



## wwPDB EM Validation Summary Report ⓘ

Aug 18, 2025 – 03:09 PM JST

PDB ID : 8YDI / pdb\_00008ydi  
EMDB ID : EMD-39172  
Title : E.coli transcription translation coupling complex in TTC-P state 1 (subclass 2) 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 : 4.60 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

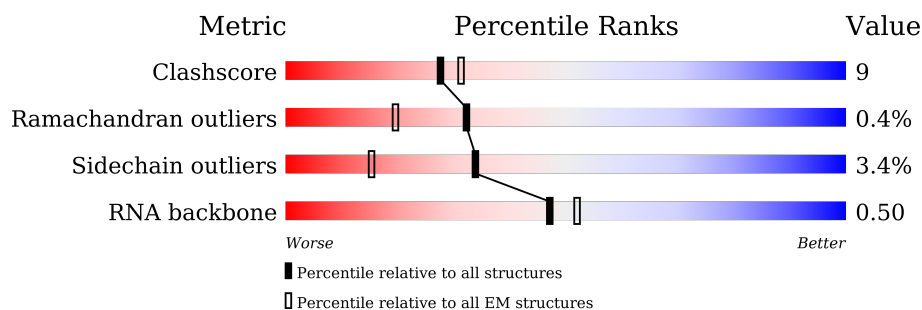
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 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.








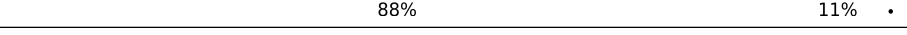

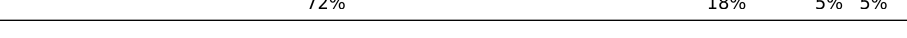
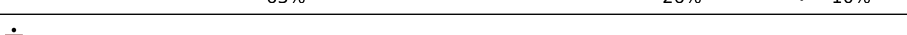
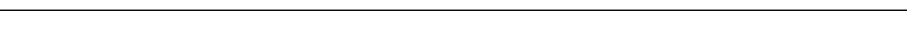















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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>7%</div> <div>81%</div> <div>13%</div> <div>6%</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>24%</div> </div>
5	E	65	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
6	F	38	<div> <div>66%</div> <div>32%</div> <div>.</div> </div>
7	G	241	<div> <div>67%</div> <div>22%</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	

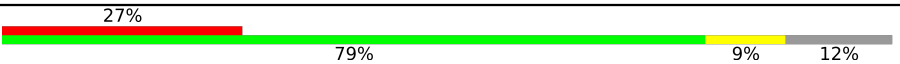

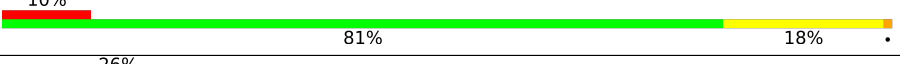
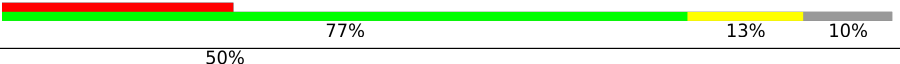
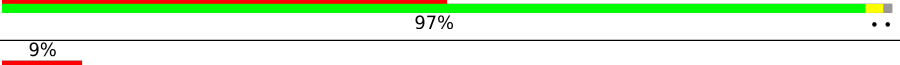
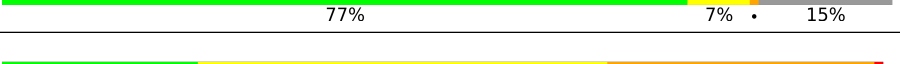
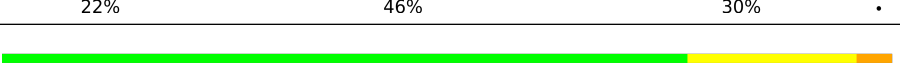
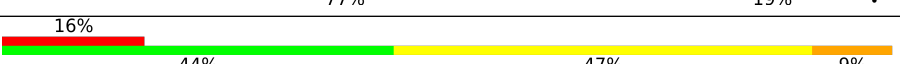


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Mol	Chain	Length	Quality of chain
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	
54	4	56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

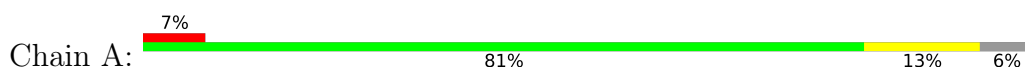
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

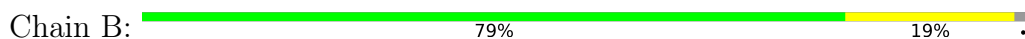
### 3 Residue-property plots [i](#)

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.

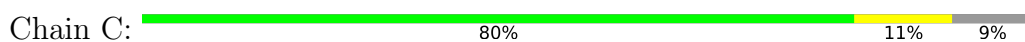
- Molecule 1: 50S ribosomal protein L31



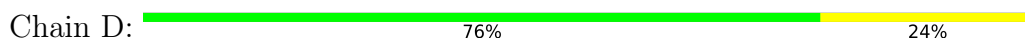
- Molecule 2: 50S ribosomal protein L32



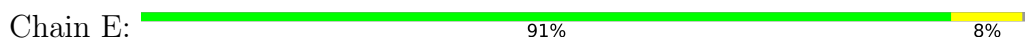
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34



- Molecule 5: 50S ribosomal protein L35



- Molecule 6: 50S ribosomal protein L36

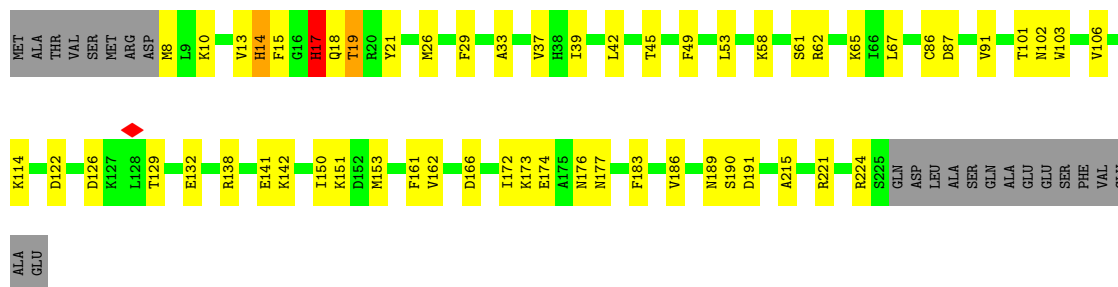


Chain F:  66% 32%



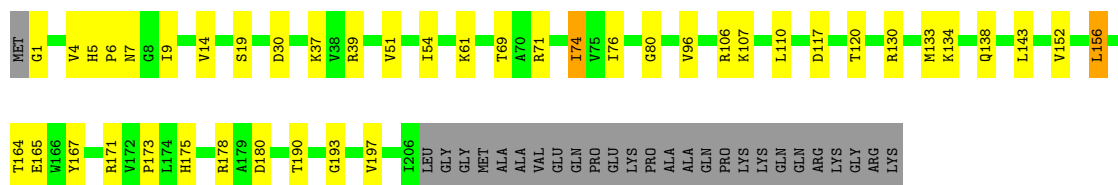
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% 10%




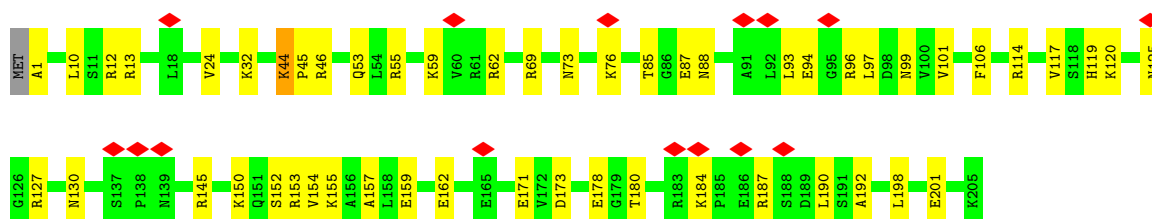
- Molecule 8: 30S ribosomal protein S3

Chain H:  70% 18% 12%




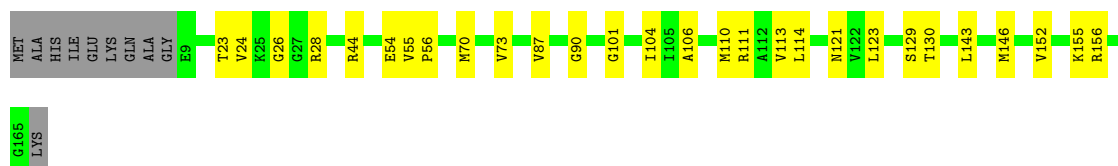
- Molecule 9: 30S ribosomal protein S4

Chain I:  7% 74% 25%



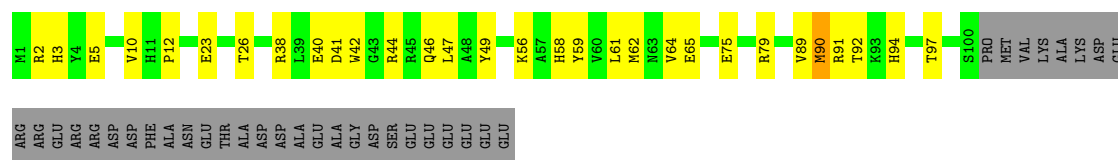
- Molecule 10: 30S ribosomal protein S5

Chain J:  77% 17% 6%



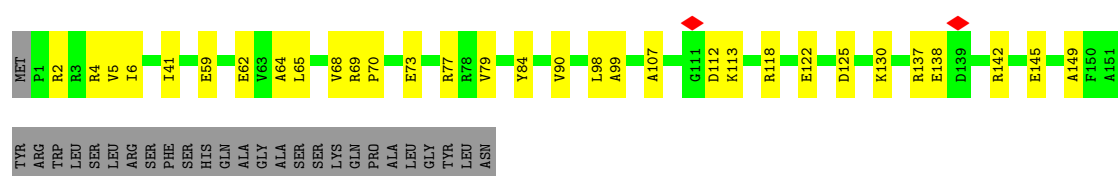
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  52% 21% 26%




- Molecule 12: 30S ribosomal protein S7

Chain L:  67% 17% 16%



- Molecule 13: 30S ribosomal protein S8

Chain M:  88% 11%



- Molecule 14: 30S ribosomal protein S9

Chain N:  66% 30%



- Molecule 15: 30S ribosomal protein S10

Chain O:  72% 18% 5% 5%



- Molecule 16: 30S ribosomal protein S11

Chain P:  63% 26% 10%





- Molecule 17: 30S ribosomal protein S12

Chain Q: 65% 32% ..



- Molecule 18: 30S ribosomal protein S13

Chain R: 69% 27% .



- Molecule 19: 30S ribosomal protein S14

Chain S: 86% 13% .



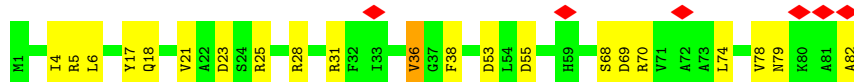
- Molecule 20: 30S ribosomal protein S15

Chain T: 84% 15% .



- Molecule 21: 30S ribosomal protein S16

Chain U: 7% 74% 24% .



