1439	G1349	U1186	U1119	G1059	U1060	A880	U894	A820	U725	U641	U562	C490	G410
A1522	U1440		G1187	G1120	U1061	A981	C982	U895	A821	G726	U642	A563	A492	G411
U1523	U1441	U1352	U1282	C1121	U1062	G1063	A983	C897	A825	A727			G493	
G1524	U1442	A1365	G1283	G1123	G1064	C1064	A984	C898	U826	C728	A644	U566	G494	C414
A1525		A1366	A1284	U1193	U1065		C985	C899	U827	G729	C645	U567	A415	U416
C1526	G1448	A1367	A1285	G1194	U1066		G989	A900	U828	A730	U646	U568		
G1527	A1449	G1368	A1286	G1195	U1067	U1066		C901	U829	C736	G647	U569	U499	U419
A1528	G1450	G1369	A1287	G1196	A1067	G1068	G993	C902	G830		G648	U570	G500	C420
G1529	G1451	G1370	G1288	U1197	G1131	G1069	C994	C903	U831	U745	U652	U571	A501	C421
G1530	G1452	G1371	C1289	U1198	U1132	A1069	C995	C904	U832	U746	U653	U572	A502	A422
	A1453	U1372	G1290	U1199	A1133	A1070	C996	A905	G833	C747	A574	A573	A503	A423
A1454	C1454	U1373	G1291	C1200	C1135	G1071	A996	U906	G834		A654	A575	A504	G424
		G1380	C1292		G1136	C1072	C1005	G907	G835	A752	G656	U580	A505	G425
A1535	C1461	G1381	U1294	A1204	G1137	A1073	A1009	C908	G836	G757			G506	C426
C1536	C1462	G1382	C1295	A1205	U1138	C1074	A1010	A910	C837		G662	A586	C510	U427
G1537	G1463	G1296	G1296	U1209	G1139	C1075	A1011	A911		C758			U511	U431
C1538	G1464	C1297	G1298	G1210	C1140	C1076	G1011		C840	C759	G669	A590	U512	A432
U1539	G1465	C1386	G1299	G1211	U1141	U1077	G1012	G914	G841	G760	A670	U591	U513	U433
G1540	U1466	A1387	G1300	G1212	A1142	U1078	C1013	C915	U842	U762	A592	U593	U514	C434
C1541	U1467	G1388	G1212	A1143	A1143	C1079	A1014		A845	G763	C671	U594	U515	C435
U1542	U1468	G1389	A1301	C1145	A1144	A1080	U1015	A918	U846	A764	C672	U595	U516	C436
G1543	A1469	U1390	C1306	U1219	C1146	U1081	U1016	U919	U847	C765	G673	C596	U517	U437
A1544	A1470			G1220	A1147	U1082	U1017		C848		A677	U596	A522	G438
A1545		U1394			U1148	U1083	A1020	G923	A849	G774		G597	A526	A439
G1546				G1225	G1149	A1084	A1021	G924	U850	G775	C678	U598	C527	A440
		U1400	G1310		C1150	A1085	G1022	A925	U851		A679	A599	A528	U441
C1550	G1483	U1401	G1311	A1230	U1151	A1086	U1023	G926	U852	U779	C680	A603	A529	C442
A1551	C1484	U1402	C1314	U1231	C1152	G1087	G1024	A927	C853	U780	G681		G530	C445
A1552	U1485	A1403	C1315	G1232	C1153	A1088	G1025	A928	U854	A781	G682	U607	C531	C446
A1553	U1486	U1404	U1316	C1233	G1154	A1089	G1026	U929	C855	U782	U683	A608	A532	U451
U1554	U1487	U1405	G1317		G1155	A1090	A1027		G858	G784	A685	A609	U534	C452
G1555		U1406	A1321	U1240	A1156	C1091	U1028	U932	U859	G785	A686	C610	U535	
	C1488	U1409	A1322		A1157	G1092	G1031		U860		A687	C611	G536	A457
C1558	G1489	G1410	A1323	U1246	G1160	U1093	U1033	G938	G864	A788	U688	G612	G537	
U1559	U1490	U1411	C1320	A1247	C1161	A1094	U1034	G940	C865	A789		A613	G538	C461
G1560	G1491	U1412	A1324		G1162	A1095	G1035	A941	U865	U790	G695	A614	A539	C462
C1561	G1492	A1413	U1325	A1253	C1163	U1096	U1036	G942	U866	C791	G696	U615	G539	C463
U1562		A1414	U1326	A1254	G1164	A1097	G1037		U867	U792	G697	A616	C540	C464
	U1497	C1415	A1327	U1255	A1165	G1099	G1038	C946	U870	A793			C541	G465
A1566	G1500	U1416	A1328	U1256	G1166	C1100	A1039	A947	U871		U703	G620	C542	A466
G1567	G1501	C1417	U1329	G1257	U1101	U1101	A1040		U872	A794	G704	A621	G543	C467
G1568	A1502	G1418	A1330	U1258	C1102	C1102	G1041	U955	C873	C796		A705	C544	G468
A1569	A1503	U1570	C1330	G1171	A1103	A1103	U1042	G956						
A1570	A1504		G1333		C1170	C1104	C1043	C957	C876		A706			
A1572	U1506			G1259	C1172	U1105								





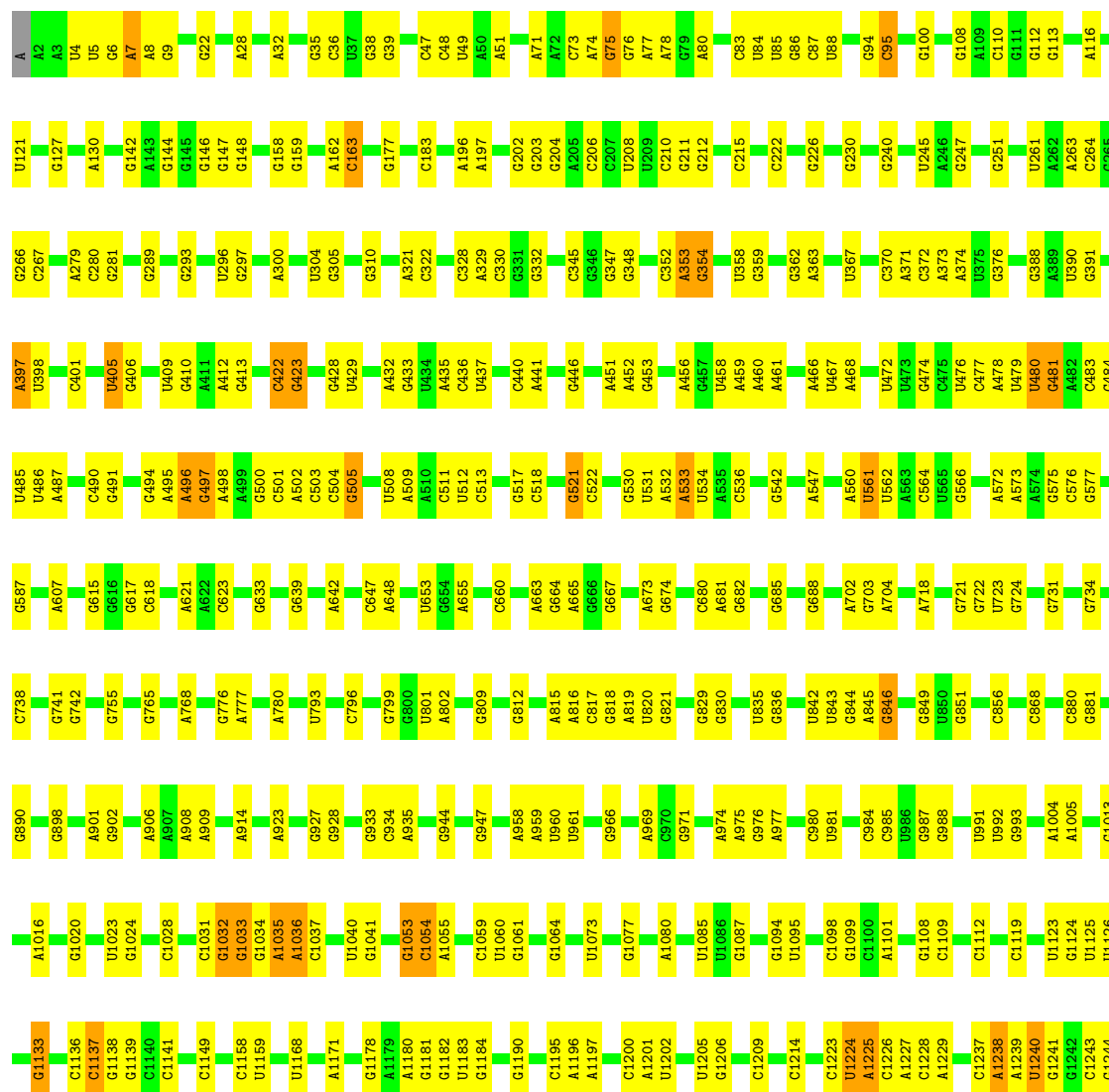
• Molecule 52: 5S rRNA

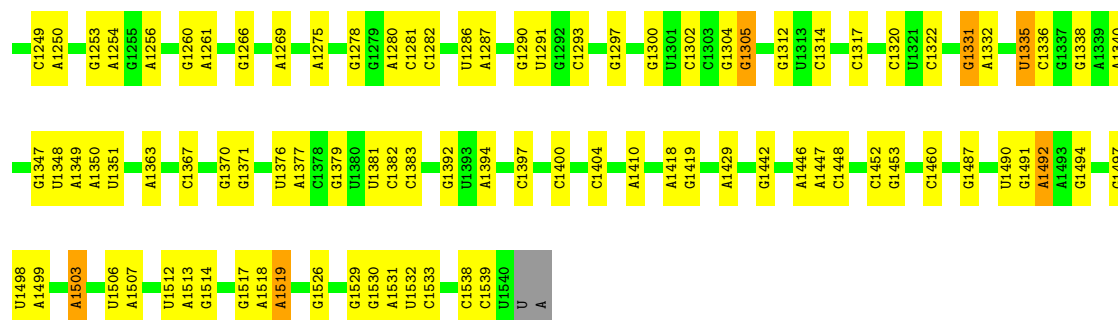
Chain 2: 76% 20%



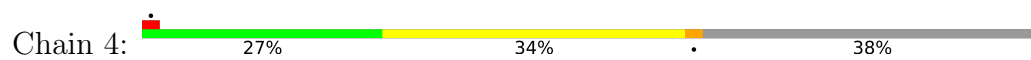
• Molecule 53: 16S rRNA

Chain 3: 68% 29%

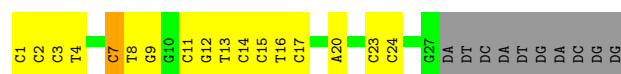
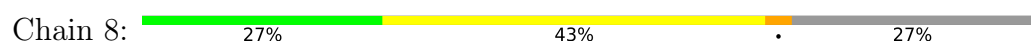




