



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 12:49 AM UTC

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

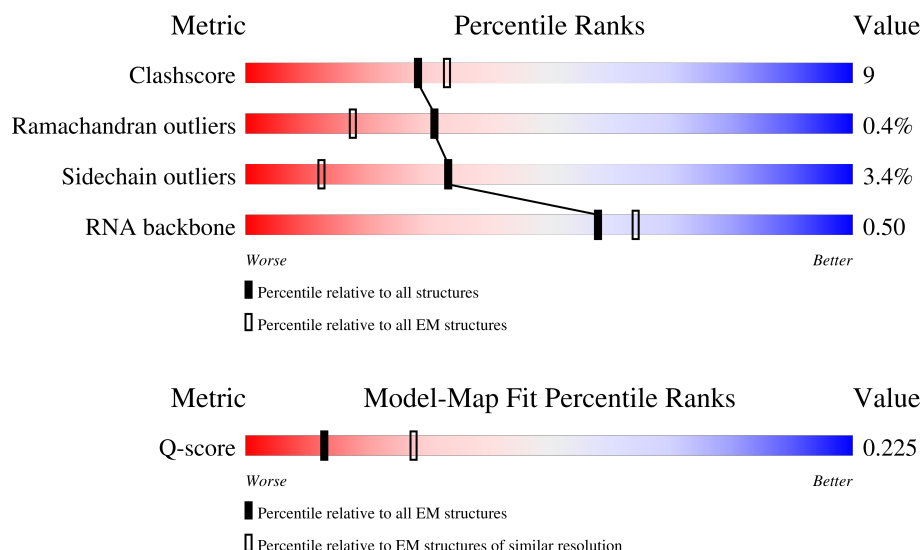
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2407 (4.10 - 5.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	70	
2	B	57	
3	C	55	

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

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

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Mol	Chain	Length	Quality of chain
54	4	56	
55	8	37	
56	9	37	
57	A1	329	
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
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		

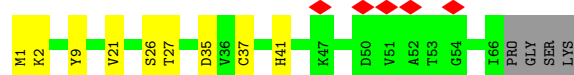
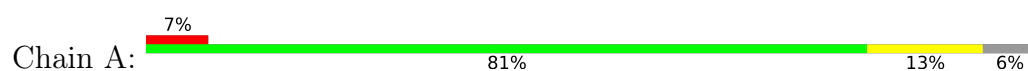
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

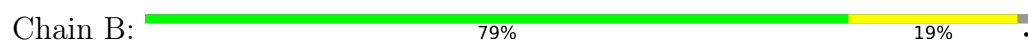
3 Residue-property plots [i](#)

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.

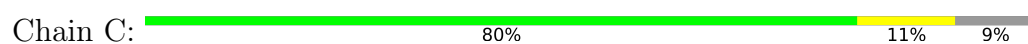
- Molecule 1: 50S ribosomal protein L31



- Molecule 2: 50S ribosomal protein L32



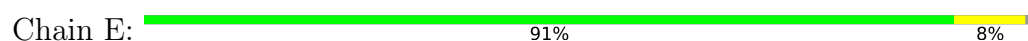
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34



- Molecule 5: 50S ribosomal protein L35



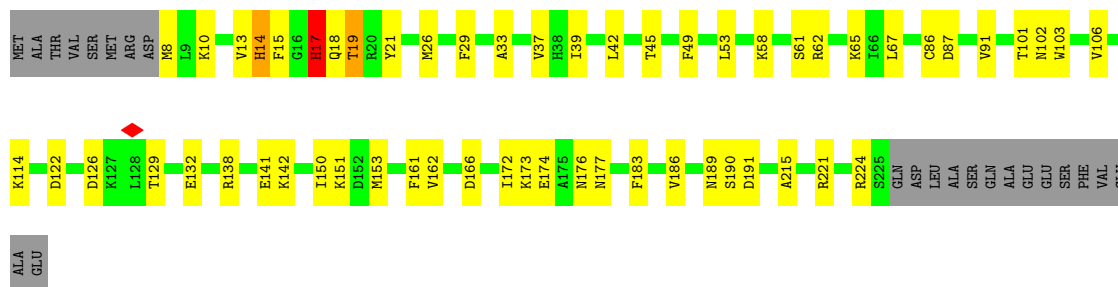
- Molecule 6: 50S ribosomal protein L36

Chain F:  66% 32% .



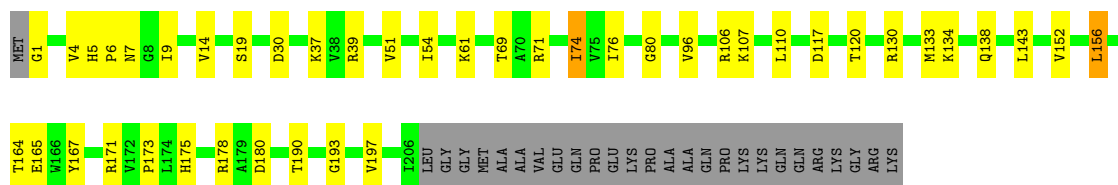
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% . 10%



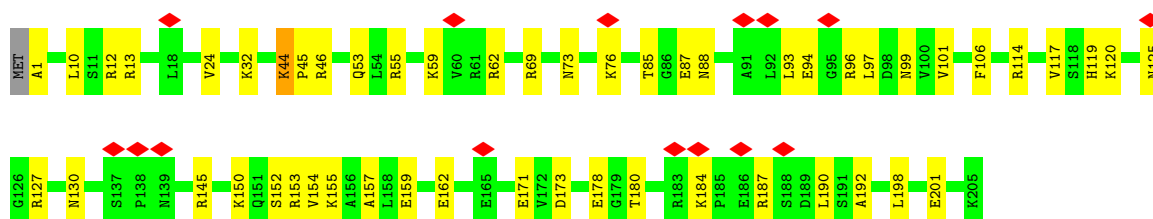
- Molecule 8: 30S ribosomal protein S3

Chain H:  70% 18% . 12%



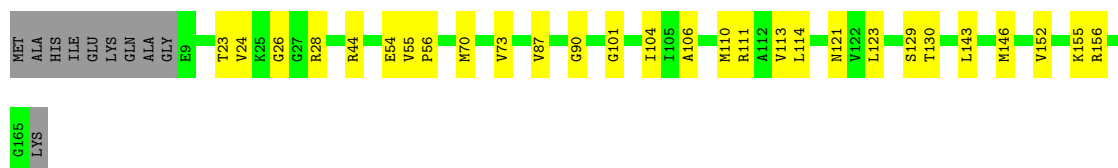
- Molecule 9: 30S ribosomal protein S4

Chain I:  7% 74% 25%



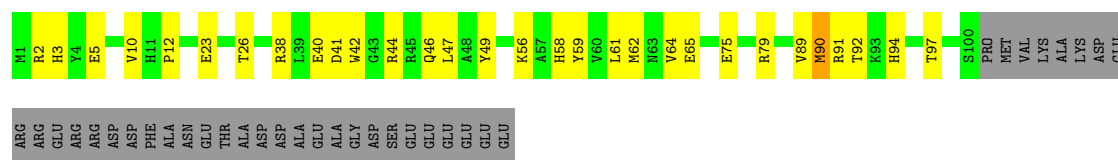
- Molecule 10: 30S ribosomal protein S5

Chain J:  77% 17% 6%



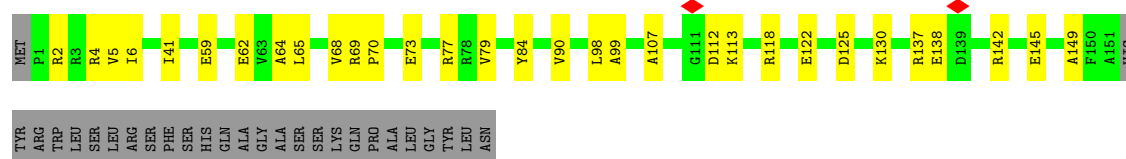
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

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%





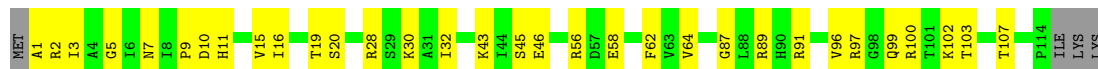
- Molecule 17: 30S ribosomal protein S12

Chain Q: 65% 32% ..



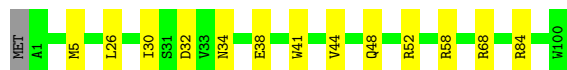
- Molecule 18: 30S ribosomal protein S13

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%



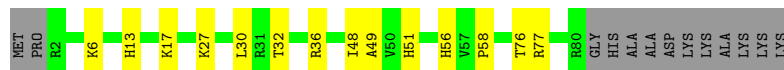
- Molecule 23: 30S ribosomal protein S18

Chain W:  65% 20% 13%



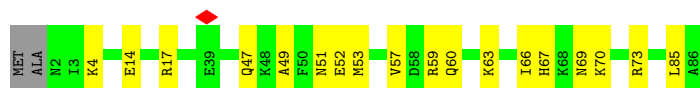
- Molecule 24: 30S ribosomal protein S19

Chain X:  71% 15% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  77% 21% 2%



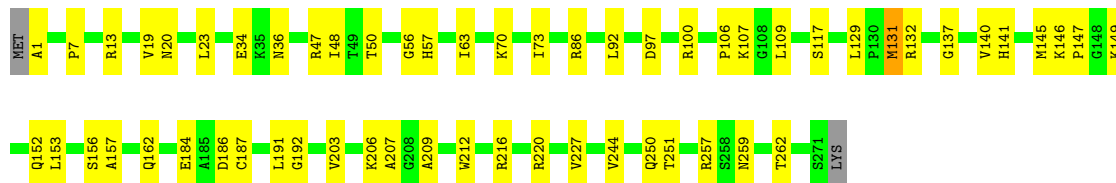
- Molecule 26: 30S ribosomal protein S21

Chain Z:  58% 32% 8%



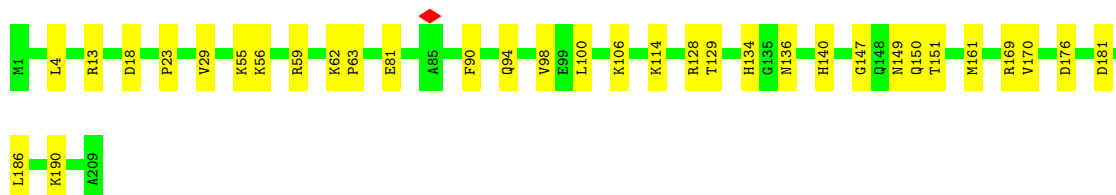
- Molecule 27: 50S ribosomal protein L2

Chain b:  78% 21% 1%



- Molecule 28: 50S ribosomal protein L3

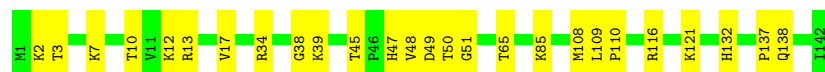
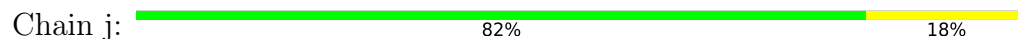
Chain c:  84% 16%



