



## wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 10:48 PM JST

PDB ID : 8Y5T / pdb\_00008y5t  
EMDB ID : EMD-38949  
Title : E.coli Transcription translation coupling complex in TTC-B state 5 (subclass 3) containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and fusidic acid  
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.  
Deposited on : 2024-01-31  
Resolution : 4.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

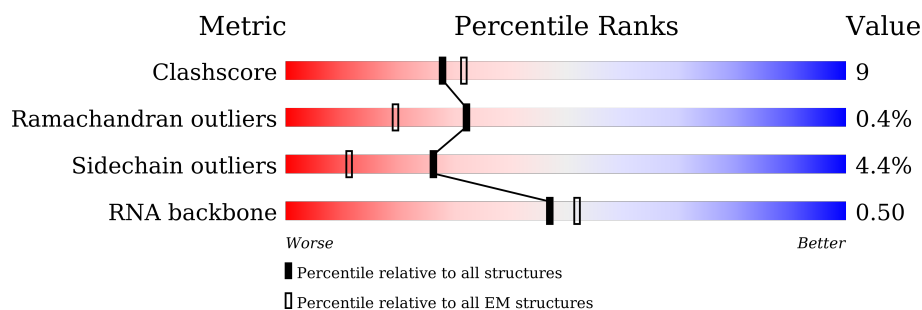
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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	




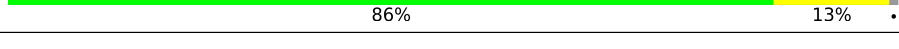
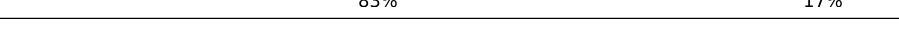
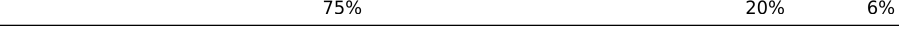
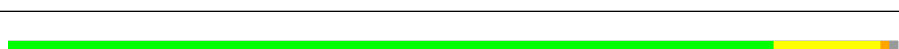










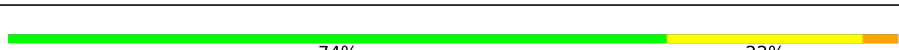


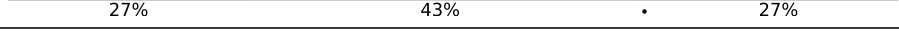




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	
27	b	273	
28	c	209	
29	d	201	
30	e	179	
31	f	177	
32	g	149	

Continued on next page...

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
65	0	716	

## 2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 179688 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
			521	323	98	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	39	Total	C	N	O	P	0	0
			809	362	113	295	39		

- 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	67	Total	C	N	O		0	0
			331	197	67	67			

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10546	6616	1839	2048	43		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NA	492	Total	C	N	O	0	0
			2432	1448	492	492		

- Molecule 62 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	NG	154	Total	C	N	O	0	0
			758	450	154	154		

- Molecule 63 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 64 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 65 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	0	673	Total	C	N	O	S	0	0
			5211	3289	900	999	23		

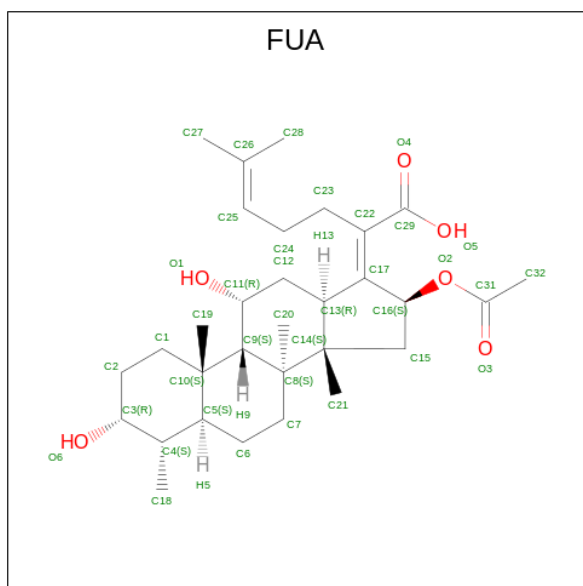
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

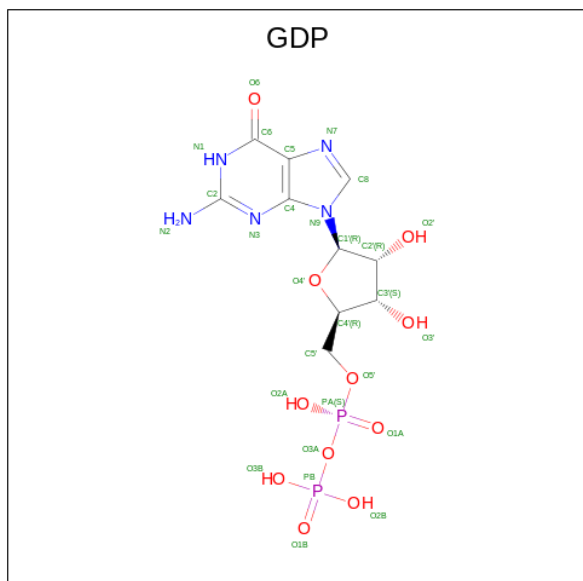
Mol	Chain	Residues	Atoms		AltConf
66	B1	1	Total	Mg	0
			1	1	

- Molecule 67 is FUSIDIC ACID (CCD ID: FUA) (formula:  $C_{31}H_{48}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
67	0	1	Total	C	O	0
			37	31	6	

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).






Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
68	0	1	28	10	5	11	2	0

### 3 Residue-property plots


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.

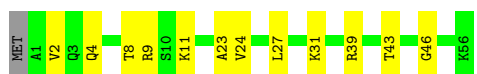
- Molecule 1: 50S ribosomal protein L31

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: 



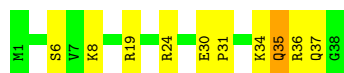
- Molecule 5: 50S ribosomal protein L35

Chain E: 



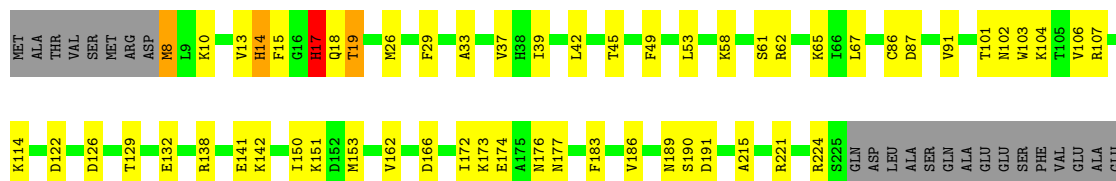
- Molecule 6: 50S ribosomal protein L36

Chain F:  74% 24% .



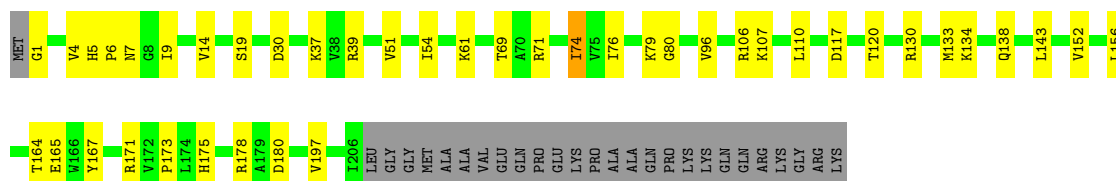
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% . 10%



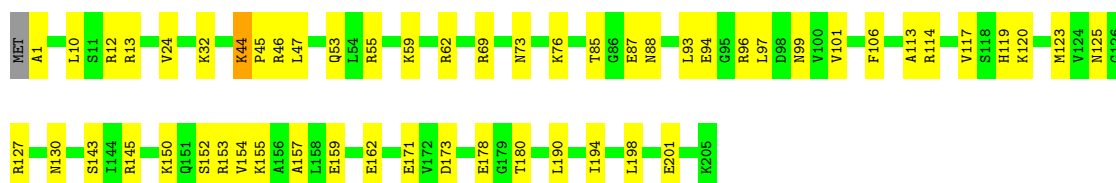
- Molecule 8: 30S ribosomal protein S3

Chain H:  70% 18% 12%




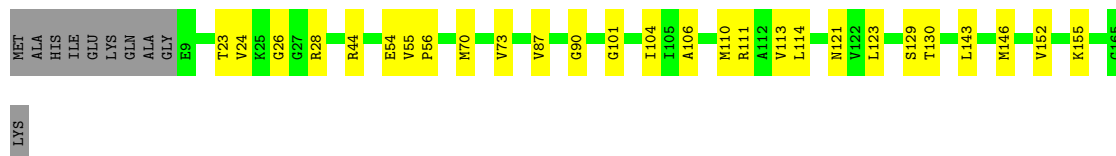
- Molecule 9: 30S ribosomal protein S4

Chain I:  73% 26%



- Molecule 10: 30S ribosomal protein S5

Chain J:  78% 16% 6%



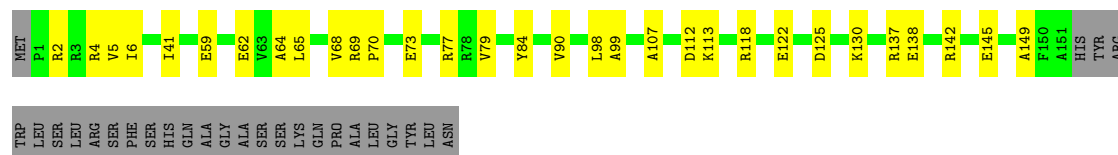
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  51% 22% 26%