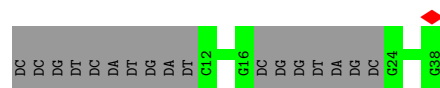
- Molecule 54: mRNA



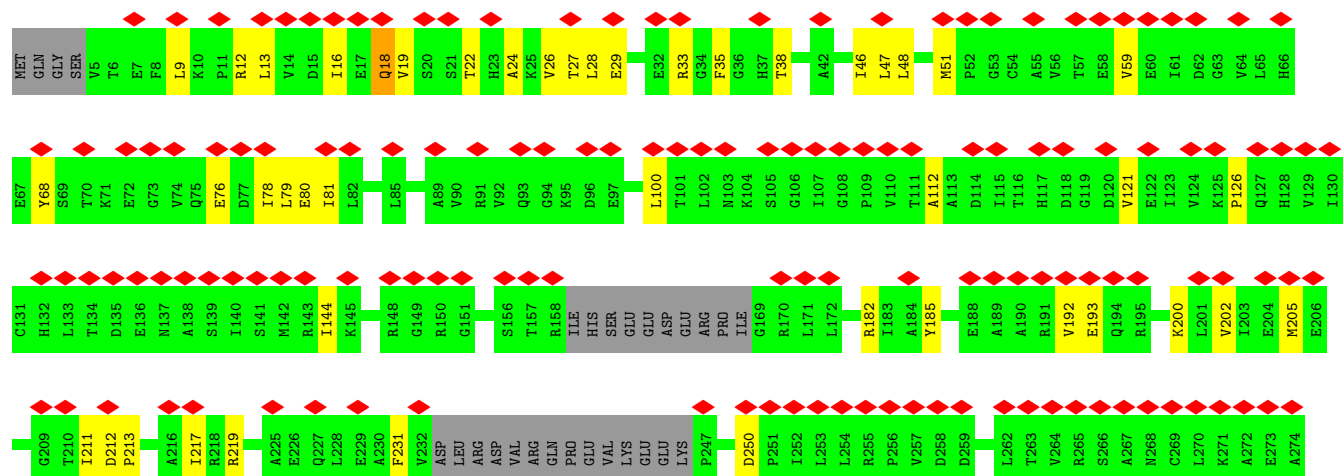
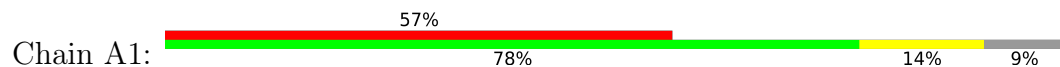
- Molecule 55: template DNA strand

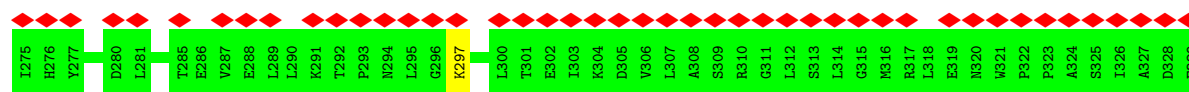


- Molecule 56: non-template DNA strand

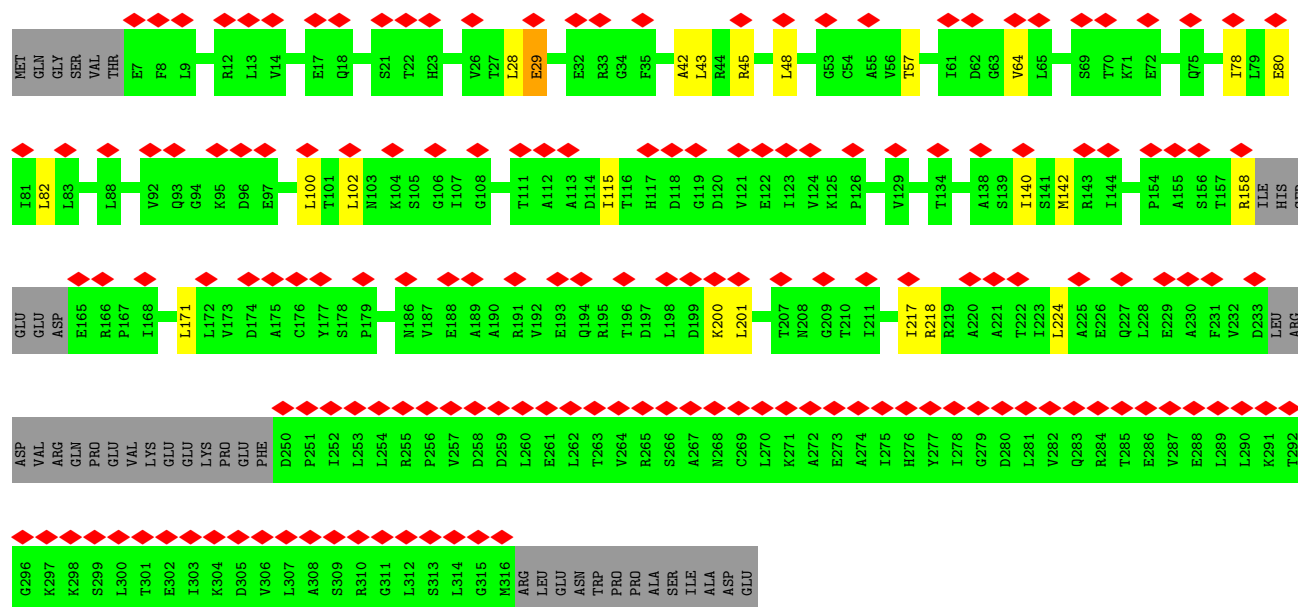
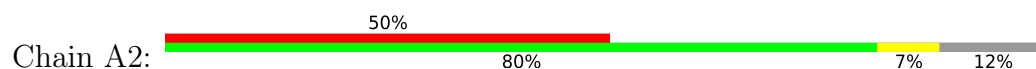


- Molecule 57: DNA-directed RNA polymerase subunit alpha

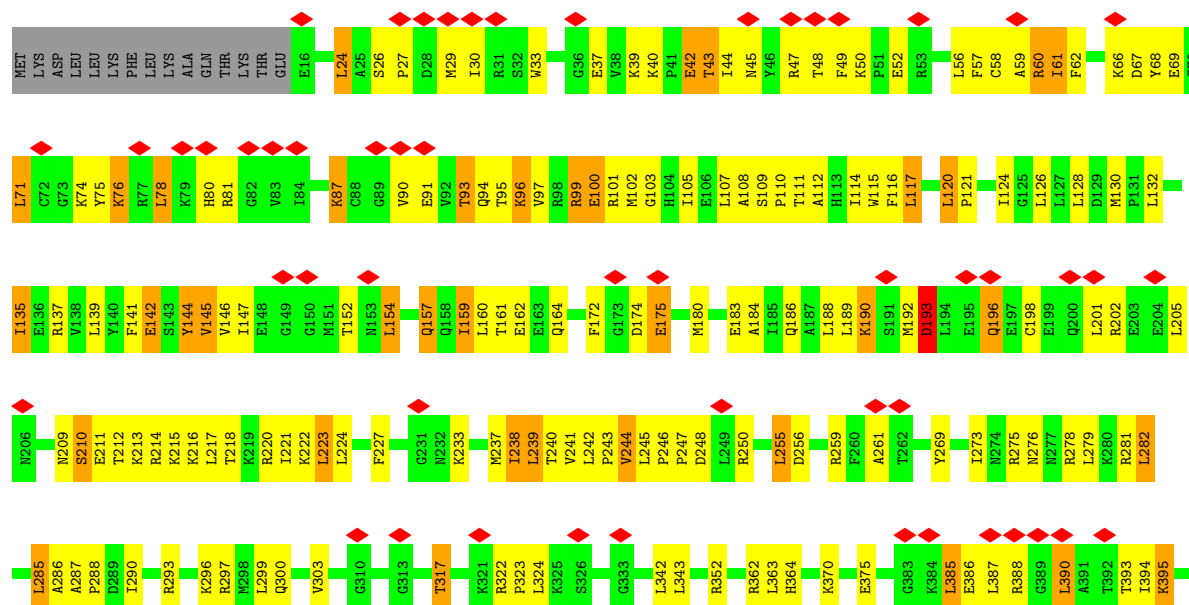


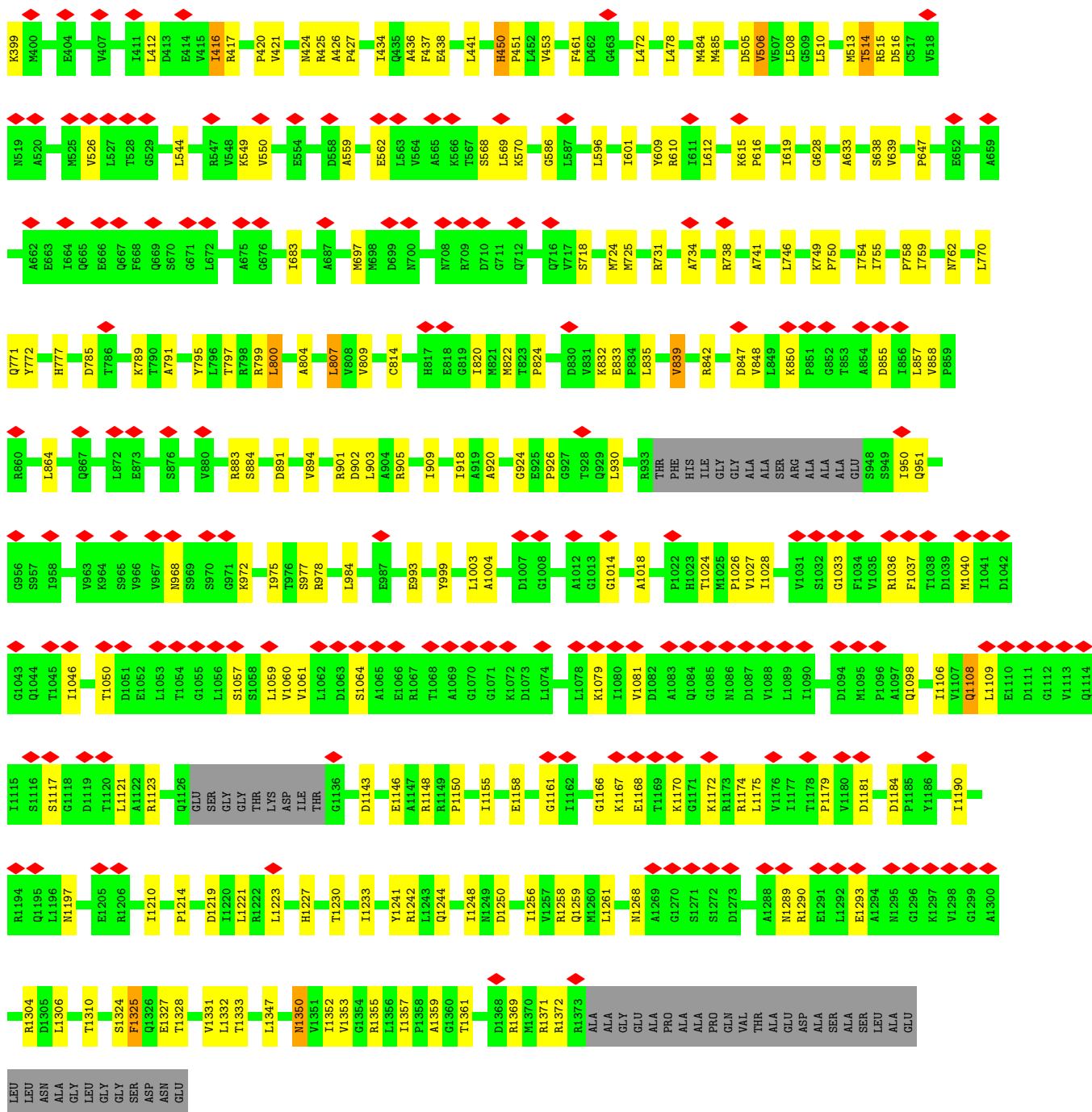


• Molecule 57: DNA-directed RNA polymerase subunit alpha



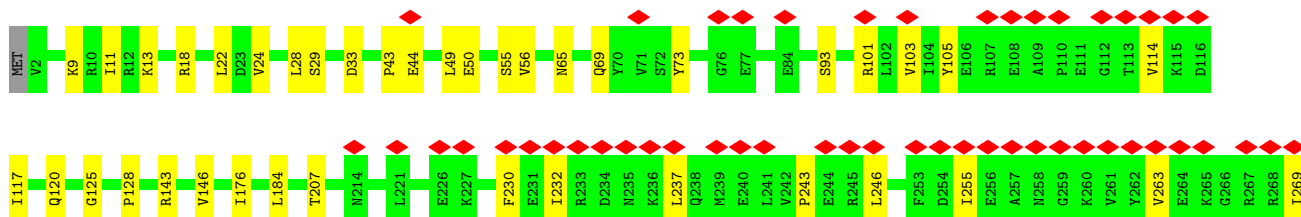
• Molecule 58: DNA-directed RNA polymerase subunit beta'