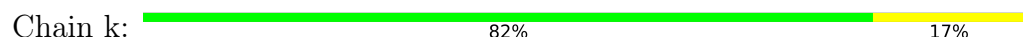
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-----	----	----	--	----	--	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	-----	-----	-----	--	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----



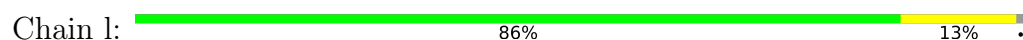
- Molecule 34: 50S ribosomal protein L13



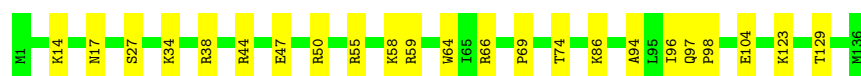
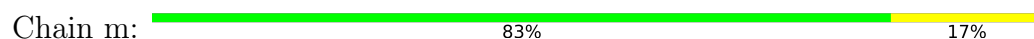
- Molecule 35: 50S ribosomal protein L14



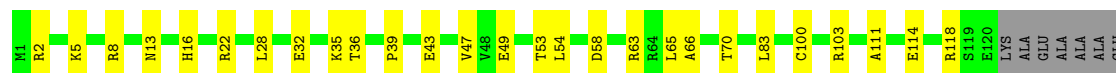
- Molecule 36: 50S ribosomal protein L15



- Molecule 37: 50S ribosomal protein L16



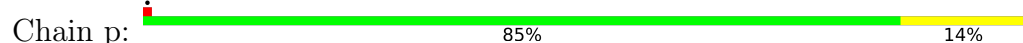
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18

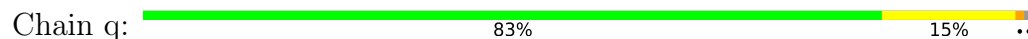


- Molecule 40: 50S ribosomal protein L19

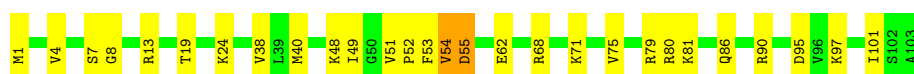




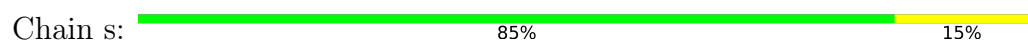
- Molecule 41: 50S ribosomal protein L20



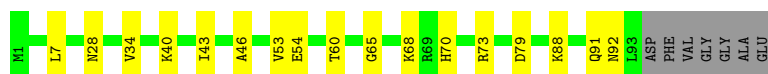
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22



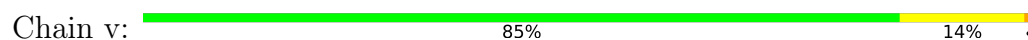
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27

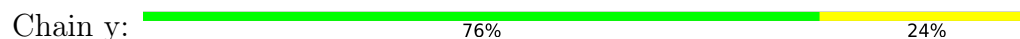




- Molecule 48: 50S ribosomal protein L28



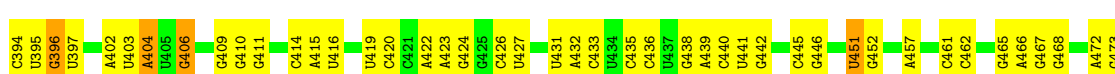
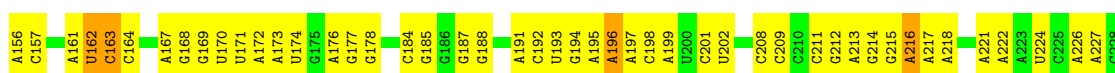
- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 23S rRNA

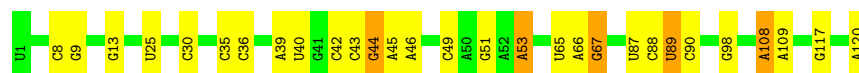


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A1580	A1580	A1515	G1435	C1345	A1275	G1182	G1112	A1050	A972	U887	U810	A718	A633	U552
G1581	G1581	G1516	G1436	A1346	C1278	U1183	U1113	A1054	A973	C888	U811	C719	C633	G553
A1583	A1583	G1517	C1437	A1347	G1279	U1184	C1114	G1055	G974	C889	C812	A720	C634	U554
G1588	G1588	C1518	A1438	C1348	G1280	G1185	G1115	G1056	A975	C890	C813	U721	G635	G555
U1589	U1589	G1519	A1439	C1349	G1281	G1187	C1117	A1057	A892	C891	C814	A722	G636	A556
U1520	U1520	U1282	G1441	U1352	U1283	U1188	C1118	U1058	A892	C892	C815	C723	C637	C557
G1521	G1521	G1283	G1442	U1352	U1284	U1119	C1119	U1059	A893	C893	A819	C724	G638	U558
U1522	U1522	A1285	G1448	A1365	A1284	G1193	U1119	U1060	A894	C894	U820	U725	G639	U559
C1523	C1523	A1286	G1449	A1366	A1285	A1194	G1120	U1061	C982	A895	C821	G726	C640	U562
A1524	A1524	A1287	G1450	G1368	C1286	G1195	C1121	G1062	A983	C897	A821	A727	U641	A563
G1525	G1525	A1287	G1451	G1368	G1289	U1130	U1130	G1063	A984	C898	A825	A728	U644	U566
C1526	C1526	G1288	G1452	G1368	G1290	G1131	G1131	C1064	C985	C899	U826	G729	C645	U567
A1527	A1527	G1289	G1453	G1368	G1291	U1132	U1132	U1065	A900	U827	U827	A730	U646	U568
G1528	G1528	G1290	A1378	A1366	U1198	A1133	U1133	U1066	C989	U828	U828	C736	G647	U569
U1529	U1529	G1291	U1379	G1368	C1200	A1134	U1134	A1067	G990	A829	G830	G745	G648	G570
G1530	G1530	C1292	G1380	G1380	C1201	C1135	C1135	G1068	G993	C902	G831	G746	G649	U571
C1461	C1461	U1294	G1381	G1381	A1204	G1136	U1136	A1069	C994	G904	C832	G747	A572	A572
C1462	C1462	C1295	G1382	A1382	A1205	G1137	G1137	A1070	C995	A905	U833	C747	U573	U573
G1463	G1463	C1296	A1383	A1383	U1209	U1138	U1138	G1071	A996	U906	U834	C748	A574	A574
A1464	A1464	C1297	G1386	C1386	G1210	G1139	C1140	C1072	C1005	C907	G835	A752	A575	A575
G1465	G1465	C1298	A1387	G1387	G1211	U1141	U1141	A1073	A910	C908	C836	G757	U580	U580
A1466	A1466	G1299	G1388	G1388	G1212	A1142	A1142	G1074	A1009	A909	G837	C758	A586	A586
U1467	U1467	A1301	G1389	G1389	A1213	A1143	A1143	C1075	A1010	A911	C840	C759	A590	A590
U1468	U1468	C1306	U1390	U1390	G1220	C1145	C1145	A1077	G1011	G914	G841	G760	U591	U591
A1469	A1469	G1307	G1390	G1390	G1221	A1146	U1146	C1078	C1013	C915	U842	A761	A592	A592
A1470	A1470	G1308	G1391	G1391	G1222	A1147	U1147	C1079	A1014	A918	A845	A762	U593	U593
C1480	C1480	G1309	G1310	G1310	G1225	U1148	U1148	A1080	U1015	U919	U846	A763	U594	U594
G1481	G1481	G1311	G1311	G1311	A1230	G1149	C1150	U1082	U1019	G923	U847	A764	C595	C595
C1482	C1482	C1314	A1403	A1403	U1231	A1151	A1151	U1083	A1020	A848	C848	A765	U596	U596
U1483	U1483	C1315	A1404	A1404	G1232	C1152	C1152	A1084	G1022	G924	A849	G774	U597	U597
A1484	A1484	U1316	U1405	U1405	C1233	C1153	C1153	A1085	A925	U850	U850	G775	U598	U598
U1485	U1485	G1317	U1406	U1406	A1237	G1154	G1154	A1086	G926	C851	C851	A779	A599	A599
U1487	U1487	U1318	U1409	U1409	G1238	A1155	A1155	A1087	A927	U852	U852	U780	A603	A603
C1488	C1488	C1319	U1410	U1410	U1239	A1156	A1156	A1088	A928	C853	C853	A781	U607	U607
A1489	A1489	C1320	U1411	U1411	U1240	G1157	G1157	A1089	G1025	C854	C854	A782	A608	A608
G1490	G1490	A1321	U1412	U1412	U1241	C1158	C1158	A1090	A1027	G855	G855	A783	A609	A609
C1491	C1491	C1322	U1413	U1413	A1245	G1160	G1160	C1092	U932	G858	G858	A784	A610	A610
G1492	G1492	G1323	A1414	A1414	A1247	G1162	G1162	C1093	A1032	U859	U859	A785	A611	A611
A1493	A1493	U1324	U1415	U1415	A1247	G1163	G1163	U1094	G938	U860	U860	A788	A612	A612
A1495	A1495	U1325	U1416	U1416	A1253	A1164	A1164	A1095	G939	C861	C861	A789	A613	A613
A1496	A1496	A1326	C1417	C1417	U1254	A1165	A1165	A1096	A941	G864	G864	A790	A614	A614
A1497	A1497	A1327	G1418	G1418	U1255	G1166	G1166	U1097	G942	C865	C865	A791	A615	A615
G1500	G1500	U1329	A1419	A1419	G1256	G1167	G1167	A1098	G1037	C866	C866	A792	A616	A616
A1501	A1501	C1330	A1420	A1420	C1257	G1170	G1170	A1099	C946	U870	U870	A793	G620	G620
U1502	U1502	G1333	G1425	G1425	U1258	C1171	C1171	C1100	A947	U871	U871	A794	A621	A621
A1503	A1503	G1334	G1426	G1426	G1259	C1172	C1172	U1101	A1040	U872	U872	A795	A622	A622
G1504	G1504	C1335	A1427	A1427	G1266	U1173	U1173	C1102	U955	C873	C873	A796	A623	A623
A1505	A1505	C1336	G1428	G1428	U1267	U1174	U1174	A1103	G956	C874	C874	A797	A624	A624
U1506	U1506	A1337	G1429	G1429	U1267	A1175	A1175	C1104	C957	C875	C875	A800	A625	A625
A1507	A1507	G1338	G1430	G1430	C1270	U1176	U1176	U1105	C1044	U877	U877	A801	A626	A626
G1508	G1508	G1339	A1431	A1431	G1271	G1177	G1177	G1106	A958	A878	A878	A801	A627	A627
A1509	A1509	G1340	G1432	G1432	U1271	C1178	C1178	G1107	A960	C879	C879	A802	A628	A628
G1510	G1510	A1433	A1433	A1433	U1273	U1180	U1180	U1108	G1047	C885	C885	A803	A629	A629

