



## wwPDB EM Validation Summary Report ⓘ

Aug 18, 2025 – 04:50 PM JST

PDB ID : 8YDH / pdb\_00008ydh  
EMDB ID : EMD-39171  
Title : E.coli transcription translation coupling complex in TTC-P state 1 (subclass1) 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 : 4.55 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

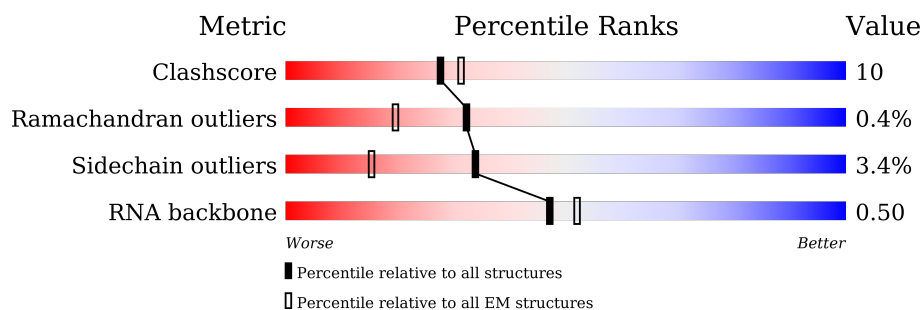
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.55 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.








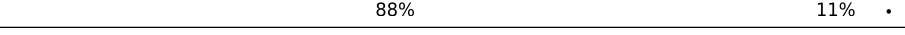

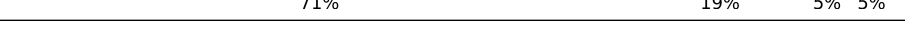
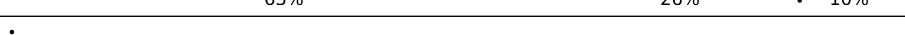
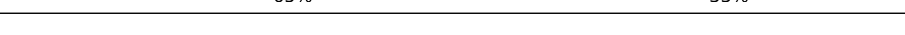
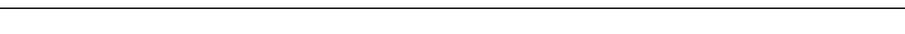

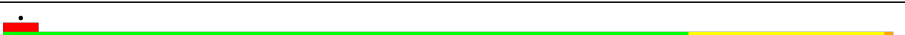












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	B	57	
3	C	55	
4	D	46	
5	E	65	
6	F	38	
7	G	241	

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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	47	
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	

## 2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 177388 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	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		
57	A2	221	Total	C	N	O	S	0	0
			1698	1060	299	333	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 tRNA(fMet).

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) (labeled as "Ligand of Interest" by depositor).

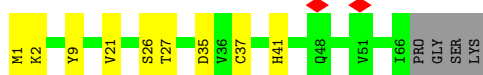
Mol	Chain	Residues	Atoms		AltConf
66	B1	1	Total	Mg	0
			1	1	

### 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

Chain A: 




- Molecule 2: 50S ribosomal protein L32

Chain B: 




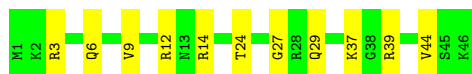
- Molecule 3: 50S ribosomal protein L33

Chain C: 




- Molecule 4: 50S ribosomal protein L34

Chain D: 



- Molecule 5: 50S ribosomal protein L35

Chain E: 



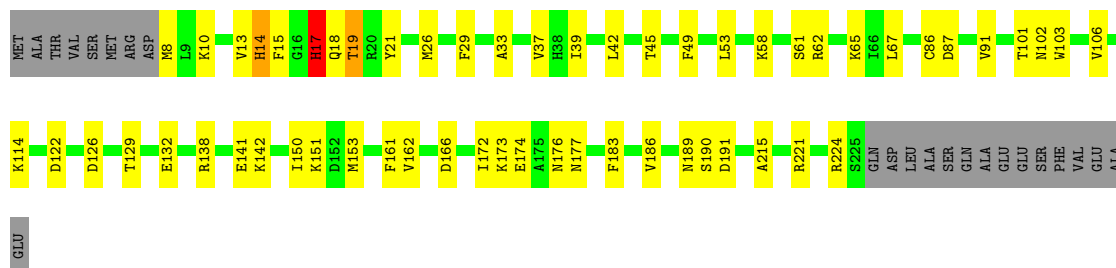
- Molecule 6: 50S ribosomal protein L36

Chain F:  66% 32% .



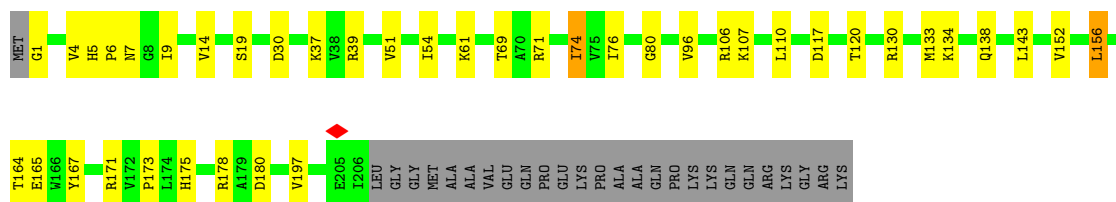
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% . 10%




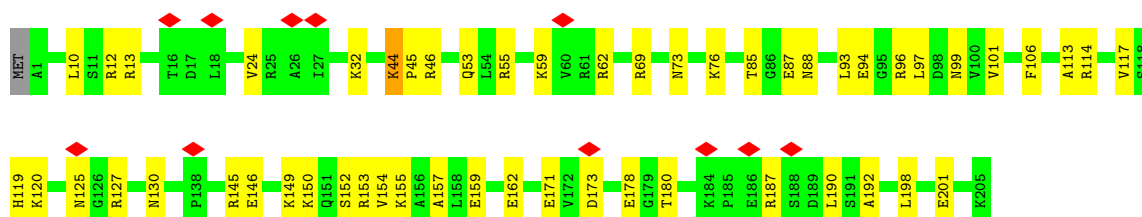
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% . 12%




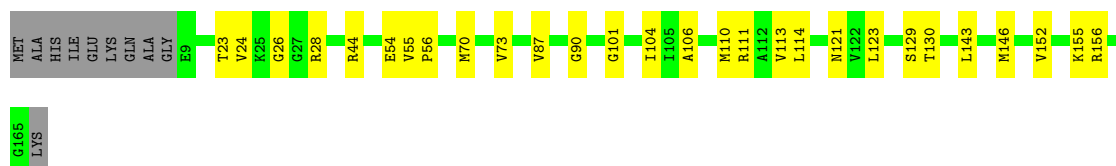
- Molecule 9: 30S ribosomal protein S4

Chain I:  5% 74% 25%



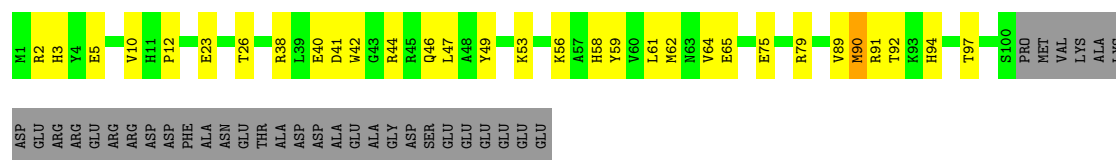
- Molecule 10: 30S ribosomal protein S5

Chain J:  77% 17% 6%



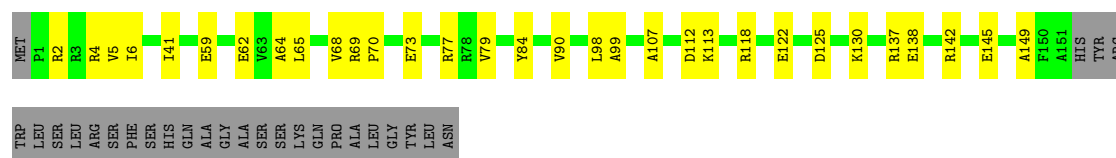
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  51% 22% 26%




- Molecule 12: 30S ribosomal protein S7

Chain L:  67% 17% 16%



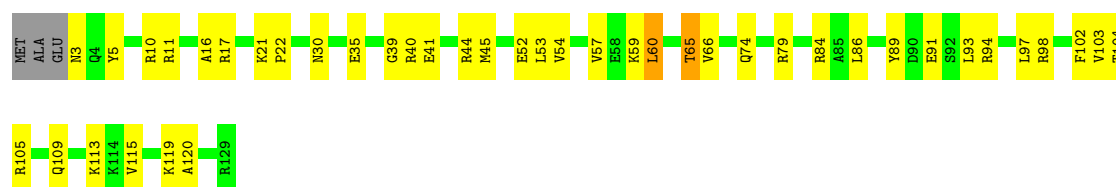
- Molecule 13: 30S ribosomal protein S8

Chain M:  88% 11%



- Molecule 14: 30S ribosomal protein S9

Chain N:  65% 31% 2%



- Molecule 15: 30S ribosomal protein S10

Chain O:  71% 19% 5%



- Molecule 16: 30S ribosomal protein S11

Chain P:  63% 26% 10%





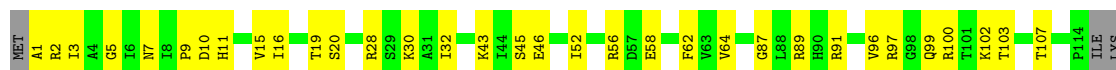
- Molecule 17: 30S ribosomal protein S12

Chain Q: 65% 33%



- Molecule 18: 30S ribosomal protein S13

Chain R: 69% 28%



- Molecule 19: 30S ribosomal protein S14

Chain S: 84% 15%



- Molecule 20: 30S ribosomal protein S15

Chain T: 84% 15%



- Molecule 21: 30S ribosomal protein S16

Chain U: 77% 22%



- Molecule 22: 30S ribosomal protein S17

Chain V: 74% 20% 5%



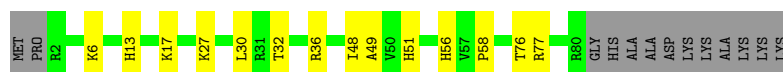
- Molecule 23: 30S ribosomal protein S18

Chain W: 65% 20% 13%



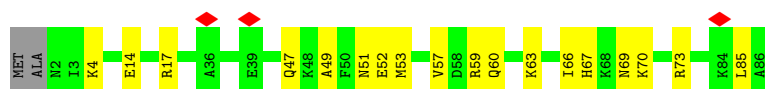
- Molecule 24: 30S ribosomal protein S19

Chain X: 71% 15% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y: 77% 21% 2%



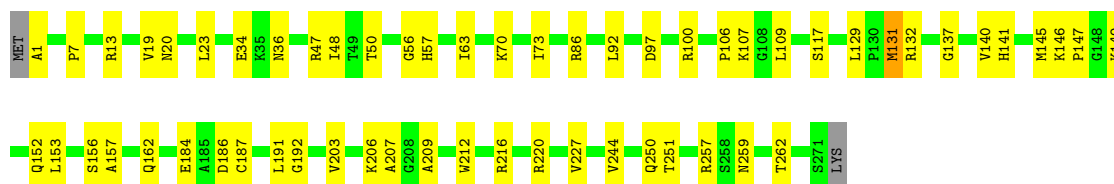
- Molecule 26: 30S ribosomal protein S21