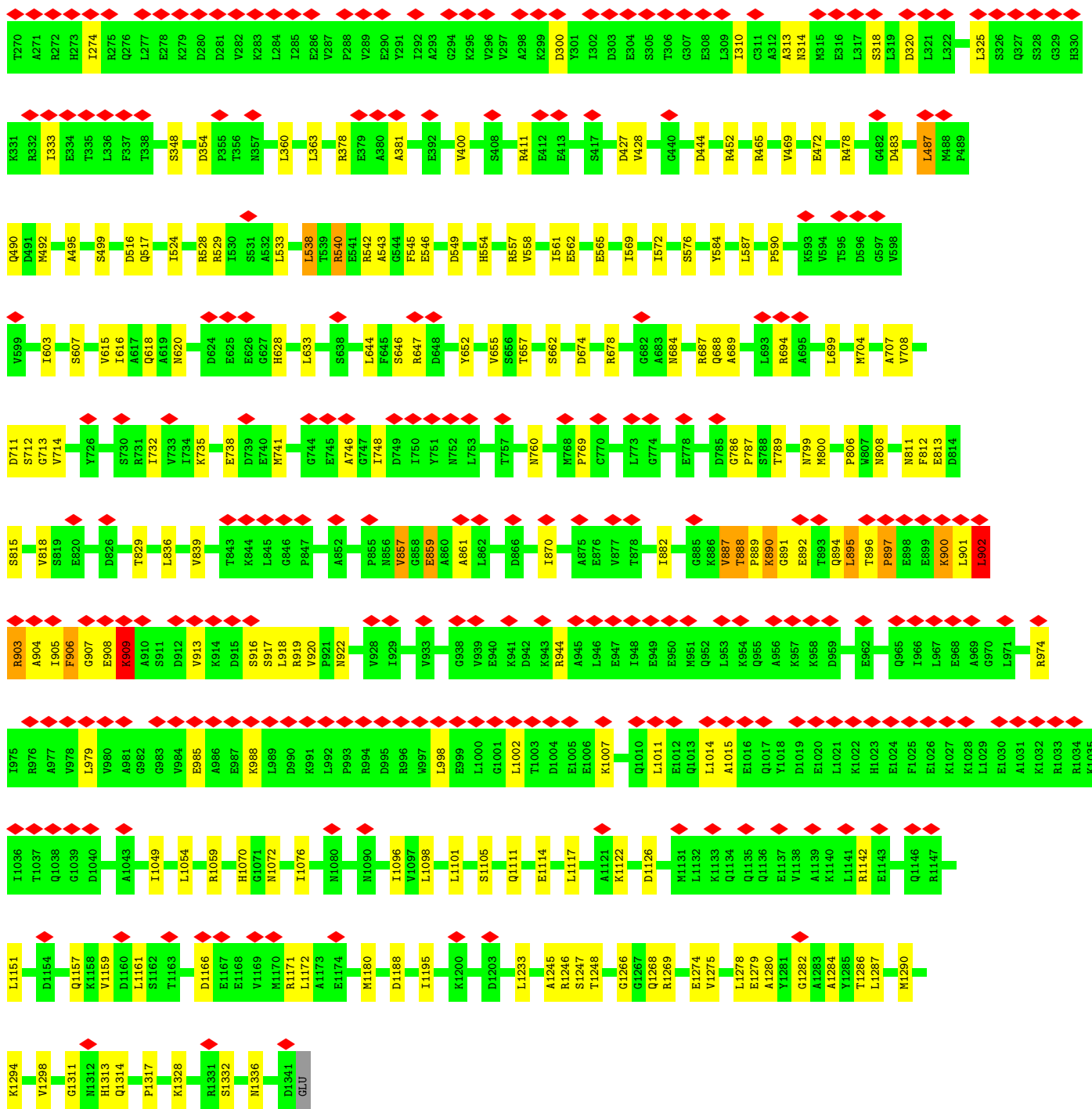


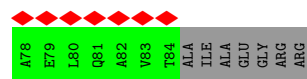


• Molecule 59: DNA-directed RNA polymerase subunit beta

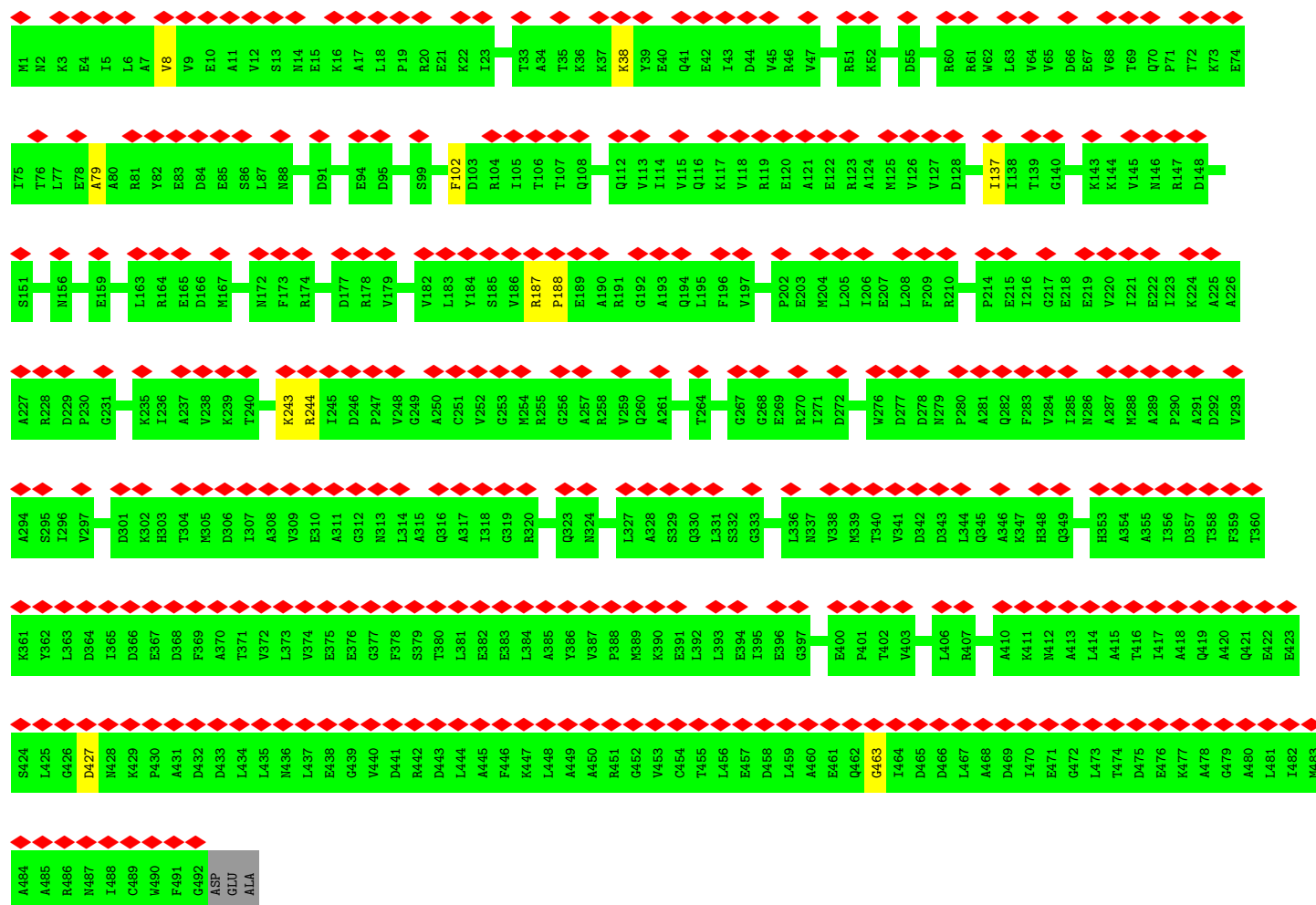
Chain B2: 23% 82% 17%



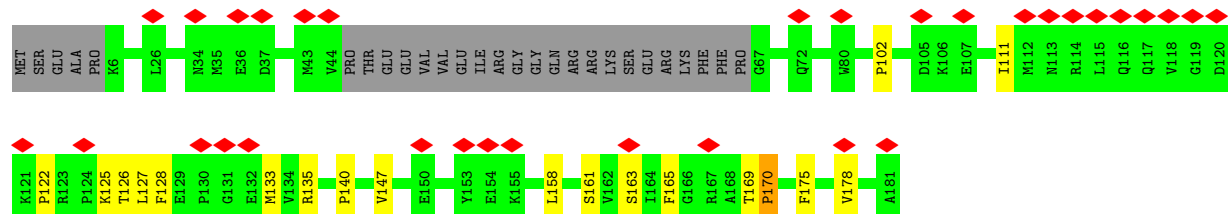
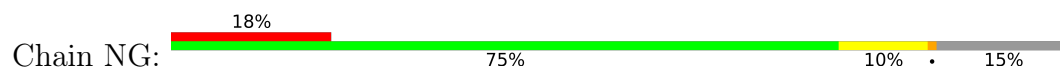




• Molecule 61: Transcription termination/antitermination protein NusA




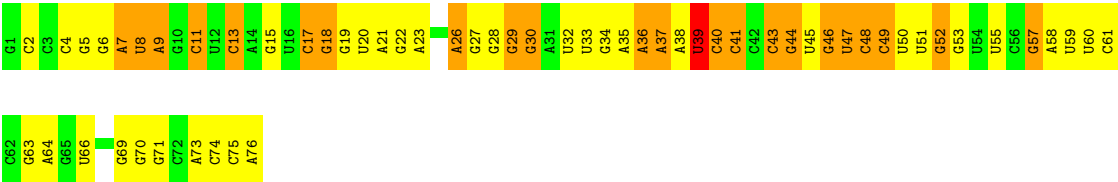
• Molecule 62: Transcription termination/antitermination protein NusG




• Molecule 63: tRNA(Phe)



Chain 5:  22% 47% 29% .



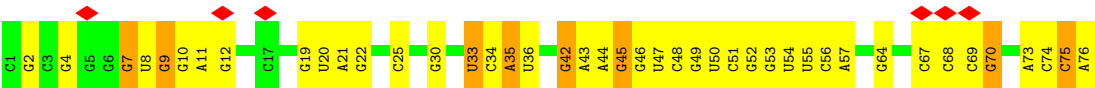
• Molecule 64: tRNA(fMet)

Chain 6:  77% 19% .