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A2900	G2816	A2741	G2659	G2576	G2396	G2315	G2237	A2170	C2102	G2012	A1917	C1761	
C2901	A2820	G2742	G2661	G2577	U2402	G2316	G2238	U2171	C2103	G2013	A1918	A1762	
C2902	G2827	G2743	A2662	G2578	U2403	U2321	G2239	U2172	C2104	A2014	A1919	G1763	
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		U2756			U2422	A2335	C2258	U2187	U2118	G2027			
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		C2762	U2684		G2428	G2345		G2193	G2125	U2034		A1785	
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		A2764			A2430	A2347	C2275	U2195	G2127	C2036	U1943	A1787	
		A2765			U2431	C2347		C2196	G2128	A2037	U1944	C1788	
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					G2436	A2352	A2281	G2201	G2133	A2051	G1954	U1797	
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						G2361	A2284	A2204	U2137	A2054	A1801	A1808	
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						G2365	A2288	G2209	G2144		G1964		
						A2366	G2289	U2210	C2145		C1965		
						G2367	U2291	A2211	G2146		A1966		
							U2292	U2212	A2147		C1967		
						G2371	G2293	C2214	G2148		G1968		
						U2372	G2294	C2215	U2149		A1969		
							C2295	G2216	C2150		U1970		
						G2379	A2296	G2217	U2151		U1971		
						A2381	A2297	G2218	G2152		G1972		
						G2382	U2298		C2153		A1978		
						G2383	U2299	G2221	U2155		G1983		
						U2384		G2222	G2156		C1984		
						A2468	U2302	G2223	G2157		G1985		
						A2469	G2303	G2224	U2158		C1986		
						G2470	U2304	A2225	G2159		G1987		
						A2471	G2305	G2226	G2160		C1988		
							C2306	A2227	A2094		G1989		
									C2161		U1990		
									G2162		G1991		
						U2390	A2309	G2230	C2163		G1992		
						G2391	C2310		A2164		U1993		
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						U2392		G2234	U2098		C1914		
						U2393		G2234	U2099				