Chain Z: 58% 30% 8%



- Molecule 27: 50S ribosomal protein L2

Chain b: 78% 21% 1%



- Molecule 28: 50S ribosomal protein L3

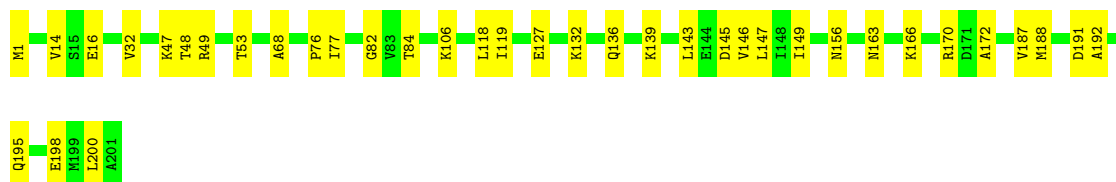
Chain c: 84% 16%





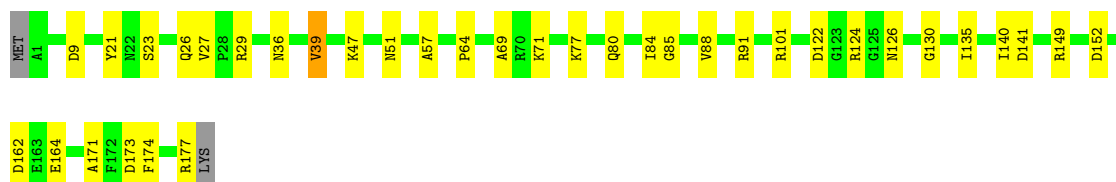
- Molecule 29: 50S ribosomal protein L4

Chain d: 82% 18%



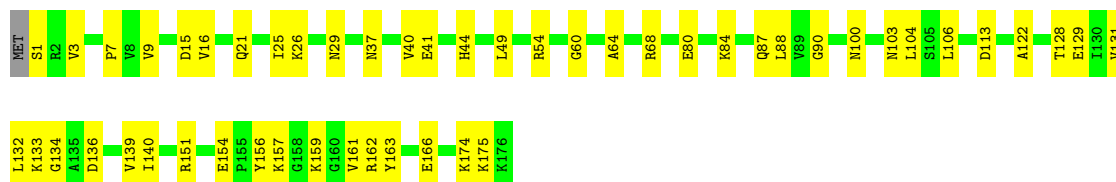
- Molecule 30: 50S ribosomal protein L5

Chain e: 79% 20% ..



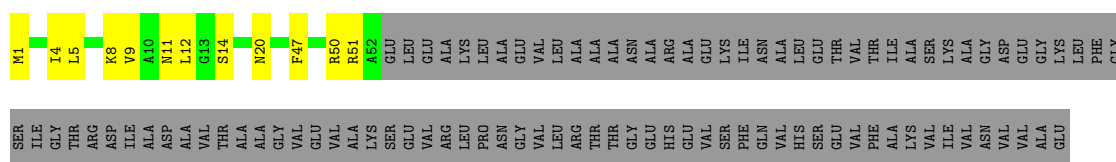
- Molecule 31: 50S ribosomal protein L6

Chain f: 71% 28% .



- Molecule 32: 50S ribosomal protein L9

Chain g: 27% 8% 65%



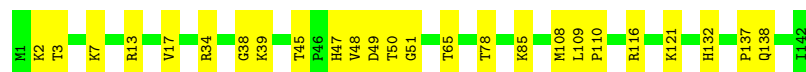
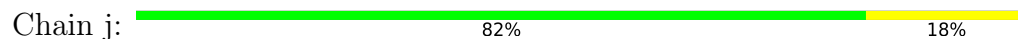
- Molecule 33: 50S ribosomal protein L11

Chain i: 9% 65% 33% ..

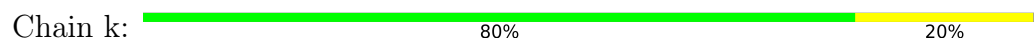




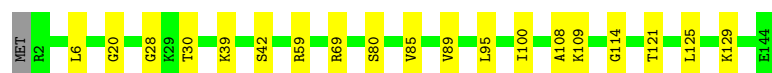
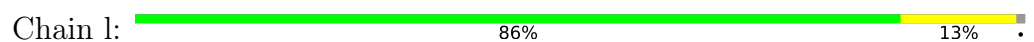
- Molecule 34: 50S ribosomal protein L13



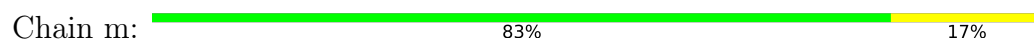
- Molecule 35: 50S ribosomal protein L14



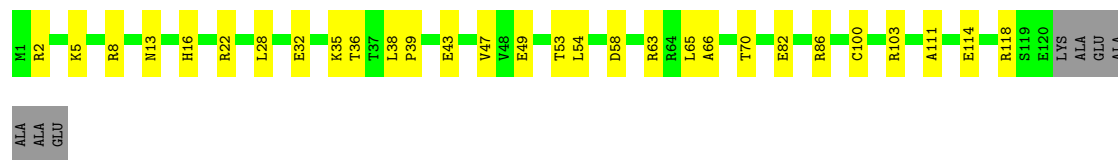
- Molecule 36: 50S ribosomal protein L15



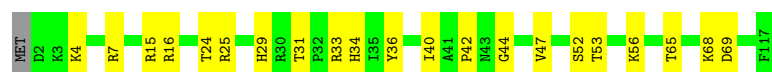
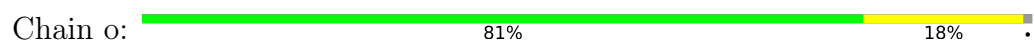
- Molecule 37: 50S ribosomal protein L16




- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18




- Molecule 40: 50S ribosomal protein L19

Chain p:  83% 17% .



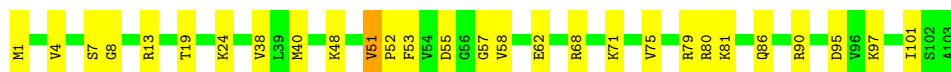
- Molecule 41: 50S ribosomal protein L20

Chain q:  83% 15% ..




- Molecule 42: 50S ribosomal protein L21

Chain r:  73% 26% .



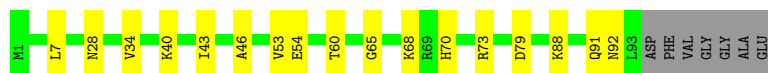
- Molecule 43: 50S ribosomal protein L22

Chain s:  85% 15%



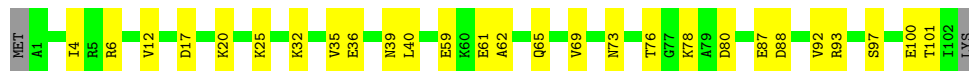
- Molecule 44: 50S ribosomal protein L23

Chain t:  76% 17% 7%




- Molecule 45: 50S ribosomal protein L24

Chain u:  72% 26% .



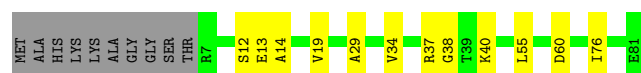
- Molecule 46: 50S ribosomal protein L25

Chain v:  86% 14%




- Molecule 47: 50S ribosomal protein L27

Chain w:  74% 14% 12%




- Molecule 48: 50S ribosomal protein L28

Chain x:  76% 22% ..



- Molecule 49: 50S ribosomal protein L29

Chain y:  76% 24%



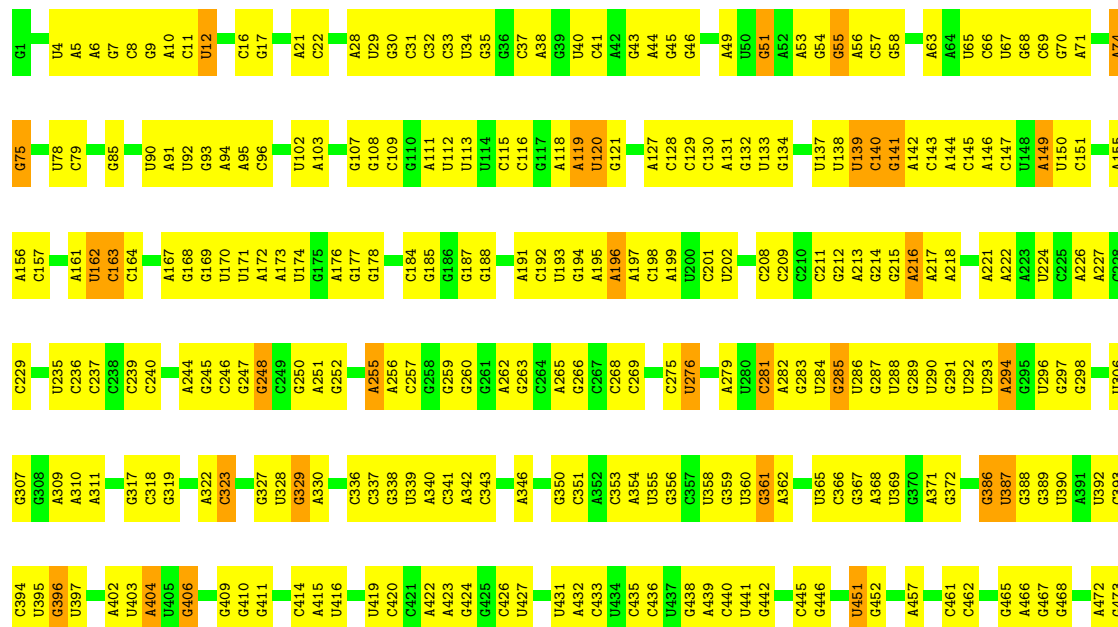
- Molecule 50: 50S ribosomal protein L30

Chain z:  76% 22% .



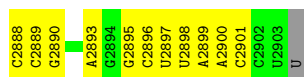
- Molecule 51: 23S rRNA

Chain 1:  42% 51% 6%

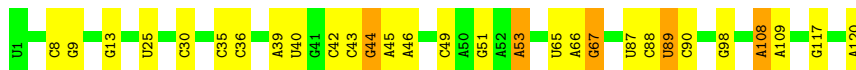


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A1579	G1511	G1338	A1431	G1177	G1107	C1045	A959	C886	G713	G629	C550	G476
A1580	C1512	G1339	A1271	C1178	U1108	A1046	C961	U887	U810	G630	G551	G481
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A1583	G1516	U1344	A1274	U1181	A1111	C1049	C968	C890	C719	C634	U554	C485
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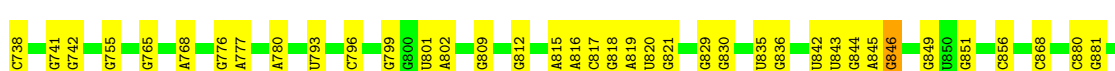
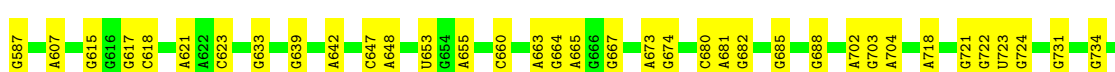
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G2872	U2713	U2555	U2555	G2459	G2373	G2293	C2214	G2149	G2062	U1971	C1893	C1741	U1742
A2873	G2714	U2556	U2556	C2462	U2374	G2294	C2215	C2150	G2069	G1972	C1894	G1816	G1743
G2876	C2717	U2557	U2557	C2463	C2375	U2295	G2216	U2151	C2073	A1978	A1901	G1817	A1744
A2879	U2720	U2558	U2558	G2464	G2383	U2297	G2217	G2152	U2074	G1983	C1902	U1818	A1745
C2880	G2723	U2561	U2561	G2467	U2384	U2298	G2218	C2153	U2085	G1984	C1905	A1819	A1746
U2884	A2799	U2562	U2562	A2468	C2385	G2303	G2222	U2155	U2086	G1985	G1906	U1747	U1747
G2885	G2801	U2563	U2563	A2469	C2386	G2304	G2223	G2156	C2091	C1986	G1907	A1821	C1748
		U2564	U2564	G2470	U2387	U2305	G2224	G2157	G2092	C1987	C1908	A1749	A1749
		G2643	G2643	A2471	A2388	C2306	A2225	A2158	G2093	C1990	C1909	G1750	G1750
										U1991	G1751	U1827	U1751
										G1992	U1911	G1828	G1753