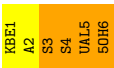
• Molecule 64: tRNA(fMet)

Chain 7:  8% 44% 45% 10%



• Molecule 65: 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	24010	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	0.175	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.011	Depositor
Map size ( $\text{\AA}$ )	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.57, 1.57, 1.57	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.27	0/531	0.54	0/709
2	B	0.40	0/450	0.60	0/599
3	C	0.28	0/416	0.52	0/554
4	D	0.47	0/380	0.76	2/498 (0.4%)
5	E	0.53	0/513	0.60	0/676
6	F	0.57	0/303	0.65	0/397
7	G	0.37	0/1735	0.64	0/2338
8	H	0.34	0/1651	0.55	0/2225
9	I	0.35	0/1665	0.71	0/2227
10	J	0.38	0/1169	0.68	2/1573 (0.1%)
11	K	0.46	0/835	0.77	0/1128
12	L	0.30	0/1195	0.67	3/1602 (0.2%)
13	M	0.35	0/989	0.52	0/1326
14	N	0.41	0/1034	0.77	0/1375
15	O	0.50	0/796	0.78	2/1077 (0.2%)
16	P	0.45	0/885	0.64	1/1195 (0.1%)
17	Q	0.50	0/969	0.86	2/1300 (0.2%)
18	R	0.33	0/892	0.73	2/1193 (0.2%)
19	S	0.32	0/817	0.61	0/1088
20	T	0.49	0/722	0.64	0/964
21	U	0.30	0/659	0.71	2/884 (0.2%)
22	V	0.44	0/657	0.71	0/881
23	W	0.54	0/544	0.74	1/731 (0.1%)
24	X	0.28	0/652	0.55	0/877
25	Y	0.28	0/671	0.52	0/888
26	Z	0.66	0/550	1.01	2/728 (0.3%)
27	b	0.49	0/2121	0.65	0/2852
28	c	0.42	0/1586	0.59	2/2134 (0.1%)
29	d	0.43	0/1571	0.62	0/2113
30	e	0.38	0/1434	0.60	2/1926 (0.1%)
31	f	0.29	0/1343	0.55	0/1816
32	g	0.32	0/405	0.74	0/544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	i	0.31	0/1046	0.77	3/1410 (0.2%)
34	j	0.41	0/1152	0.55	1/1551 (0.1%)
35	k	0.45	0/947	0.66	0/1268
36	l	0.40	0/1054	0.63	0/1403
37	m	0.56	0/1093	0.74	0/1460
38	n	0.46	0/973	0.72	1/1301 (0.1%)
39	o	0.32	0/902	0.51	0/1209
40	p	0.42	0/929	0.61	0/1242
41	q	0.52	0/960	0.62	1/1278 (0.1%)
42	r	0.43	0/829	0.69	0/1107
43	s	0.44	0/864	0.58	0/1156
44	t	0.33	0/744	0.52	0/994
45	u	0.45	0/787	0.75	0/1051
46	v	0.34	0/766	0.51	0/1025
47	w	0.40	0/582	0.52	0/769
48	x	0.43	0/635	0.63	1/848 (0.1%)
49	y	0.29	0/510	0.64	0/677
50	z	0.41	0/453	0.53	0/605
51	1	0.51	0/69796	0.62	22/108888 (0.0%)
52	2	0.43	0/2872	0.46	0/4479
53	3	0.42	0/36963	0.43	0/57662
54	4	0.52	0/808	0.65	0/1251
55	8	0.56	0/599	0.70	1/919 (0.1%)
56	9	0.49	0/468	0.56	0/719
57	A1	0.55	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.75	0/2786
58	B1	0.57	4/10510 (0.0%)	0.75	8/14196 (0.1%)
59	B2	0.46	0/10714	0.67	1/14459 (0.0%)
60	W0	0.30	0/652	0.61	0/879
61	NA	0.76	0/2431	1.22	1/3385 (0.0%)
62	NG	1.10	0/756	1.06	0/1048
63	5	0.57	0/1812	0.86	3/2823 (0.1%)
64	6	0.40	0/1832	0.48	0/2855
64	7	0.39	0/1832	0.57	1/2855 (0.0%)
65	h	3.16	2/11 (18.2%)	0.75	0/13
All	All	0.48	6/191576 (0.0%)	0.62	67/282857 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	3	SER	CA-C	-6.71	1.38	1.52
65	h	4	SER	CA-C	-6.16	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.36	1.22	1.33
58	B1	424	ASN	CG-ND2	-5.17	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.11	1.33	1.23

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	73	VAL	N-CA-C	-9.03	104.53	113.20
41	q	33	VAL	N-CA-C	-8.80	104.72	112.12
12	L	64	ALA	N-CA-C	-7.70	105.05	114.75
51	1	1130	U	C2'-C3'-O3'	7.58	120.88	109.50
64	7	33	U	C2'-C3'-O3'	7.28	120.42	109.50

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	7	0
2	B	444	0	461	9	0
3	C	409	0	440	4	0
4	D	377	0	418	9	0
5	E	504	0	574	3	0
6	F	302	0	343	7	0
7	G	1704	0	1732	36	0
8	H	1624	0	1699	26	0
9	I	1643	0	1710	34	0
10	J	1156	0	1199	18	0
11	K	817	0	808	16	0
12	L	1181	0	1240	19	0
13	M	979	0	1034	8	0
14	N	1022	0	1070	23	0
15	O	786	0	828	15	0
16	P	869	0	878	21	0
17	Q	955	0	1019	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	883	0	944	20	0
19	S	805	0	847	10	0
20	T	714	0	737	6	0
21	U	649	0	666	15	0
22	V	648	0	691	8	0
23	W	535	0	552	8	0
24	X	637	0	665	7	0
25	Y	665	0	714	11	0
26	Z	544	0	579	12	0
27	b	2082	0	2157	46	0
28	c	1565	0	1616	28	0
29	d	1552	0	1619	27	0
30	e	1410	0	1447	23	0
31	f	1323	0	1374	31	0
32	g	400	0	423	7	0
33	i	1032	0	1088	41	0
34	j	1129	0	1162	22	0
35	k	938	0	1012	17	0
36	l	1045	0	1117	17	0
37	m	1074	0	1157	13	0
38	n	960	0	1000	19	0
39	o	892	0	923	16	0
40	p	917	0	965	17	0
41	q	947	0	1022	9	0
42	r	816	0	839	19	0
43	s	857	0	922	11	0
44	t	738	0	807	10	0
45	u	779	0	834	13	0
46	v	753	0	780	9	0
47	w	575	0	592	8	0
48	x	625	0	655	12	0
49	y	509	0	543	12	0
50	z	449	0	491	9	0
51	1	62317	0	31346	1462	0
52	2	2568	0	1303	15	0
53	3	33012	0	16618	188	0
54	4	729	0	364	5	0
55	8	539	0	305	29	0
56	9	417	0	224	0	0
57	A1	2088	0	1895	22	0
57	A2	2029	0	1864	17	0
58	B1	10353	0	10548	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B2	10546	0	10550	167	0
60	W0	650	0	658	11	0
61	NA	2432	0	1171	10	0
62	NG	758	0	334	14	0
63	5	1622	0	821	26	0
64	6	1640	0	837	7	0
64	7	1640	0	837	21	0
65	h	48	0	40	9	0
66	B1	1	0	0	0	0
All	All	178130	0	126632	2811	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 2811 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)
40:p:52:ARG:HH21	51:1:2720:U:H5''	0.95	1.09
51:1:275:C:H2'	51:1:276:U:H4'	1.37	1.07
51:1:1666:G:H2'	51:1:1667:G:H5'	1.41	1.03
51:1:2713:U:H3'	51:1:2714:G:H5'	1.41	1.03
51:1:1672:A:C2	51:1:2582:G:H5'	1.95	1.02

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%)	59 (92%)	5 (8%)	0	100	100
2	B	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
4	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
5	E	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
6	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	51
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	25	64
10	J	155/167 (93%)	138 (89%)	17 (11%)	0	100	100
11	K	98/135 (73%)	85 (87%)	13 (13%)	0	100	100
12	L	149/179 (83%)	129 (87%)	20 (13%)	0	100	100
13	M	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
14	N	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
15	O	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	13	49
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	51
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	51
19	S	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
20	T	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
21	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
22	V	78/84 (93%)	69 (88%)	8 (10%)	1 (1%)	10	42
23	W	63/75 (84%)	56 (89%)	5 (8%)	2 (3%)	3	21
24	X	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
25	Y	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
26	Z	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	8	37
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
31	f	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
32	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	6	31
33	i	139/142 (98%)	116 (84%)	23 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
35	k	120/123 (98%)	106 (88%)	14 (12%)	0	100	100
36	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
37	m	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
38	n	118/127 (93%)	103 (87%)	15 (13%)	0	100	100
39	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	p	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
41	q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	35
42	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	49
43	s	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
44	t	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
45	u	100/104 (96%)	84 (84%)	15 (15%)	1 (1%)	13	49
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	10	42
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	21 (7%)	1 (0%)	37	72
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1202 (90%)	123 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1201 (90%)	131 (10%)	6 (0%)	30	68
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	472 (96%)	15 (3%)	3 (1%)	22	60
62	NG	150/181 (83%)	132 (88%)	12 (8%)	6 (4%)	2	18
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9586/10235 (94%)	8662 (90%)	885 (9%)	39 (0%)	32	68

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	r	54	VAL
48	x	25	LYS
58	B1	121	PRO

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Mol	Chain	Res	Type
59	B2	897	PRO
61	NA	187	ARG

### 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%)	58 (98%)	1 (2%)	56	72
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	47	65
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	60
5	E	51/52 (98%)	49 (96%)	2 (4%)	27	48
6	F	34/34 (100%)	30 (88%)	4 (12%)	4	16
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	53
8	H	170/190 (90%)	167 (98%)	3 (2%)	54	71
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	64
10	J	119/126 (94%)	117 (98%)	2 (2%)	56	72
11	K	87/116 (75%)	82 (94%)	5 (6%)	17	39
12	L	124/147 (84%)	124 (100%)	0	100	100
13	M	104/105 (99%)	103 (99%)	1 (1%)	73	82
14	N	105/107 (98%)	98 (93%)	7 (7%)	13	34
15	O	86/90 (96%)	78 (91%)	8 (9%)	7	23
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	52
17	Q	103/104 (99%)	98 (95%)	5 (5%)	21	42
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	83 (100%)	0	100	100
20	T	76/77 (99%)	73 (96%)	3 (4%)	27	48
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	72 (97%)	2 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	56/65 (86%)	52 (93%)	4 (7%)	12	32
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	64 (98%)	1 (2%)	60	75
26	Z	55/61 (90%)	47 (86%)	8 (14%)	2	12
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	70
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	54	71
30	e	148/150 (99%)	145 (98%)	3 (2%)	50	68
31	f	137/138 (99%)	135 (98%)	2 (2%)	60	75
32	g	41/114 (36%)	38 (93%)	3 (7%)	11	31
33	i	109/110 (99%)	108 (99%)	1 (1%)	75	83
34	j	116/116 (100%)	116 (100%)	0	100	100
35	k	103/104 (99%)	103 (100%)	0	100	100
36	l	102/103 (99%)	101 (99%)	1 (1%)	73	82
37	m	109/109 (100%)	103 (94%)	6 (6%)	18	40
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	82
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	99 (100%)	0	100	100
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	52
42	r	84/84 (100%)	82 (98%)	2 (2%)	44	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	70	80
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	21	43
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	57 (100%)	0	100	100
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
57	A2	186/286 (65%)	185 (100%)	1 (0%)	86	89
58	B1	1110/1168 (95%)	1017 (92%)	93 (8%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	B2	1150/1157 (99%)	1117 (97%)	33 (3%)	37	57
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	76
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7132 (97%)	249 (3%)	34	52