- Molecule 12: 30S ribosomal protein S7

Chain L: 67% 17% 16%



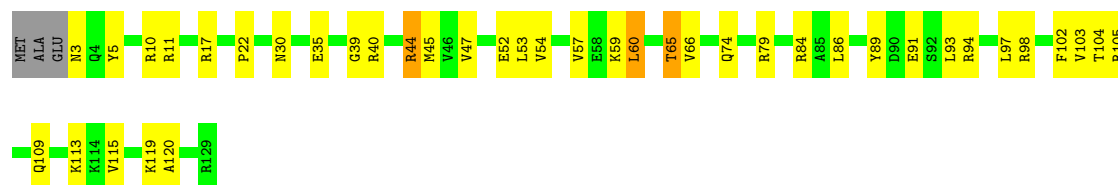
- Molecule 13: 30S ribosomal protein S8

Chain M: 88% 12%



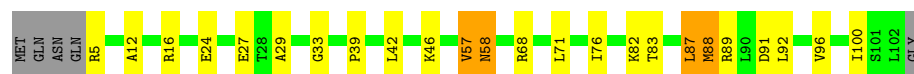
- Molecule 14: 30S ribosomal protein S9

Chain N: 67% 28% 5%



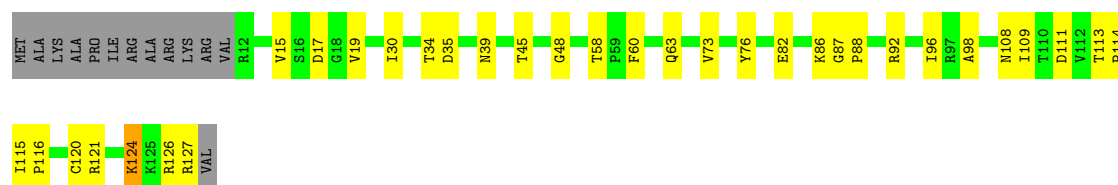
- Molecule 15: 30S ribosomal protein S10

Chain O: 72% 19% 9%



- Molecule 16: 30S ribosomal protein S11

Chain P: 64% 25% 11%



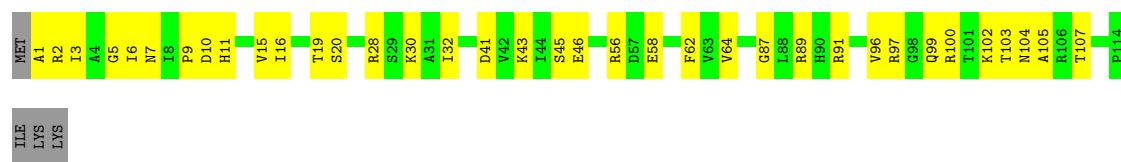
- Molecule 17: 30S ribosomal protein S12

Chain Q:  66% 32%




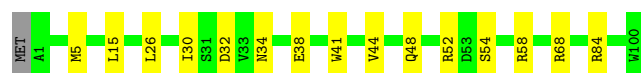
- Molecule 18: 30S ribosomal protein S13

Chain R:  66% 31%




- Molecule 19: 30S ribosomal protein S14

Chain S:  84% 15%



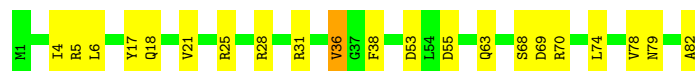
- Molecule 20: 30S ribosomal protein S15

Chain T:  83% 16%



- Molecule 21: 30S ribosomal protein S16

Chain U:  74% 24%



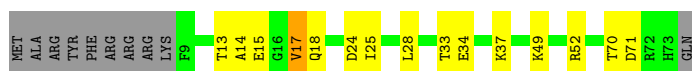
- Molecule 22: 30S ribosomal protein S17

Chain V:  75% 19% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  67% 19% 13%



- Molecule 24: 30S ribosomal protein S19

Chain X: 73% 13% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y: 76% 22% .



- Molecule 26: 30S ribosomal protein S21

Chain Z: 56% 32% . 8%



- Molecule 27: 50S ribosomal protein L2

Chain b: 78% 21% .



- Molecule 28: 50S ribosomal protein L3

Chain c: 83% 17%

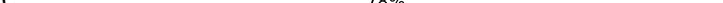


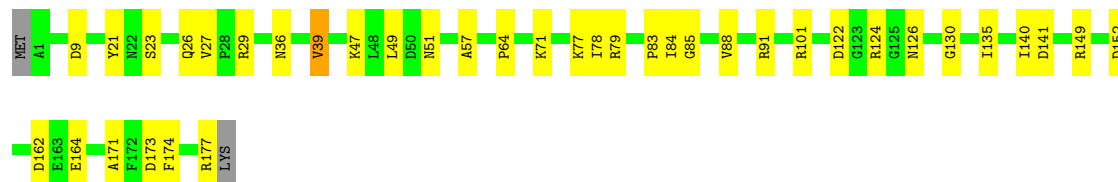
- Molecule 29: 50S ribosomal protein L4

Chain d: 81% 19%



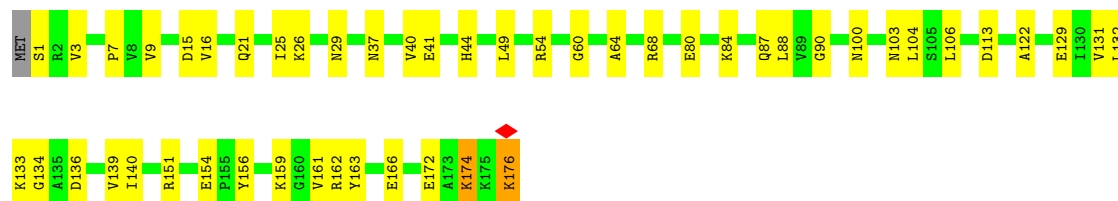
- Molecule 30: 50S ribosomal protein L5

Chain e:  78% 21% ..



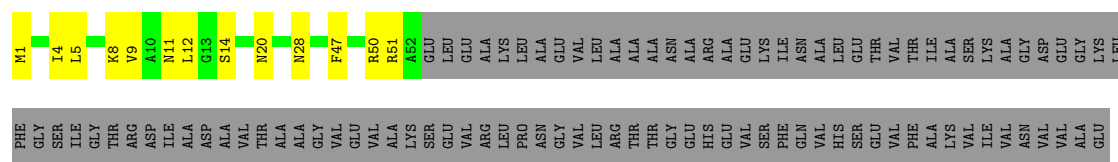
- Molecule 31: 50S ribosomal protein L6

Chain f:  72% 27% ..



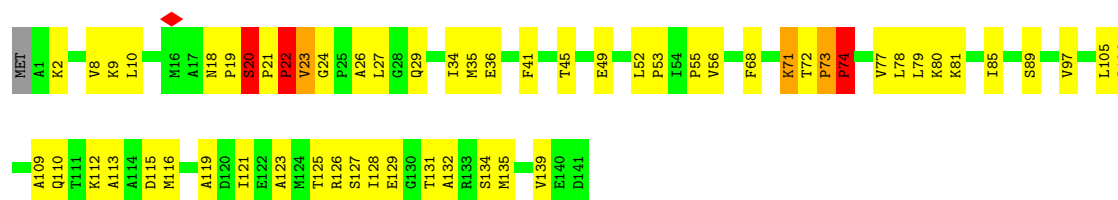
- Molecule 32: 50S ribosomal protein L9

Chain g:  26% 9% 65%




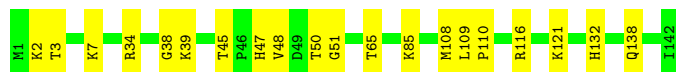
- Molecule 33: 50S ribosomal protein L11

Chain i:  58% 37% ...