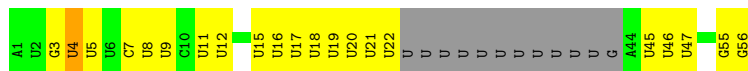
• Molecule 52: 5S rRNA



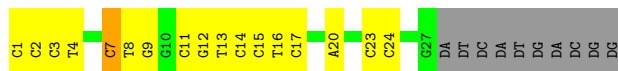
• Molecule 53: 16S rRNA



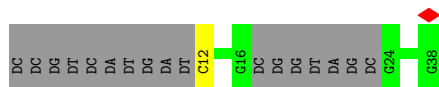
- Molecule 54: mRNA



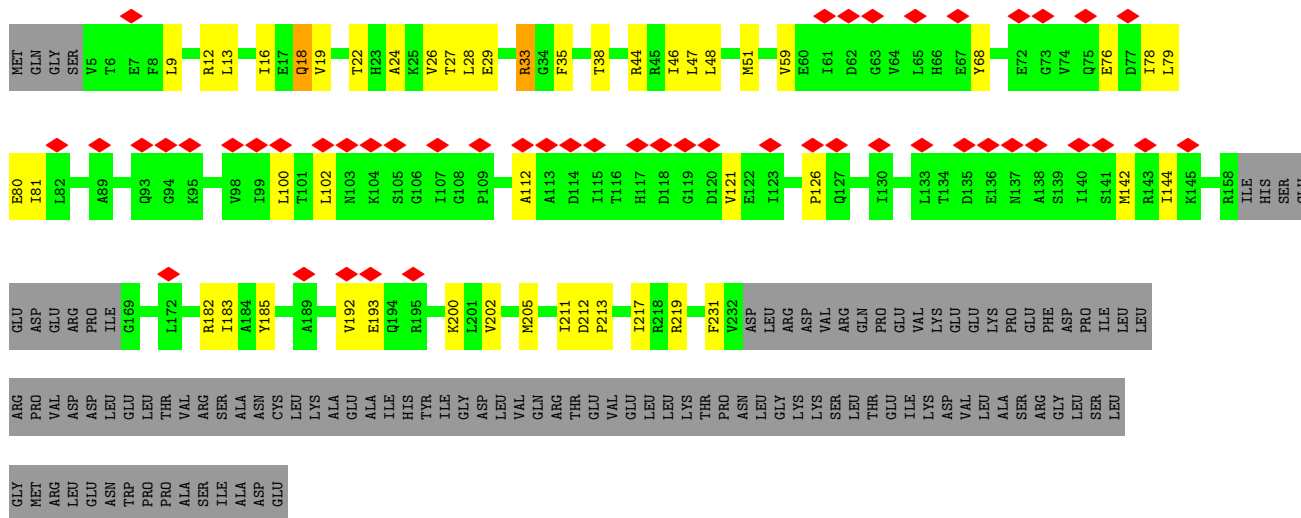
- Molecule 55: template DNA strand



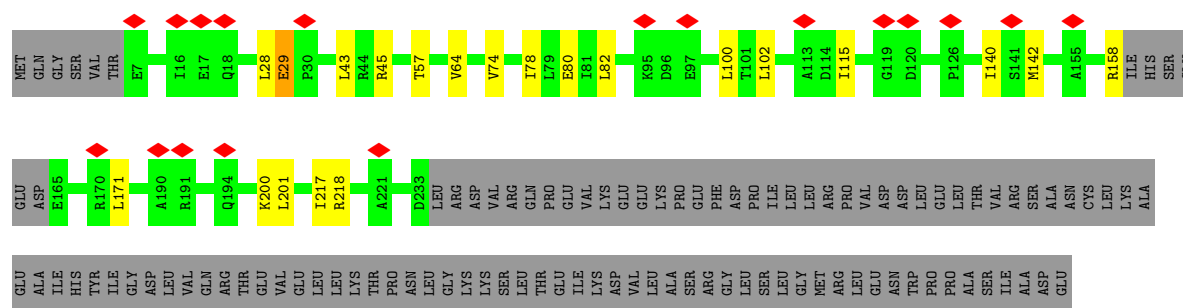
- Molecule 56: non-templete DNA strand



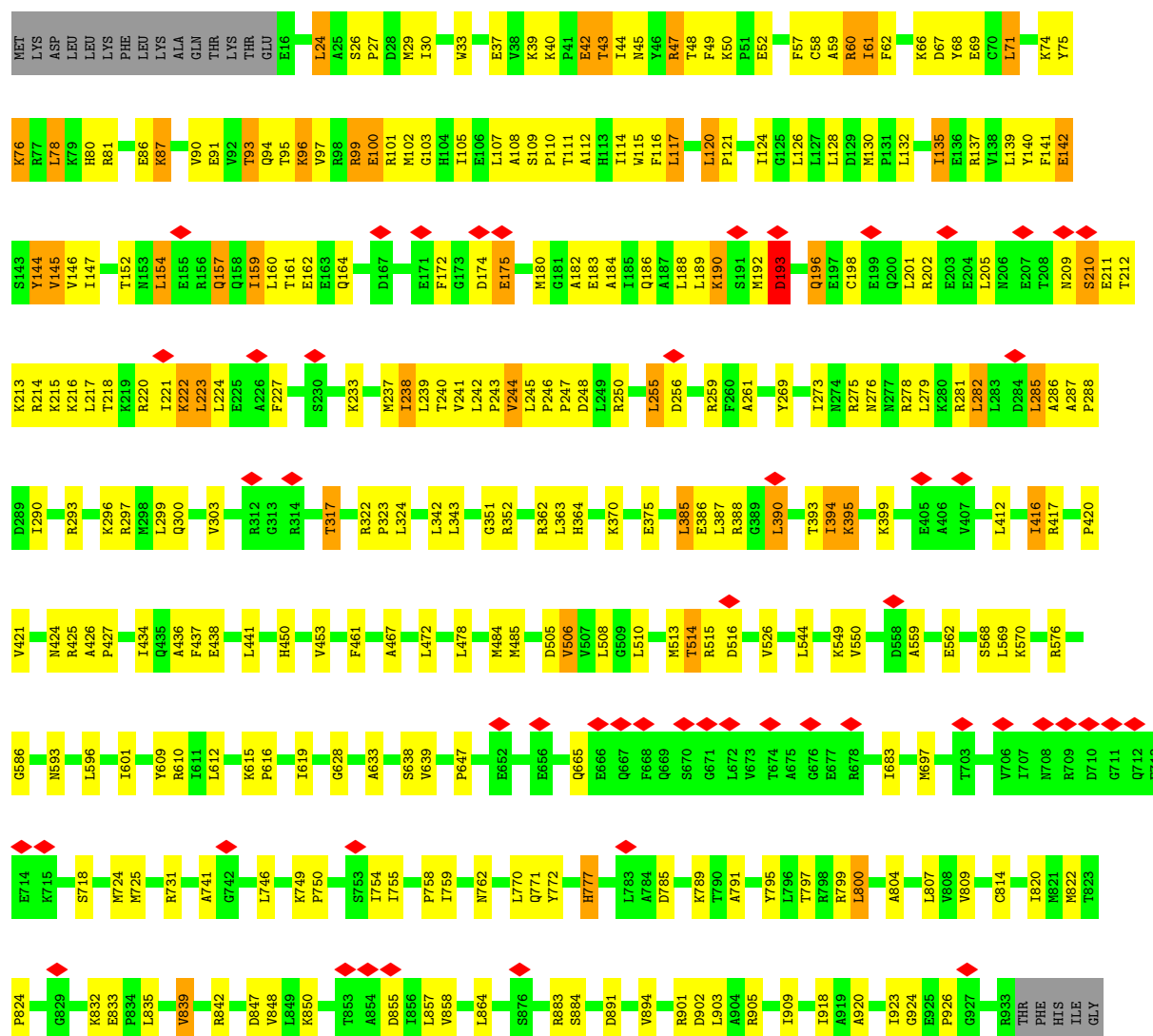
- Molecule 57: DNA-directed RNA polymerase subunit alpha



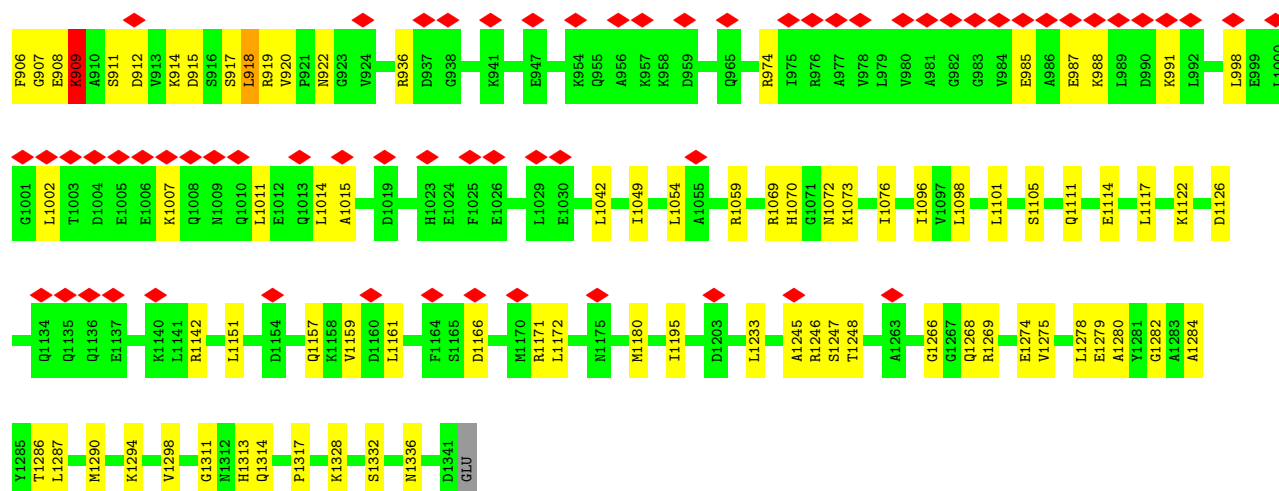
- Molecule 57: DNA-directed RNA polymerase subunit alpha



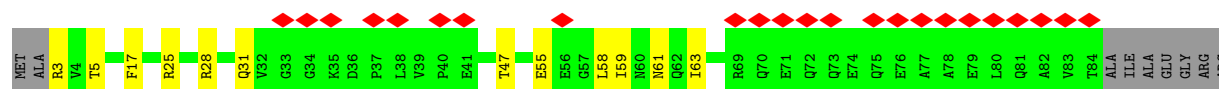
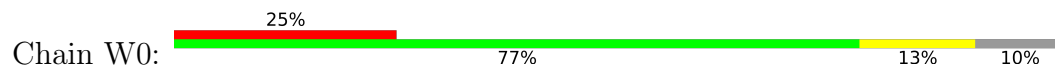
• Molecule 58: DNA-directed RNA polymerase subunit beta'