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	A1	22	THR
59	B2	516	ASP
58	B1	96	LYS
59	B2	483	ASP
59	B2	902	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
29	d	90	GLN
58	B1	1238	GLN
36	l	104	GLN
58	B1	1195	GLN
59	B2	688	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	399 (13%)	16 (0%)
52	2	119/120 (99%)	17 (14%)	1 (0%)
53	3	1538/1542 (99%)	253 (16%)	4 (0%)
54	4	33/56 (58%)	16 (48%)	2 (6%)
63	5	75/76 (98%)	43 (57%)	7 (9%)
64	6	76/77 (98%)	10 (13%)	0
64	7	76/77 (98%)	27 (35%)	2 (2%)
All	All	4819/4852 (99%)	765 (15%)	32 (0%)

5 of 765 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
51	1	12	U
51	1	34	U
51	1	35	G
51	1	46	G

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	57	G
63	5	60	U
51	1	1930	G
51	1	1801	A
64	7	33	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	$\# Z  > 2$
65	DPP	h	2	65	3,5,6	0.56	0	1,5,7	0.09	0
65	KBE	h	1	65	8,8,9	0.61	0	7,8,10	1.21	1 (14%)
65	5OH	h	6	65	8,12,13	0.76	0	3,16,18	1.52	1 (33%)
65	UAL	h	5	65	7,8,9	2.31	3 (42%)	5,9,11	2.91	2 (40%)

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
65	DPP	h	2	65	-	0/2/4/6	-
65	KBE	h	1	65	-	0/7/7/8	-
65	5OH	h	6	65	-	0/2/18/20	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	UAL	h	5	65	-	0/3/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	5	UAL	C1-N1	-4.88	1.32	1.40
65	h	5	UAL	C-CA	-2.90	1.40	1.45
65	h	5	UAL	CA-N	2.03	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	h	5	UAL	CA-CB-N1	-5.28	115.63	125.60
65	h	5	UAL	O-C-CA	-3.23	121.28	125.39
65	h	6	5OH	CR-CB-CA	-2.38	110.04	112.61
65	h	1	KBE	CB-CA-C	-2.07	109.22	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

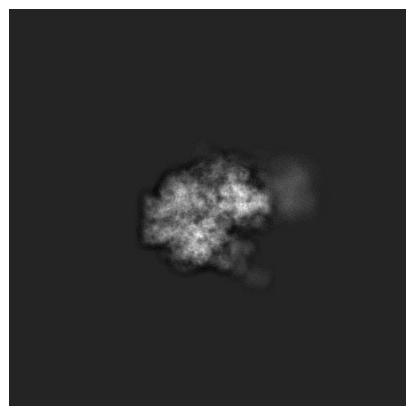
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39168. These allow visual inspection of the internal detail of the map and identification of artifacts.

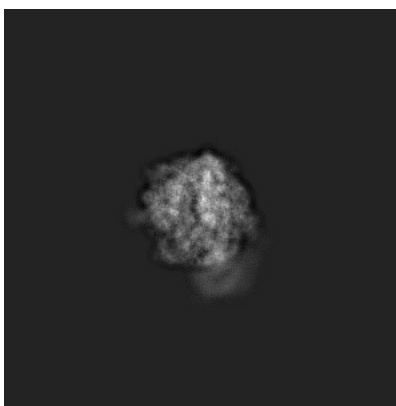
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

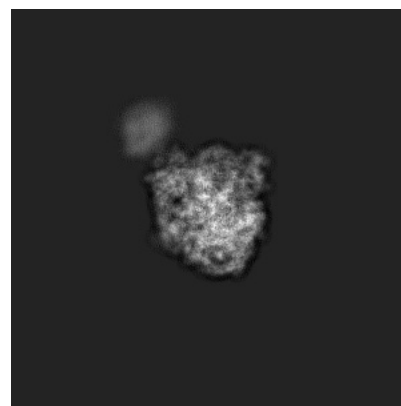
#### 6.1.1 Primary map



X

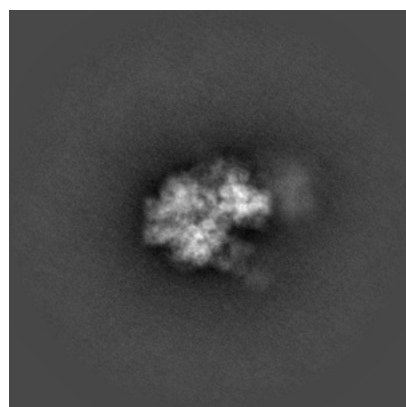


Y

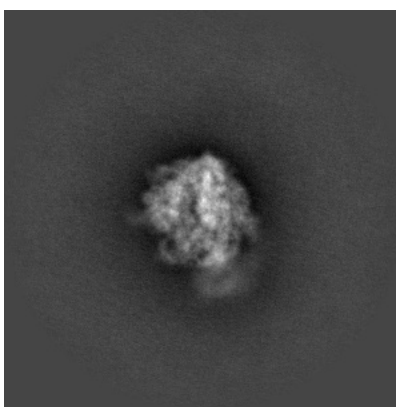


Z

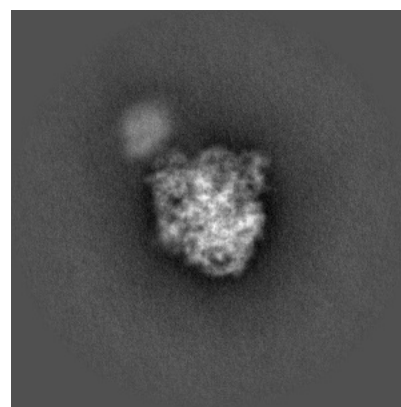
#### 6.1.2 Raw map



X



Y



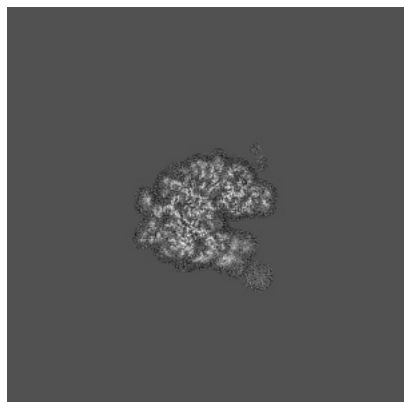
Z

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

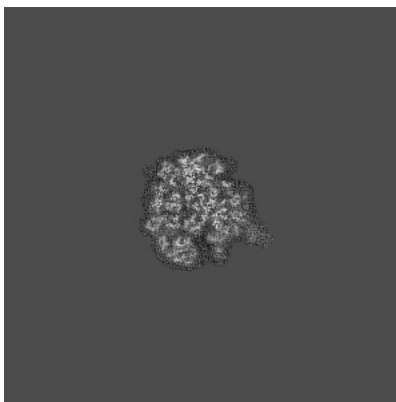


## 6.2 Central slices [i](#)

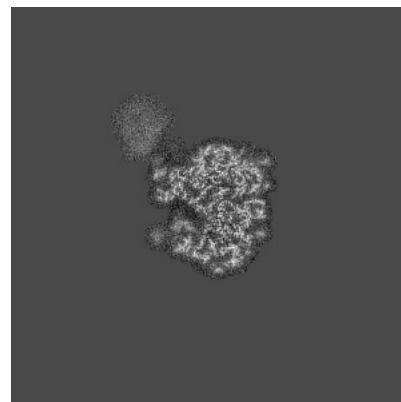
### 6.2.1 Primary map



X Index: 240

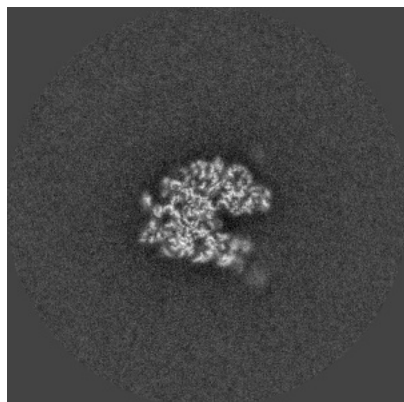


Y Index: 240

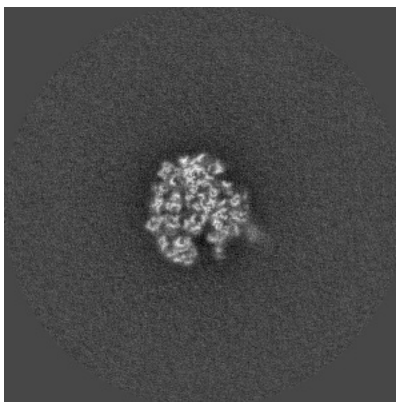


Z Index: 240

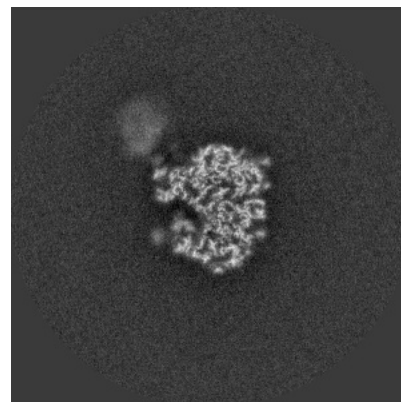
### 6.2.2 Raw map



X Index: 240



Y Index: 240

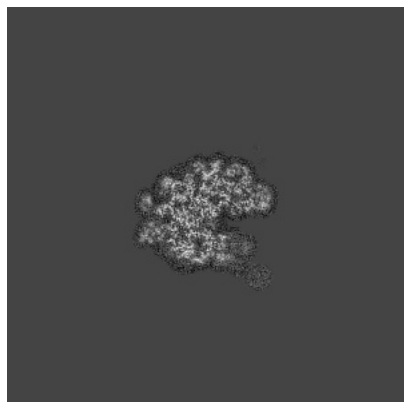


Z Index: 240

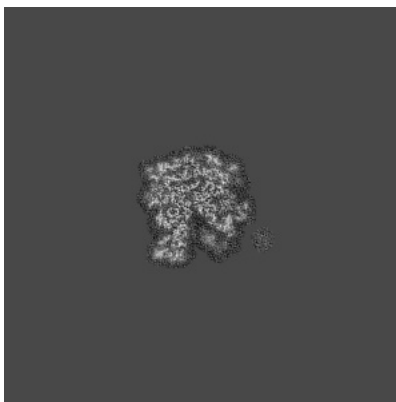
The images above show central slices of the map in three orthogonal directions.