- Molecule 22: 30S ribosomal protein S17

Chain V: 74% 21% 5%



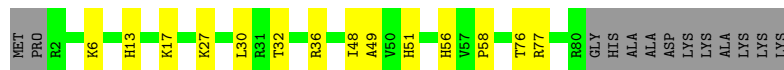
- Molecule 23: 30S ribosomal protein S18

Chain W:  65% 20% 13%




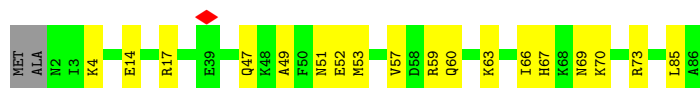
- Molecule 24: 30S ribosomal protein S19

Chain X:  71% 15% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  77% 21% 2%




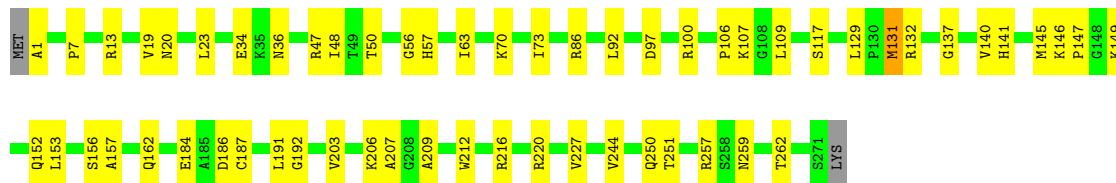
- Molecule 26: 30S ribosomal protein S21

Chain Z:  58% 32% 8%




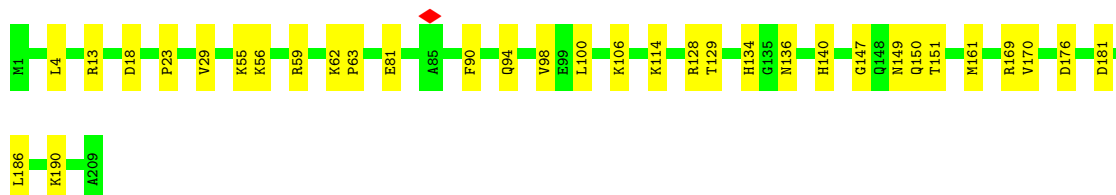
- Molecule 27: 50S ribosomal protein L2

Chain b:  78% 21% 1%

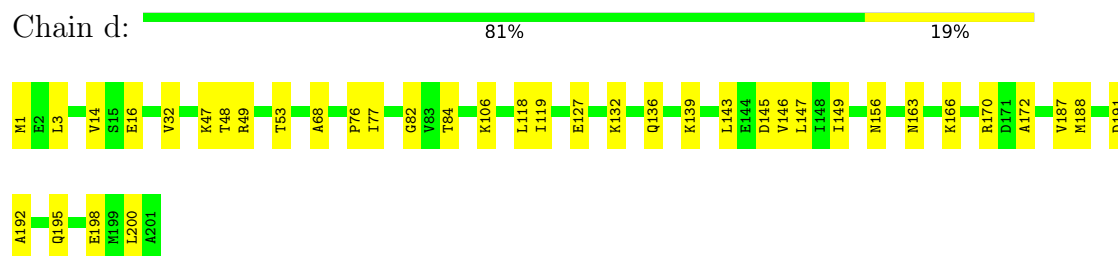


- Molecule 28: 50S ribosomal protein L3

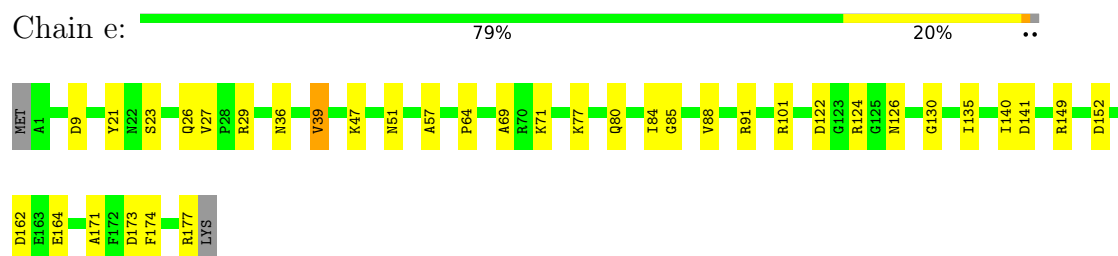
Chain c:  84% 16%



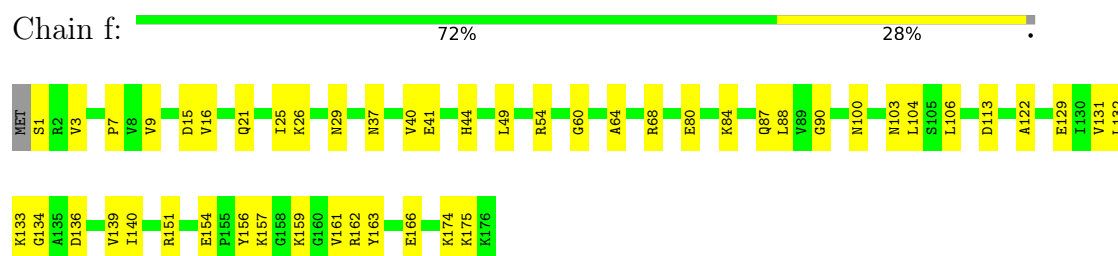
- Molecule 29: 50S ribosomal protein L4



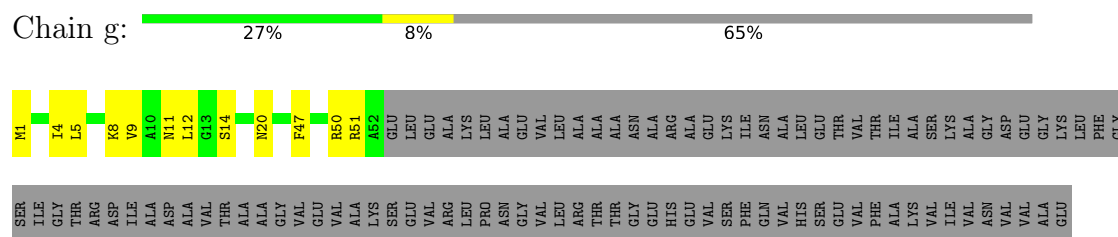
- Molecule 30: 50S ribosomal protein L5



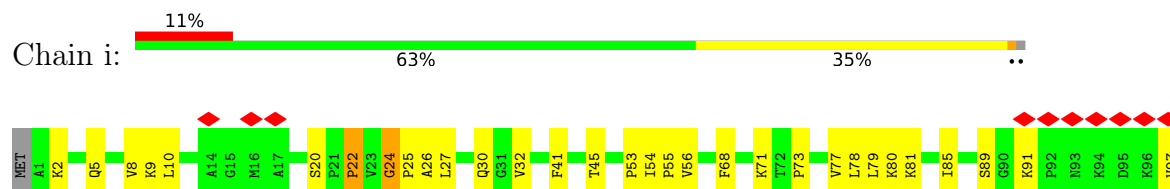
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

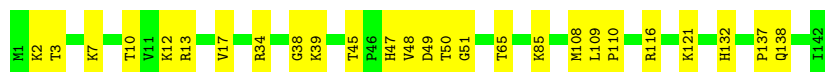
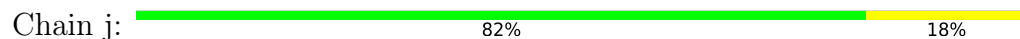


- Molecule 33: 50S ribosomal protein L11

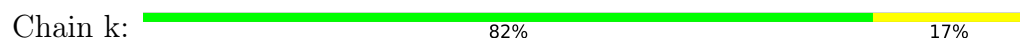




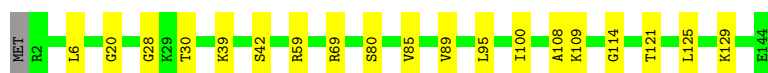
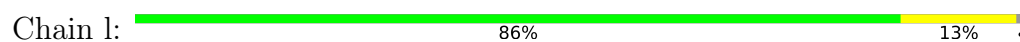
- Molecule 34: 50S ribosomal protein L13



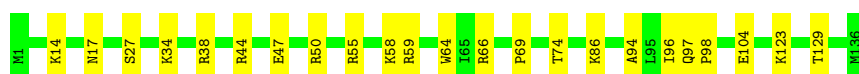
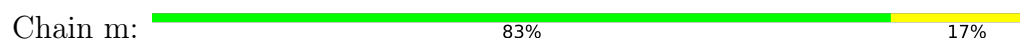
- Molecule 35: 50S ribosomal protein L14



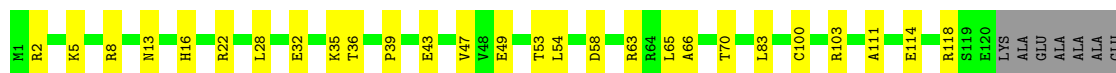
- Molecule 36: 50S ribosomal protein L15



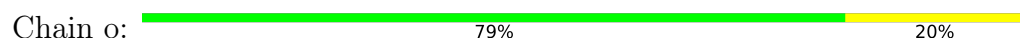
- Molecule 37: 50S ribosomal protein L16



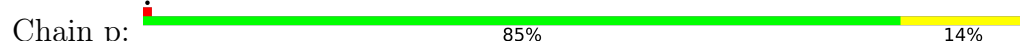
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19





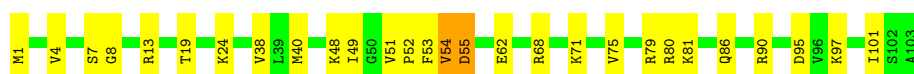
- Molecule 41: 50S ribosomal protein L20

Chain q: 83% 15% ..



- Molecule 42: 50S ribosomal protein L21

Chain r: 73% 25% .



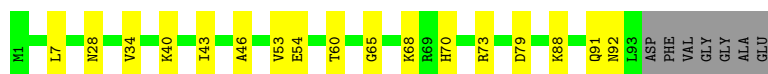
- Molecule 43: 50S ribosomal protein L22

Chain s: 85% 15%



- Molecule 44: 50S ribosomal protein L23

Chain t: 76% 17% 7%



- Molecule 45: 50S ribosomal protein L24

Chain u: 72% 26% .



- Molecule 46: 50S ribosomal protein L25

Chain v: 85% 14% .

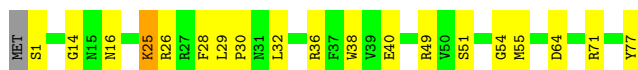


- Molecule 47: 50S ribosomal protein L27

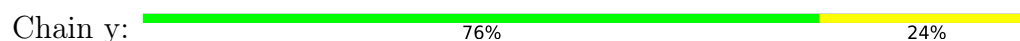
Chain w: 74% 14% 12%



• Molecule 48: 50S ribosomal protein L28



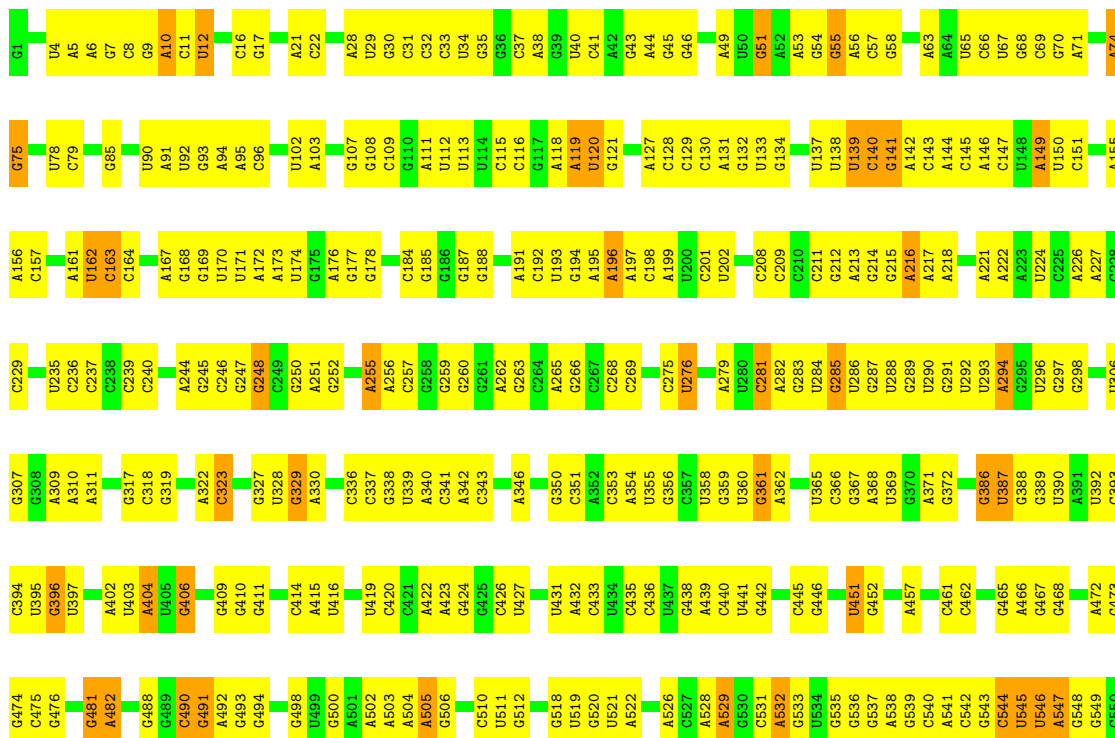
• Molecule 49: 50S ribosomal protein L29