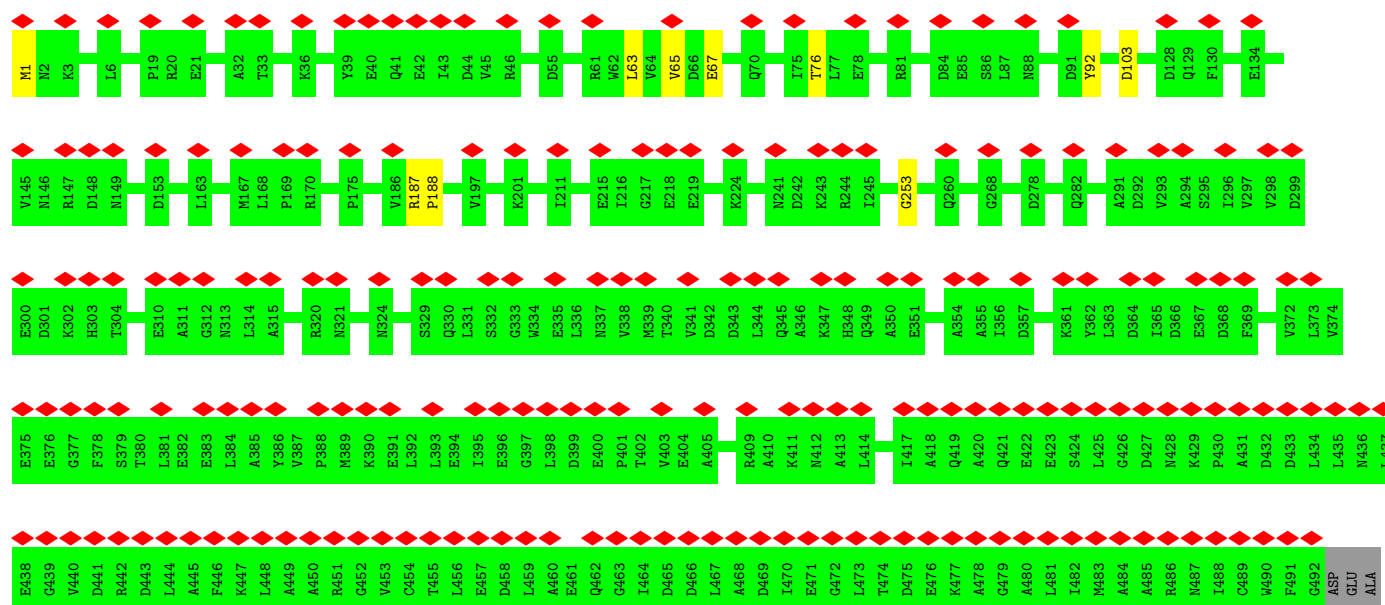
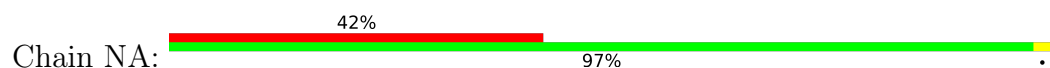




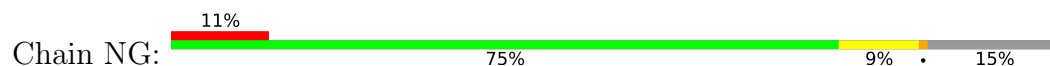
- Molecule 60: DNA-directed RNA polymerase subunit omega

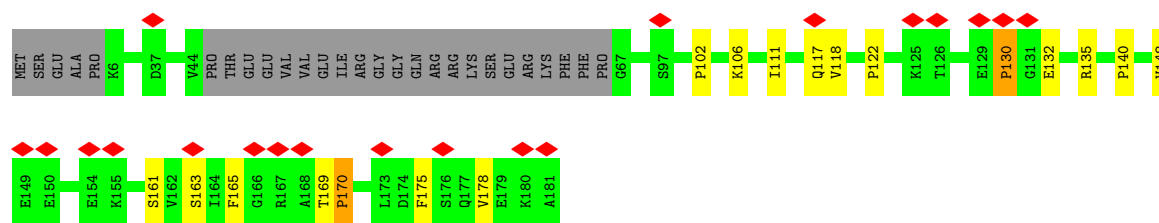


- Molecule 61: Transcription termination/antitermination protein NusA



- Molecule 62: Transcription termination/antitermination protein NusG





• Molecule 63: tRNA(Phe)

Chain 5: 21% 47% 30% .



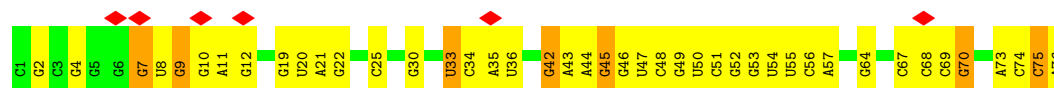
• Molecule 64: tRNA(fMet)

Chain 6: 77% 19% .



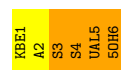
• Molecule 64: tRNA(fMet)

Chain 7: 8% 44% 47% 9%



• Molecule 65: tRNA(fMet)

Chain h: 33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23023	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	0.188	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.011	Depositor
Map size ( $\text{\AA}$ )	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.57, 1.57, 1.57	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.27	0/531	0.54	0/709
2	B	0.41	0/450	0.60	2/599 (0.3%)
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	0.31	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	0.85	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	0.65	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	0.67	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	0.38	0/1434	0.60	2/1926 (0.1%)
31	f	0.29	0/1343	0.55	0/1816
32	g	0.32	0/405	0.75	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	0.42	0/1152	0.56	1/1551 (0.1%)
35	k	0.45	0/947	0.66	0/1268
36	l	0.40	0/1054	0.63	0/1403
37	m	0.56	0/1093	0.74	0/1460
38	n	0.46	0/973	0.72	1/1301 (0.1%)
39	o	0.32	0/902	0.51	0/1209
40	p	0.42	0/929	0.62	0/1242
41	q	0.52	0/960	0.62	1/1278 (0.1%)
42	r	0.47	0/829	0.66	0/1107
43	s	0.44	0/864	0.58	0/1156
44	t	0.33	0/744	0.52	0/994
45	u	0.45	0/787	0.75	0/1051
46	v	0.34	0/766	0.51	0/1025
47	w	0.40	0/582	0.52	0/769
48	x	0.43	0/635	0.63	1/848 (0.1%)
49	y	0.29	0/510	0.64	0/677
50	z	0.41	0/453	0.54	0/605
51	1	0.51	0/69796	0.62	20/108888 (0.0%)
52	2	0.44	0/2872	0.46	0/4479
53	3	0.42	0/36963	0.43	1/57662 (0.0%)
54	4	0.53	0/808	0.67	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	0.49	0/1696	0.69	0/2298
57	A2	0.43	0/1718	0.63	0/2328
58	B1	0.57	4/10510 (0.0%)	0.75	8/14196 (0.1%)
59	B2	0.46	0/10714	0.67	1/14459 (0.0%)
60	W0	0.30	0/652	0.61	0/879
61	NA	0.87	0/2431	1.26	1/3385 (0.0%)
62	NG	1.11	0/756	1.03	0/1048
63	5	0.57	0/1812	0.86	3/2823 (0.1%)
64	6	0.41	0/1832	0.48	0/2855
64	7	0.39	0/1832	0.57	1/2855 (0.0%)
65	h	3.17	2/11 (18.2%)	0.75	0/13
All	All	0.48	6/190836 (0.0%)	0.62	66/281829 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	3	SER	CA-C	-6.73	1.38	1.52
65	h	4	SER	CA-C	-6.15	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.24	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.09	1.33	1.23
58	B1	424	ASN	CG-ND2	-5.06	1.22	1.33

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	73	VAL	N-CA-C	-9.04	104.53	113.20
41	q	33	VAL	N-CA-C	-8.79	104.73	112.12
12	L	64	ALA	N-CA-C	-7.70	105.05	114.75
51	1	1130	U	C2'-C3'-O3'	7.58	120.87	109.50
64	7	33	U	C2'-C3'-O3'	7.24	120.35	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	8	0
3	C	409	0	440	3	0
4	D	377	0	418	9	0
5	E	504	0	574	3	0
6	F	302	0	343	7	0
7	G	1704	0	1732	35	0
8	H	1624	0	1699	28	0
9	I	1643	0	1710	32	0
10	J	1156	0	1199	18	0
11	K	817	0	808	17	0
12	L	1181	0	1240	19	0
13	M	979	0	1034	9	0
14	N	1022	0	1070	25	0
15	O	786	0	828	16	0
16	P	869	0	878	22	0
17	Q	955	0	1019	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	883	0	944	19	0
19	S	805	0	847	10	0
20	T	714	0	737	6	0
21	U	649	0	666	14	0
22	V	648	0	691	10	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	13	0
27	b	2082	0	2157	46	0
28	c	1565	0	1616	29	0
29	d	1552	0	1619	27	0
30	e	1410	0	1447	23	0
31	f	1323	0	1374	34	0
32	g	400	0	423	6	0
33	i	1032	0	1088	40	0
34	j	1129	0	1162	22	0
35	k	938	0	1012	17	0
36	l	1045	0	1117	16	0
37	m	1074	0	1157	13	0
38	n	960	0	1000	20	0
39	o	892	0	923	15	0
40	p	917	0	965	18	0
41	q	947	0	1022	10	0
42	r	816	0	839	17	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	8	0
47	w	575	0	592	8	0
48	x	625	0	655	11	0
49	y	509	0	543	11	0
50	z	449	0	491	8	0
51	1	62317	0	31346	1468	0
52	2	2568	0	1303	15	0
53	3	33012	0	16618	180	0
54	4	729	0	364	7	0
55	8	539	0	305	27	0
56	9	417	0	224	1	0
57	A1	1677	0	1713	25	0
57	A2	1698	0	1718	13	0
58	B1	10353	0	10548	327	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	4	0
62	NG	758	0	334	16	0
63	5	1622	0	821	29	0
64	6	1640	0	837	7	0
64	7	1640	0	837	20	0
65	h	48	0	40	7	0
66	B1	1	0	0	0	0
All	All	177388	0	126304	2824	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 10.