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

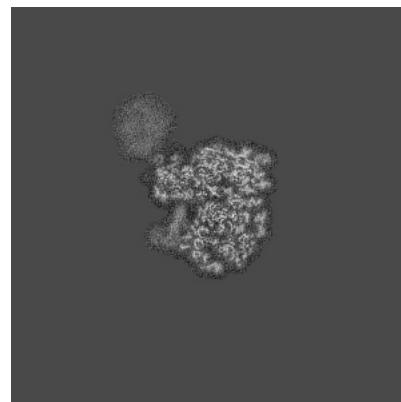
### 6.3.1 Primary map



X Index: 243

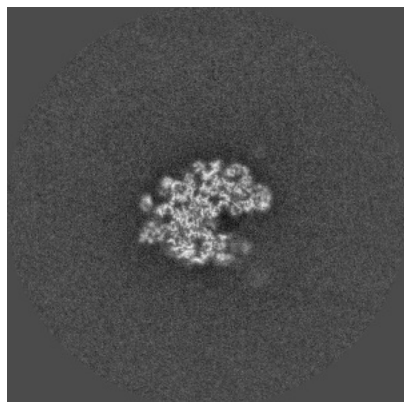


Y Index: 224

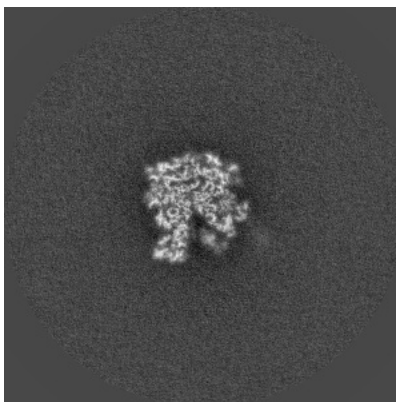


Z Index: 245

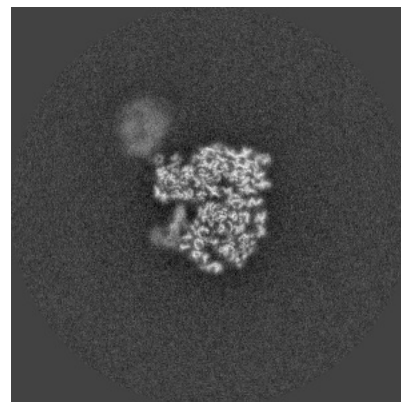
### 6.3.2 Raw map



X Index: 243



Y Index: 224

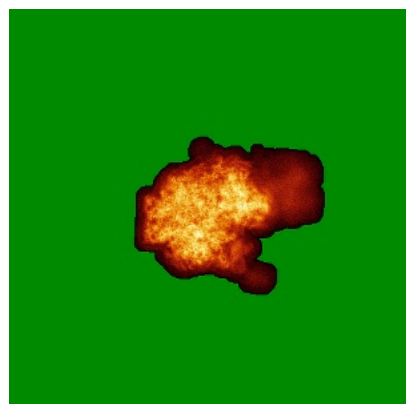


Z Index: 245

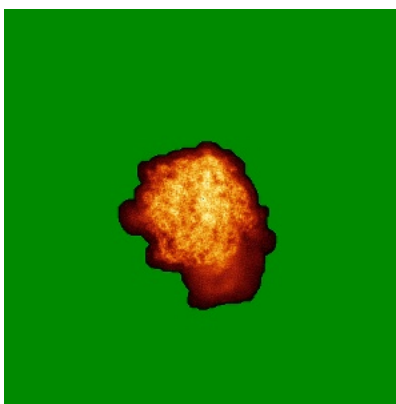
The images above show the largest variance slices of the map in three orthogonal directions.

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

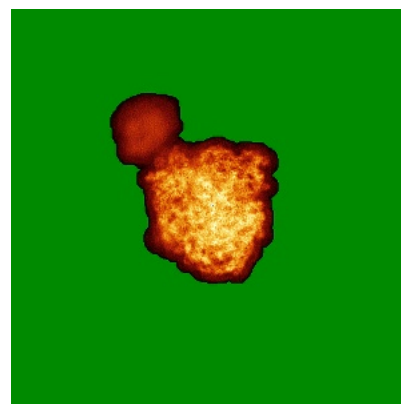
### 6.4.1 Primary map



X

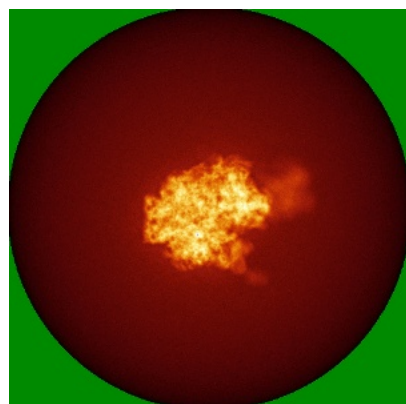


Y

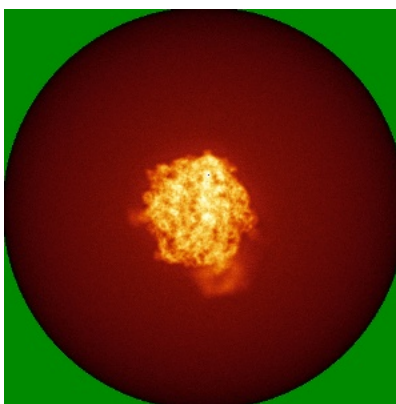


Z

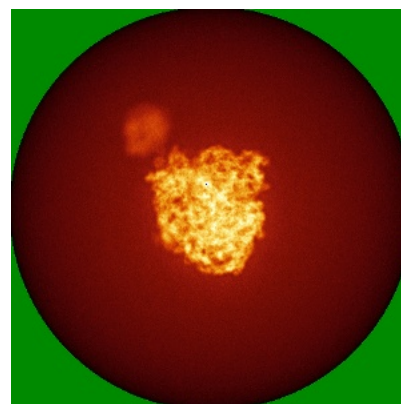
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

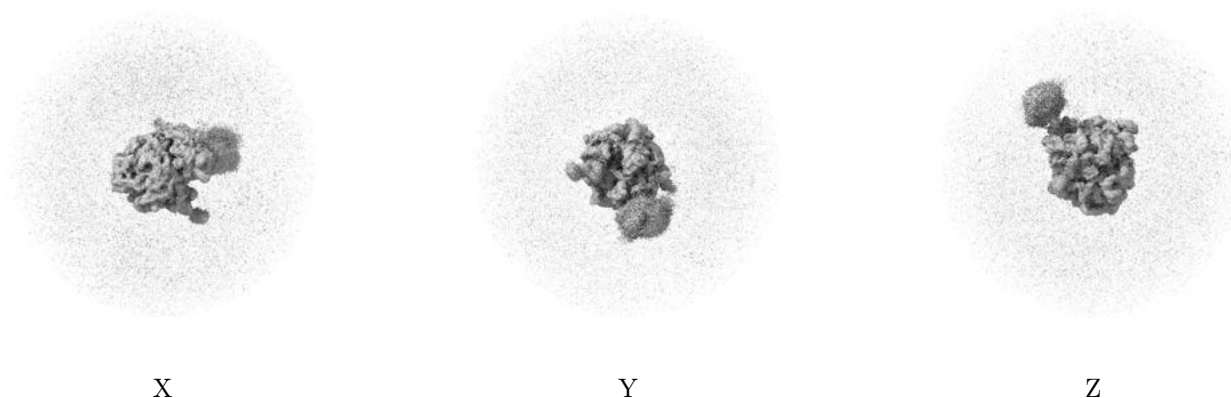
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

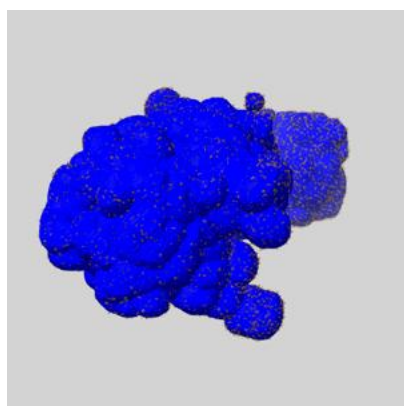
## 6.6 Mask visualisation [i](#)

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

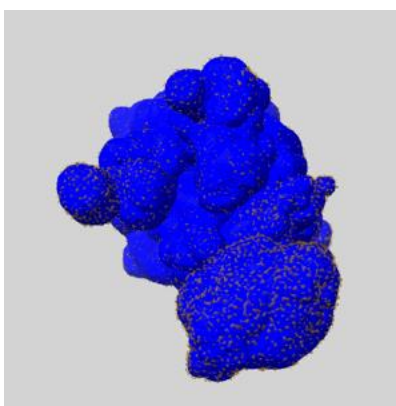
A mask typically either:

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

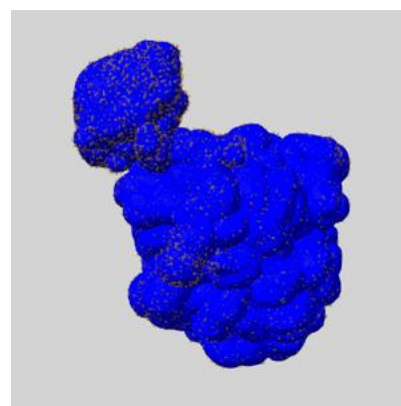
### 6.6.1 emd\_39168\_msk\_1.map [i](#)