• Molecule 50: 50S ribosomal protein L30



• Molecule 51: 23S rRNA




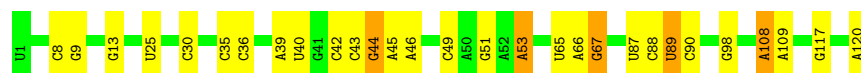


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G1581	G1581	G1516	G1436	C1346	C1278	U1183	U1113	A1054	A973	C888	U811	C719	C633	G553
A1583	A1583	C1517	C1437	A1347	G1279	U1184	C1114	G1055	C890	C889	C812	A718	C634	U554
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G1521	G1521	U1520	G1441	U1352	U1283	C1119	U1119	U1059	A893	C893	A819	C723	G638	U558
A1522	A1522	U1521	U1442	C1365	G1284	U1190	G1120	U1060	A894	U894	A819	C724	G639	U559
C1523	C1523	U1522	G1448	A1366	A1285	G1193	G1121	U1061	C982	U895	A821	G725	C640	U562
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C1526	C1526	C1451	C1451	G1368	G1288	G1197	G1131	C1064	C985	U899	U826	G728	C645	U567
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	G2846	G2763	G2529	A2602	G2429	A2351	A2281	U2194	A2126	U2034	C1942	G1869	A1786
	U2847	A2764	C2517	A2602	G2430	A2352	C2282	U2195	G2127	G2035	U1943	G1870	A1787
	G2848	A2765	A2518		A2431	C2347	C2275	C2196	G2128	A2037	U1944	A1871	C1788
	U2849		G2525	U2609	U2432	U2348	C2278	U2197	C2129		G1945	A1872	G1789
	A2850	U2768	G2526	C2610	A2433	G2349	A2278	A2198	U2130	C2043	G1948	A1873	C1790
	A2851		U2527	G2611	G2434	A2350	G2279	A2199	U2131		A1952	G1874	
	G2852	C2773	U2528	U2612	A2435	G2351	G2280	C2200	U2132	C2047	A1953	C1795	A1794
	C2853		G2529	U2613	G2436	A2352	A2281	G2201	G2133	G2048	A1954	U1796	C1795
			A2530		G2437	A2352	C2282	U2202	A2134	G2049	A1955	U1797	U1796
			U2533	U2617		G2360	C2283	U2203		C2050	U1956	U1798	
	U2701		A2534	G2618	C2440	G2361	C2284	U2204	G2137	A2051	C1955	G1882	
	G2702			C2619	U2441	G2362	C2285	A2205	U2138	G2052	A1956	U1883	C1800
						G2363	C2286			G2053		G1884	A1801
	U2707		C2539	G2625	G2445	G2364	A2287	C2208	G2141	A2054	U1963	A1885	A1802
	G2708			C2626	G2446	G2365	A2288	G2209	G2144	G2055	G1964	U1886	
	G2709		G2545	G2627	G2447	G2366	G2289	U2210	C2145	G2056	C1965	G1887	G1807
	C2710		U2546	U2628	A2448	A2367	U2291	A2211	G2146	A2060	A1966	A1888	A1808
	A2711		A2547	U2629		C2368	U2292	U2212	A2147	G1968	C1967	A1889	A1809
	G2712			G2630	G2455		G2293	C2214	G2148		A1969	A1890	
	U2713		U2553	G2631	C2456	G2371	G2294	C2215	U2149	G2069	A1970	U1812	U1812
	G2714		U2554	A2632	U2457	U2372	G2295	G2216	C2150		U1971	G1813	G1813
			U2555	A2634	G2458		C2296	G2217	U2151		U1972	C1816	
	C2717		C2556	G2635	C2462	G2379	A2297	U2218	G2152	C2073		A1901	G1817
	G2718		G2557	U2636	C2463	A2381	A2298	G2219	C2153	U2074	A1978	C1902	U1818
	U2720		U2561	G2638	G2464	G2382	U2299	G2221	A2154	U2085		A1819	A1819
			U2562			G2383		C2222	U2155	U2086	G1983	U1820	
	C2723		U2563	G2642	C2467	U2384	U2302	G2223	G2156		G1984	G1905	
			A2564	G2643	A2468	C2385	G2303	G2224	G2157	C2091	C1985	G1906	
	A2726		A2565	G2644	A2469	A2386	G2304	A2225	A2158	U2092	C1986	G1907	A1821
			A2566	G2645	G2470	U2387	U2305	G2226	G2159	G2093	C1987	G1908	C1822
	G2729		G2567	U2646	A2471	A2388	C2306	A2227	C2160	A2094	C1990	G1909	C1823
						A2389			C2161	A2095	G1991	G1910	
	G2731		G2570	G2647		U2390	A2309	G2230	G2162	C2096	G1992	U1911	U1827
			U2571	G2648	A2476	G2391	C2310		A2163	A2097	U1993	A1912	G1828
	G2732		A2572	G2649		A2392	G2311	U2233	C2164	U2098		A1913	A1829
	A2733		U2573	G2650	A2482	G2393	U2312	G2234	C2165	U2099	C1997	C1914	C1832
	A2734		C2573		C2483								
	G2735		C2573										