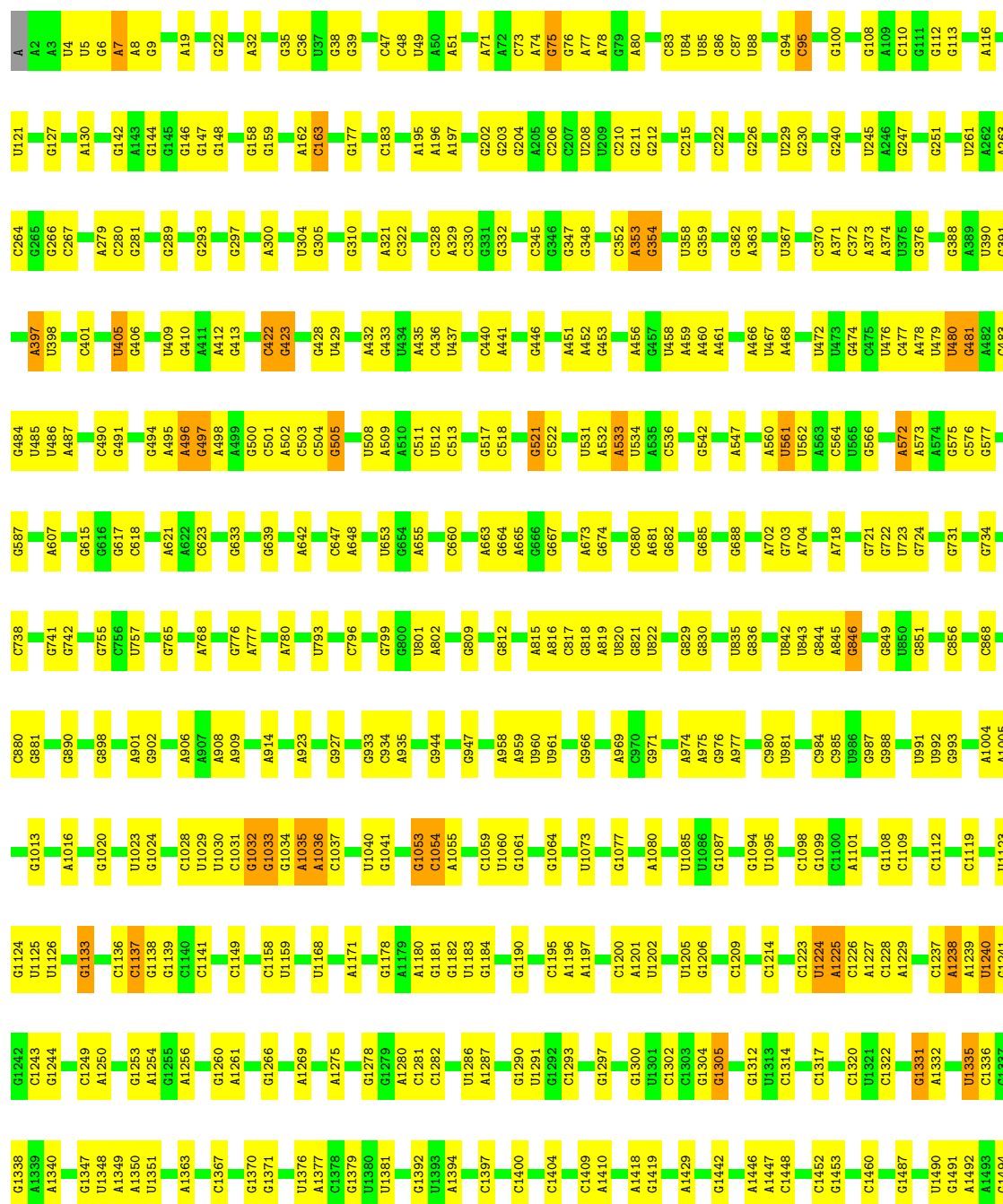
- Molecule 52: 5S rRNA

Chain 2:  76% 20%

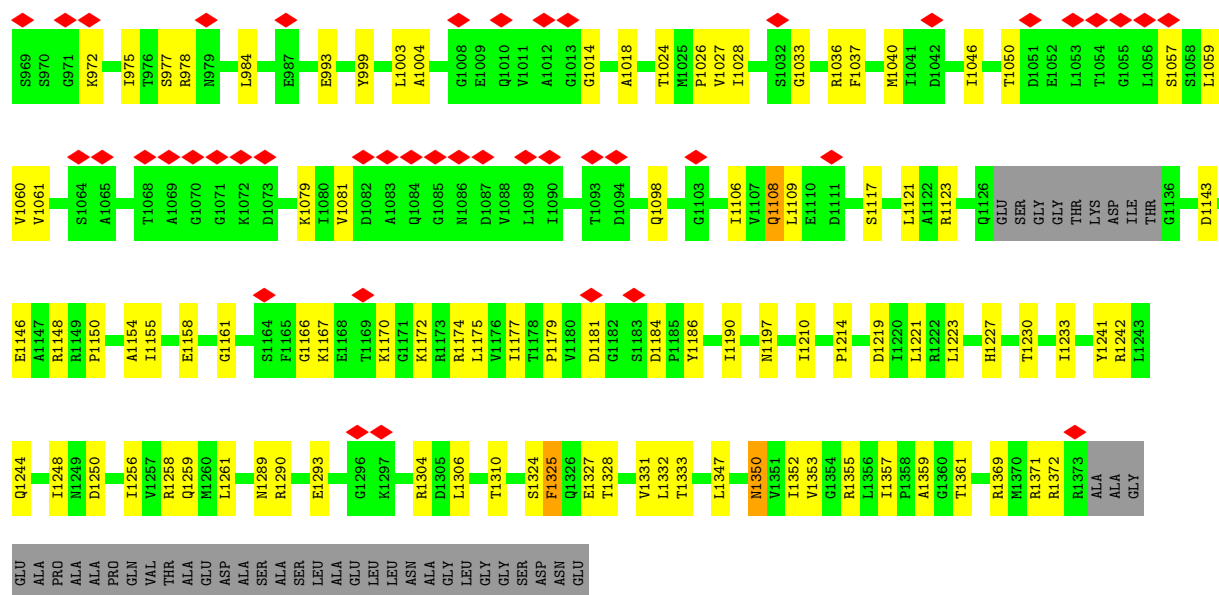


- Molecule 53: 16S rRNA

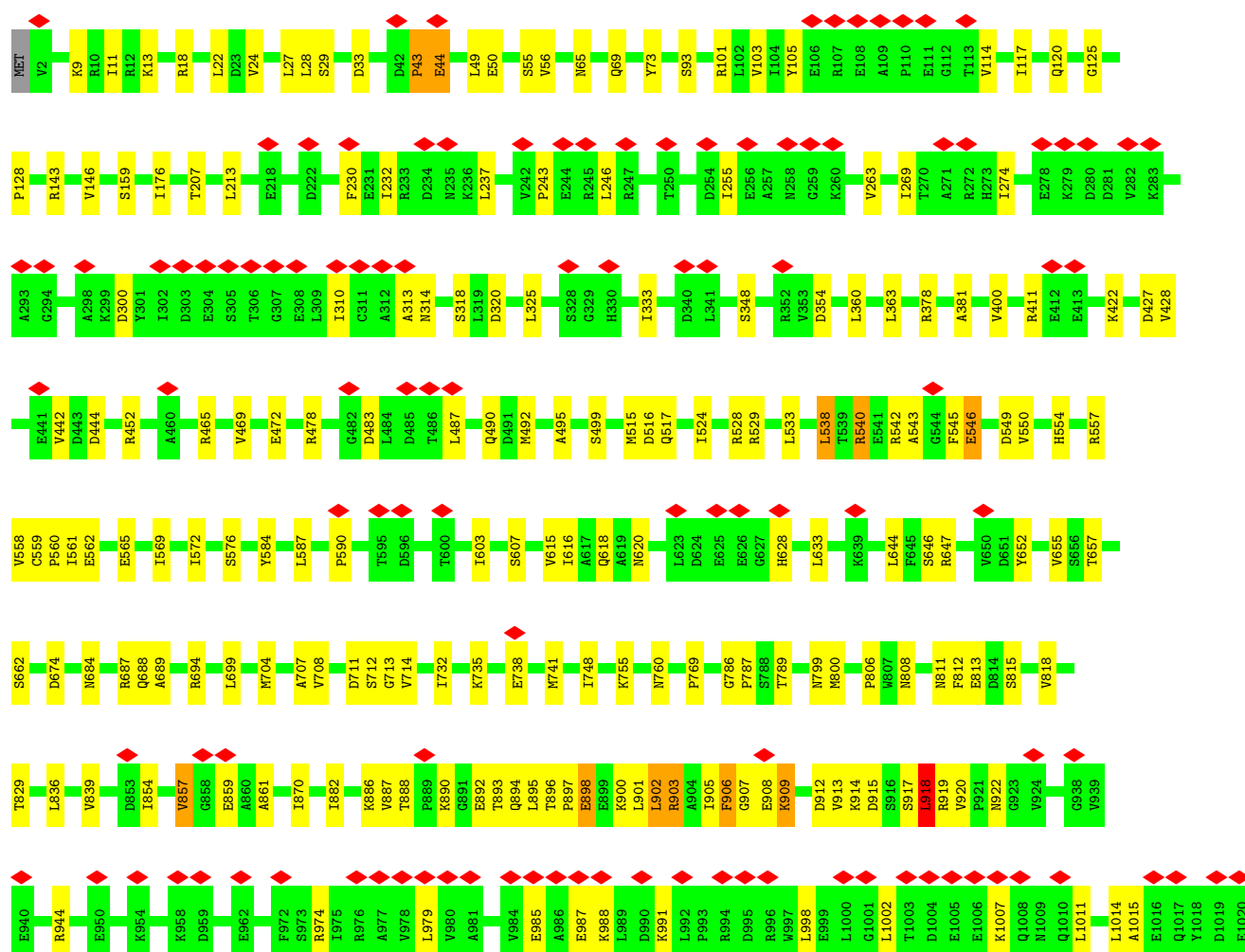
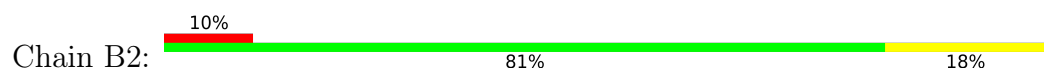
Chain 3:  68% 29%

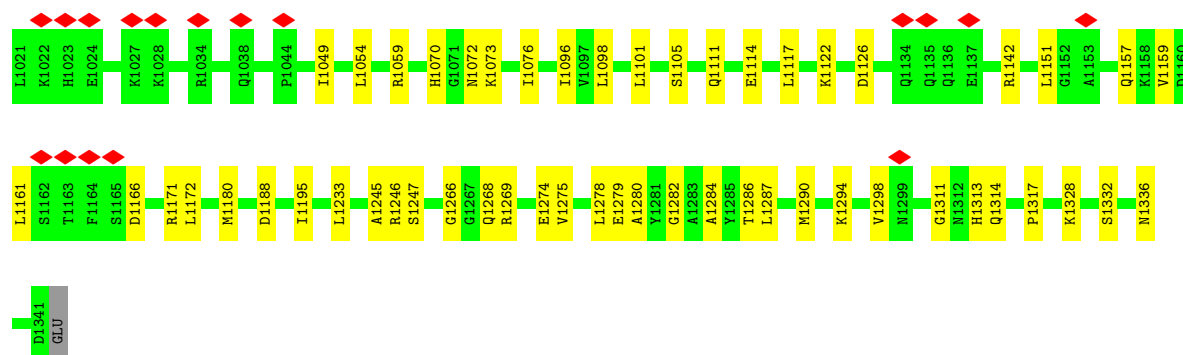




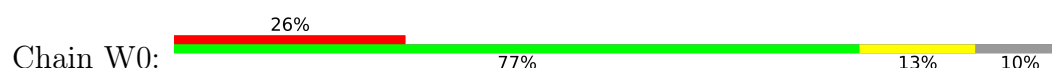


• Molecule 59: DNA-directed RNA polymerase subunit beta





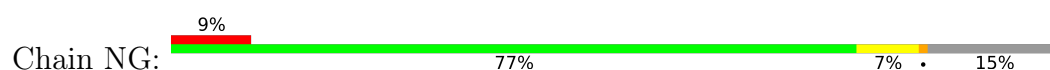
- Molecule 60: DNA-directed RNA polymerase subunit omega

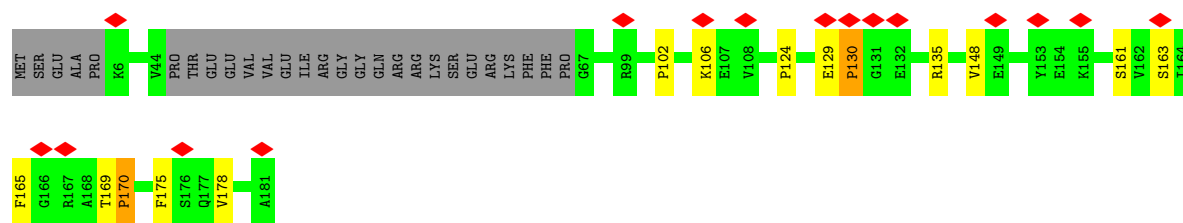


- Molecule 61: Transcription termination/antitermination protein NusA

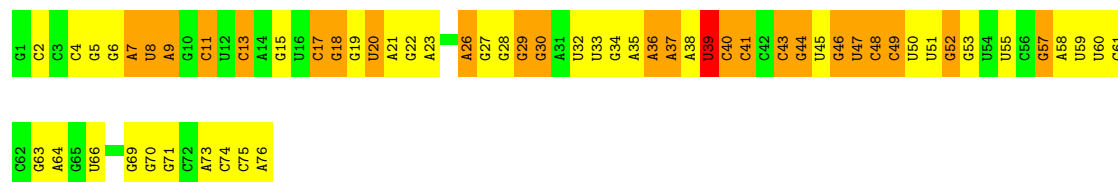
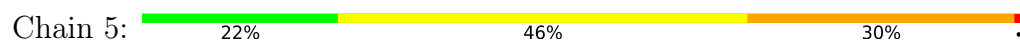


- Molecule 62: Transcription termination/antitermination protein NusG

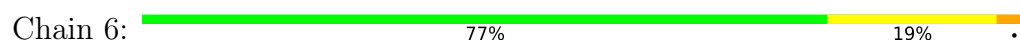




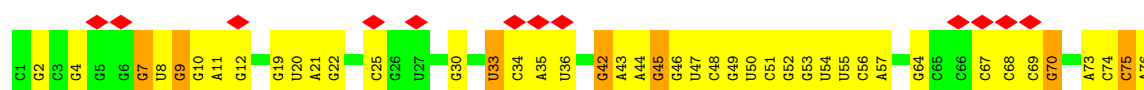
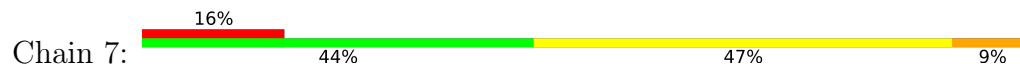
• Molecule 63: tRNA(Phe)



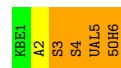
• Molecule 64: tRNA(fMet)



• 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, UAL, DPP, 5OH, 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	19

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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	49
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	172 (85%)	30 (15%)	1 (0%)	24	63
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%)	12	47
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	49
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	49
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%)	9	41
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%)	7	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	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%)	12	47
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%)	12	47
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%)	9	41
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%)	36	71
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1203 (90%)	122 (9%)	4 (0%)	36	71
59	B2	1338/1342 (100%)	1203 (90%)	131 (10%)	4 (0%)	36	71
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	469 (96%)	17 (4%)	4 (1%)	16	53
62	NG	150/181 (83%)	129 (86%)	14 (9%)	7 (5%)	2	16
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9586/10235 (94%)	8659 (90%)	888 (9%)	39 (0%)	31	67

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
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%)	53	67
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	45	64
4	D	38/38 (100%)	37 (97%)	1 (3%)	40	60
5	E	51/52 (98%)	49 (96%)	2 (4%)	28	49
6	F	34/34 (100%)	30 (88%)	4 (12%)	5	19
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	55
8	H	170/190 (90%)	167 (98%)	3 (2%)	51	67
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	63
10	J	119/126 (94%)	117 (98%)	2 (2%)	53	67
11	K	87/116 (75%)	82 (94%)	5 (6%)	18	40
12	L	124/147 (84%)	124 (100%)	0	100	100
13	M	104/105 (99%)	103 (99%)	1 (1%)	68	76
14	N	105/107 (98%)	98 (93%)	7 (7%)	15	36
15	O	86/90 (96%)	78 (91%)	8 (9%)	8	26
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	54
17	Q	103/104 (99%)	98 (95%)	5 (5%)	22	44
18	R	92/96 (96%)	91 (99%)	1 (1%)	65	74
19	S	83/84 (99%)	83 (100%)	0	100	100
20	T	76/77 (99%)	73 (96%)	3 (4%)	28	49
21	U	65/65 (100%)	64 (98%)	1 (2%)	57	70
22	V	74/78 (95%)	72 (97%)	2 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	56/65 (86%)	52 (93%)	4 (7%)	13	35
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	64 (98%)	1 (2%)	57	70
26	Z	55/61 (90%)	47 (86%)	8 (14%)	3	14
27	b	216/218 (99%)	212 (98%)	4 (2%)	50	66
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	51	67
30	e	148/150 (99%)	145 (98%)	3 (2%)	48	65
31	f	137/138 (99%)	135 (98%)	2 (2%)	57	70
32	g	41/114 (36%)	38 (93%)	3 (7%)	13	34
33	i	109/110 (99%)	108 (99%)	1 (1%)	70	76
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%)	68	76
37	m	109/109 (100%)	103 (94%)	6 (6%)	19	42
38	n	100/103 (97%)	99 (99%)	1 (1%)	68	76
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	99 (100%)	0	100	100
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	54
42	r	84/84 (100%)	82 (98%)	2 (2%)	43	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	65	74
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	23	45
46	v	78/78 (100%)	77 (99%)	1 (1%)	61	72
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%)	26	48
57	A1	185/286 (65%)	174 (94%)	11 (6%)	18	40
57	A2	186/286 (65%)	184 (99%)	2 (1%)	65	74
58	B1	1110/1168 (95%)	1018 (92%)	92 (8%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	B2	1150/1157 (99%)	1116 (97%)	34 (3%)	36	57
60	W0	70/75 (93%)	69 (99%)	1 (1%)	59	71
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7131 (97%)	250 (3%)	33	54