- Molecule 34: 50S ribosomal protein L13

Chain j:  86% 14%




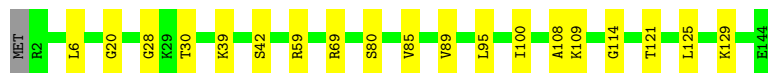
- Molecule 35: 50S ribosomal protein L14

Chain k:  80% 20%




- Molecule 36: 50S ribosomal protein L15

Chain l:  86% 13%



- Molecule 37: 50S ribosomal protein L16

Chain m:  83% 17%




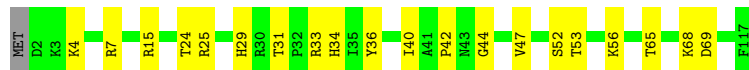
- Molecule 38: 50S ribosomal protein L17

Chain n:  75% 20% 6%




- Molecule 39: 50S ribosomal protein L18

Chain o:  82% 17%




- Molecule 40: 50S ribosomal protein L19

Chain p:  86% 12%




- Molecule 41: 50S ribosomal protein L20



Chain q:  83% 15% ..




- Molecule 42: 50S ribosomal protein L21

Chain r:  77% 23%



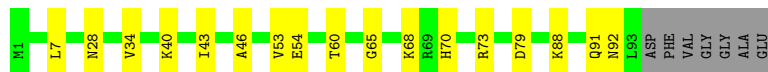
- Molecule 43: 50S ribosomal protein L22

Chain s:  85% 15%



- Molecule 44: 50S ribosomal protein L23

Chain t:  76% 17% 7%




- Molecule 45: 50S ribosomal protein L24

Chain u:  72% 26%



- Molecule 46: 50S ribosomal protein L25

Chain v:  85% 15%




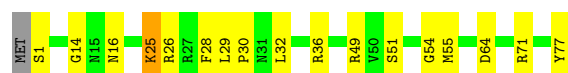
- Molecule 47: 50S ribosomal protein L27

Chain w:  73% 15% 12%




- Molecule 48: 50S ribosomal protein L28

Chain x:  77% 21% ..



- Molecule 49: 50S ribosomal protein L29

Chain y:  78% 22%



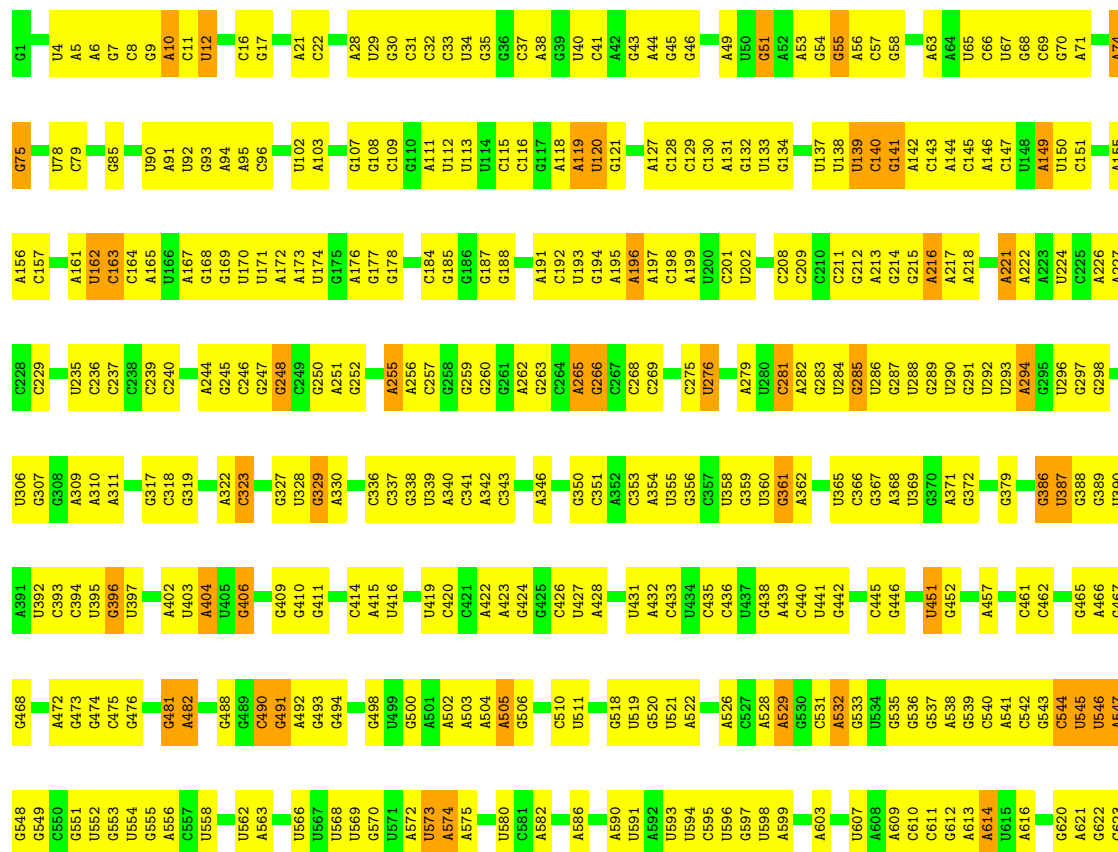
- Molecule 50: 50S ribosomal protein L30

Chain z:  76% 22% .



- Molecule 51: 23S rRNA

Chain 1:  43% 51% 7%





G2890	C2805	G2729	G2642	A2564	C2467	G2383	G2303	G2224	G2157	C2091	C1985	G1906	A1821
G2893	C2806	G2730	G2643	A2565	C2468	U2384	G2304	A2225	A2158	U2092	C1986	G1907	A1822
G2894	A2810	G2731	G2644	A2566	A2469	G2385	C2305	G2226	G2159	G2093	C1987	G1908	G1823
G2895	G2811	G2732	G2645	A2567	A2470	A2386	C2306	A2227	C2160	A2094	C1990	C1909	U1827
G2896	G2812	G2733	G2646	G2568	A2471	A2387	A2309	G2230	C2161	A2095	U1991	G1910	U1828
G2897	G2813	A2734	G2647	G2569	G2471	A2388	G2310	G2231	A2163	A2097	U1993	U1911	A1829
G2898	A2814	G2735	G2648	G2570	A2476	G2389	G2311	U2233	C2164	U2098	A1913	A1912	
G2899	G2815	A2736	G2649	U2571	U2477	U2390	A2312	G2234	G2165	U2099	C1997	A1914	C1832
A2900	G2816	G2737	G2650	A2572	G2490	G2391	U2313	G2235	A2166	G2100	A1998	U1915	C1833
C2901	G2817	G2738	G2651	G2573	U2491	U2392	A2314	G2236	U2167	A2101	C1999	A1916	U1834
C2902	A2820	A2741	G2652	G2574	A2482	U2393	G2315	G2237	G2170	G2102	G2012	U1917	G1845
U2903	G2827	U2742	G2658	G2575	G2488	G2394	G2316	G2238	A2171	C2103	A2013	A1918	G1846
U	G2828	U2743	G2659	A2577	U2489	U2395	U2321	G2239	A2172	G2104	A2014	A1919	A1847
	A2829	G2744	G2660	G2578	G2490	U2402	G2325	U2240	U2173	U2105	A2015	G1920	A1848
	C2830	G2745	G2661	G2579	U2492	C2403	G2326	G2241	A2174	G2107	U2016	G1921	G1922
	G2834	G2746	G2662	U2580	U2493	U2404	A2327	G2242	C2174	G2110	A2020	U1923	U1851
	A2835	A2747	G2663	G2581	C2496	G2405	A2328	U2243	U2180	G2111	C2021	C1924	U1852
	U2836	G2748	G2670	G2582	A2497	A2406	A2329	A2247	U2181	U2112	G2022	A1927	A1853
	G2837	G2750	G2671	U2583	C2498	A2407	G2330	G2248	U2182	U2113	C2023	A1928	U1854
	G2838	G2751	U2672	U2584	C2499	A2411	G2331	G2249	A2183	U2114	G2024	G1929	U1855
	G2839	U2754	G2676	U2585	G2502	A2412	G2332	G2250	A2184	G2115	C2025	G1930	G1857
	C2840	C2755	G2677	U2593	G2506	A2420	A2333	U2257	U2185	G2118	U2026	U1931	A1858
	G2843	A2758	A2679	G2594	G2507	G2421	U2334	C2258	U2187	A2119	G2027	G1935	G1863
	G2844	G2759	U2680	G2595	U2506	G2422	A2335	C2259	U2188	G2122	A2030	A1936	U1864
	U2845	G2760	G2681	A2598	C2507	U2423	A2336	G2260	U2189	G2123	G2031	A1937	U1865
	G2846	A2761	A2682	G2599	U2510	U2424	G2337	A2267	G2190	G2124	G2032	A1938	A1866
	G2847	G2762	G2683	A2600	G2511	G2425	C2338	A2268	U2191	G2125	U2034	U1939	G1867
	U2847	G2763	U2684	G2601	U2512	A2426	A2340	G2269	U2192	C2126	G2035	C1942	C1868
	G2848	A2764	U2687	A2602	A2516	C2427	G2345	G2271	U2194	G2127	G2036	U1943	C1870
	U2849	G2765	G2688	U2609	A2517	G2428	A2346	C2275	U2195	U1944	A2037	G1945	A1871
	G2850	U2768	U2689	C2610	G2518	G2429	G2347	C2276	C2196	G2128	C2043	G1948	A1872
	G2851	C2773	U2690	C2611	G2525	A2430	U2348	A2278	U2197	U2130	C2047		C1874
	C2852	G2776	G2691	G2612	G2526	U2431	G2349	G2279	A2198	U2131	G2048	A1952	G1875
	G2853	A2777	G2692	U2613	G2527	A2432	C2350	G2280	A2199	G2132	G2049	A1953	C1878
	C2854	G2778	A2700	A2614	U2528	A2433	G2351	A2281	G2200	U2133	C2050	G1954	C1879
	G2855	U2779	U2701	U2615	G2529	A2434	A2352	G2282	G2201	A2134	A2051	U1955	
	U2856	G2780	G2702	G2616	A2530	G2435	G2357	C2283	U2202	U2137	A2052	U1956	U1882
	G2857	G2781	U2703	G2617	U2533	G2436	G2358	A2284	G2204	G2138	G2053	U1963	U1883
	A2858	U2782	G2704	U2618	A2534	U2440	G2359	C2285	A2205	G2141	A2054	U1964	G1884
	G2859	U2783	G2705	G2619	G2535	U2441	G2360	G2286	C2208	G2144	C2055	G1965	U1885
	C2860	U2784	C2706	G2620	C2536	G2442	G2361	A2287	G2209	G2145	G2056	C1966	U1886
	U2861	G2785	C2707	C2621	C2537	G2443	G2362	A2288	G2210	C2146	A2057	A1967	G1887
	G2862	C2786	A2711	G2622	G2538	G2444	C2363	G2289	A2211	C2147	G2060	G1968	G1888
	A2863	G2787	G2712	C2623	G2539	G2445	G2364	G2290	U2212	A2148	G2061	U1969	A1889
	G2864	C2788	C2713	U2624	G2540	G2446	C2365	G2291	G2213	U2149	G2062	A1970	A1890
	U2865	G2789	U2714	U2625	A2541	G2447	G2366	U2292	G2214	C2150	G2069	U1971	C1893
	G2866	A2792	C2715	G2626	U2542	G2448	G2367	U2293	G2215	U2151	C2073	G1972	C1894
	A2867	C2793	G2716	C2627	U2543	A2449	G2368	G2294	G2216	G2152	U2074		A1901
	C2868	G2794	C2717	U2627	U2544	G2450	C2369	C2295	C2217	C2153		A1978	C1902
	G2869	U2795	G2718	G2628	U2545	G2451	G2370	G2296	G2218	A2154	U2085	G1983	C1905
	U2870	U2796	G2719	C2629	C2546	U2452	G2371	U2297	G2219	G2155	U2086		
	A2871	G2797	U2720	U2630	A2547	G2453	G2372	A2298	G2221	G2156			
	G2872	C2798	C2721	G2631	U2548	G2454	G2373	U2299	G2222				
	U2873	A2799	G2722	G2632	U2549	G2455	G2374	U2300	G2223				
	A2874	U2800	G2723	A2633	C2550	G2456	G2375	U2301					
	G2875	G2801	U2804	A2634	C2551	U2457	G2376	A2298					
	C2876	C2802		C2635	U2552	G2458	G2377	U2302					
	A2877	G2803		G2636	U2553	G2459	G2378	U2303					
	G2878	U2804		G2637	U2554	G2460	G2379	U2304					
	U2879	C2805		G2638	U2555	G2461	G2380						
	A2880	G2806			U2556	G2462	A2381						
	C2881	A2881			C2557	G2463	G2382						
	G2882	G2882			U2558	G2464	G2383						
	U2883	C2883			U2559								
	A2884	G2884			U2560								
	G2885	C2885			U2561								
	C2886	U2886			U2562								
	A2887	G2887			U2563								
	U2888	C2888											
	G2889	U2889											