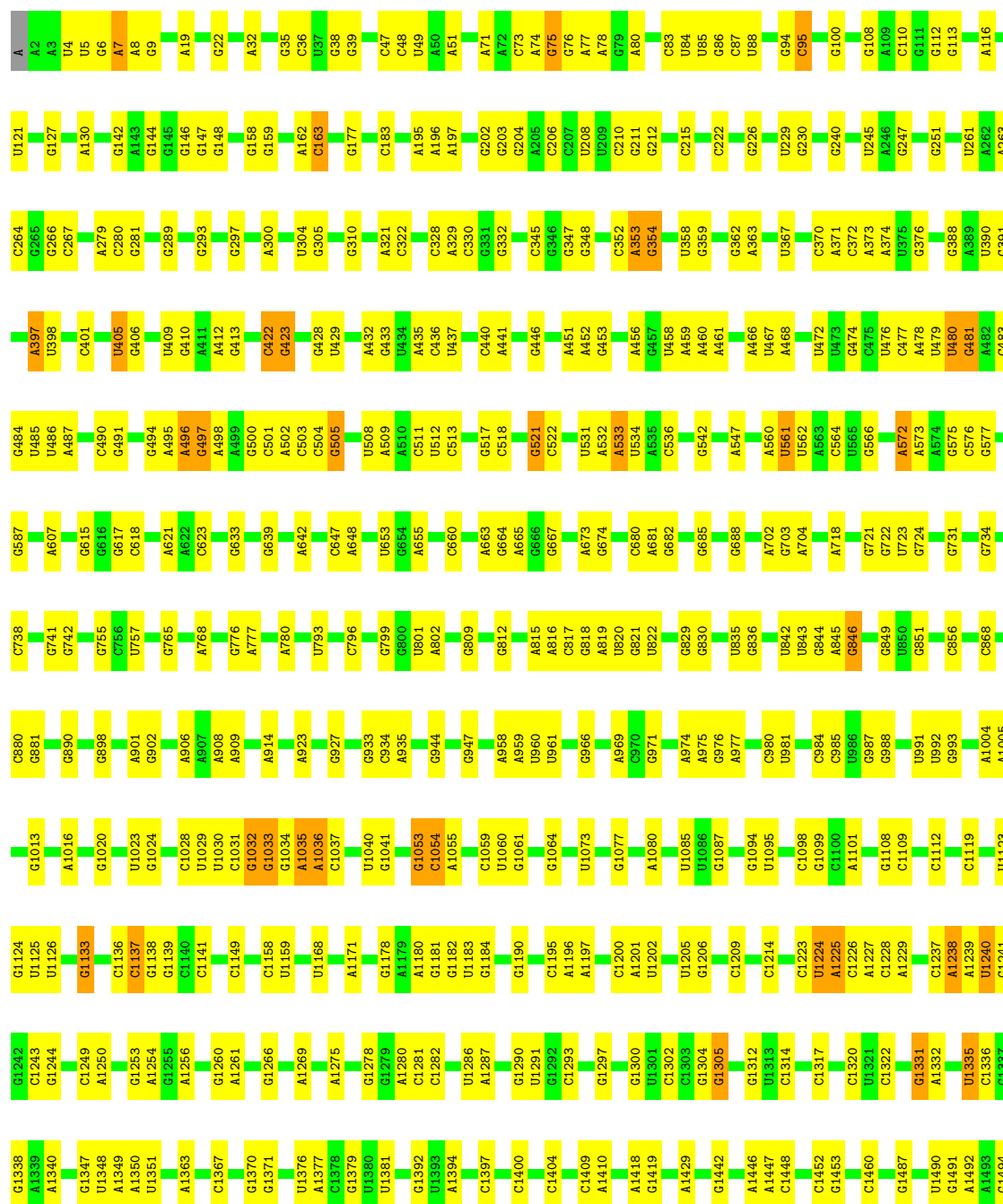
- Molecule 52: 5S rRNA

Chain 2:  76% 20%



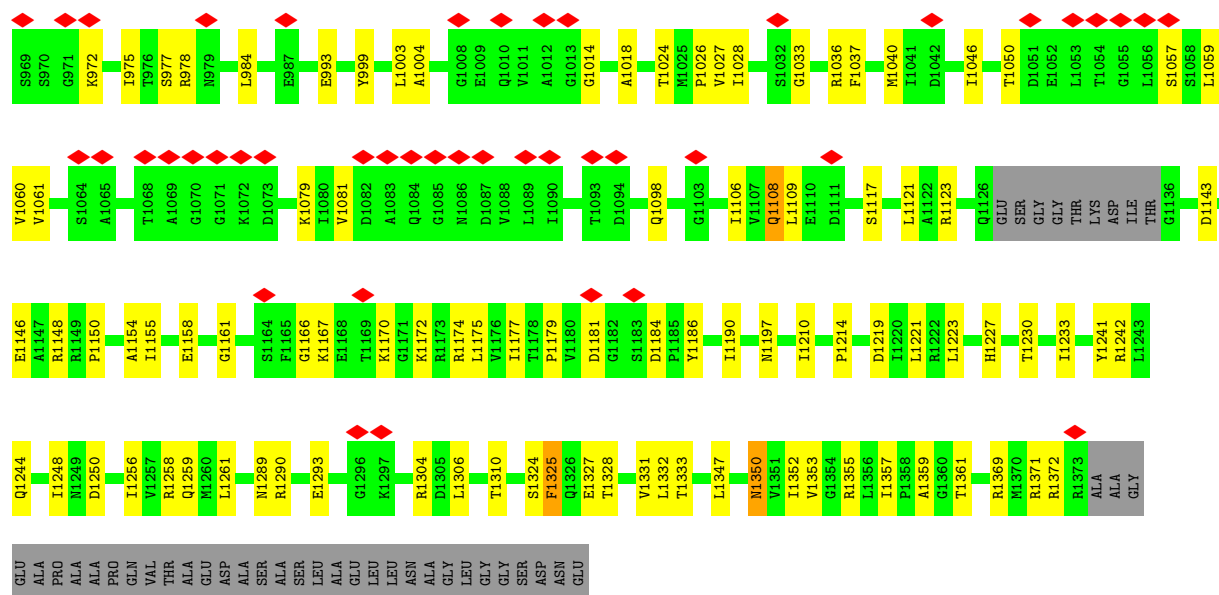
- Molecule 53: 16S rRNA

Chain 3:  68% 29%

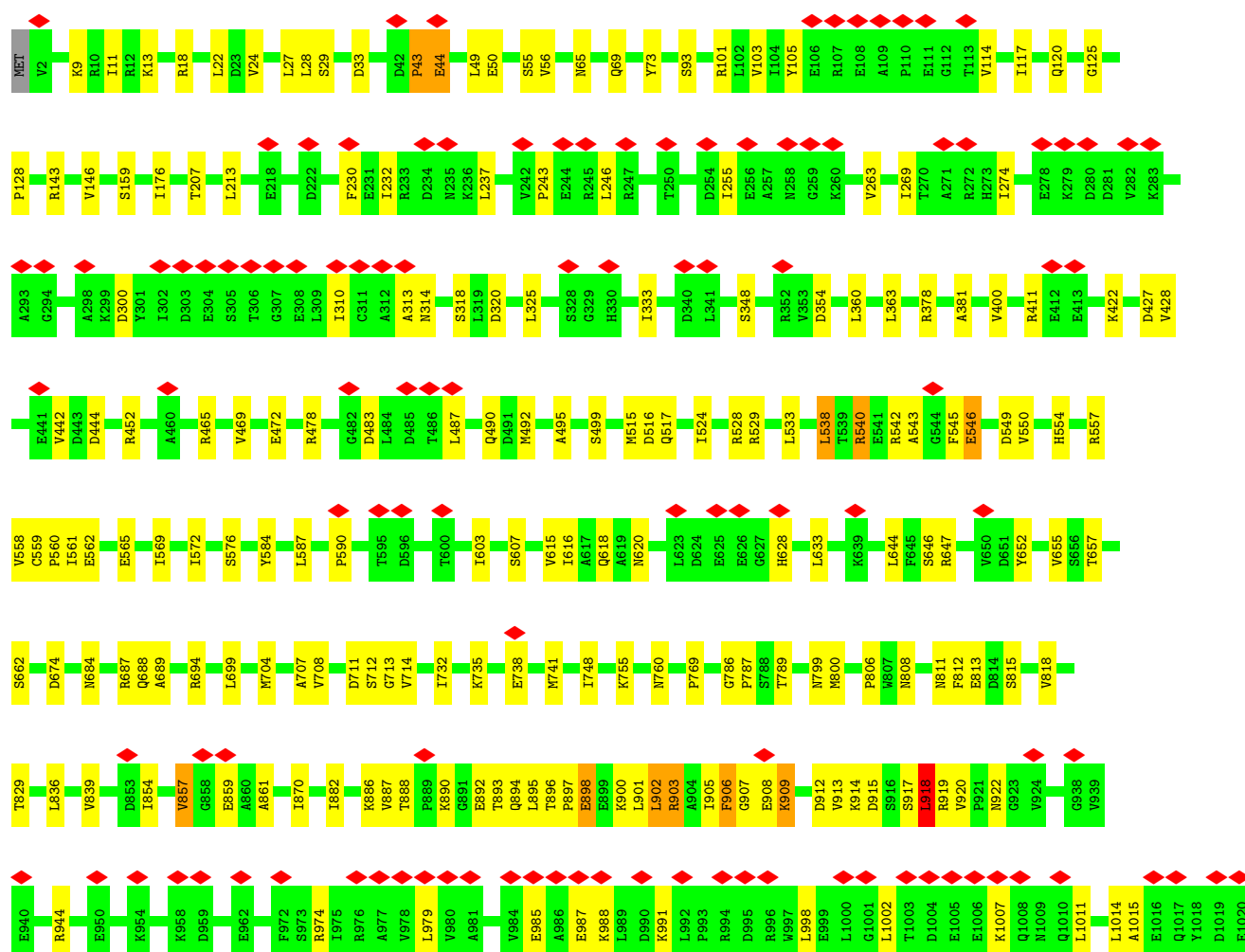
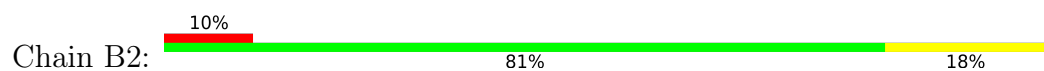


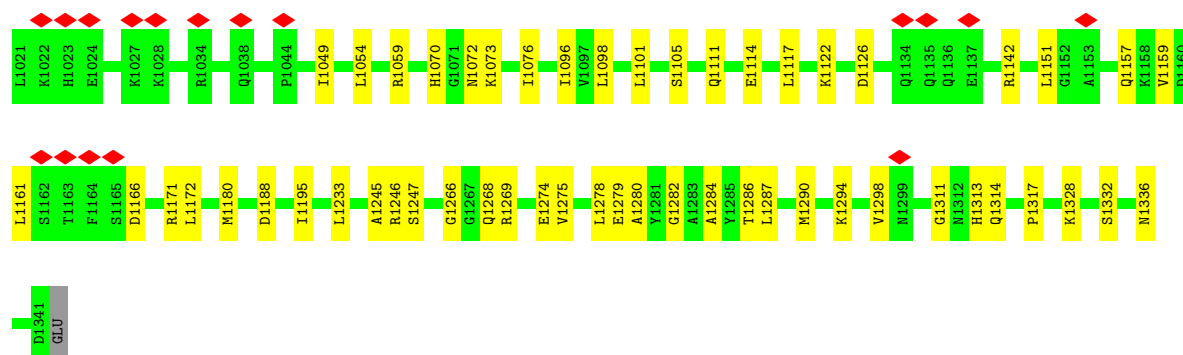




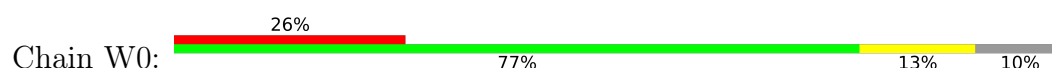


• Molecule 59: DNA-directed RNA polymerase subunit beta





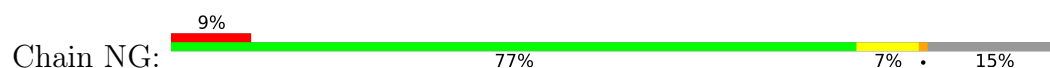
- Molecule 60: DNA-directed RNA polymerase subunit omega

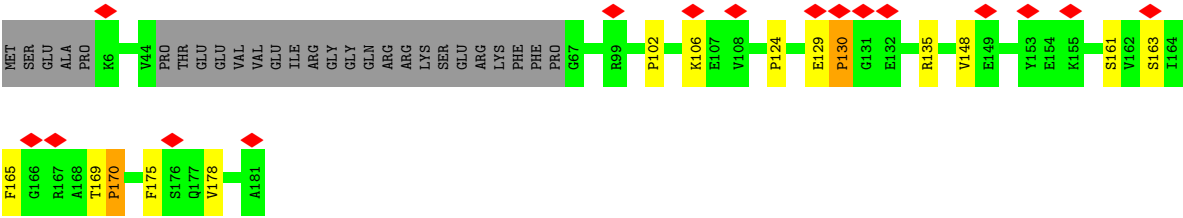


- Molecule 61: Transcription termination/antitermination protein NusA

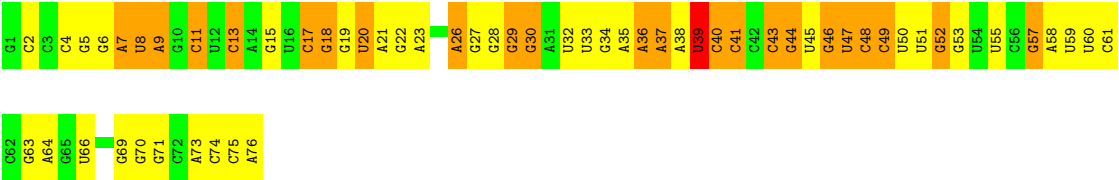
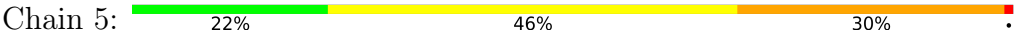


- Molecule 62: Transcription termination/antitermination protein NusG

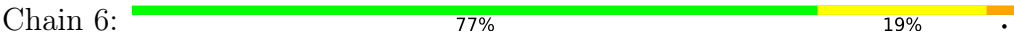




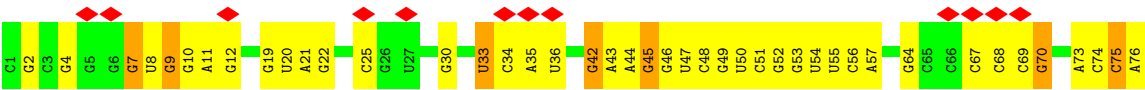
• Molecule 63: tRNA(Phe)



• Molecule 64: tRNA(fMet)



• Molecule 64: tRNA(fMet)



• Molecule 65: viomycin





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35000	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	0.161	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.012	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, 5OH, UAL, DPP, MG

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	0.26	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	0.69	0/498
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	0.66	3/1602 (0.2%)
13	M	0.35	0/989	0.53	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	0.33	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	0.64	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	0.37	0/1434	0.60	2/1926 (0.1%)
31	f	0.29	0/1343	0.55	0/1816
32	g	0.32	0/405	0.75	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	0.41	0/929	0.62	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	0.43	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	0.63	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	0.53	0/719
57	A1	0.55	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.57	6/10510 (0.1%)	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	0.84	0/2431	1.24	0/3385
62	NG	1.11	0/756	1.07	1/1048 (0.1%)
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%)	0.74	0/13
All	All	0.48	8/191576 (0.0%)	0.62	65/282857 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	3	SER	CA-C	-6.70	1.38	1.52
65	h	4	SER	CA-C	-6.18	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.28	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.17	1.33	1.23
58	B1	424	ASN	CG-ND2	-5.14	1.22	1.33

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	73	VAL	N-CA-C	-9.00	104.56	113.20
41	q	33	VAL	N-CA-C	-8.81	104.72	112.12
12	L	64	ALA	N-CA-C	-7.67	105.09	114.75
51	1	1130	U	C2'-C3'-O3'	7.59	120.88	109.50
64	7	33	U	C2'-C3'-O3'	7.25	120.38	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	2	0
6	F	302	0	343	7	0
7	G	1704	0	1732	35	0
8	H	1624	0	1699	29	0
9	I	1643	0	1710	32	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	9	0
14	N	1022	0	1070	24	0
15	O	786	0	828	14	0
16	P	869	0	878	22	0
17	Q	955	0	1019	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	883	0	944	18	0
19	S	805	0	847	9	0
20	T	714	0	737	6	0
21	U	649	0	666	16	0
22	V	648	0	691	9	0
23	W	535	0	552	9	0
24	X	637	0	665	9	0
25	Y	665	0	714	11	0
26	Z	544	0	579	11	0
27	b	2082	0	2157	46	0
28	c	1565	0	1616	29	0
29	d	1552	0	1619	28	0
30	e	1410	0	1447	23	0
31	f	1323	0	1374	33	0
32	g	400	0	423	6	0
33	i	1032	0	1088	42	0
34	j	1129	0	1162	22	0
35	k	938	0	1012	16	0
36	l	1045	0	1117	16	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	16	0
41	q	947	0	1022	10	0
42	r	816	0	839	18	0
43	s	857	0	922	11	0
44	t	738	0	807	9	0
45	u	779	0	834	14	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	11	0
50	z	449	0	491	9	0
51	1	62317	0	31346	1464	0
52	2	2568	0	1303	15	0
53	3	33012	0	16618	188	0
54	4	729	0	364	6	0
55	8	539	0	305	29	0
56	9	417	0	224	2	0
57	A1	2088	0	1895	25	0
57	A2	2029	0	1864	20	0
58	B1	10353	0	10548	322	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B2	10546	0	10550	169	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	9	0
62	NG	758	0	334	9	0
63	5	1622	0	821	28	0
64	6	1640	0	837	7	0
64	7	1640	0	837	20	0
65	h	48	0	40	9	0
66	B1	1	0	0	0	0
All	All	178130	0	126632	2826	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 2826 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	1.08
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	1.02
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%)	172 (85%)	30 (15%)	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%)	130 (87%)	19 (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	48
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%)	190 (92%)	17 (8%)	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%)	158 (91%)	16 (9%)	0	100	100
32	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	6	32
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	36
42	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	48
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	48
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%)	1203 (90%)	122 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1203 (90%)	131 (10%)	4 (0%)	37	72
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	469 (96%)	17 (4%)	4 (1%)	16	54
62	NG	150/181 (83%)	129 (86%)	14 (9%)	7 (5%)	2	17
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9586/10235 (94%)	8659 (90%)	888 (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