The worst 5 of 2824 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	1.03
51:1:1672:A:C2	51:1:2582:G:H5'	1.95	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
2	B	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
4	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
5	E	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
6	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	51
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	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%)	129 (87%)	20 (13%)	0	100	100
13	M	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
14	N	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
15	O	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	13	49
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	51
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	98 (88%)	13 (12%)	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	38
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
31	f	174/177 (98%)	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%)	89 (88%)	12 (12%)	0	100	100
43	s	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
44	t	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
45	u	100/104 (96%)	84 (84%)	15 (15%)	1 (1%)	13	49
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	10	42
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	214/329 (65%)	195 (91%)	19 (9%)	0	100	100
57	A2	217/329 (66%)	206 (95%)	11 (5%)	0	100	100
58	B1	1329/1407 (94%)	1203 (90%)	122 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1207 (90%)	126 (9%)	5 (0%)	30	68
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	451 (92%)	36 (7%)	3 (1%)	22	60
62	NG	150/181 (83%)	131 (87%)	13 (9%)	6 (4%)	2	18
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9440/10235 (92%)	8500 (90%)	904 (10%)	36 (0%)	32	68

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	x	25	LYS
58	B1	121	PRO
61	NA	187	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
61	NA	188	PRO
62	NG	102	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	60

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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%)	102 (99%)	1 (1%)	73	81
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%)	80 (95%)	4 (5%)	21	43
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%)	1017 (92%)	93 (8%)	9	28

*Continued on next page...*

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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	76
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7127 (97%)	254 (3%)	34	53

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	A1	13	LEU
59	B2	56	VAL
58	B1	91	GLU
59	B2	44	GLU
59	B2	892	GLU

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

Mol	Chain	Res	Type
29	d	165	HIS
59	B2	69	GLN
37	m	13	HIS
58	B1	1259	GLN
59	B2	808	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	398 (13%)	16 (0%)
52	2	119/120 (99%)	17 (14%)	1 (0%)
53	3	1538/1542 (99%)	255 (16%)	4 (0%)
54	4	33/47 (70%)	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	4819/4843 (99%)	766 (15%)	32 (0%)

5 of 766 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A

*Continued on next page...*

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

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	57	G
63	5	60	U
51	1	1930	G
51	1	1801	A
64	7	33	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
65	DPP	h	2	65	3,5,6	0.56	0	1,5,7	0.09	0
65	UAL	h	5	65	7,8,9	2.31	3 (42%)	5,9,11	2.90	2 (40%)
65	5OH	h	6	65	8,12,13	0.76	0	3,16,18	1.53	1 (33%)
65	KBE	h	1	65	8,8,9	0.61	0	7,8,10	1.21	1 (14%)

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	UAL	h	5	65	-	0/3/7/9	-
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	KBE	h	1	65	-	0/7/7/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	5	UAL	C1-N1	-4.92	1.32	1.40
65	h	5	UAL	C-CA	-2.87	1.40	1.45
65	h	5	UAL	CA-N	2.01	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	h	5	UAL	CA-CB-N1	-5.28	115.65	125.60
65	h	5	UAL	O-C-CA	-3.23	121.28	125.39
65	h	6	5OH	CR-CB-CA	-2.40	110.02	112.61
65	h	1	KBE	CB-CA-C	-2.07	109.21	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

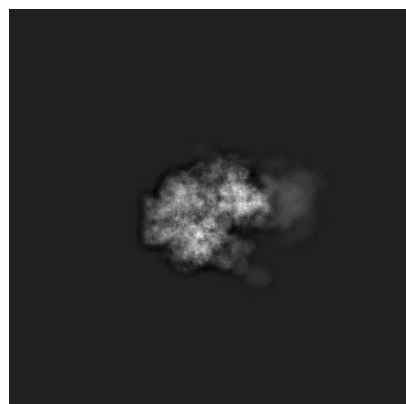
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39171. These allow visual inspection of the internal detail of the map and identification of artifacts.

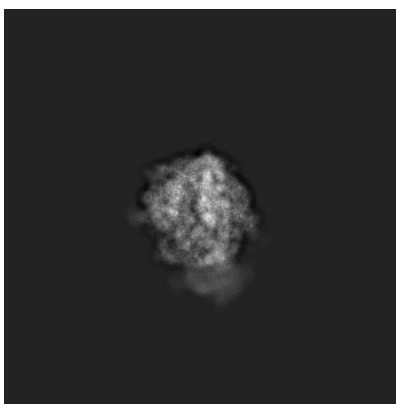
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

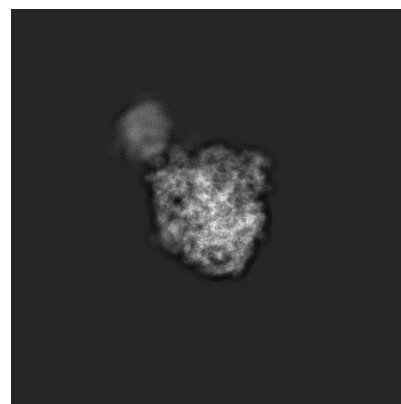
#### 6.1.1 Primary map



X

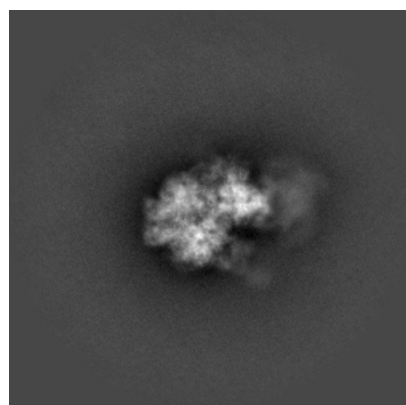


Y

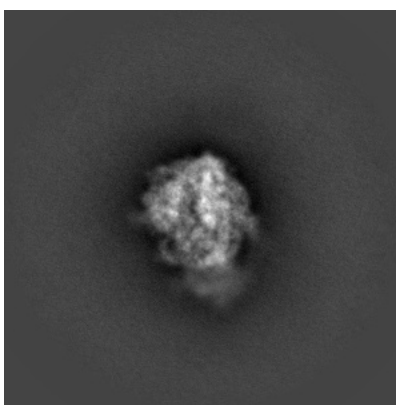


Z

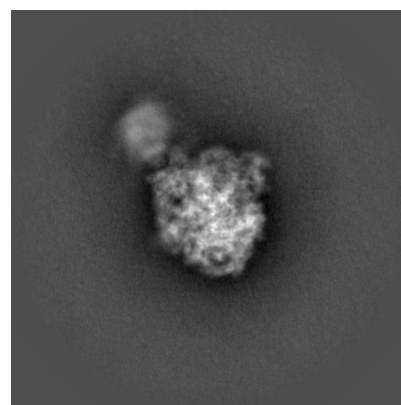
#### 6.1.2 Raw map



X



Y

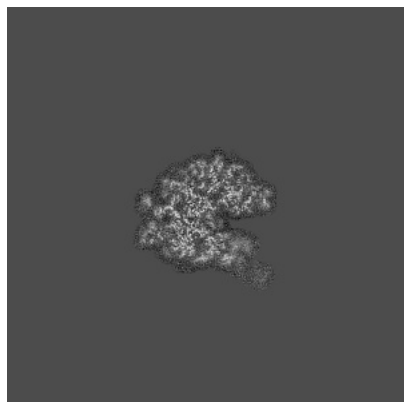


Z

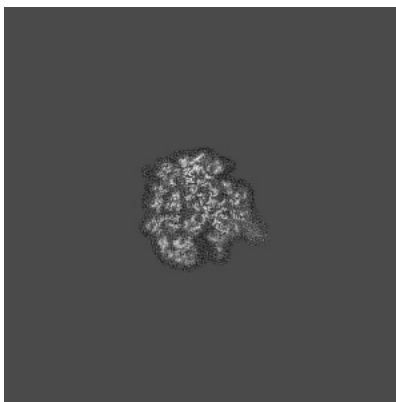
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

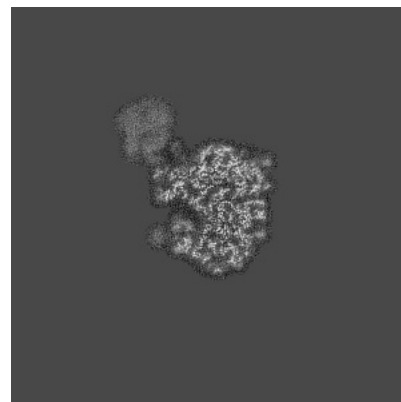
### 6.2.1 Primary map



X Index: 240

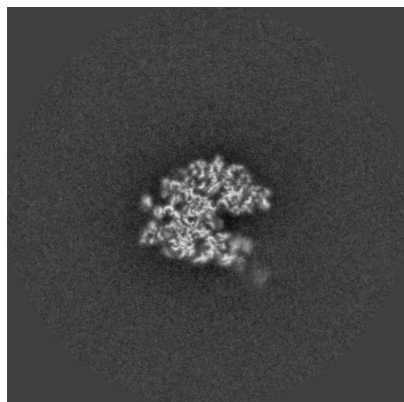


Y Index: 240

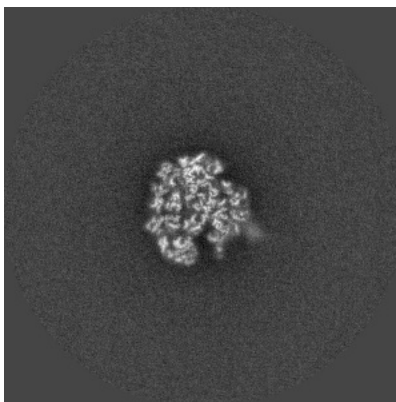


Z Index: 240

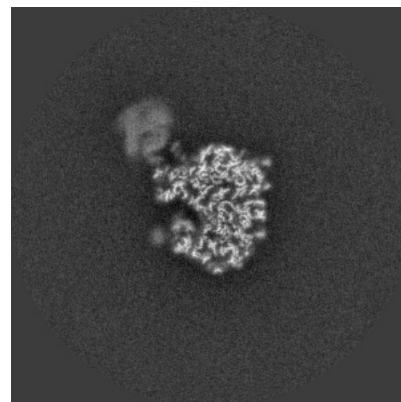
### 6.2.2 Raw map



X Index: 240



Y Index: 240

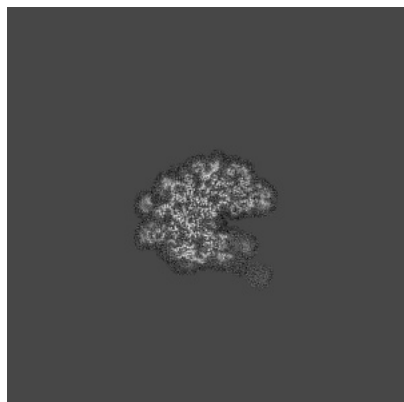


Z Index: 240

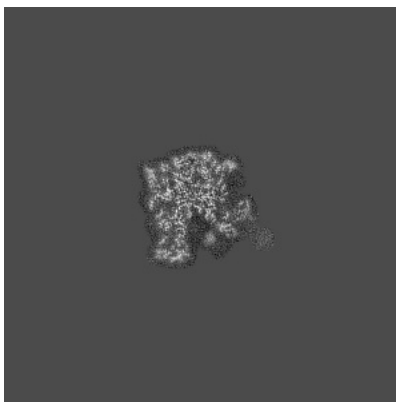
The images above show central slices of the map in three orthogonal directions.