X



Y

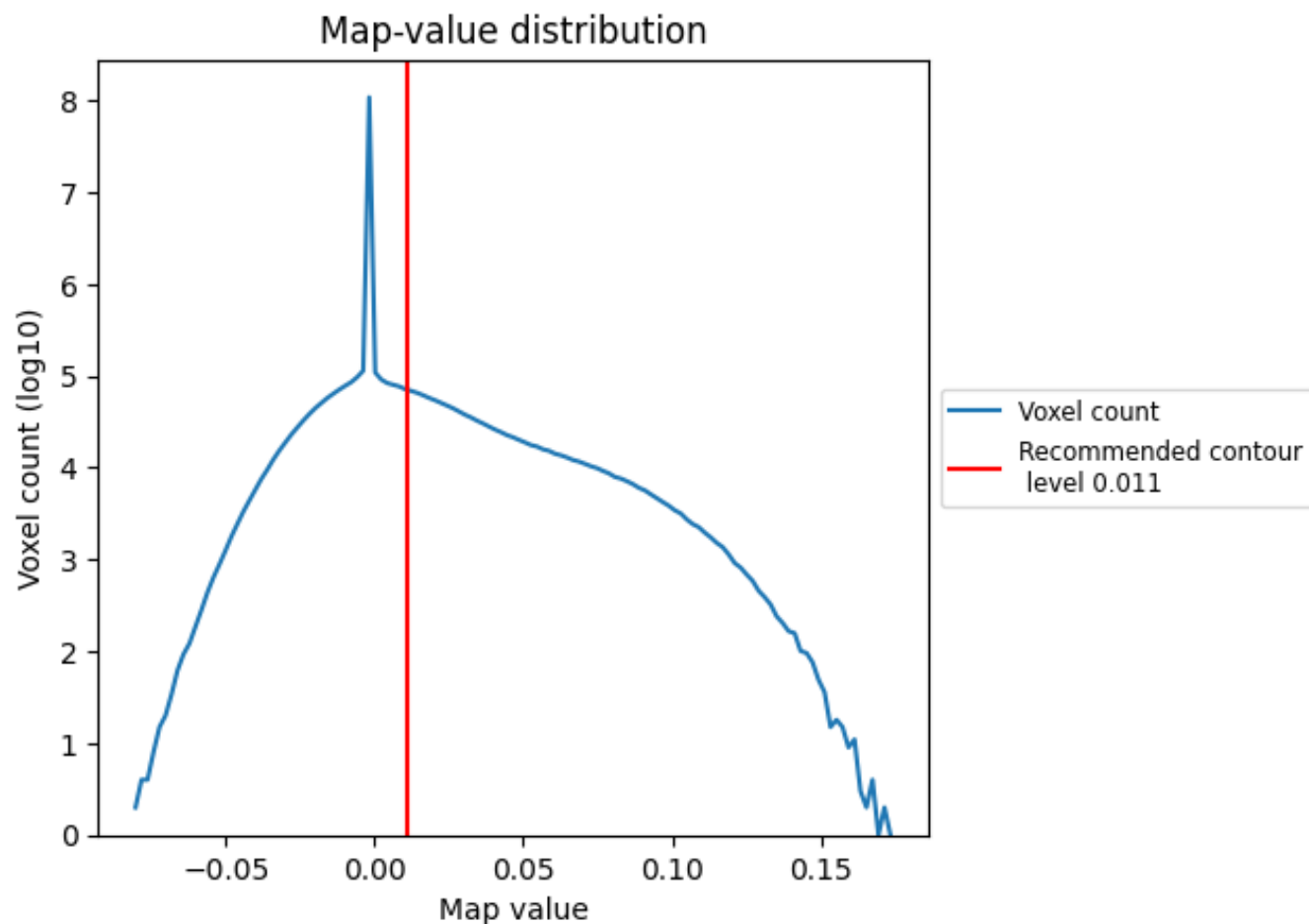


Z

## 7 Map analysis [i](#)

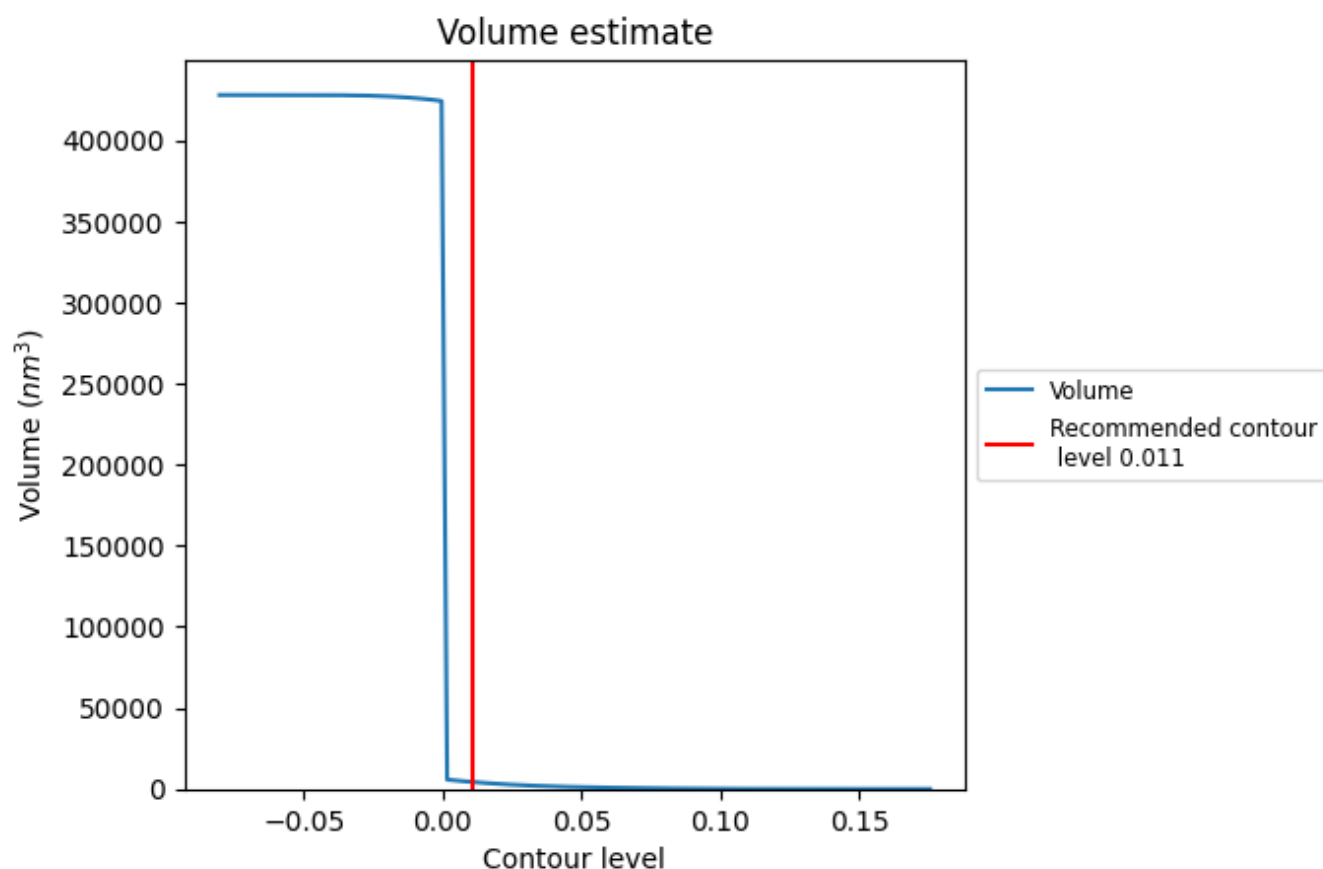
This section contains the results of statistical analysis of the map.

### 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.

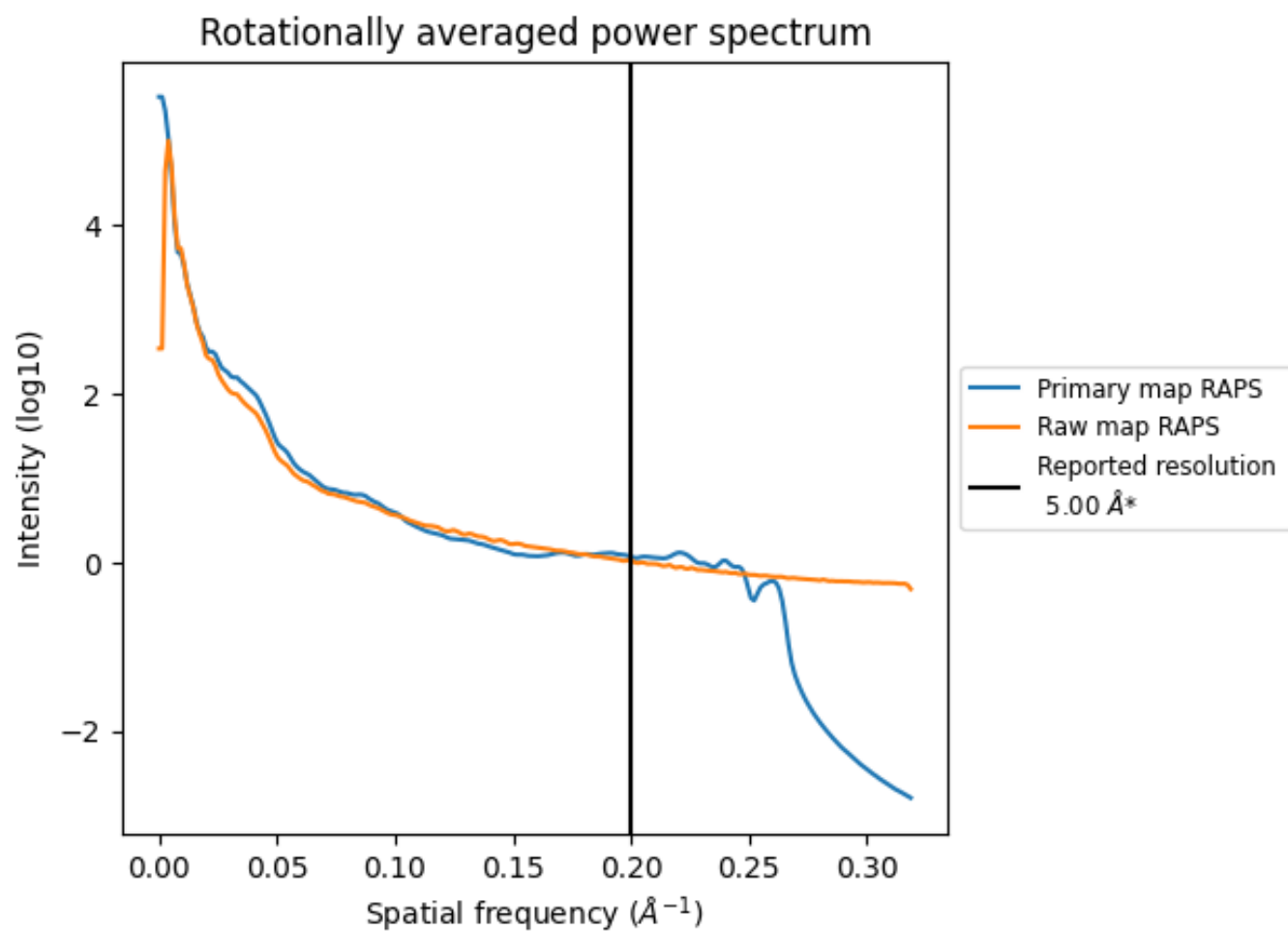
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4264  $\text{nm}^3$ ; this corresponds to an approximate mass of 3852 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



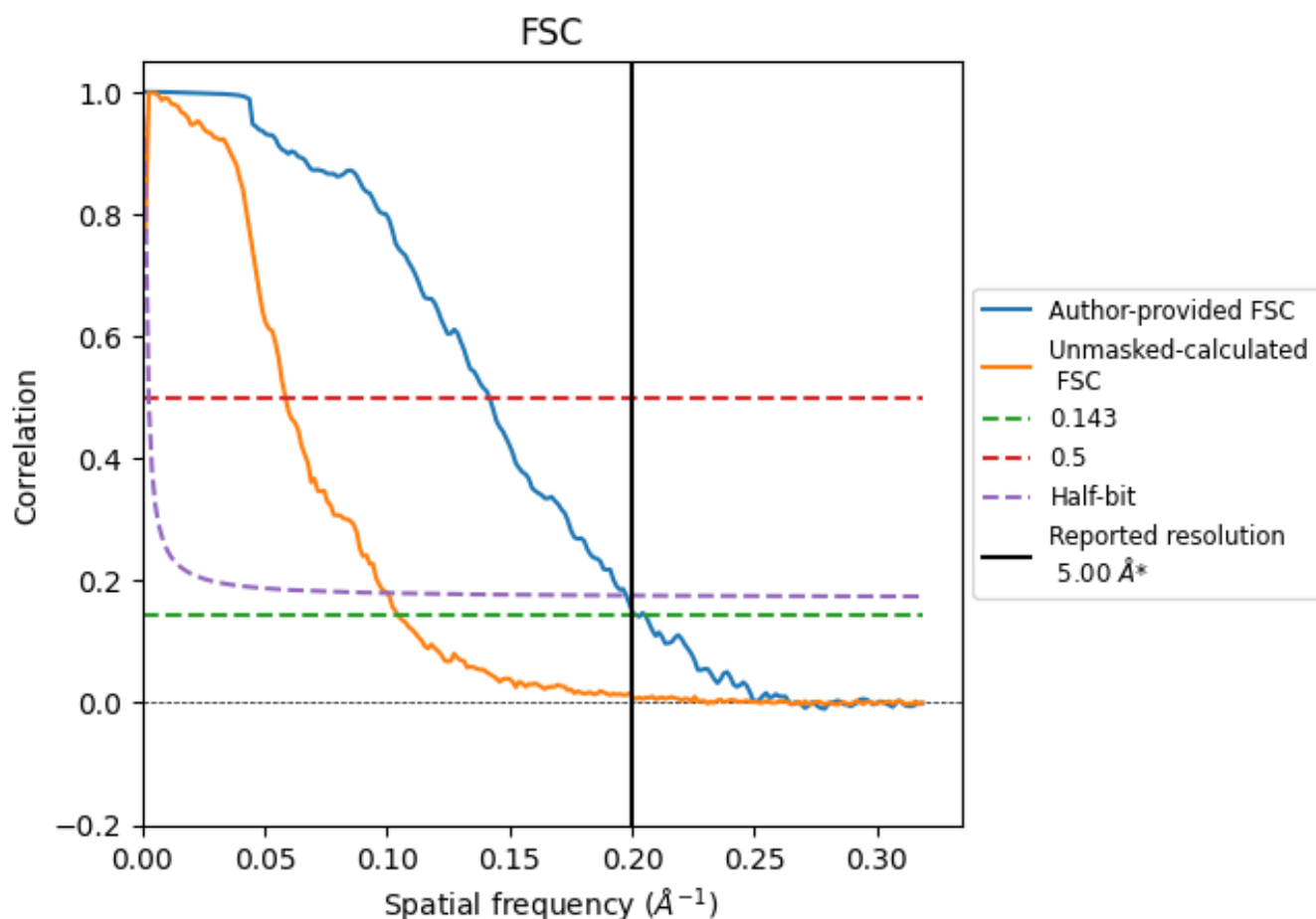
\*Reported resolution corresponds to spatial frequency of 0.200  $\text{\AA}^{-1}$