*Continued on next page...*



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Mol	Chain	Res	Type
61	NA	187	ARG
61	NA	188	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	49
6	F	34/34 (100%)	30 (88%)	4 (12%)	4	17
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	54
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	81
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	53
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	49
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	13
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
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	81
37	m	109/109 (100%)	103 (94%)	6 (6%)	18	40
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%)	99 (100%)	0	100	100
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
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%)	184 (99%)	2 (1%)	70	80
58	B1	1110/1168 (95%)	1018 (92%)	92 (8%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	B2	1150/1157 (99%)	1116 (97%)	34 (3%)	36	56
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7131 (97%)	250 (3%)	34	53

5 of 250 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	901	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
29	d	165	HIS
59	B2	314	ASN
36	l	99	ASN
59	B2	69	GLN
59	B2	1080	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	397 (13%)	16 (0%)
52	2	119/120 (99%)	17 (14%)	1 (0%)
53	3	1538/1542 (99%)	254 (16%)	5 (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%)	764 (15%)	33 (0%)

5 of 764 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A

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*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 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	48	C
63	5	57	G
64	7	56	C
51	1	1930	G
51	1	1801	A

## 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	0.08	0
65	5OH	h	6	65	8,12,13	0.76	0	3,16,18	1.51	1 (33%)
65	KBE	h	1	65	8,8,9	0.60	0	7,8,10	1.20	1 (14%)
65	UAL	h	5	65	7,8,9	2.32	3 (42%)	5,9,11	2.90	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	5OH	h	6	65	-	0/2/18/20	0/1/1/1
65	KBE	h	1	65	-	0/7/7/8	-

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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	-4.90	1.32	1.40
65	h	5	UAL	C-CA	-2.91	1.40	1.45
65	h	5	UAL	CA-N	2.04	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	-5.27	115.66	125.60
65	h	5	UAL	O-C-CA	-3.22	121.30	125.39
65	h	6	5OH	CR-CB-CA	-2.36	110.06	112.61
65	h	1	KBE	CB-CA-C	-2.06	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.

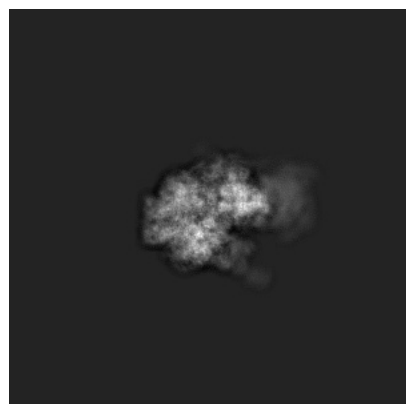
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39172. These allow visual inspection of the internal detail of the map and identification of artifacts.

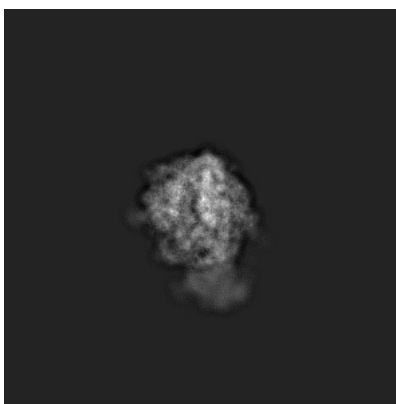
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

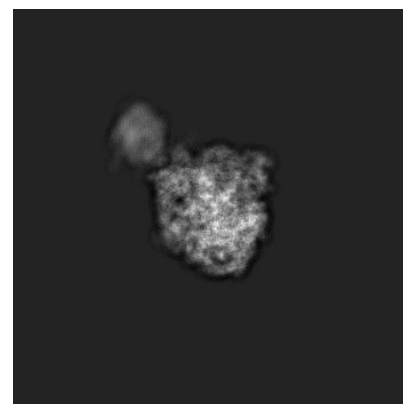
#### 6.1.1 Primary map



X

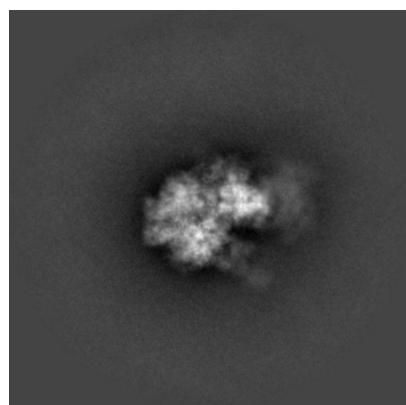


Y

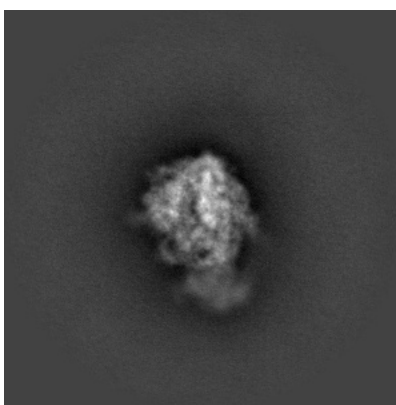


Z

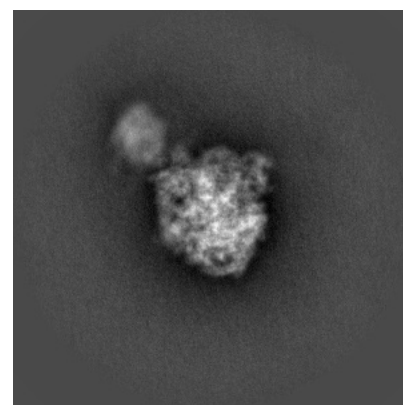
#### 6.1.2 Raw map



X



Y

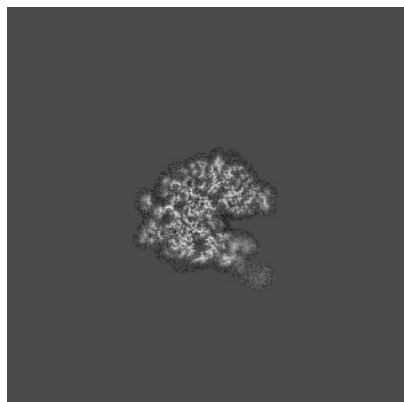


Z

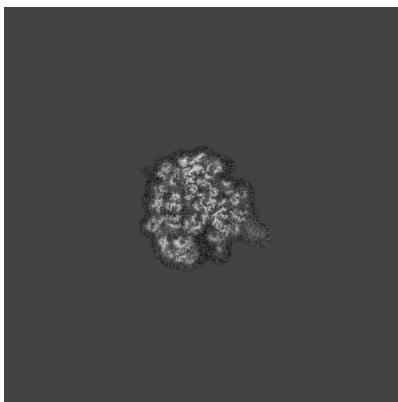
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