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

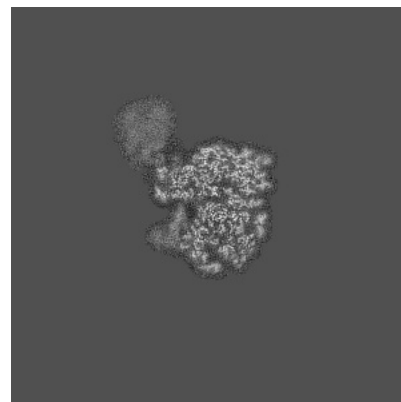
### 6.3.1 Primary map



X Index: 243

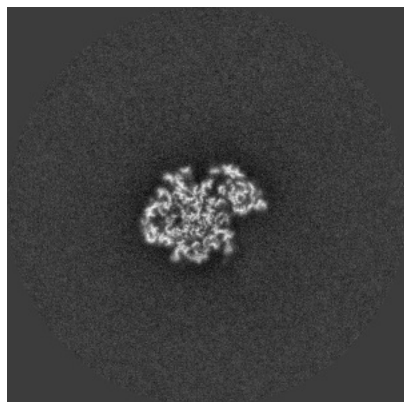


Y Index: 228

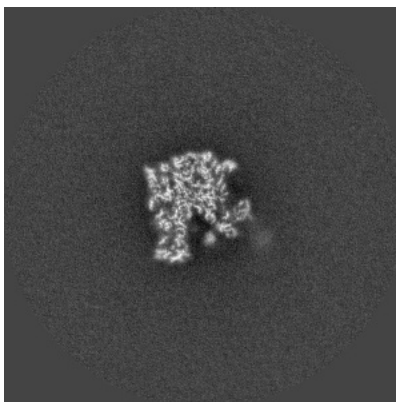


Z Index: 245

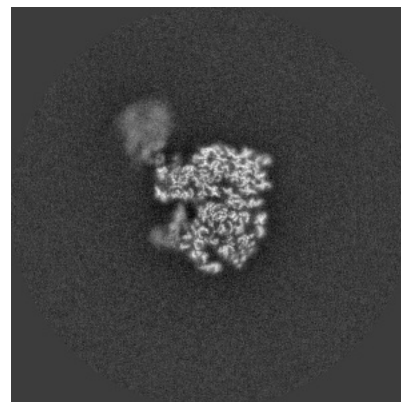
### 6.3.2 Raw map



X Index: 265



Y Index: 228

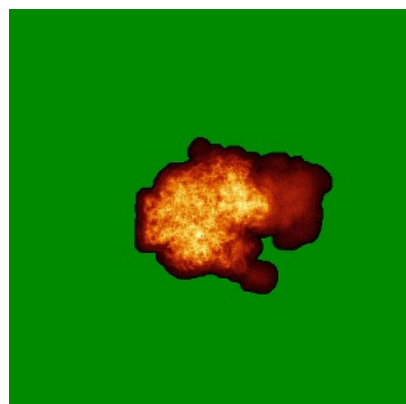


Z Index: 245

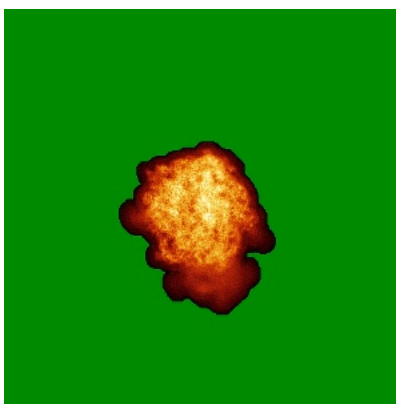
The images above show the largest variance slices of the map in three orthogonal directions.

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

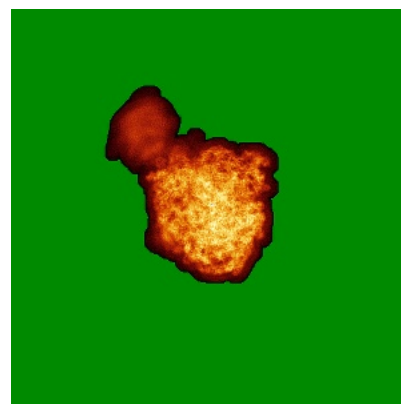
### 6.4.1 Primary map



X

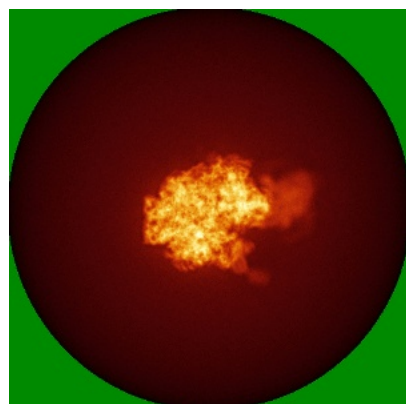


Y

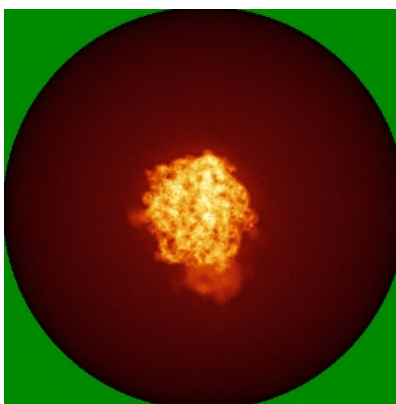


Z

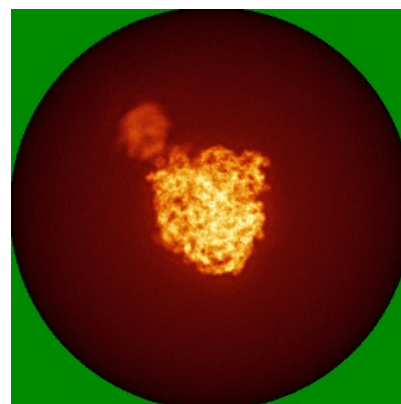
### 6.4.2 Raw map



X



Y



Z

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

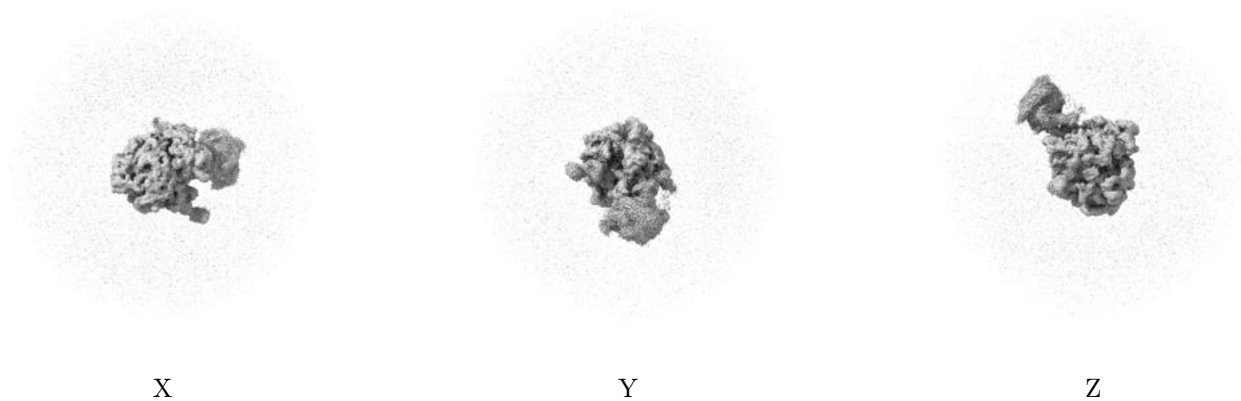
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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

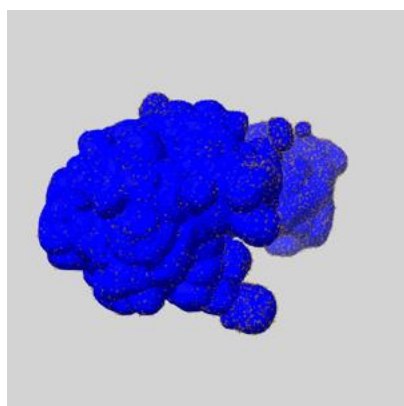
## 6.6 Mask visualisation [i](#)

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

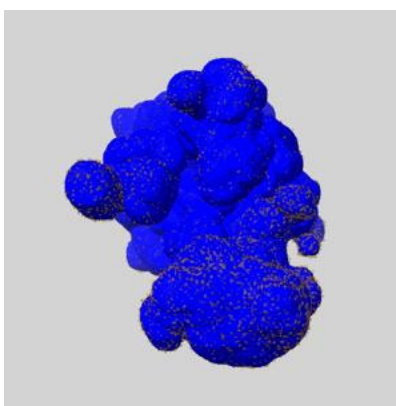
A mask typically either:

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

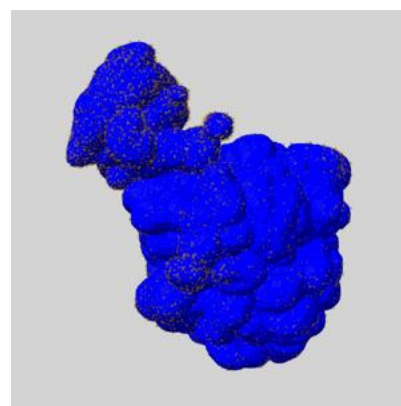
### 6.6.1 emd\_39171\_msk\_1.map [i](#)