## 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 0.200  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

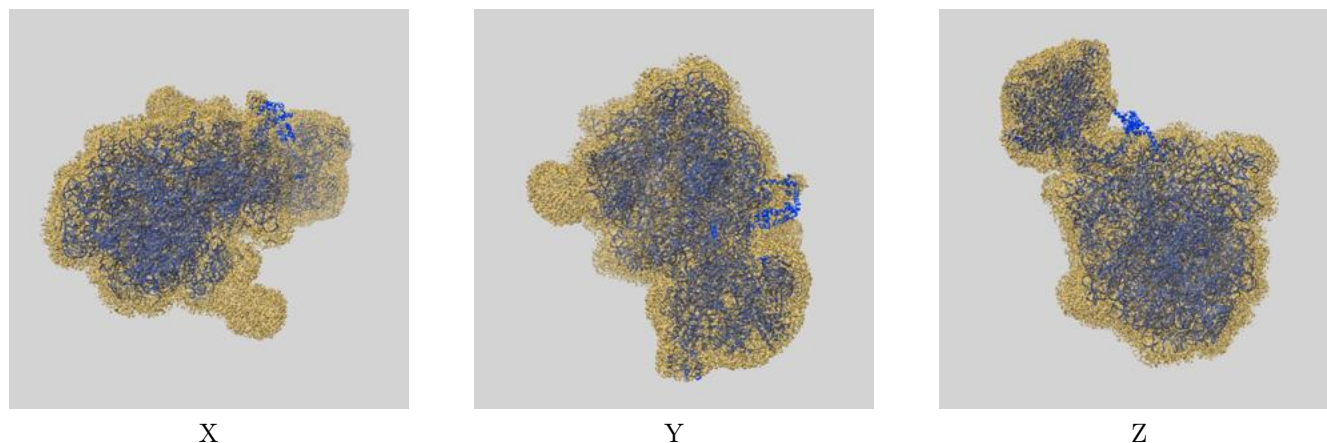
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.95	7.06	5.06
Unmasked-calculated*	9.57	17.09	666.67

\*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 9.57 differs from the reported value 5.0 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39168 and PDB model 8YDE. Per-residue inclusion information can be found in section 3 on page 16.

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



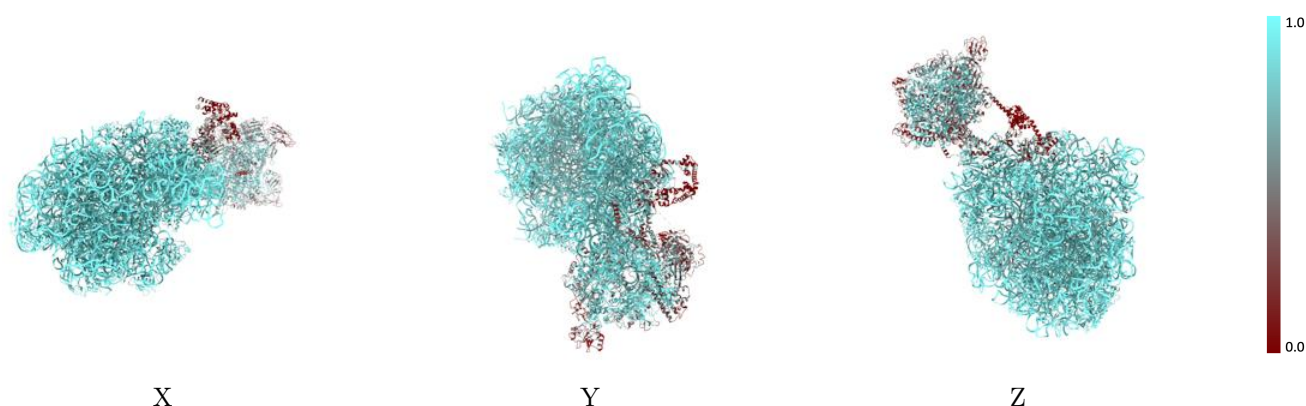
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



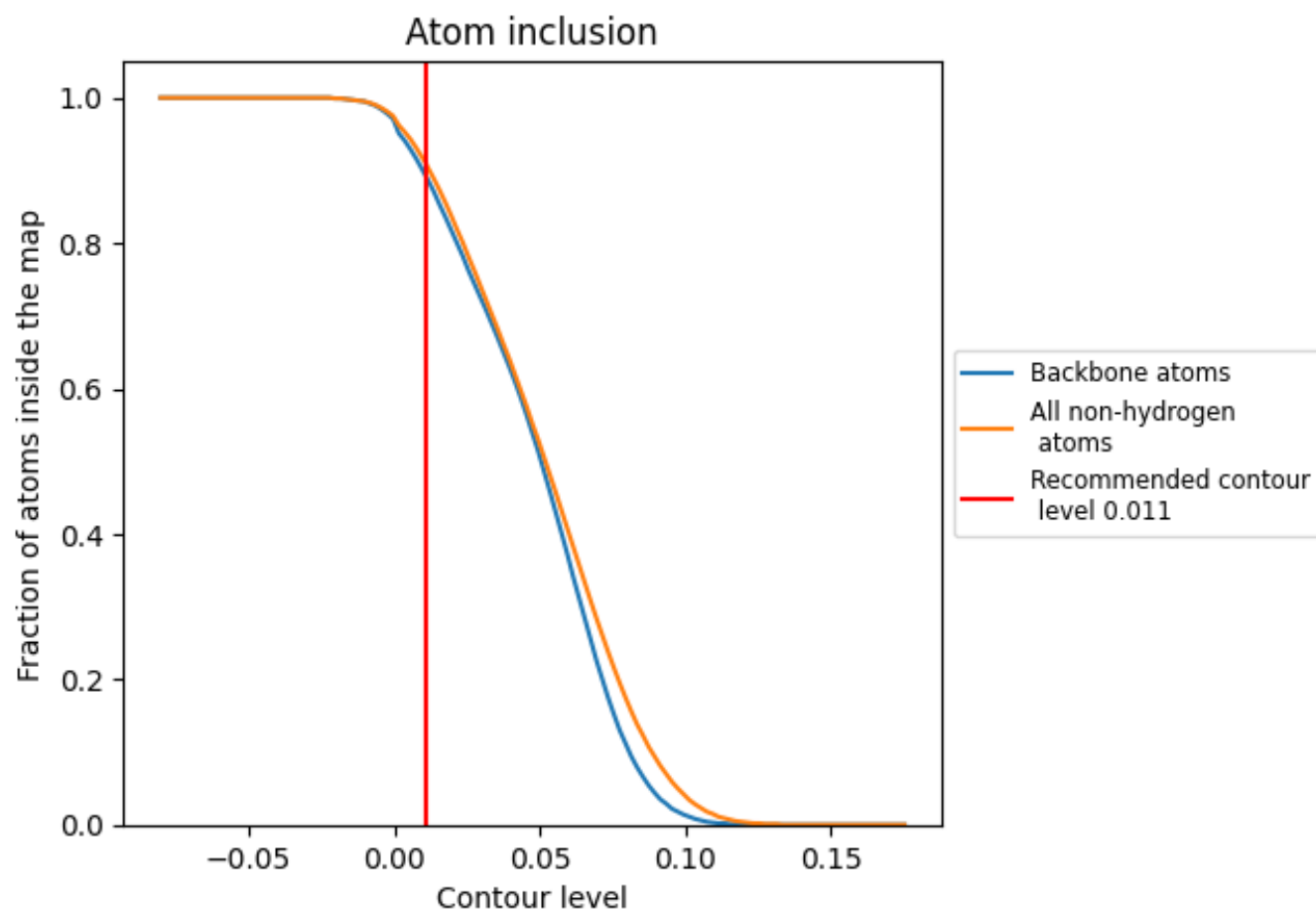
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



































































The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.2050
1	 0.9900	 0.2870
2	 0.9940	 0.2410
3	 0.9850	 0.2310
4	 0.7830	 0.0350
5	 0.9180	 0.0970
6	 0.9840	 0.2870
7	 0.7850	 0.0720
8	 0.8050	 0.0210
9	 0.7840	 0.0180
A	 0.8920	 0.1370
A1	 0.3580	 0.0100
A2	 0.3940	 0.0010
B	 0.9490	 0.2720
B1	 0.7120	 0.0000
B2	 0.6820	 -0.0070
C	 0.9350	 0.2470
D	 0.9410	 0.3120
E	 0.9450	 0.3080
F	 0.9490	 0.2430
G	 0.9190	 0.1650
H	 0.9080	 0.2190
I	 0.8090	 0.0590
J	 0.9300	 0.2570
K	 0.9350	 0.1620
L	 0.9340	 0.1930
M	 0.9450	 0.2460
N	 0.9640	 0.1760
NA	 0.3260	 0.0200
NG	 0.7490	 0.0140
O	 0.8940	 0.1390
P	 0.9390	 0.2150
Q	 0.8870	 0.1910
R	 0.9360	 0.1580
S	 0.9350	 0.2000



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Chain	Atom inclusion	Q-score
T	 0.9380	 0.2080
U	 0.8260	 0.0950
V	 0.8960	 0.1270
W	 0.9420	 0.1980
W0	 0.4180	 -0.0170
X	 0.9320	 0.1540
Y	 0.9030	 0.1380
Z	 0.8470	 0.1280
b	 0.9520	 0.3240
c	 0.9510	 0.2750
d	 0.9590	 0.2500
e	 0.9510	 0.2170
f	 0.9450	 0.1520
g	 0.9470	 0.1660
h	 0.9580	 0.2930
i	 0.8450	 0.0000
j	 0.9490	 0.2820
k	 0.8920	 0.2490
l	 0.9580	 0.2790
m	 0.9320	 0.2880
n	 0.9490	 0.2520
o	 0.9710	 0.2180
p	 0.9110	 0.1910
q	 0.9580	 0.2990
r	 0.9690	 0.2980
s	 0.9320	 0.2810
t	 0.9210	 0.1940
u	 0.9670	 0.2250
v	 0.9500	 0.2270
w	 0.9460	 0.2820
x	 0.9500	 0.3090
y	 0.9520	 0.1600
z	 0.9660	 0.2910