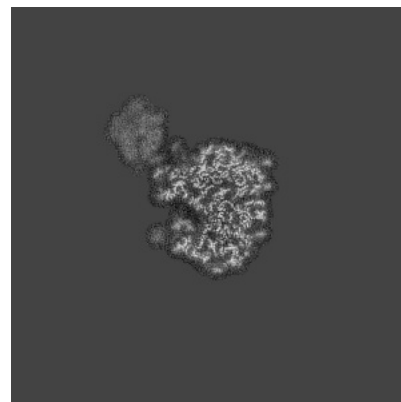
### 6.2.1 Primary map



X Index: 240

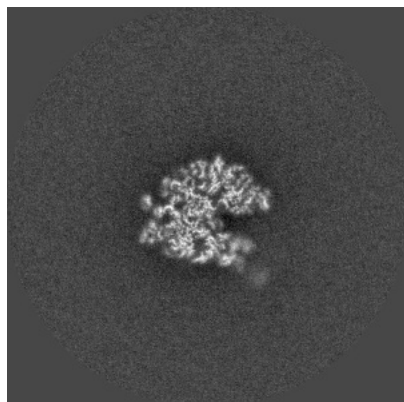


Y Index: 240

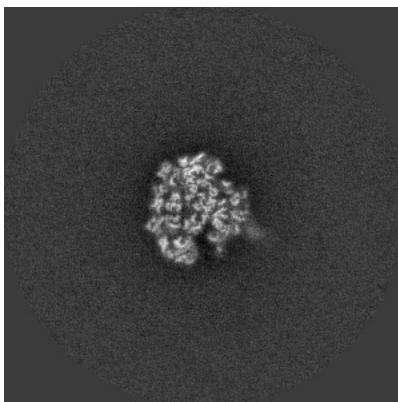


Z Index: 240

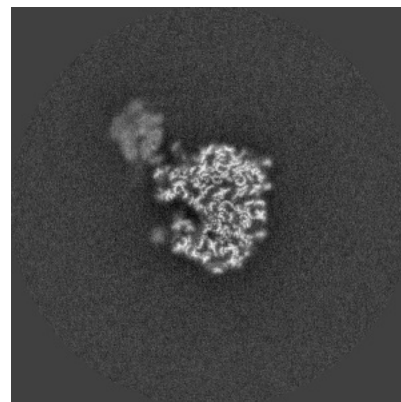
### 6.2.2 Raw map



X Index: 240



Y Index: 240



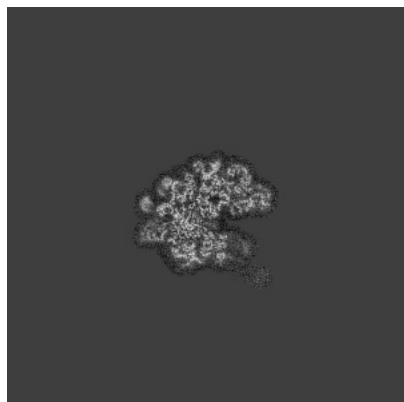
Z Index: 240

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

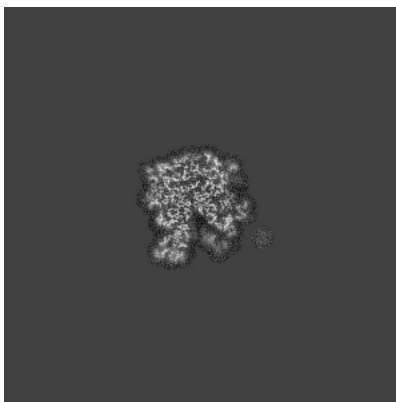


## 6.3 Largest variance slices [i](#)

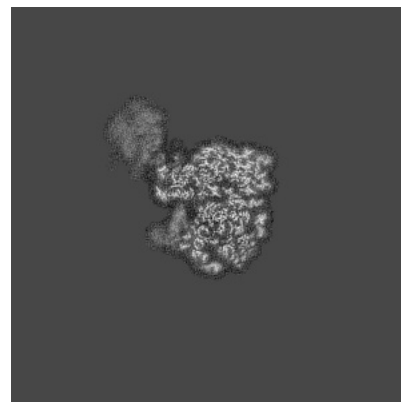
### 6.3.1 Primary map



X Index: 244

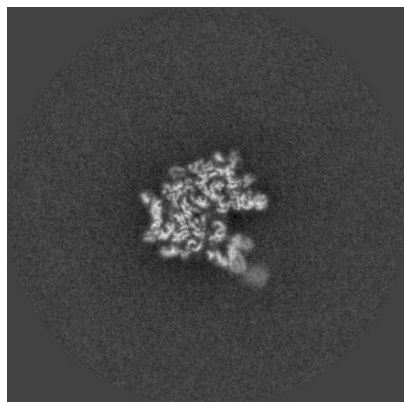


Y Index: 224

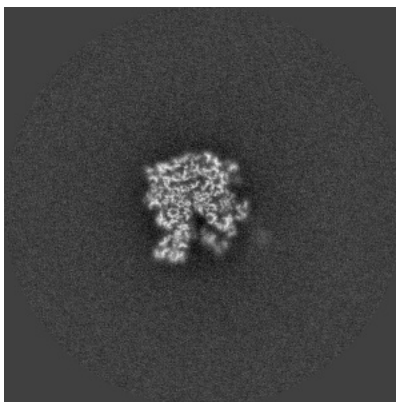


Z Index: 245

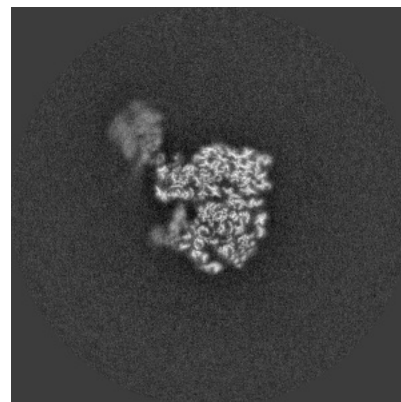
### 6.3.2 Raw map



X Index: 233



Y Index: 224

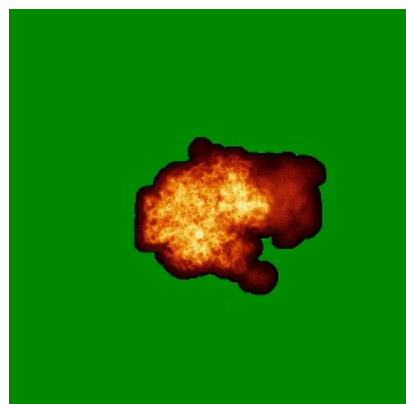


Z Index: 245

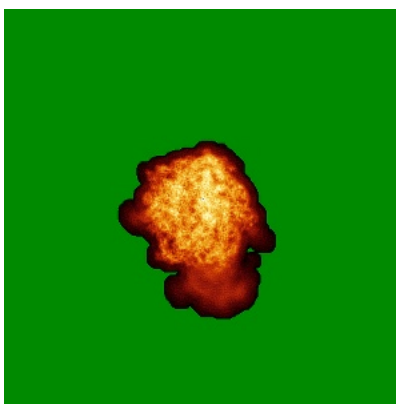
The images above show the largest variance slices of the map in three orthogonal directions.

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

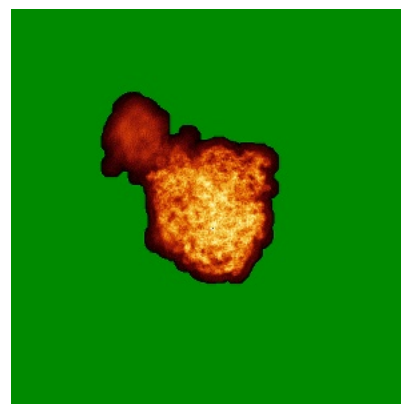
### 6.4.1 Primary map



X

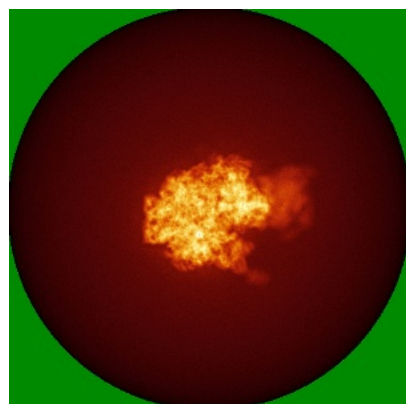


Y

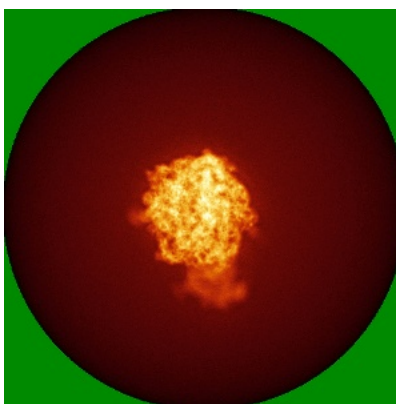


Z

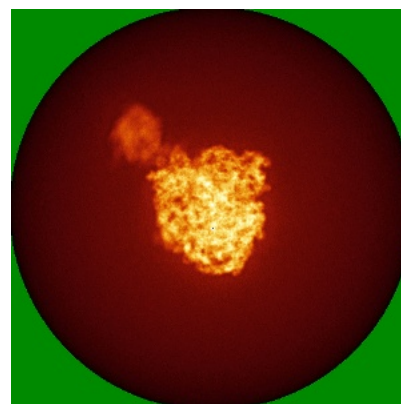
### 6.4.2 Raw map



X



Y

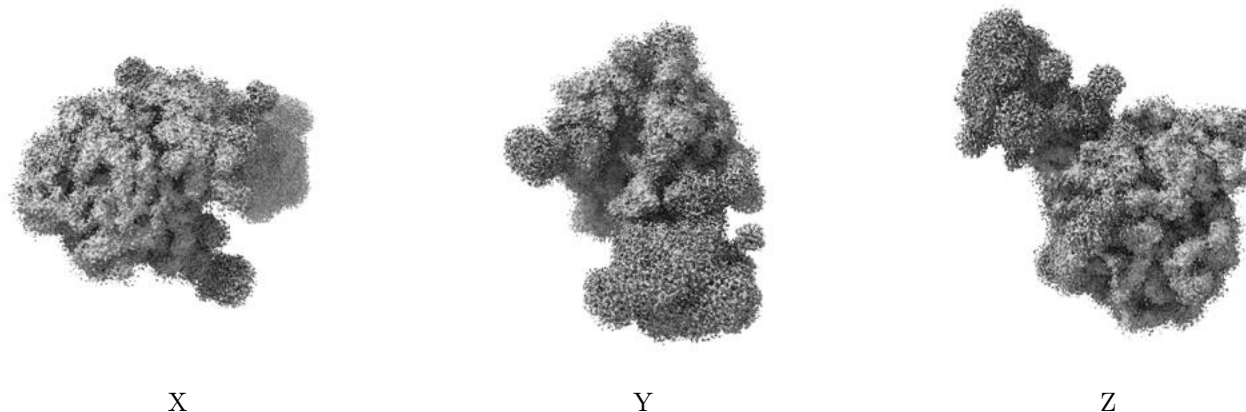


Z

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.

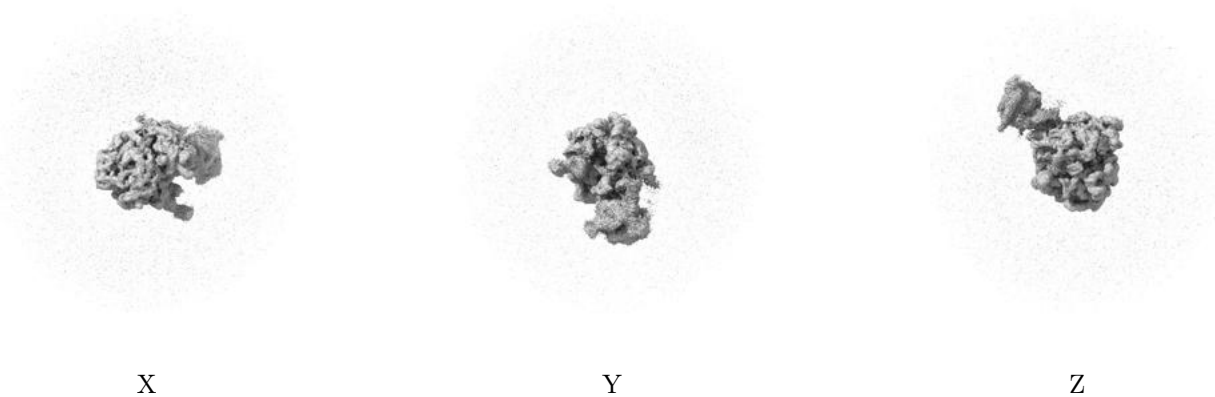
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

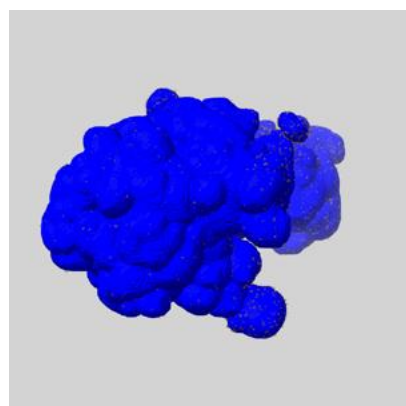
## 6.6 Mask visualisation [i](#)

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

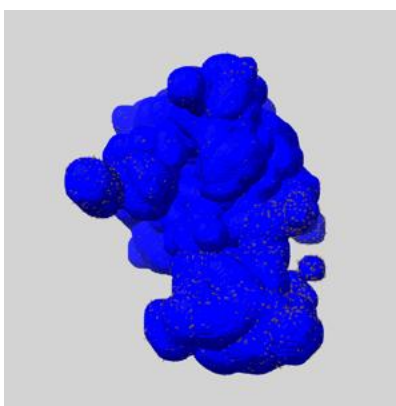
A mask typically either:

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

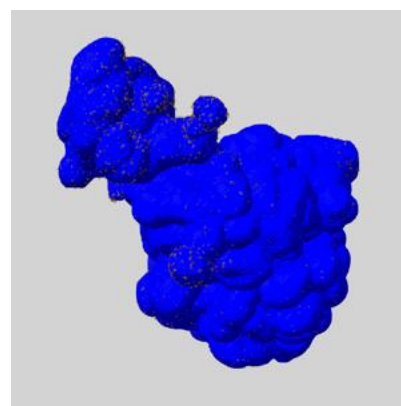
### 6.6.1 emd\_39172\_msk\_1.map [i](#)