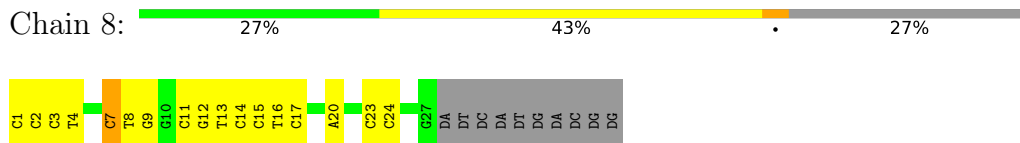
• Molecule 52: 5S rRNA

Chain 2:





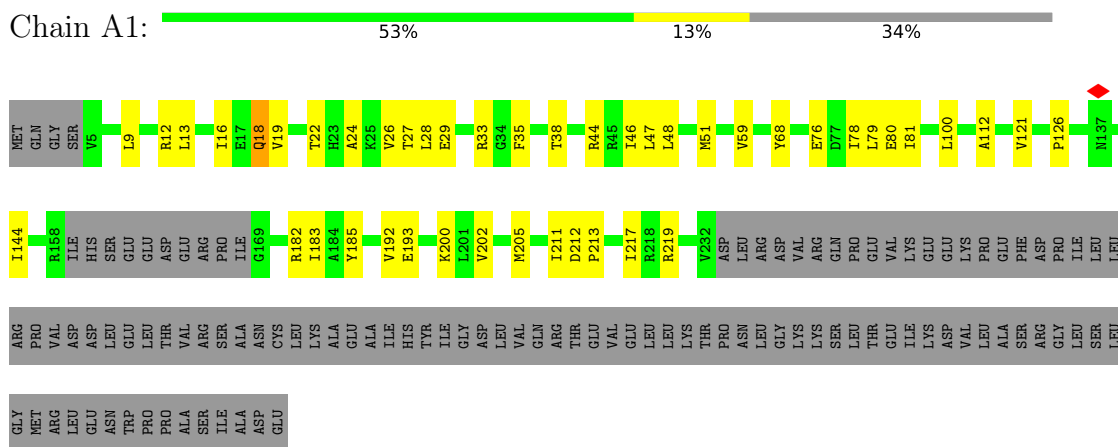
- Molecule 55: template DNA strand



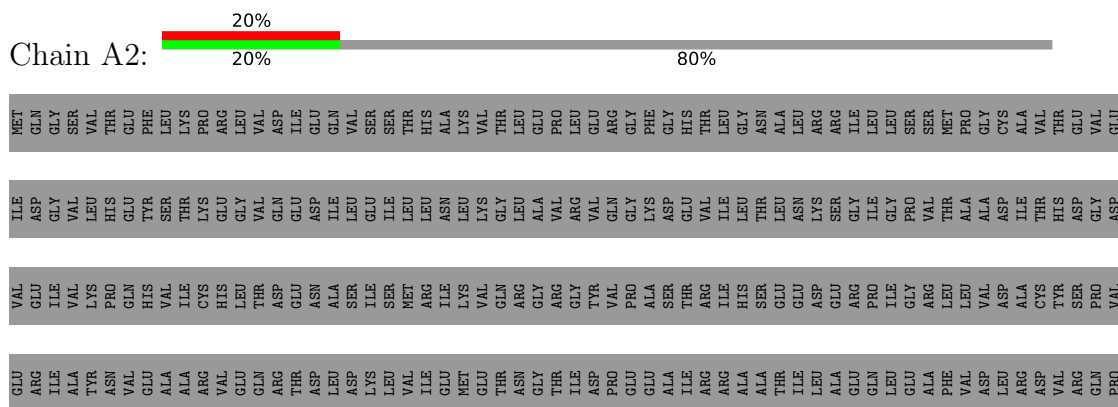
- Molecule 56: non-template DNA strand



- Molecule 57: DNA-directed RNA polymerase subunit alpha

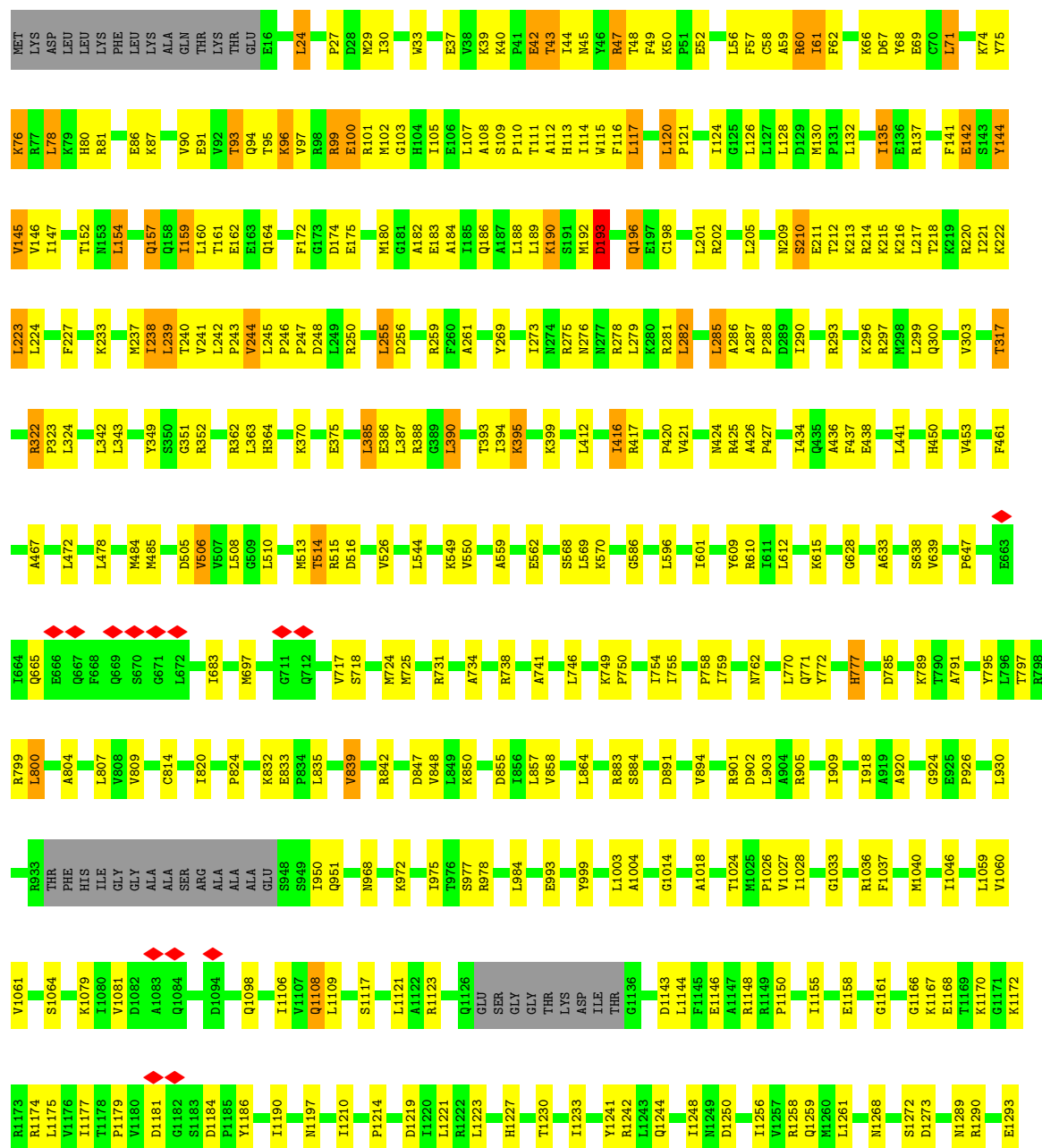


- Molecule 57: DNA-directed RNA polymerase subunit alpha



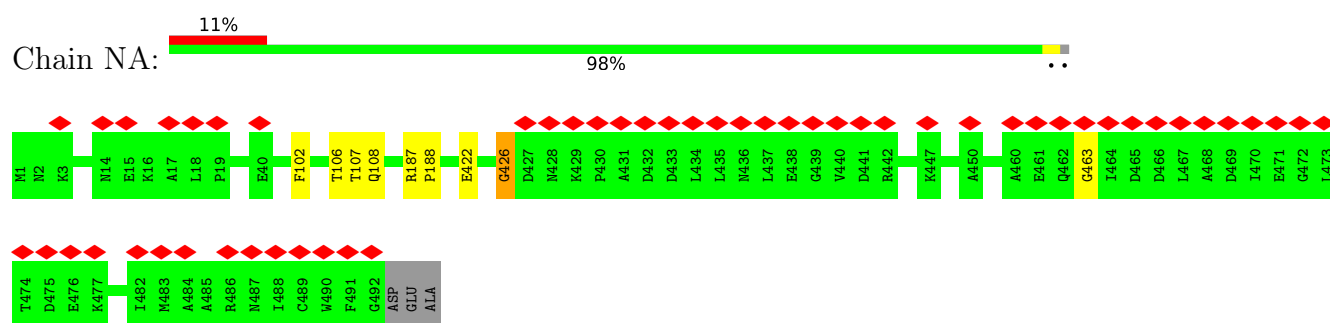
- Molecule 58: DNA-directed RNA polymerase subunit beta'

Chain B1:  67% 25% 5%

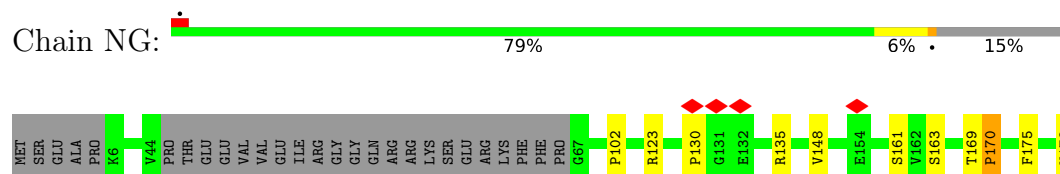