X



Y

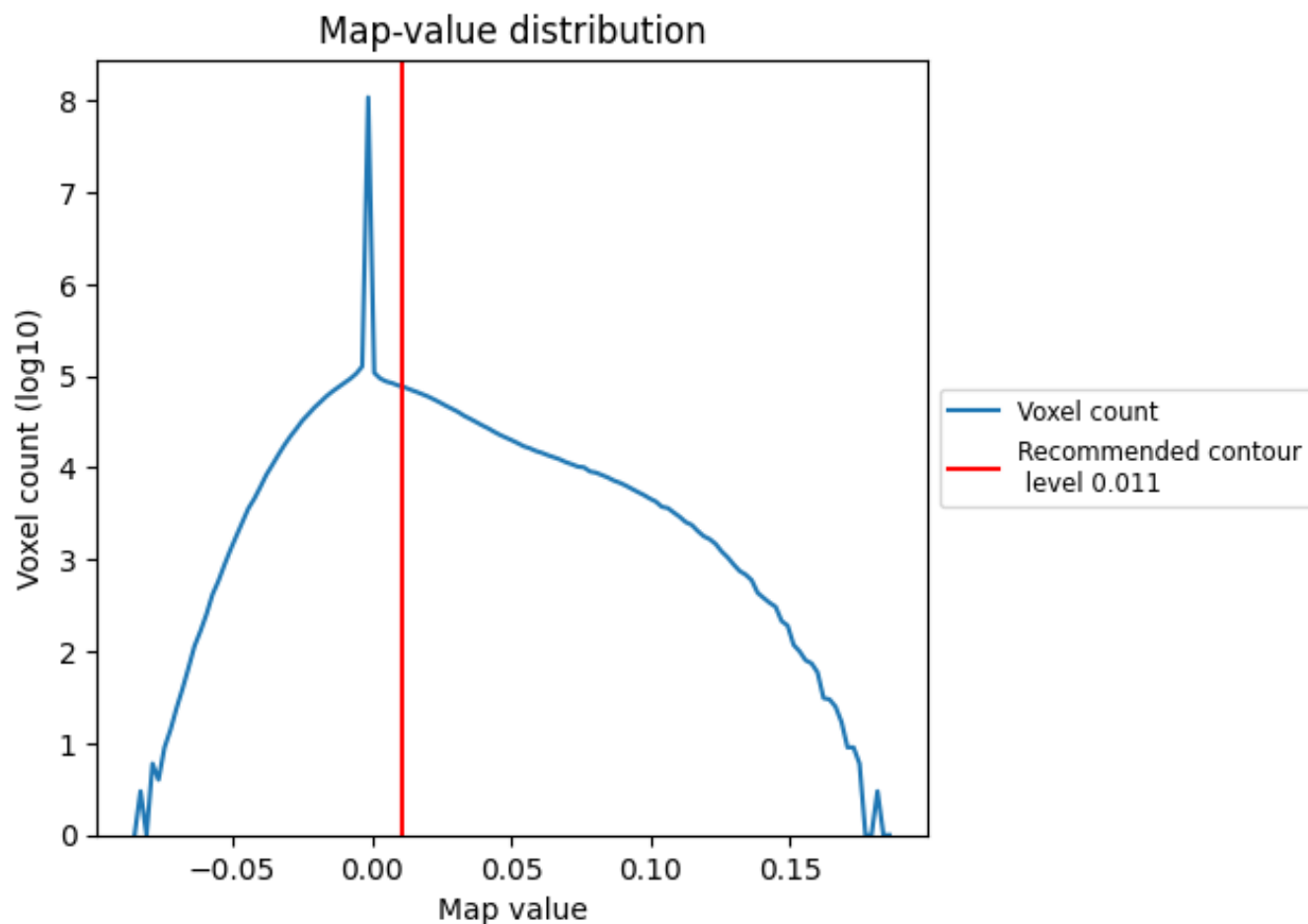


Z

## 7 Map analysis [i](#)

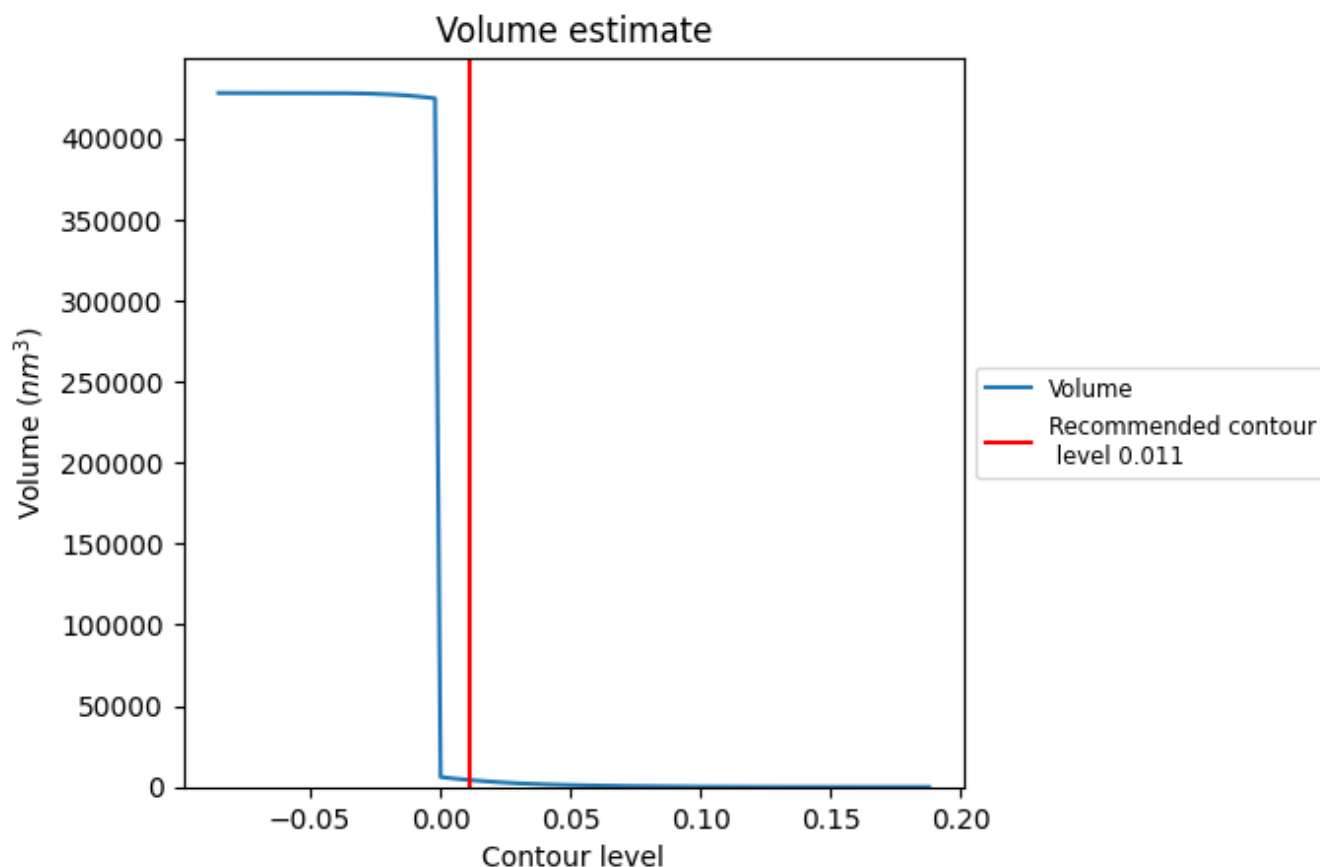
This section contains the results of statistical analysis of the map.

### 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.

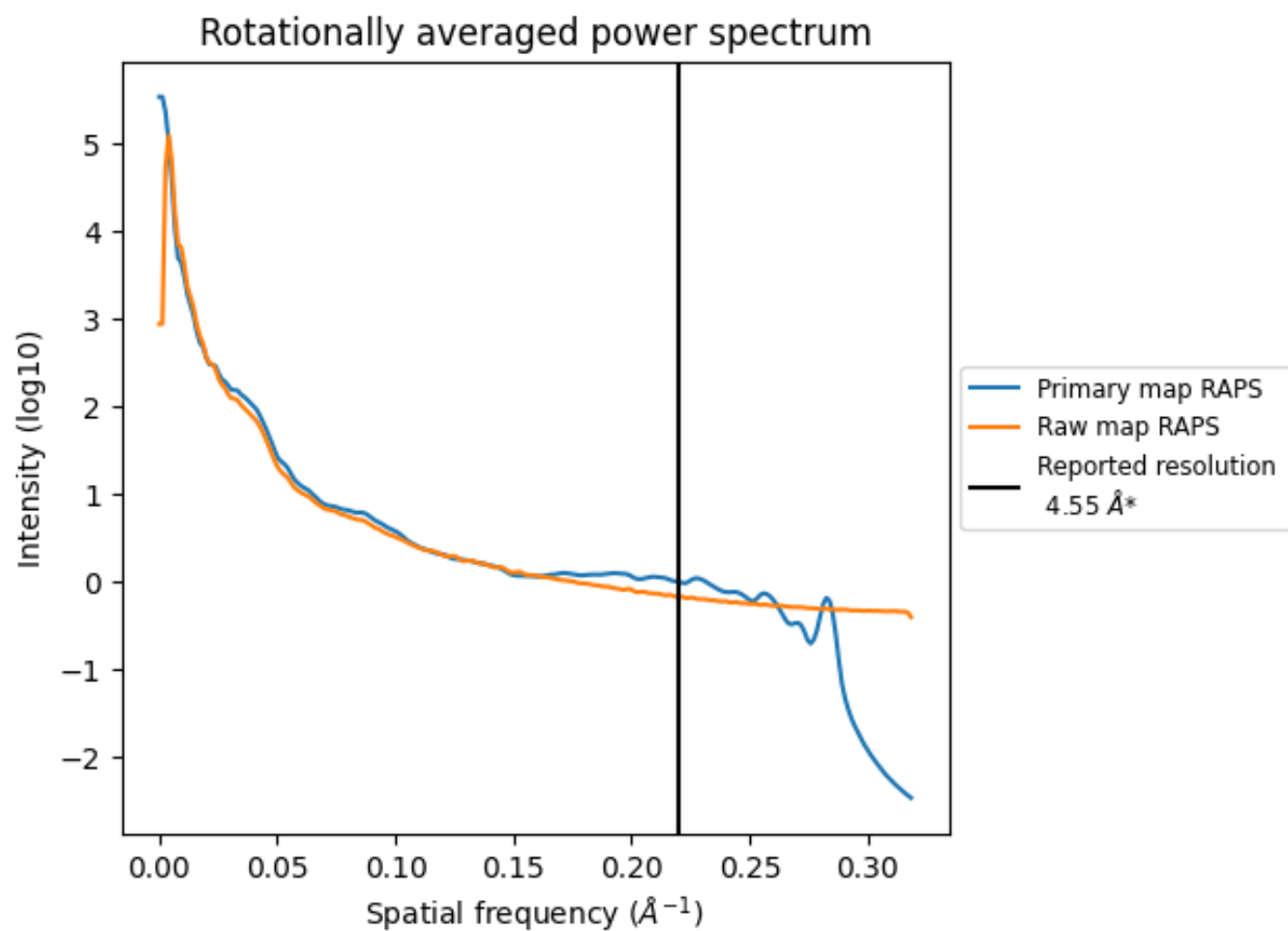
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4328  $\text{nm}^3$ ; this corresponds to an approximate mass of 3910 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 ⓘ

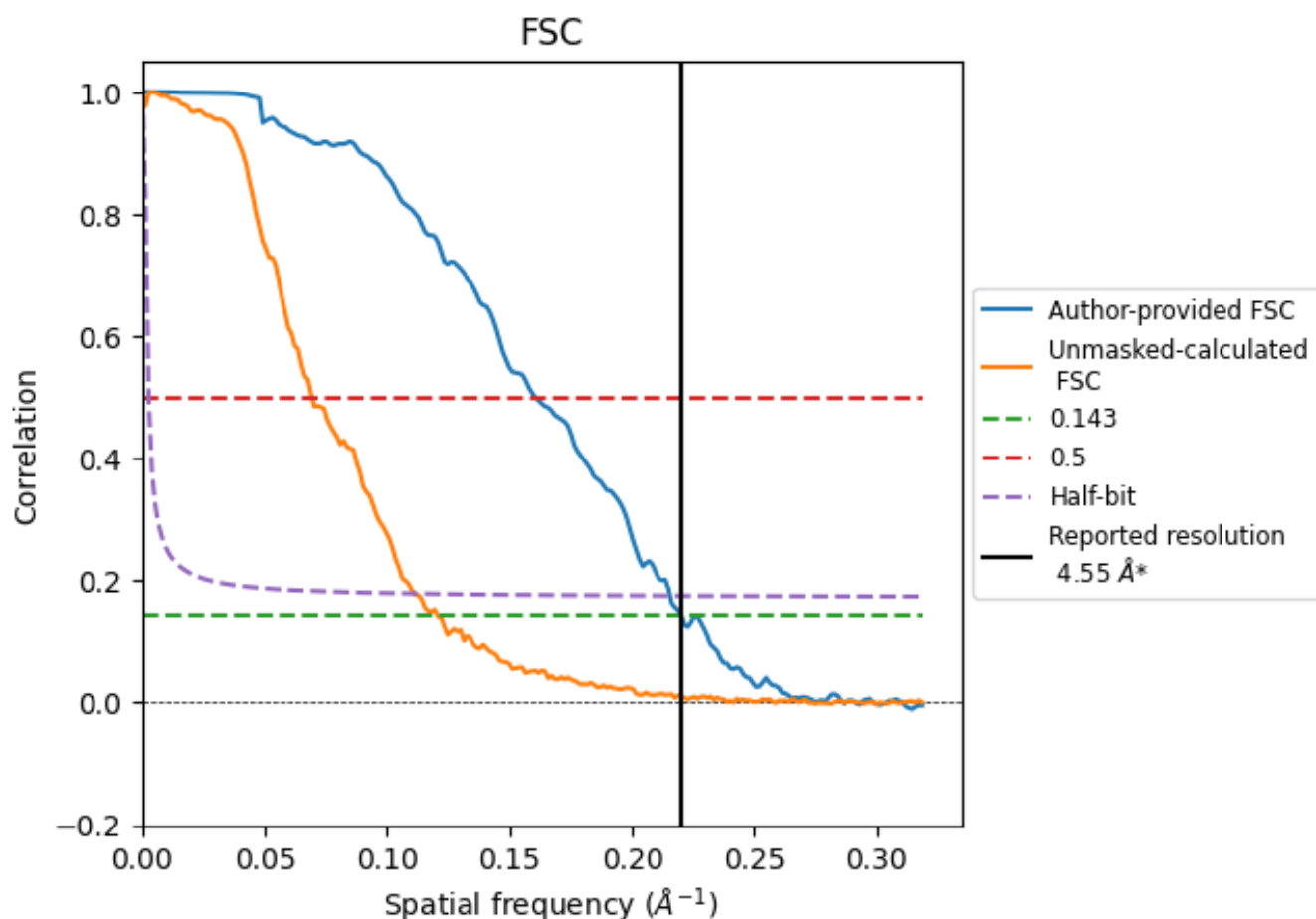


\*Reported resolution corresponds to spatial frequency of 0.220 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