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

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 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	UAL	h	5	65	6,8,9	2.39	2 (33%)	4,9,11	1.87	1 (25%)
65	KBE	h	1	65	8,8,9	0.57	0	6,8,10	1.18	0
65	5OH	h	6	65	7,12,13	0.70	0	4,16,18	1.34	1 (25%)
65	DPP	h	2	65	4,5,6	0.50	0	1,5,7	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	UAL	h	5	65	-	0/3/7/9	-
65	KBE	h	1	65	-	0/7/7/8	-
65	5OH	h	6	65	-	0/2/18/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	DPP	h	2	65	-	0/2/4/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	5	UAL	C1-N1	-5.02	1.32	1.40
65	h	5	UAL	C-CA	-2.84	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	h	5	UAL	O-C-CA	-3.26	121.30	125.39
65	h	6	5OH	CR-CB-CA	-2.40	110.06	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	h	5	UAL	1	0
65	h	6	5OH	6	0
65	h	2	DPP	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

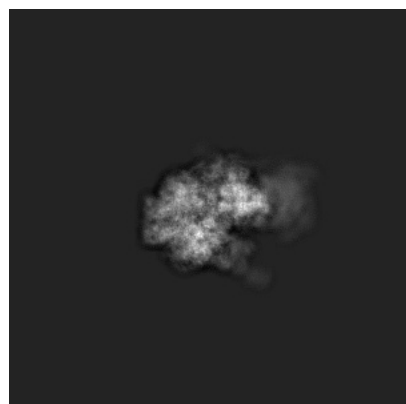
6 Map visualisation [i](#)

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

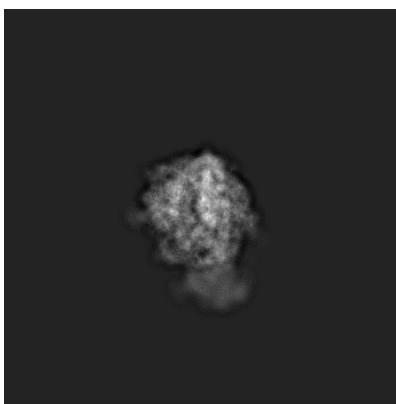
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

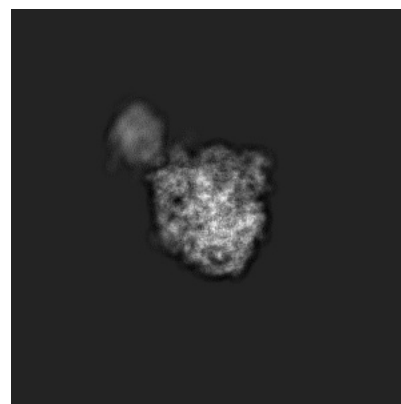
6.1.1 Primary map



X

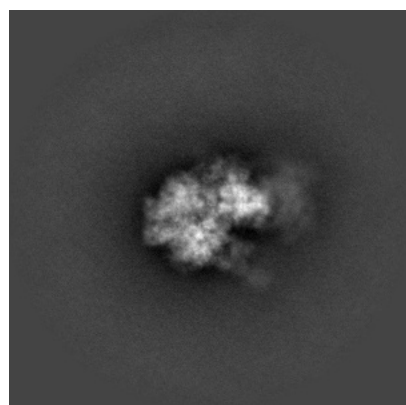


Y

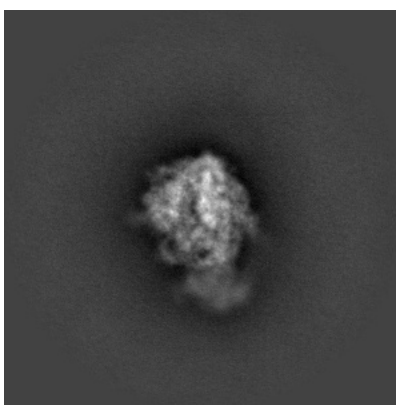


Z

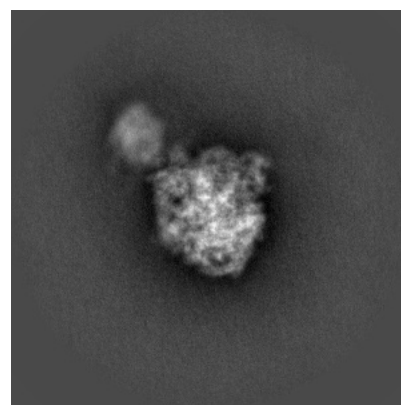
6.1.2 Raw map



X



Y

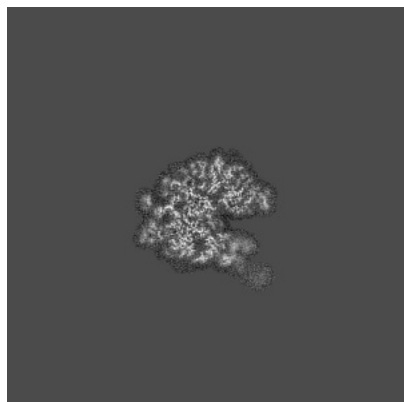


Z

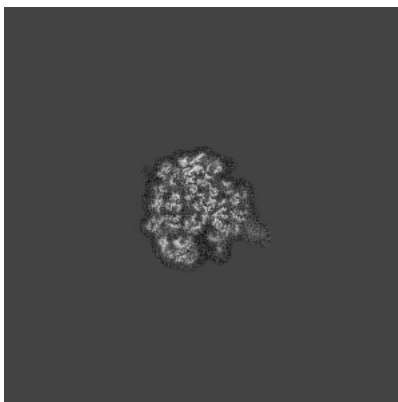
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

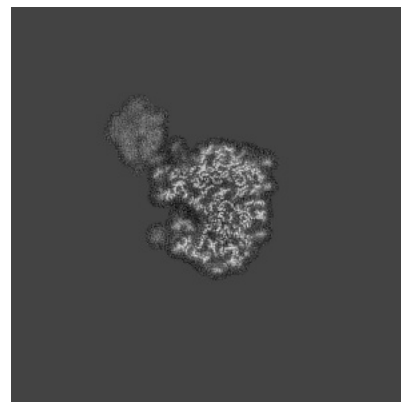
6.2.1 Primary map



X Index: 240

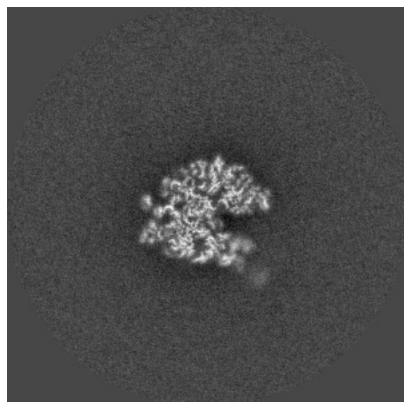


Y Index: 240

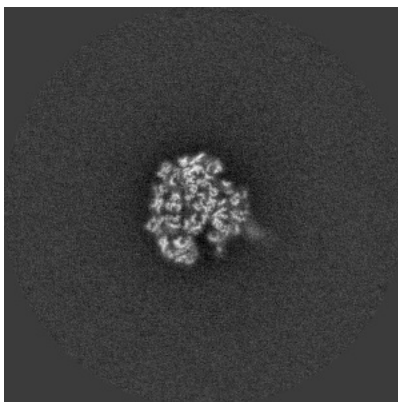


Z Index: 240

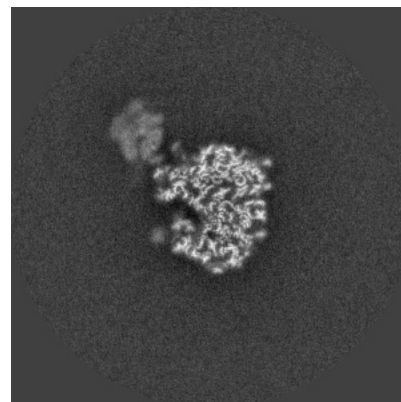
6.2.2 Raw map



X Index: 240



Y Index: 240

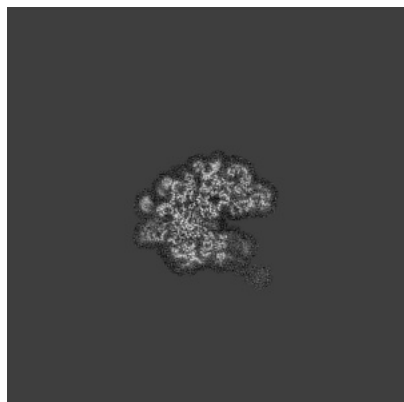


Z Index: 240

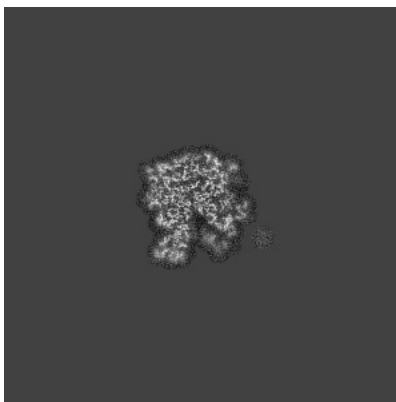
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