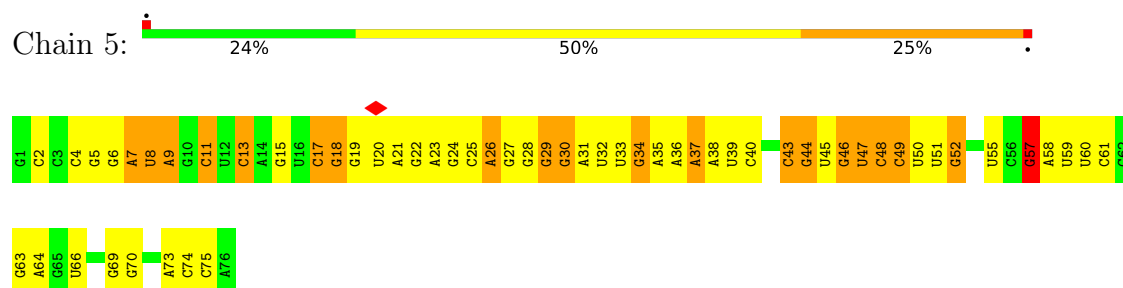




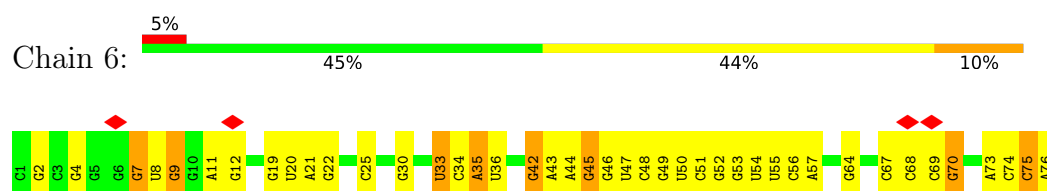
- Molecule 62: Transcription termination/antitermination protein NusG



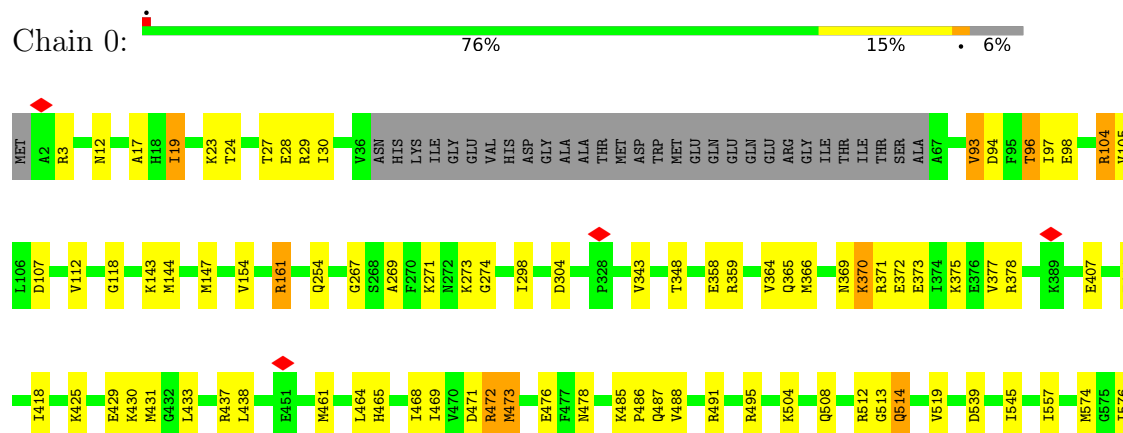
- Molecule 63: tRNA(Phe)



- Molecule 64: tRNA(fMet)



- Molecule 65: Elongation factor G





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	609587	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	0.088	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	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, FUA, GDP