X



Y

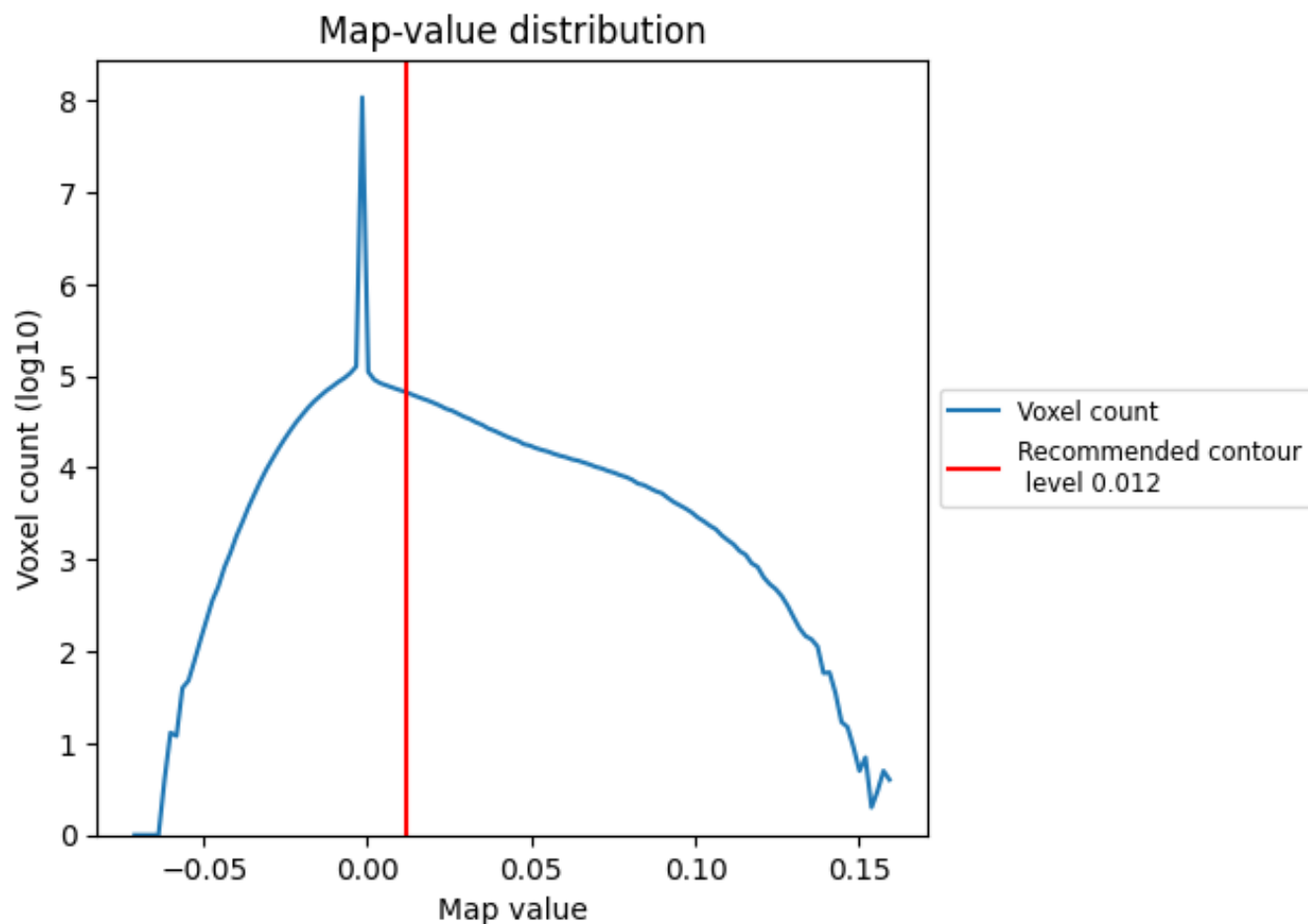


Z

## 7 Map analysis [i](#)

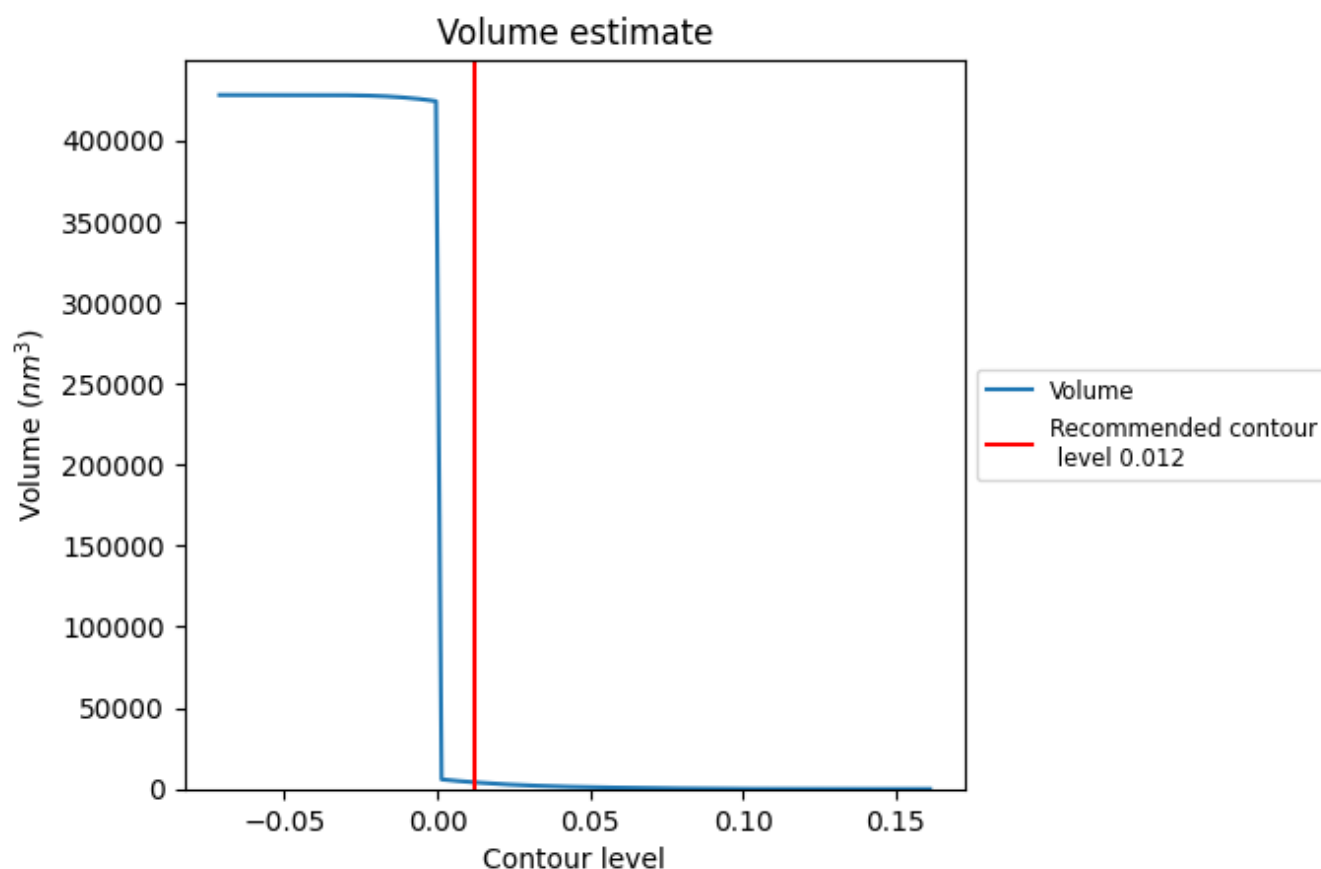
This section contains the results of statistical analysis of the map.

### 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.

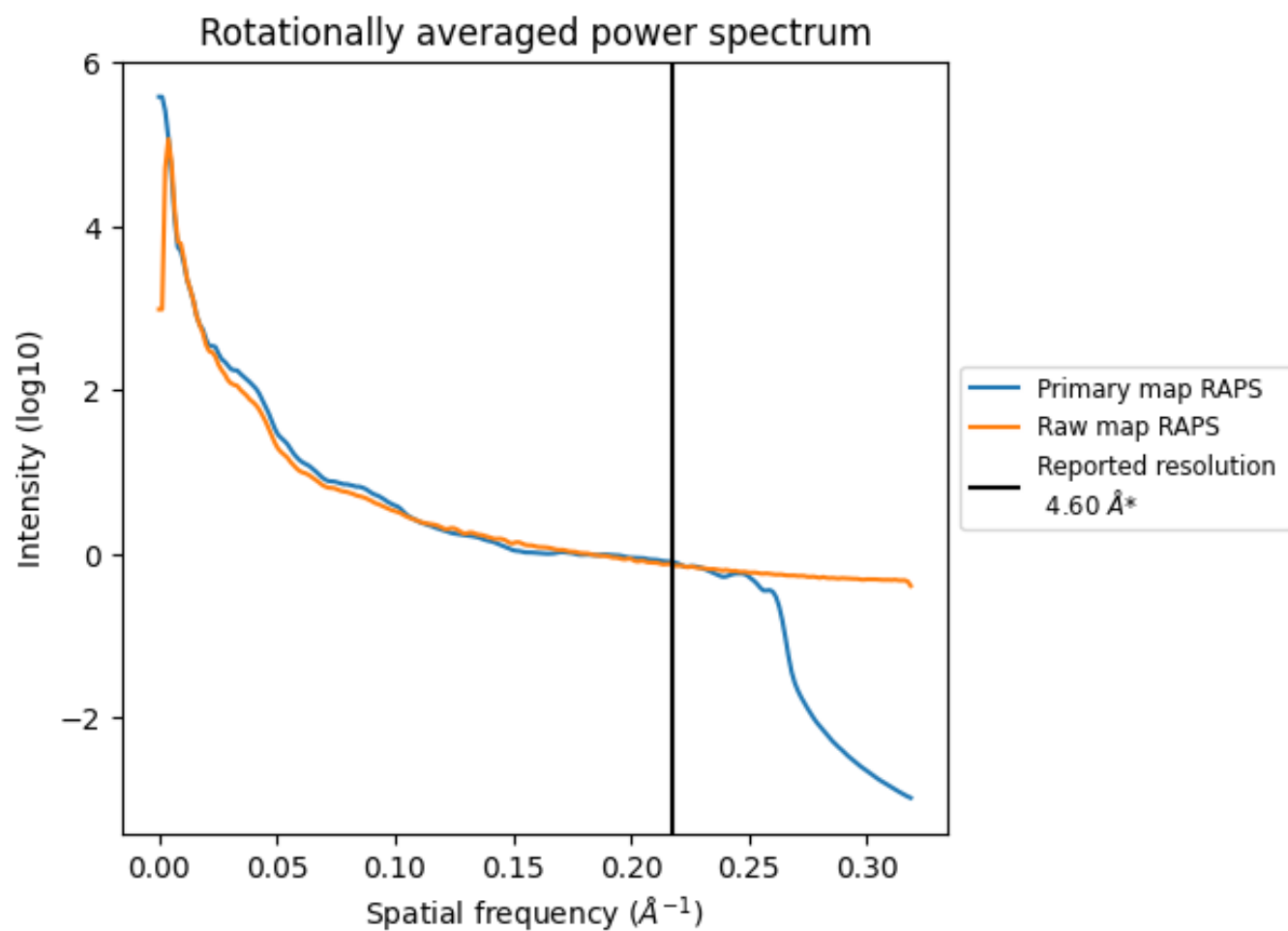
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4127  $\text{nm}^3$ ; this corresponds to an approximate mass of 3728 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 ⓘ