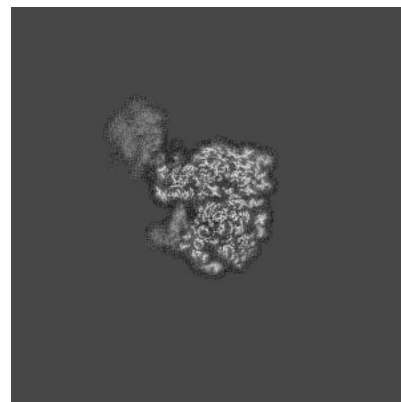
6.3.1 Primary map



X Index: 244

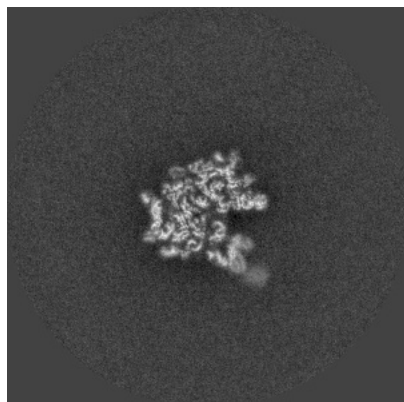


Y Index: 224

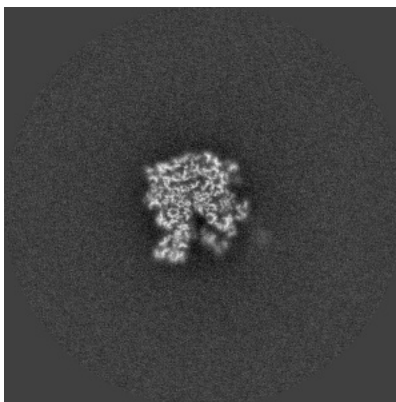


Z Index: 245

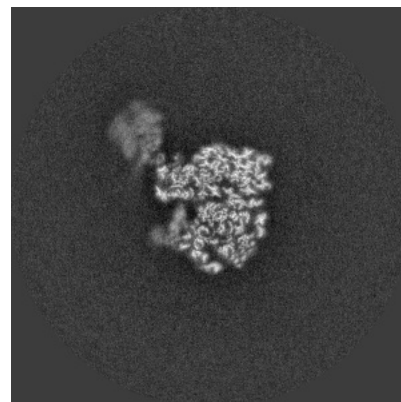
6.3.2 Raw map



X Index: 233



Y Index: 224

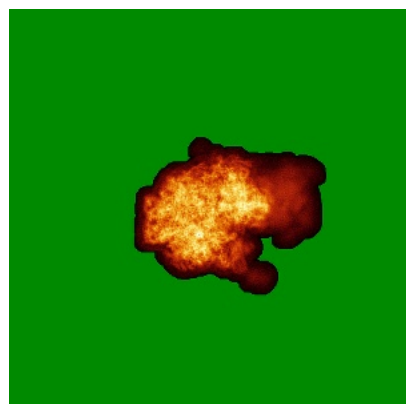


Z Index: 245

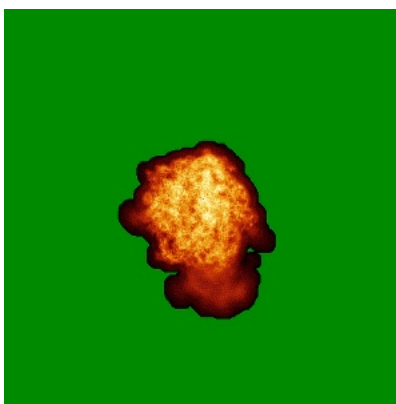
The images above show the largest variance slices of the map in three orthogonal directions.

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

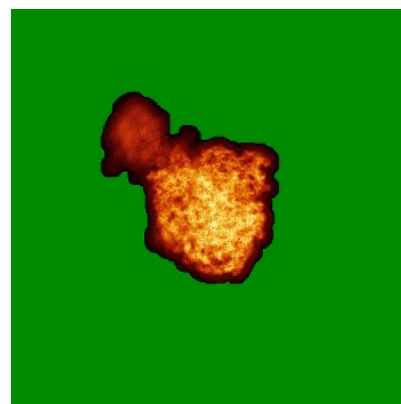
6.4.1 Primary map



X

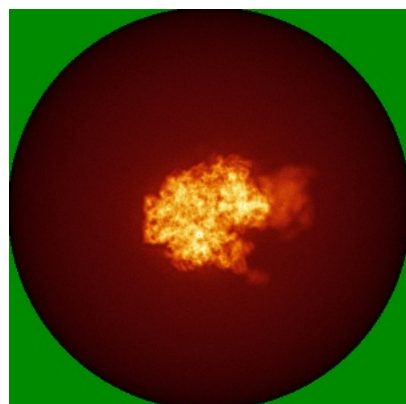


Y

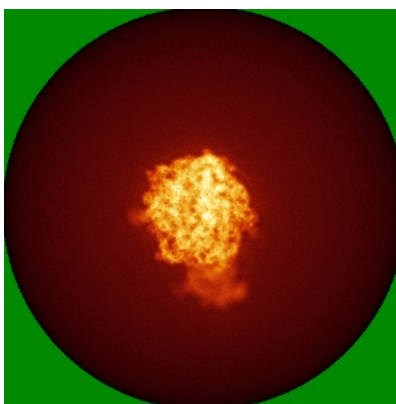


Z

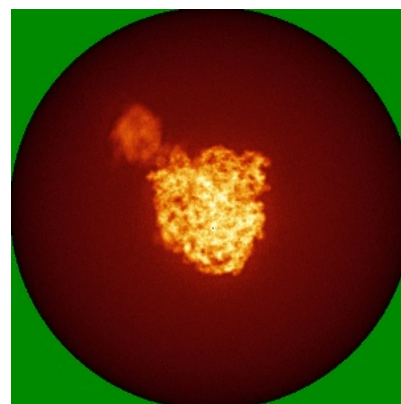
6.4.2 Raw map



X



Y

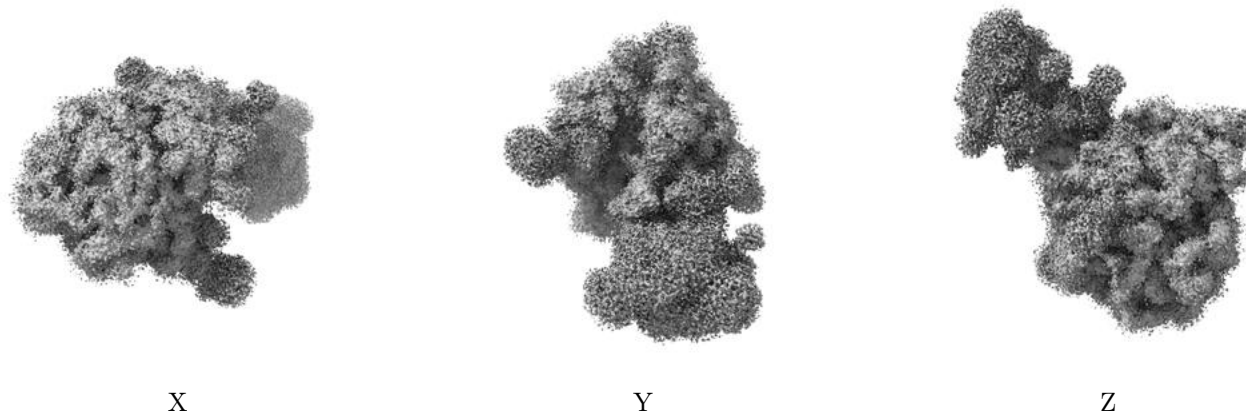


Z

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.

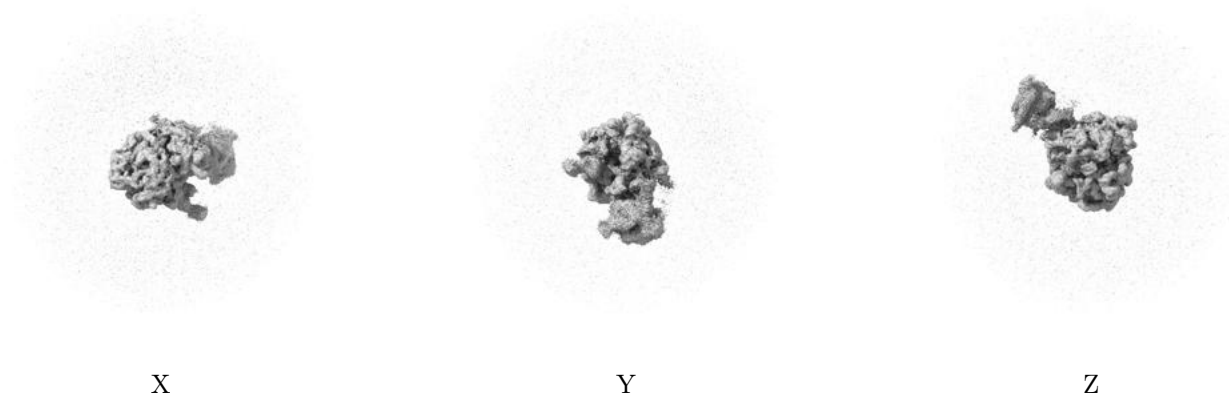
6.5 Orthogonal surface views [i](#)

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.

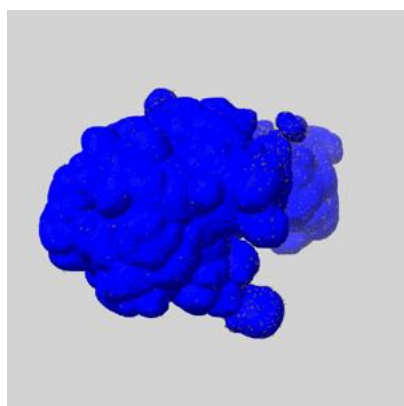
6.6 Mask visualisation [i](#)

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

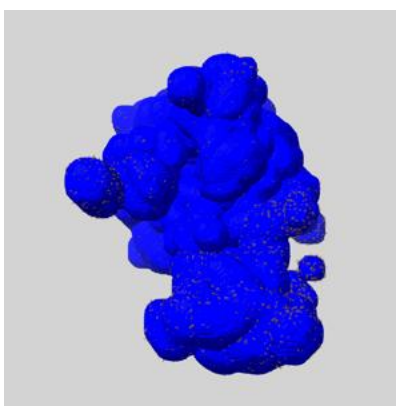
A mask typically either:

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

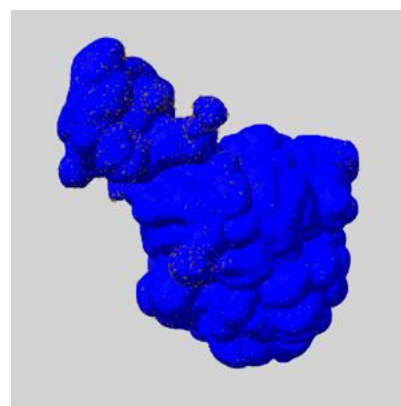
6.6.1 emd_39172_msk_1.map [i](#)