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	0/530	0.54	0/707
2	B	0.40	0/450	0.60	0/599
3	C	0.27	0/416	0.52	0/554
4	D	0.47	0/380	0.76	2/498 (0.4%)
5	E	0.53	0/513	0.60	0/676
6	F	0.57	0/303	0.66	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	0.47	0/1034	0.77	0/1375
15	O	0.49	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	4/1193 (0.3%)
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	0.43	0/1434	0.65	2/1926 (0.1%)
31	f	0.35	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	0.55	0/1046	0.93	4/1410 (0.3%)
34	j	0.41	0/1152	0.55	1/1551 (0.1%)
35	k	0.45	0/947	0.66	0/1268
36	l	0.40	0/1054	0.63	0/1403
37	m	0.56	0/1093	0.74	0/1460
38	n	0.46	0/973	0.72	1/1301 (0.1%)
39	o	0.32	0/902	0.51	0/1209
40	p	0.42	0/929	0.63	0/1242
41	q	0.52	0/960	0.62	1/1278 (0.1%)
42	r	0.45	0/829	0.69	0/1107
43	s	0.44	0/864	0.58	0/1156
44	t	0.33	0/744	0.52	0/994
45	u	0.46	0/787	0.75	0/1051
46	v	0.34	0/766	0.51	0/1025
47	w	0.40	0/582	0.52	0/769
48	x	0.43	0/635	0.63	1/848 (0.1%)
49	y	0.29	0/510	0.64	0/677
50	z	0.41	0/453	0.53	0/605
51	1	0.51	0/69796	0.62	21/108888 (0.0%)
52	2	0.43	0/2872	0.46	0/4479
53	3	0.42	0/36963	0.43	0/57662
54	4	0.55	0/896	0.74	0/1387
55	8	0.56	0/599	0.71	1/919 (0.1%)
56	9	0.49	0/468	0.53	0/719
57	A1	0.48	0/1696	0.69	0/2298
57	A2	0.75	0/330	1.20	0/458
58	B1	0.57	5/10510 (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	0.60	0/879
61	NA	0.78	0/2431	1.22	0/3385
62	NG	1.11	0/756	1.05	0/1048
63	5	0.57	0/1812	0.85	1/2823 (0.0%)
64	6	0.39	0/1832	0.57	1/2855 (0.0%)
65	0	0.84	0/5308	1.17	6/7181 (0.1%)
All	All	0.49	5/193000 (0.0%)	0.64	72/284406 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
65	0	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.26	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.18	1.33	1.23
58	B1	424	ASN	CG-ND2	-5.14	1.22	1.33
58	B1	665	GLN	CD-OE1	5.03	1.33	1.23
58	B1	1268	ASN	CG-OD1	5.00	1.33	1.23

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	i	74	PRO	N-CA-CB	-11.05	91.64	103.25
65	0	580	PHE	CA-CB-CG	9.59	123.39	113.80
16	P	73	VAL	N-CA-C	-9.08	104.48	113.20
41	q	33	VAL	N-CA-C	-8.69	104.82	112.12
12	L	64	ALA	N-CA-C	-7.71	105.04	114.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
65	0	161	ARG	Sidechain

## 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	521	0	520	8	0
2	B	444	0	461	10	0
3	C	409	0	440	3	0
4	D	377	0	418	9	0
5	E	504	0	574	2	0
6	F	302	0	343	5	0
7	G	1704	0	1732	37	0
8	H	1624	0	1699	29	0
9	I	1643	0	1710	34	0
10	J	1156	0	1199	17	0
11	K	817	0	808	17	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1181	0	1240	19	0
13	M	979	0	1034	9	0
14	N	1022	0	1070	21	0
15	O	786	0	828	12	0
16	P	869	0	878	20	0
17	Q	955	0	1019	26	0
18	R	883	0	944	20	0
19	S	805	0	847	10	0
20	T	714	0	737	7	0
21	U	649	0	666	16	0
22	V	648	0	691	10	0
23	W	535	0	552	7	0
24	X	637	0	665	8	0
25	Y	665	0	714	12	0
26	Z	544	0	579	13	0
27	b	2082	0	2157	47	0
28	c	1565	0	1616	32	0
29	d	1552	0	1619	27	0
30	e	1410	0	1447	22	0
31	f	1323	0	1374	28	0
32	g	400	0	423	6	0
33	i	1032	0	1088	43	0
34	j	1129	0	1162	19	0
35	k	938	0	1012	18	0
36	l	1045	0	1117	15	0
37	m	1074	0	1157	13	0
38	n	960	0	1000	18	0
39	o	892	0	923	14	0
40	p	917	0	965	12	0
41	q	947	0	1022	10	0
42	r	816	0	839	14	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	10	0
47	w	575	0	592	9	0
48	x	625	0	655	11	0
49	y	509	0	543	11	0
50	z	449	0	491	9	0
51	1	62317	0	31346	1454	0
52	2	2568	0	1303	16	0
53	3	33012	0	16618	187	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	4	809	0	404	12	0
55	8	539	0	305	28	0
56	9	417	0	224	1	0
57	A1	1677	0	1713	23	0
57	A2	331	0	146	2	0
58	B1	10353	0	10548	324	0
59	B2	10546	0	10550	181	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	16	0
62	NG	758	0	334	8	0
63	5	1622	0	821	28	0
64	6	1640	0	837	20	0
65	0	5211	0	5200	51	0
66	B1	1	0	0	0	0
67	0	37	0	47	7	0
68	0	28	0	12	0	0
All	All	179688	0	129150	2841	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 2841 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)
54:4:26:U:O2'	58:B1:78:LEU:HB3	1.46	1.12
59:B2:901:LEU:HD13	61:NA:107:THR:CB	1.82	1.08
59:B2:901:LEU:HD11	61:NA:107:THR:C	1.77	1.08
51:1:275:C:H2'	51:1:276:U:H4'	1.37	1.07
51:1:1672:A:C2	51:1:2582:G:H5'	1.95	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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
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%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	50
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	25	63
10	J	155/167 (93%)	138 (89%)	17 (11%)	0	100	100
11	K	98/135 (73%)	84 (86%)	14 (14%)	0	100	100
12	L	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
13	M	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
14	N	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
15	O	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	13	48
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	50
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	98 (88%)	13 (12%)	1 (1%)	14	50
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	22
24	X	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
25	Y	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
26	Z	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	8	37
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
32	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	6	32
33	i	139/142 (98%)	109 (78%)	27 (19%)	3 (2%)	5	30
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%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	36
42	r	101/103 (98%)	88 (87%)	13 (13%)	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	48
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	10	42
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	214/329 (65%)	195 (91%)	19 (9%)	0	100	100
57	A2	65/329 (20%)	65 (100%)	0	0	100	100
58	B1	1329/1407 (94%)	1202 (90%)	123 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1205 (90%)	129 (10%)	4 (0%)	37	72
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	472 (96%)	15 (3%)	3 (1%)	22	59
62	NG	150/181 (83%)	132 (88%)	13 (9%)	5 (3%)	3	21
65	0	669/716 (93%)	625 (93%)	43 (6%)	1 (0%)	48	83
All	All	9955/10945 (91%)	8997 (90%)	921 (9%)	37 (0%)	32	67

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	x	25	LYS
58	B1	121	PRO
61	NA	187	ARG
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	58/62 (94%)	57 (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	66
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	61
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	65
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%)	95 (90%)	10 (10%)	7	23
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	43
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	72 (97%)	2 (3%)	40	60
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	70
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	54	71
30	e	148/150 (99%)	142 (96%)	6 (4%)	26	48
31	f	137/138 (99%)	132 (96%)	5 (4%)	30	52
32	g	41/114 (36%)	38 (93%)	3 (7%)	11	31
33	i	109/110 (99%)	98 (90%)	11 (10%)	6	21
34	j	116/116 (100%)	116 (100%)	0	100	100
35	k	103/104 (99%)	103 (100%)	0	100	100
36	l	102/103 (99%)	101 (99%)	1 (1%)	73	81
37	m	109/109 (100%)	103 (94%)	6 (6%)	18	40
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	81
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	98 (99%)	1 (1%)	73	81
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
42	r	84/84 (100%)	82 (98%)	2 (2%)	44	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	70	80
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	21	43
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	25	47
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	B1	1110/1168 (95%)	1016 (92%)	94 (8%)	8	28
59	B2	1150/1157 (99%)	1118 (97%)	32 (3%)	38	59
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	76
65	0	553/588 (94%)	481 (87%)	72 (13%)	3	15
All	All	7745/8214 (94%)	7405 (96%)	340 (4%)	26	46

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	B1	1327	GLU
65	0	365	GLN
59	B2	146	VAL
59	B2	913	VAL
65	0	461	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
59	B2	314	ASN
59	B2	554	HIS
65	0	496	GLN
26	Z	8	ASN
25	Y	77	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%)	2 (1%)
53	3	1538/1542 (99%)	253 (16%)	4 (0%)
54	4	37/44 (84%)	21 (56%)	3 (8%)
63	5	75/76 (98%)	39 (52%)	6 (8%)
64	6	76/77 (98%)	27 (35%)	2 (2%)
All	All	4747/4763 (99%)	755 (15%)	33 (0%)