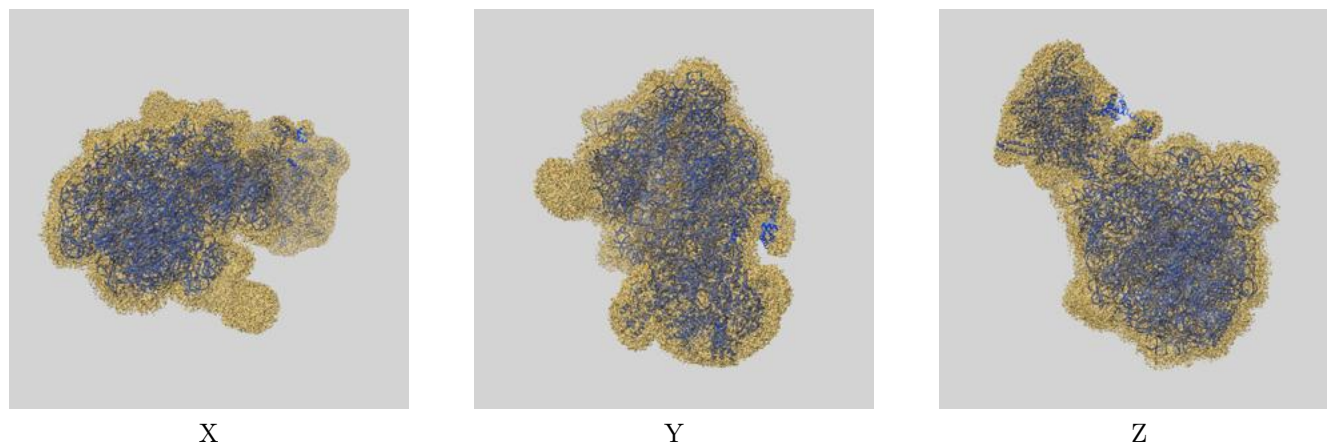
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	4.54	6.23	4.64
Unmasked-calculated*	8.29	14.43	8.99

\*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 8.29 differs from the reported value 4.55 by more than 10 %

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

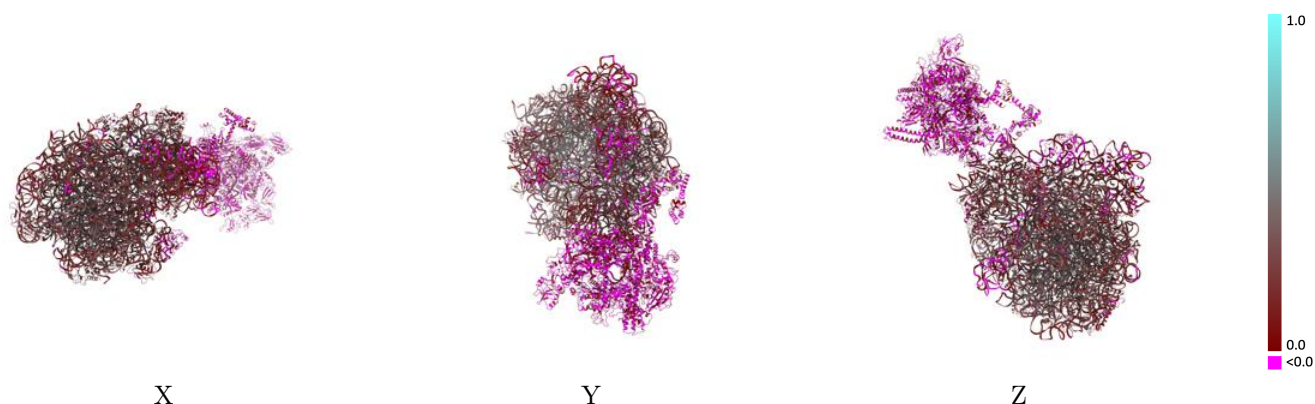
This section contains information regarding the fit between EMDB map EMD-39171 and PDB model 8YDH. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

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



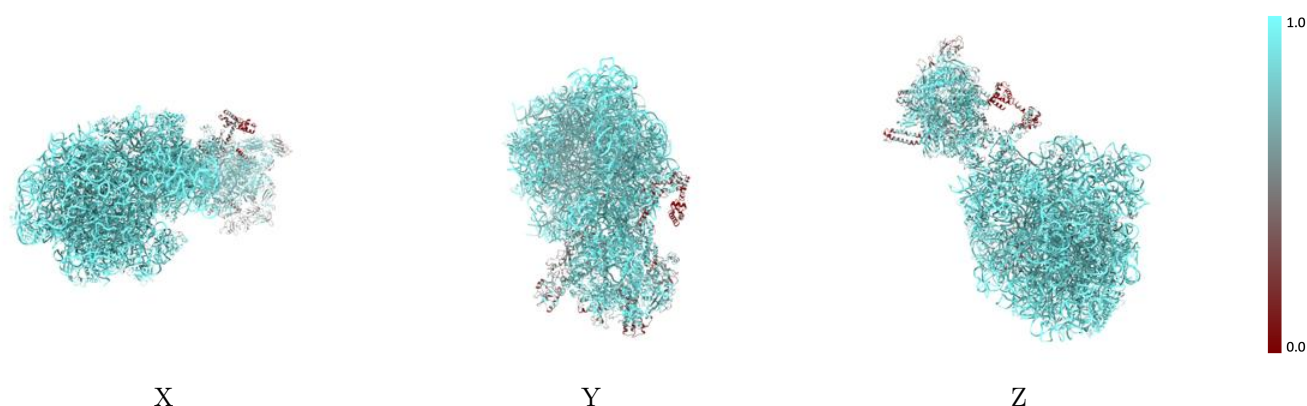
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



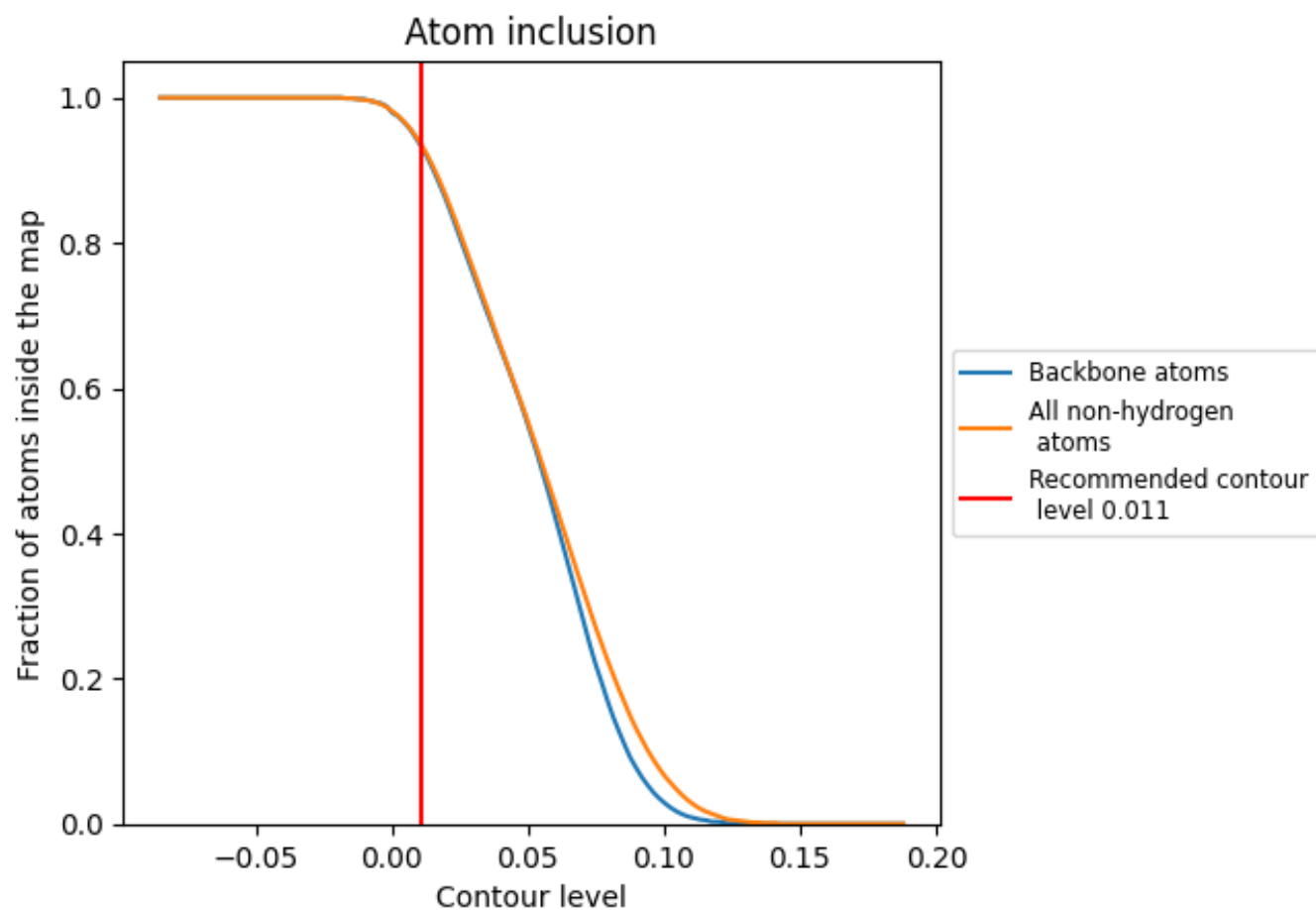
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



































































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

Chain	Atom inclusion	Q-score
All	 0.9340	 0.2260
1	 0.9900	 0.3100
2	 0.9910	 0.2590
3	 0.9830	 0.2500
4	 0.8270	 0.0830
5	 0.9240	 0.1000
6	 0.9870	 0.3050
7	 0.7770	 0.0540
8	 0.8570	 0.0020
9	 0.9230	 0.0700
A	 0.8900	 0.1890
A1	 0.6540	 -0.0010
A2	 0.7980	 0.0170
B	 0.9600	 0.3140
B1	 0.7830	 0.0090
B2	 0.7870	 0.0140
C	 0.9300	 0.2990
D	 0.9490	 0.3370
E	 0.9490	 0.3470
F	 0.9280	 0.2270
G	 0.9270	 0.1850
H	 0.9190	 0.2580
I	 0.8260	 0.0500
J	 0.9500	 0.2820
K	 0.9360	 0.2160
L	 0.9290	 0.2040
M	 0.9430	 0.2750
N	 0.9540	 0.1940
NA	 0.5560	 0.0200
NG	 0.8290	 0.0140
O	 0.9240	 0.1910
P	 0.9440	 0.2610
Q	 0.8950	 0.2090
R	 0.9540	 0.2150
S	 0.9470	 0.2240



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Chain	Atom inclusion	Q-score
T	 0.9460	 0.2380
U	 0.8740	 0.1020
V	 0.8970	 0.1510
W	 0.9610	 0.2360
W0	 0.5790	 0.0370
X	 0.9400	 0.1940
Y	 0.9010	 0.1440
Z	 0.8700	 0.1690
b	 0.9530	 0.3590
c	 0.9380	 0.2780
d	 0.9570	 0.2770
e	 0.9550	 0.2630
f	 0.9550	 0.1620
g	 0.9520	 0.2110
h	 0.9380	 0.2200
i	 0.8340	 0.0160
j	 0.9620	 0.2990
k	 0.8860	 0.2660
l	 0.9680	 0.3070
m	 0.9300	 0.2990
n	 0.9630	 0.2950
o	 0.9660	 0.2310
p	 0.9200	 0.2140
q	 0.9600	 0.3200
r	 0.9690	 0.2970
s	 0.9230	 0.2970
t	 0.9240	 0.1900
u	 0.9610	 0.2110
v	 0.9580	 0.2300
w	 0.9360	 0.3050
x	 0.9530	 0.3240
y	 0.9540	 0.1810
z	 0.9630	 0.2960