X



Y

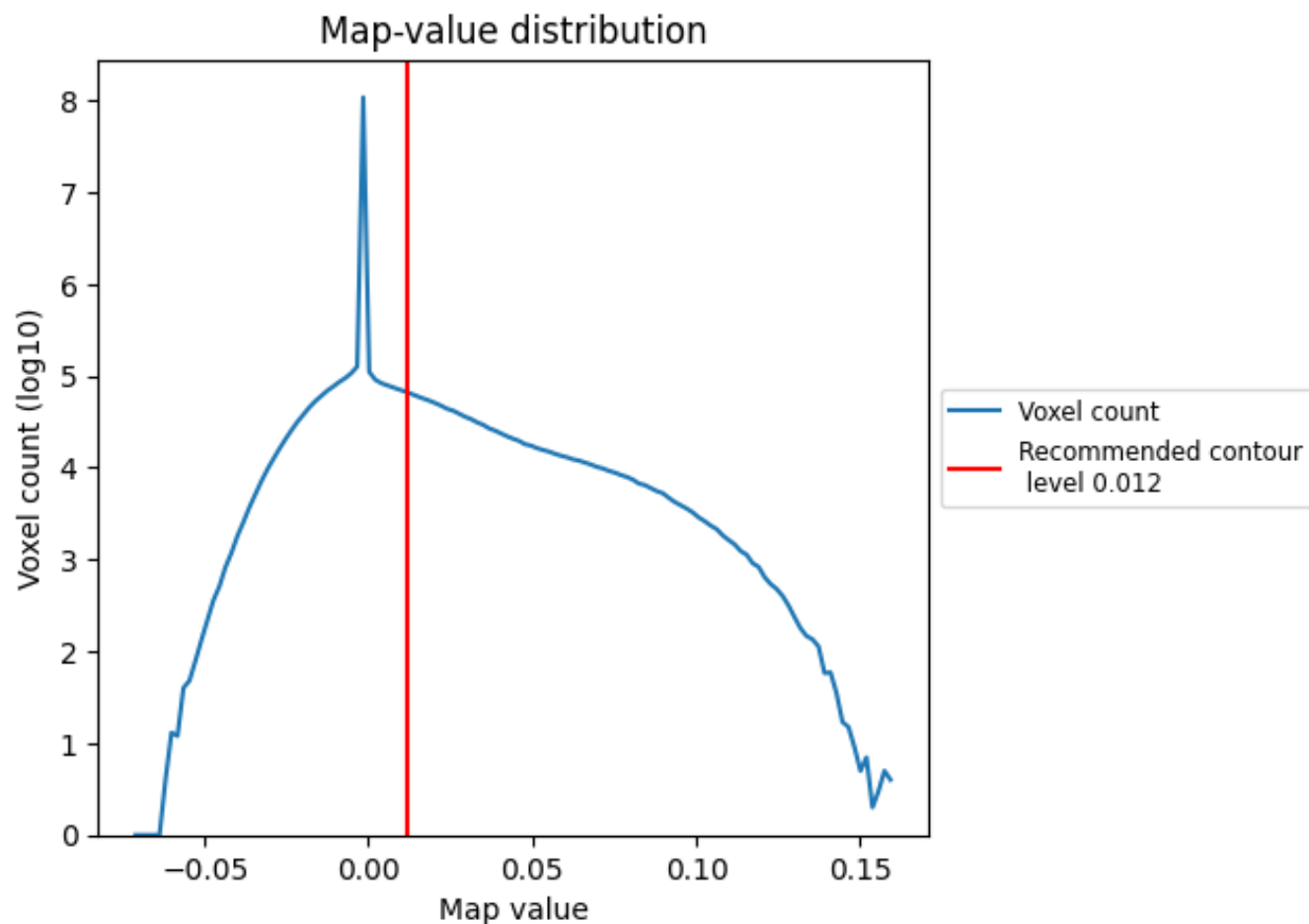


Z

7 Map analysis [i](#)

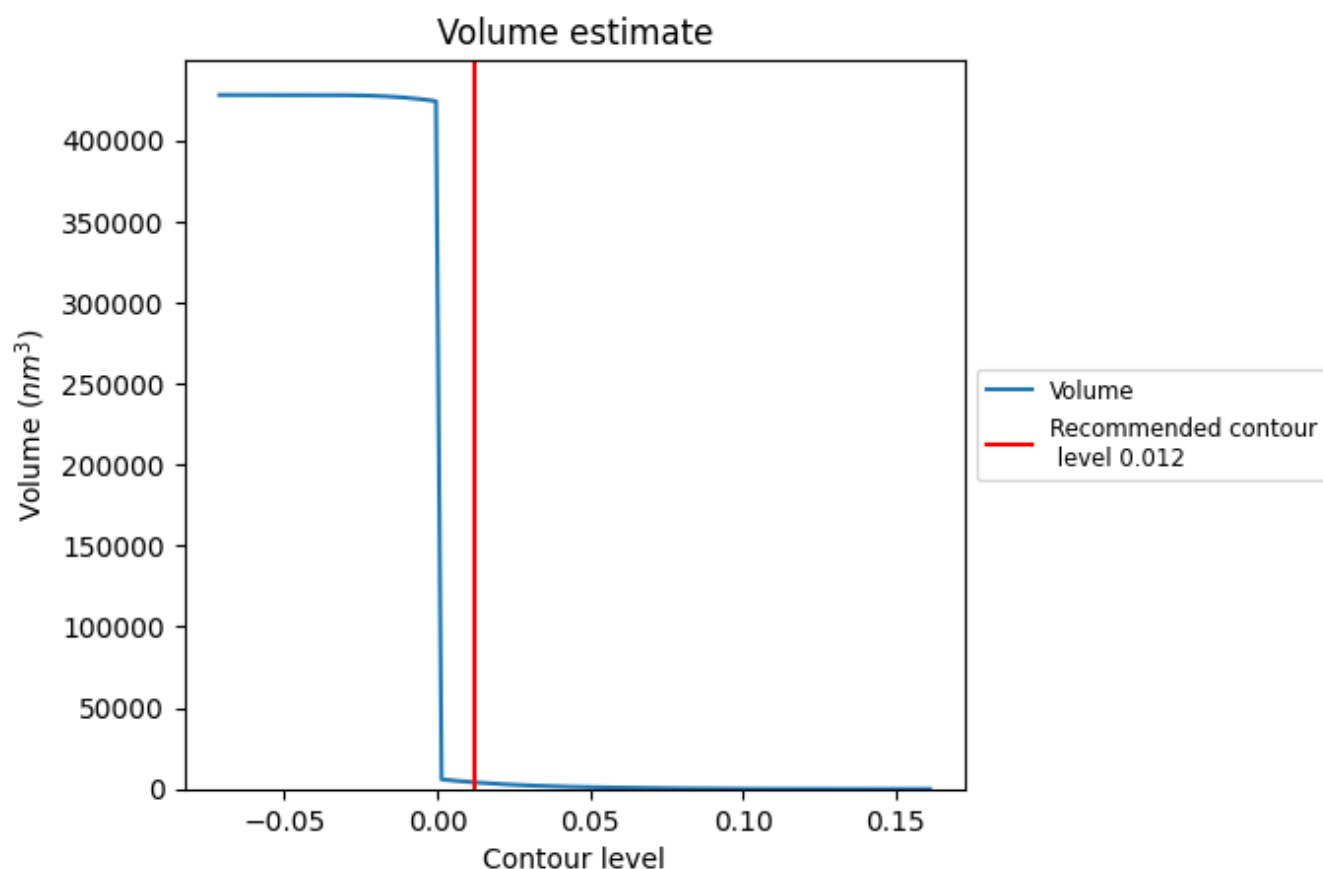
This section contains the results of statistical analysis of the map.

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.

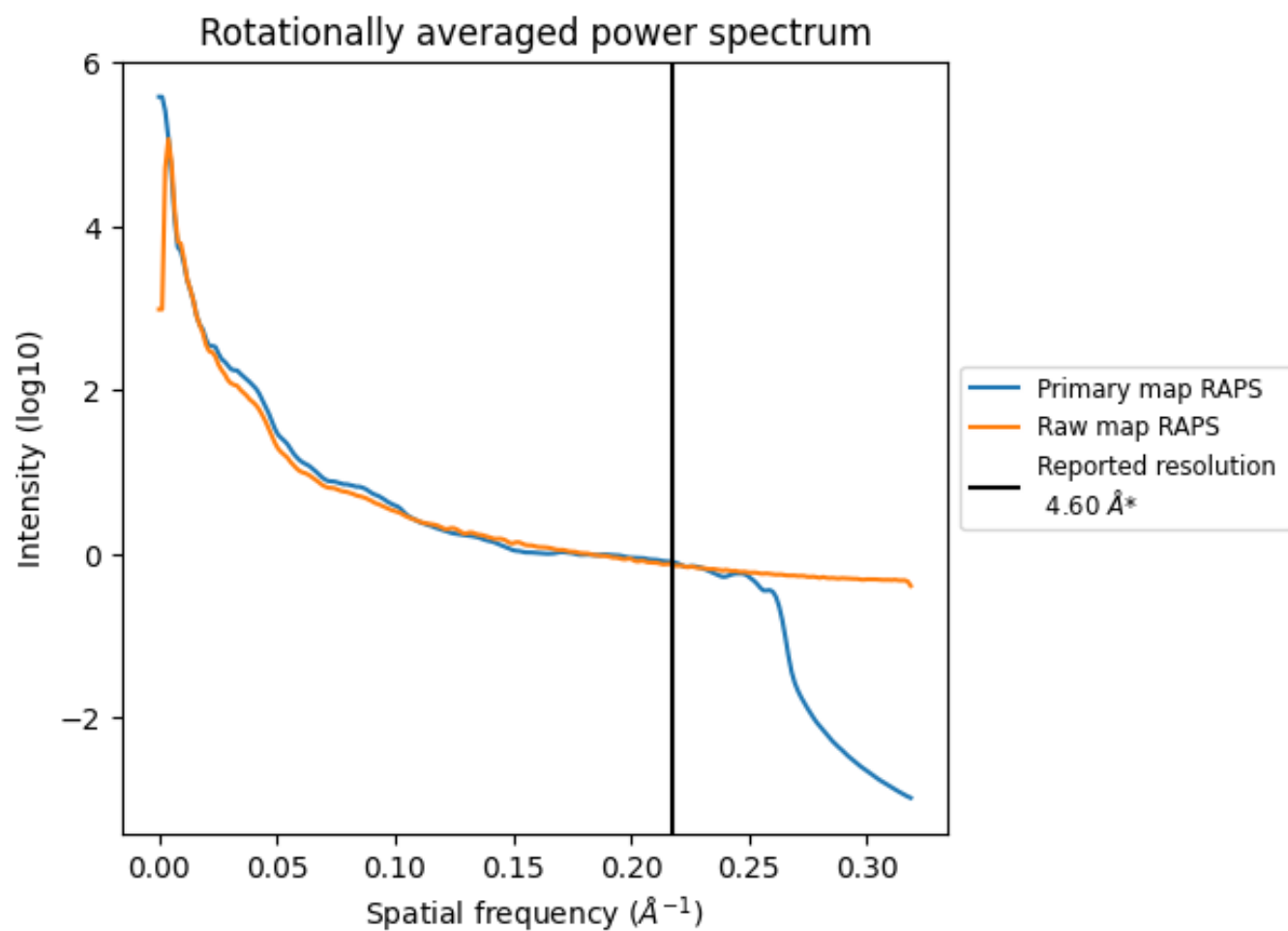
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4127 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 ⓘ