5 of 755 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
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	6	56	C
51	1	1930	G
51	1	1801	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
67	FUA	0	800	-	39,40,40	1.63	3 (7%)	49,64,64	1.16	4 (8%)
68	GDP	0	801	-	24,30,30	0.90	1 (4%)	30,47,47	1.39	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	FUA	0	800	-	-	10/15/92/92	0/4/4/4
68	GDP	0	801	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	0	800	FUA	C29-C22	-9.25	1.34	1.47
67	0	800	FUA	O5-C29	-2.41	1.23	1.30
67	0	800	FUA	C9-C11	2.40	1.57	1.54
68	0	801	GDP	C6-N1	-2.31	1.34	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	0	801	GDP	C3'-C2'-C1'	2.88	105.31	100.98
68	0	801	GDP	PA-O3A-PB	-2.62	123.84	132.83
68	0	801	GDP	C5-C6-N1	2.59	118.52	113.95
67	0	800	FUA	C14-C8-C9	-2.48	104.53	109.40
67	0	800	FUA	C8-C9-C10	2.48	118.89	116.34

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	0	800	FUA	C13-C17-C22-C29
67	0	800	FUA	C23-C22-C29-O4
67	0	800	FUA	C23-C22-C29-O5
67	0	800	FUA	C22-C23-C24-C25
67	0	800	FUA	C32-C31-O2-C16

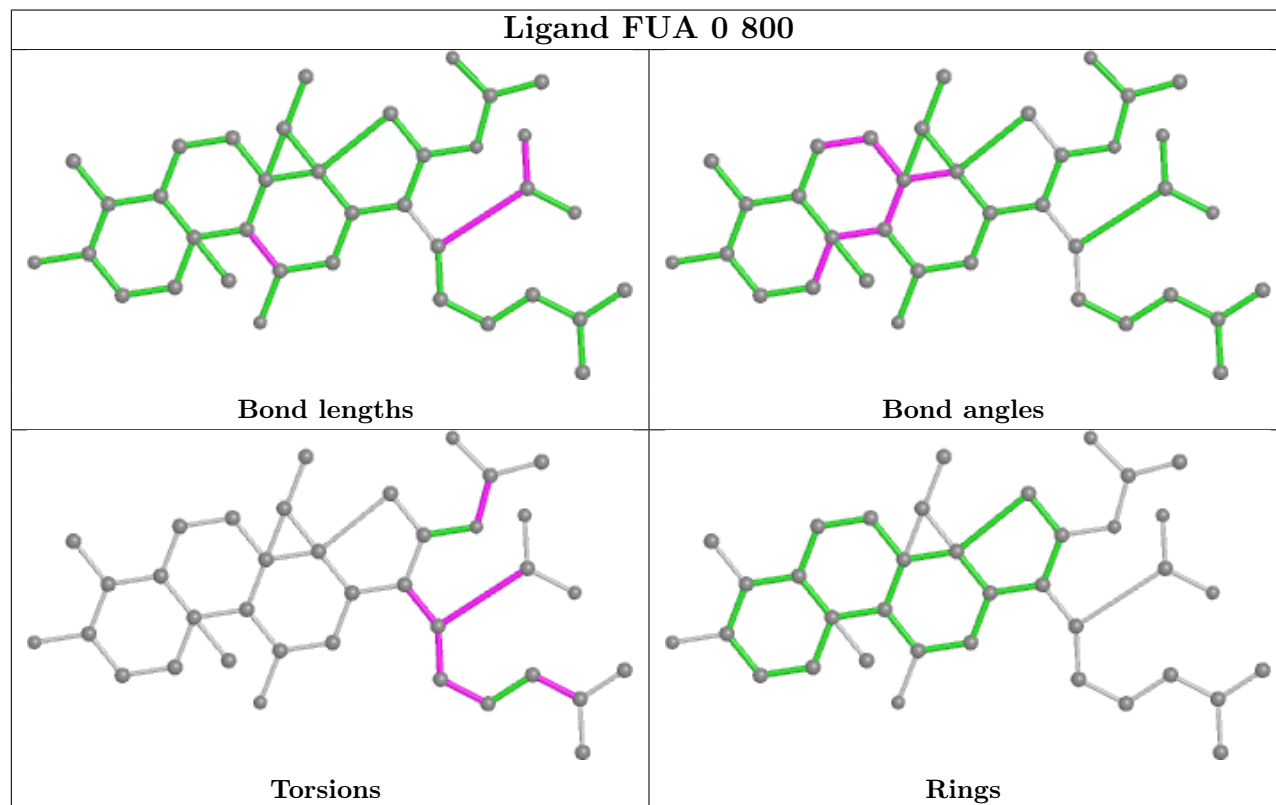
There are no ring outliers.

1 monomer is involved in 7 short contacts:

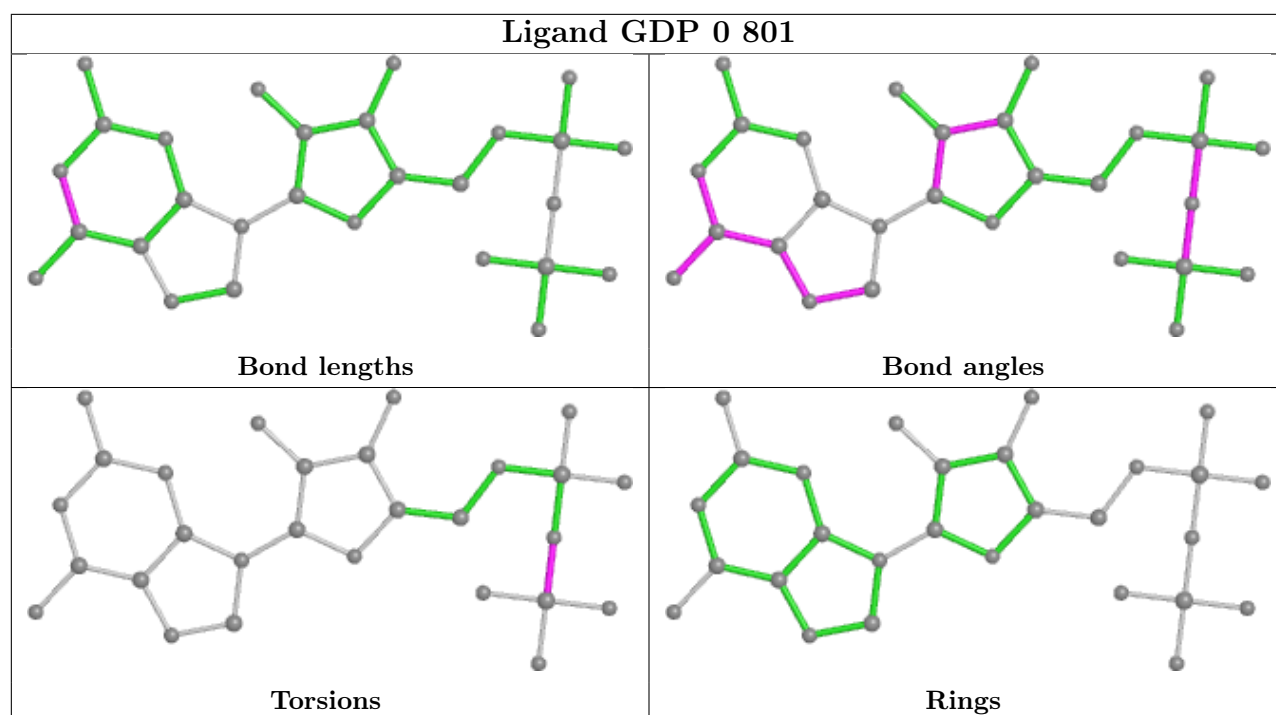
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	0	800	FUA	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

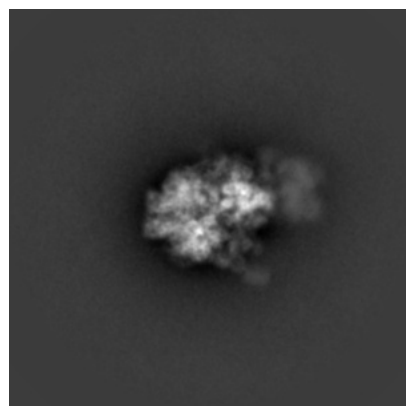
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38949. These allow visual inspection of the internal detail of the map and identification of artifacts.