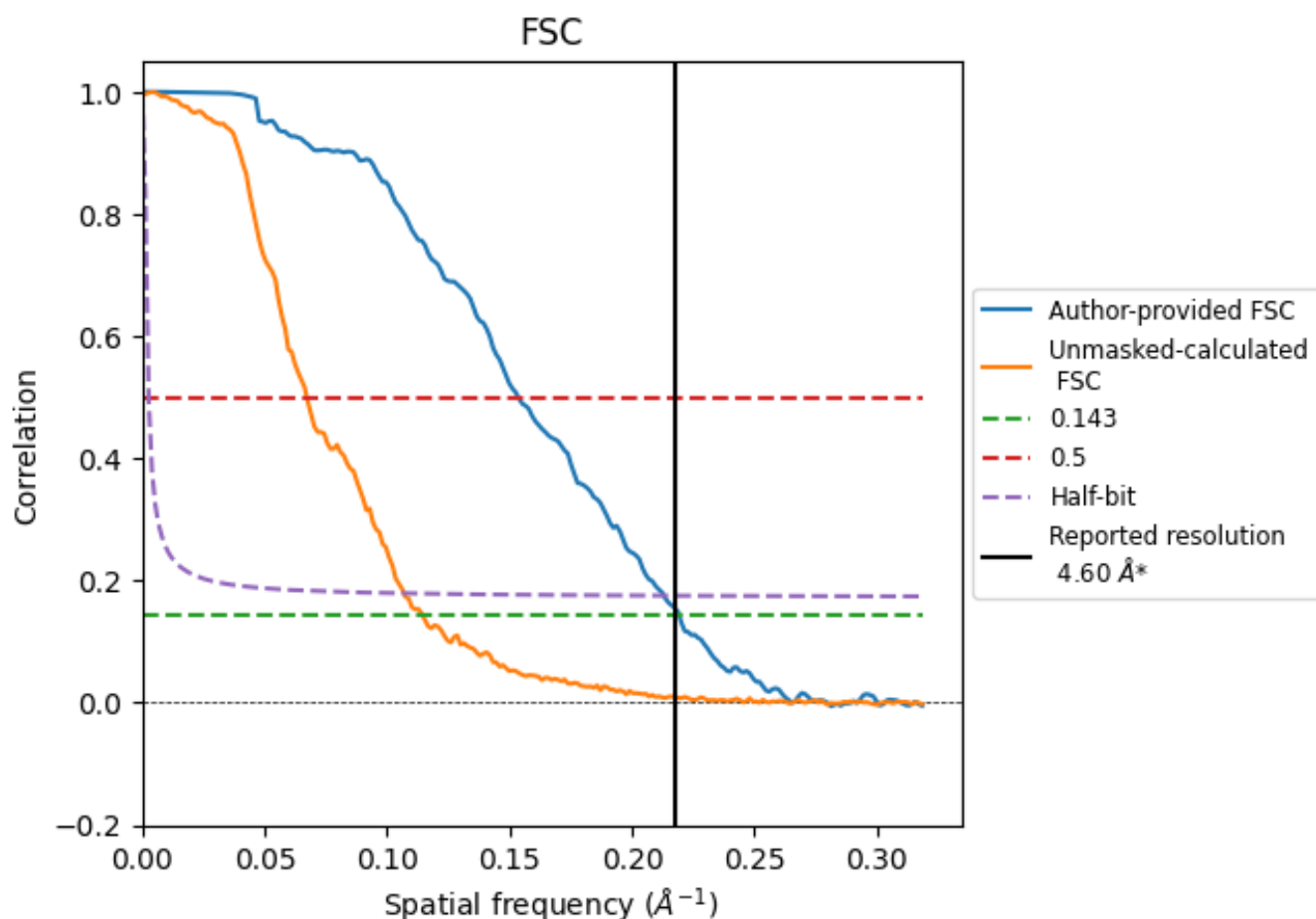


\*Reported resolution corresponds to spatial frequency of 0.217 Å<sup>-1</sup>

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



## 8.2 Resolution estimates [i](#)

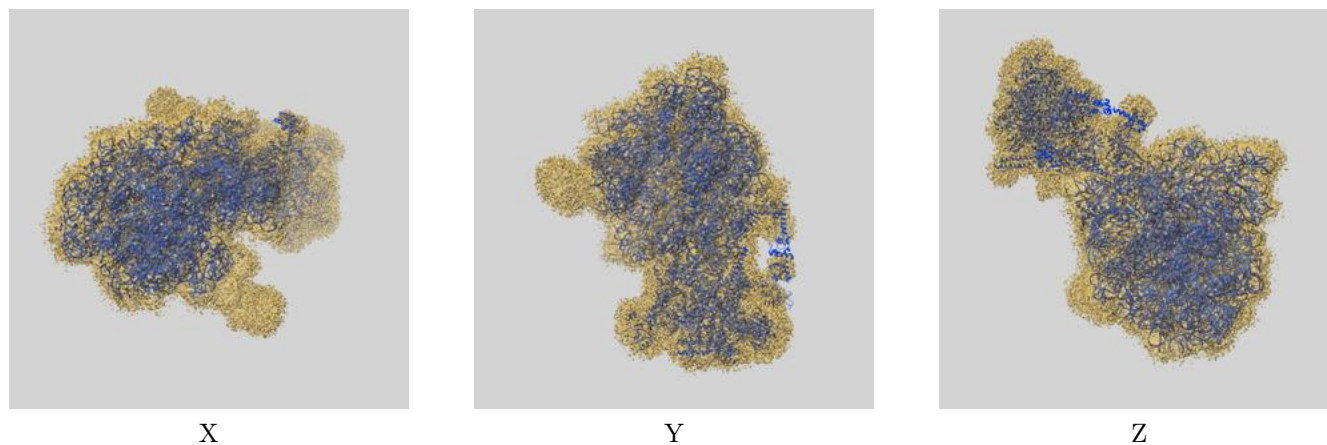
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.51	4.69
Unmasked-calculated*	8.73	14.88	9.35

\*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 8.73 differs from the reported value 4.6 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-39172 and PDB model 8YDI. Per-residue inclusion information can be found in section [3](#) on page [16](#).

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



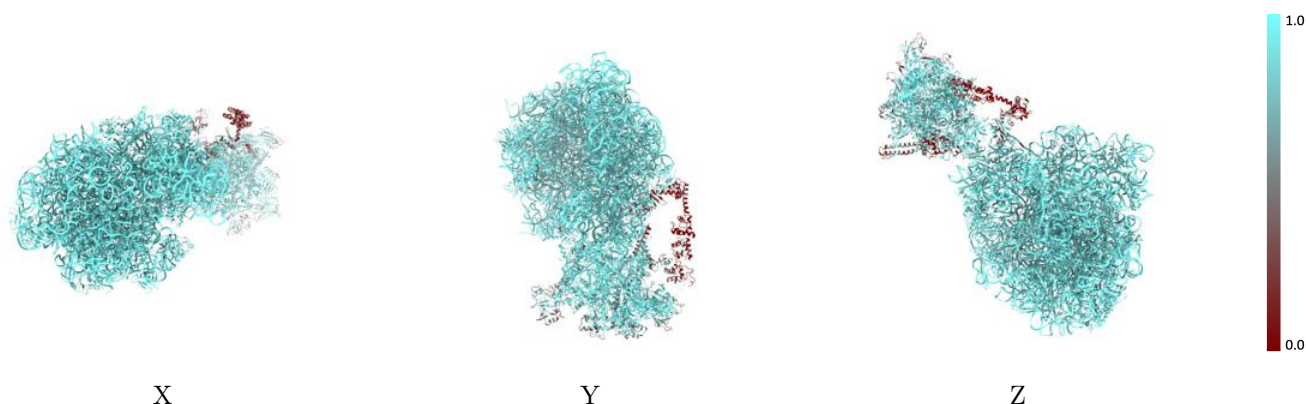
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



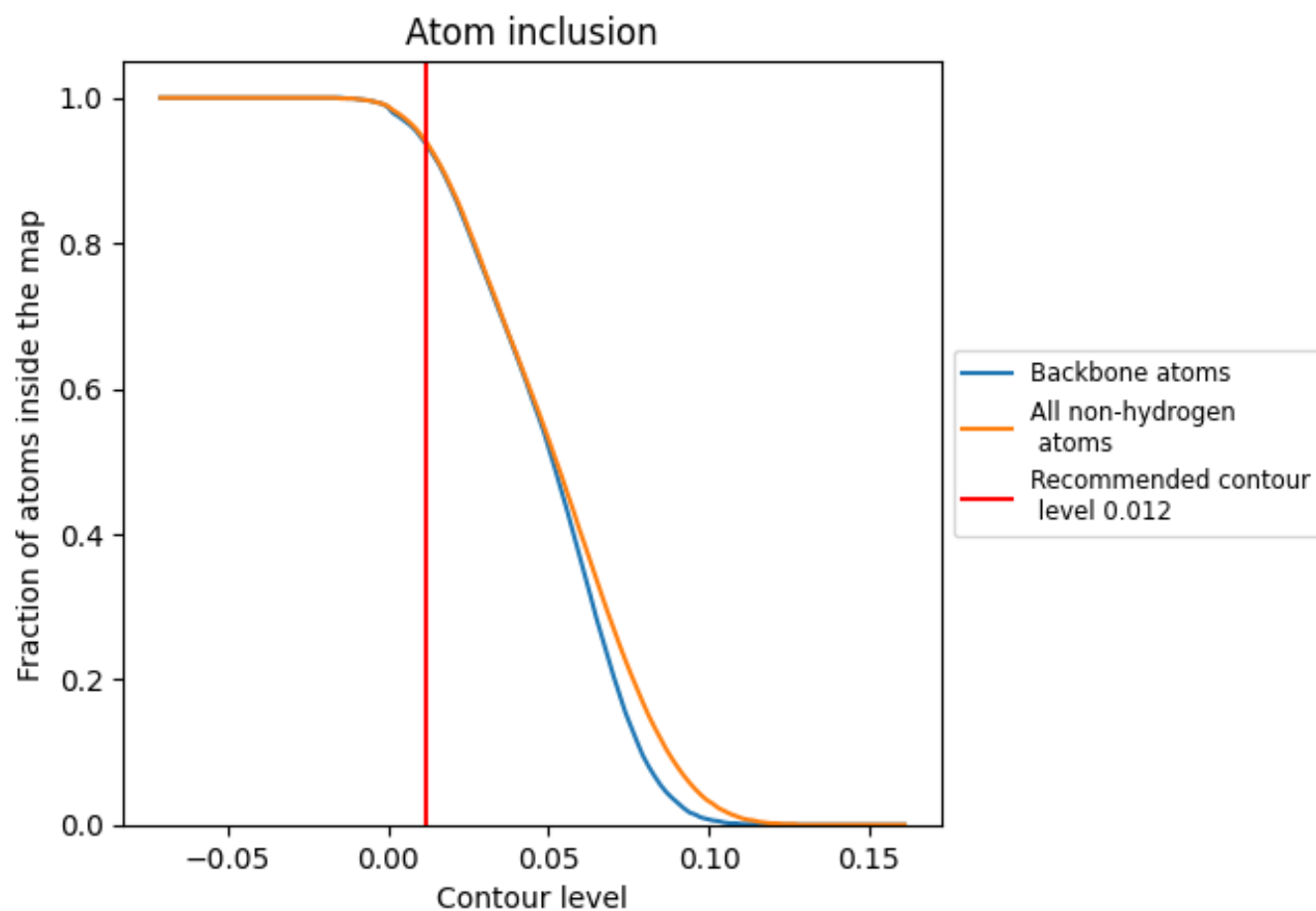
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9380	 0.2250
1	 0.9920	 0.3080
2	 0.9960	 0.2630
3	 0.9860	 0.2470
4	 0.8160	 0.0330
5	 0.9190	 0.0940
6	 0.9900	 0.3120
7	 0.7340	 0.0600
8	 0.9500	 0.0360
9	 0.9260	 0.0410
A	 0.8670	 0.1360
A1	 0.6580	 0.0200
A2	 0.6840	 0.0220
B	 0.9510	 0.3070
B1	 0.8600	 0.0200
B2	 0.8110	 0.0200
C	 0.9600	 0.2970
D	 0.9410	 0.3440
E	 0.9610	 0.3560
F	 0.9450	 0.2510
G	 0.9340	 0.2080
H	 0.9230	 0.2590
I	 0.8250	 0.0490
J	 0.9410	 0.2720
K	 0.9380	 0.2180
L	 0.9240	 0.2040
M	 0.9490	 0.2780
N	 0.9570	 0.1880
NA	 0.4720	 -0.0140
NG	 0.8710	 0.0480
O	 0.9130	 0.1880
P	 0.9520	 0.2350
Q	 0.8990	 0.1910
R	 0.9520	 0.2130
S	 0.9510	 0.2190



*Continued on next page...*

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Chain	Atom inclusion	Q-score
T	 0.9580	 0.2540
U	 0.8250	 0.0870
V	 0.9070	 0.1540
W	 0.9460	 0.2290
W0	 0.6370	 0.0030
X	 0.9570	 0.1940
Y	 0.9340	 0.1700
Z	 0.8200	 0.1370
b	 0.9550	 0.3540
c	 0.9470	 0.2800
d	 0.9560	 0.2780
e	 0.9530	 0.2490
f	 0.9510	 0.1770
g	 0.9590	 0.2220
h	 0.9380	 0.2650
i	 0.8550	 0.0460
j	 0.9590	 0.2960
k	 0.8950	 0.2780
l	 0.9640	 0.3160
m	 0.9260	 0.3060
n	 0.9570	 0.2820
o	 0.9730	 0.2220
p	 0.9210	 0.2360
q	 0.9580	 0.3140
r	 0.9640	 0.3140
s	 0.9380	 0.3090
t	 0.9330	 0.1930
u	 0.9640	 0.2250
v	 0.9590	 0.2280
w	 0.9520	 0.3030
x	 0.9580	 0.3360
y	 0.9560	 0.1740
z	 0.9610	 0.3010