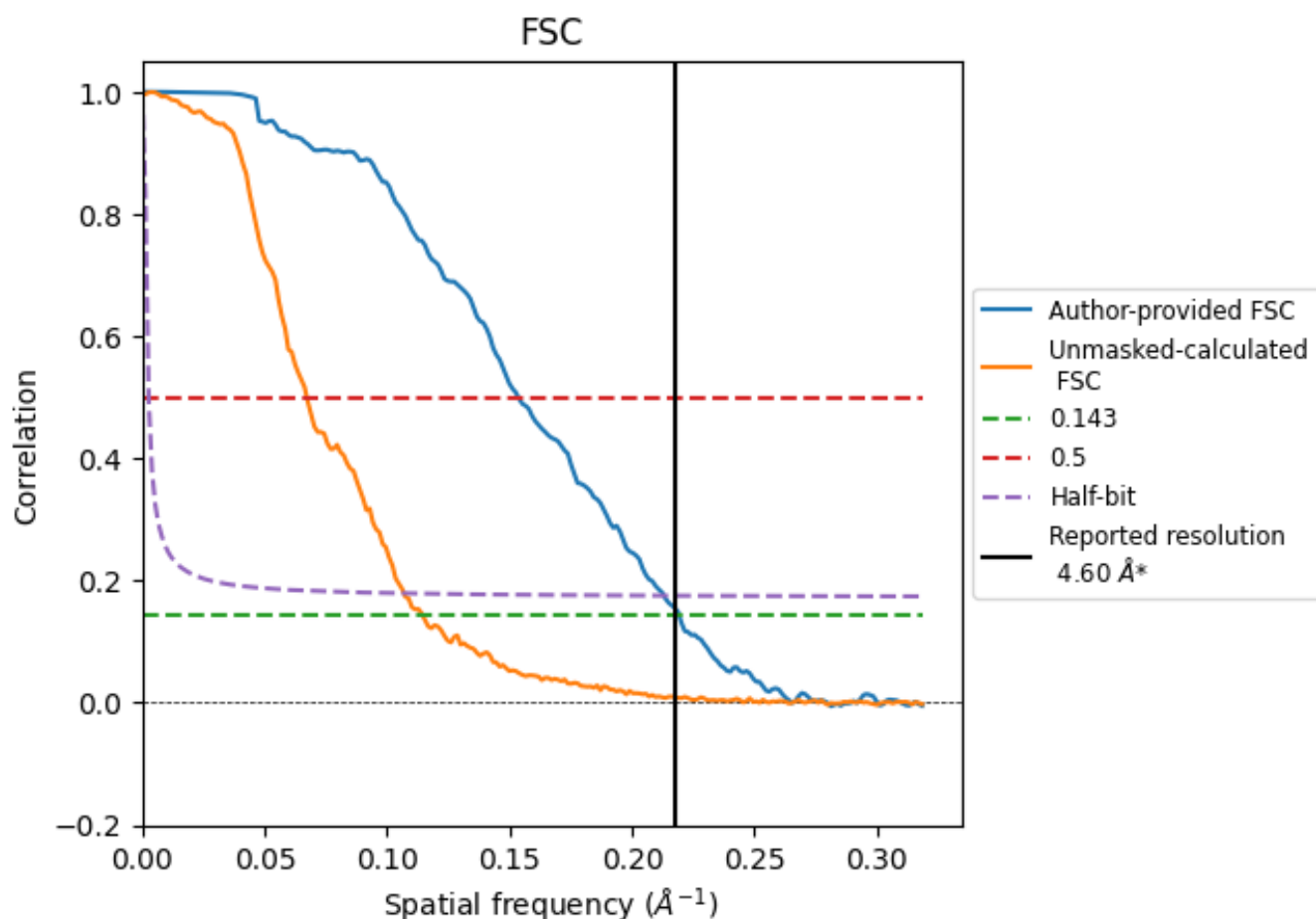


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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

8.2 Resolution estimates [i](#)

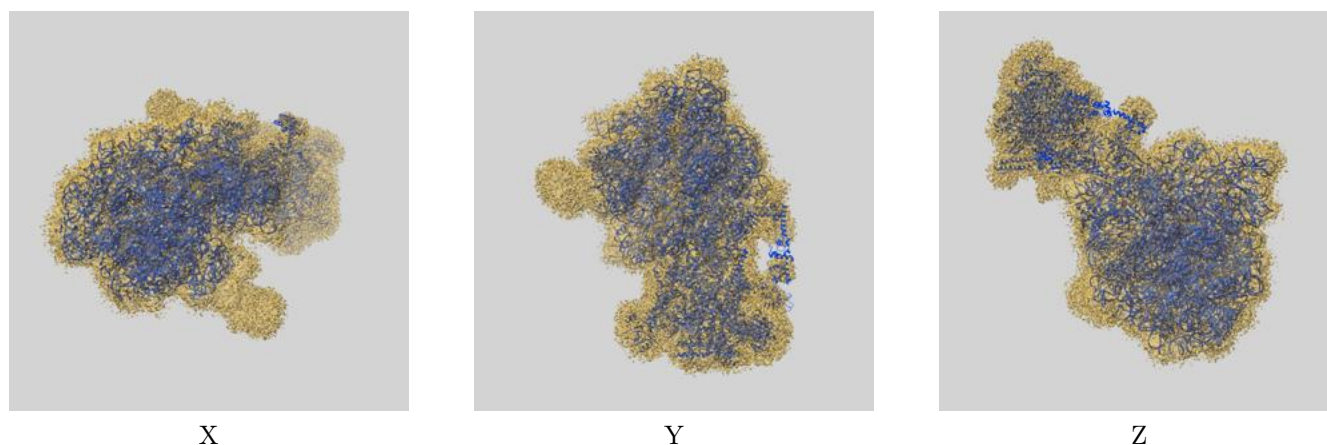
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.51	4.69
Unmasked-calculated*	8.73	14.88	9.35

*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](#)



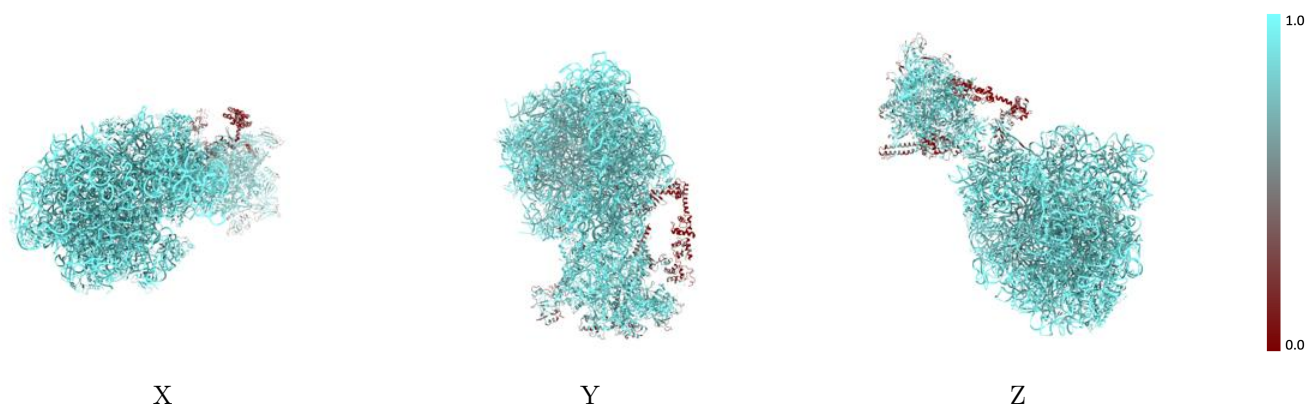
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



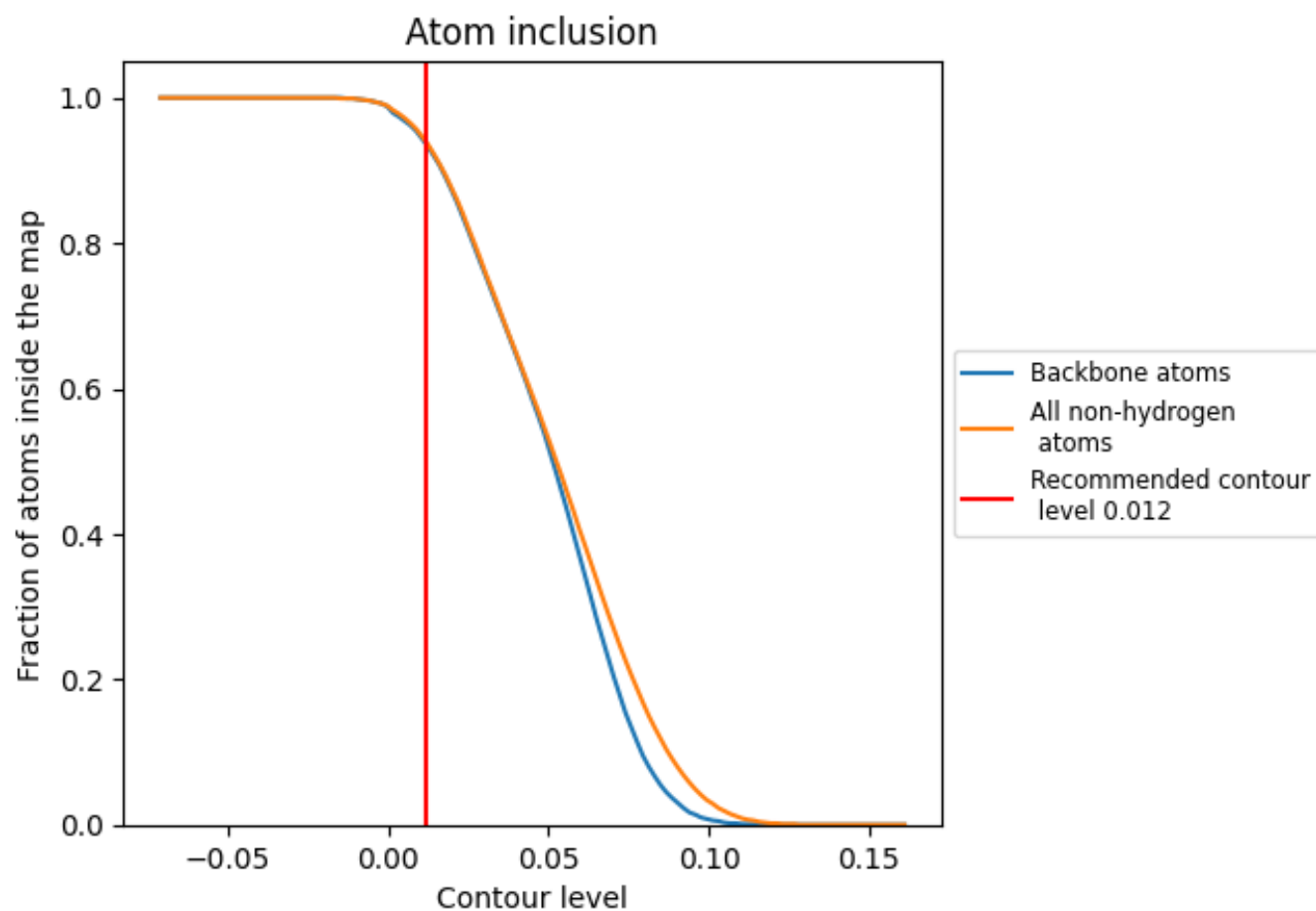
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.0210
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



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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	 0.0020
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