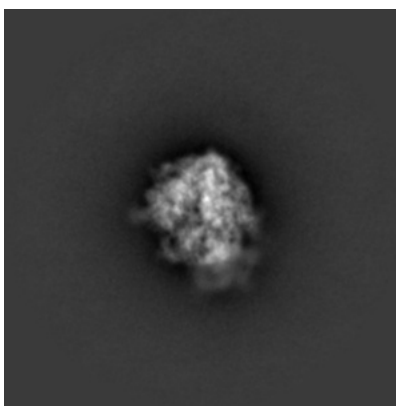
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

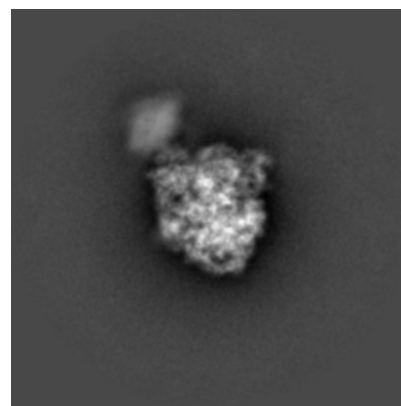
#### 6.1.1 Primary map



X

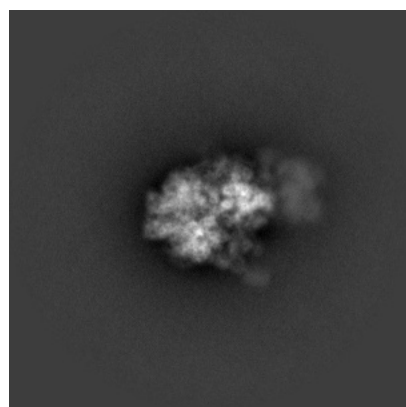


Y

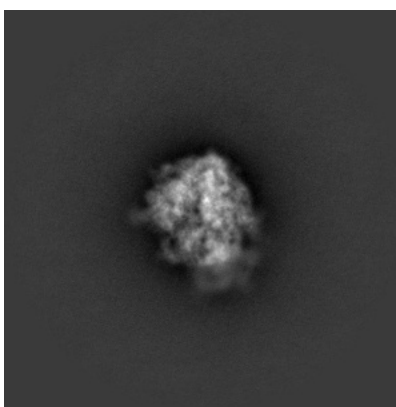


Z

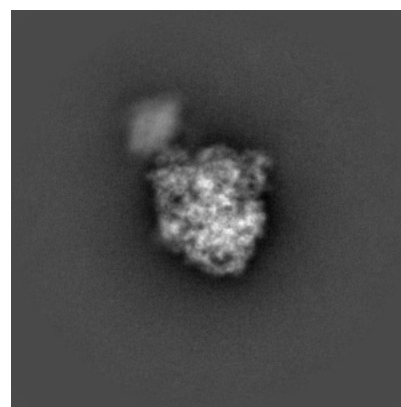
#### 6.1.2 Raw map



X



Y

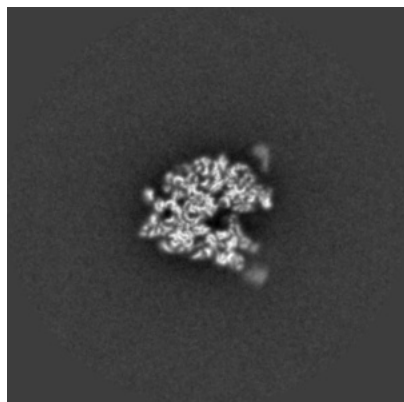


Z

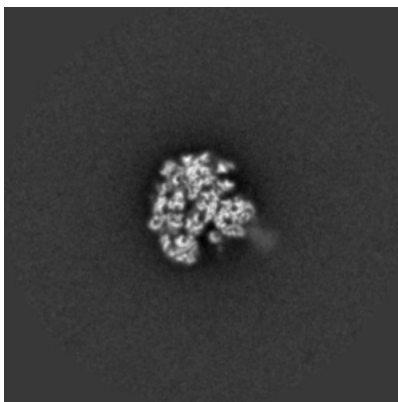
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

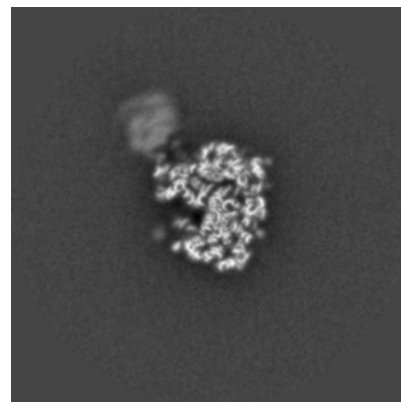
### 6.2.1 Primary map



X Index: 240

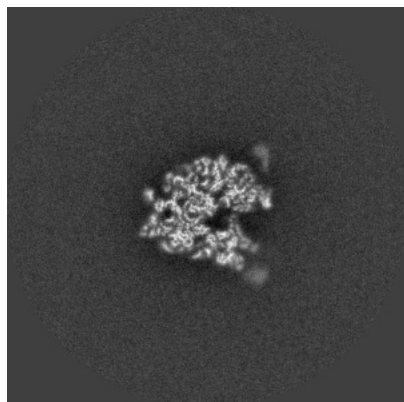


Y Index: 240

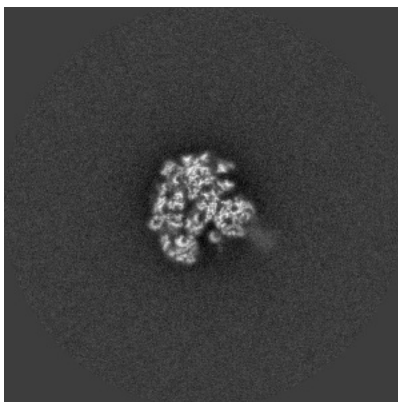


Z Index: 240

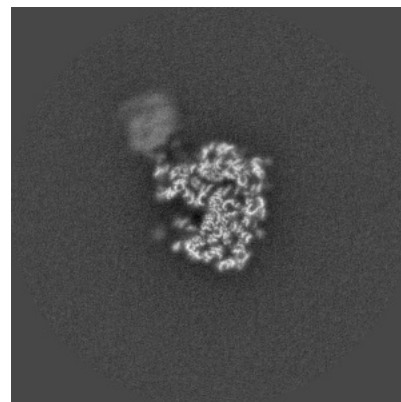
### 6.2.2 Raw map



X Index: 240



Y Index: 240

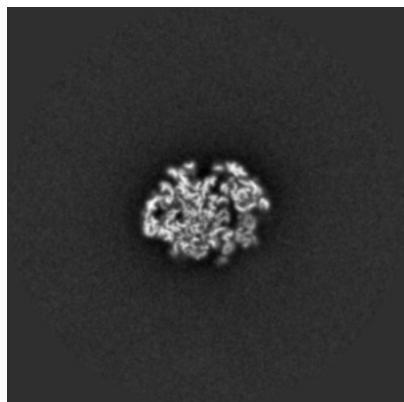


Z Index: 240

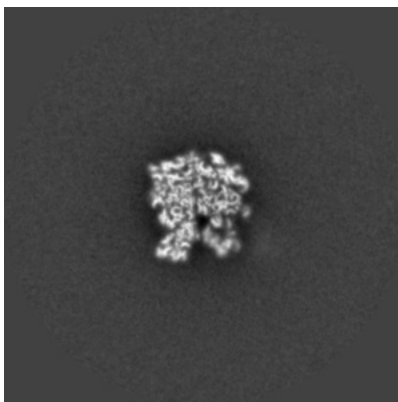
The images above show central slices of the map in three orthogonal directions.

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

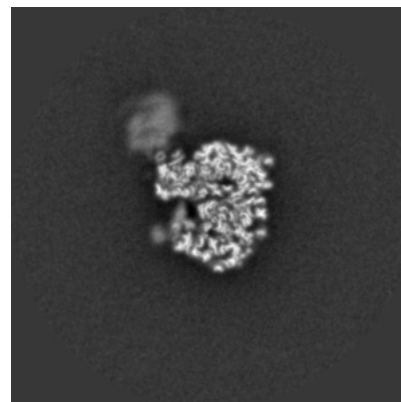
### 6.3.1 Primary map



X Index: 265

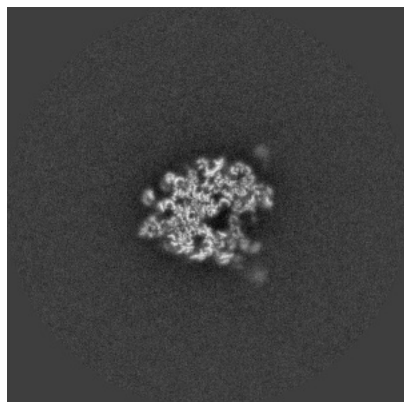


Y Index: 223

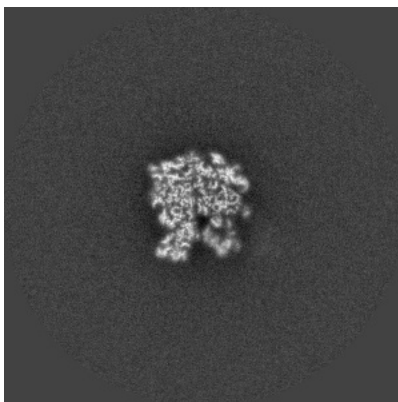


Z Index: 246

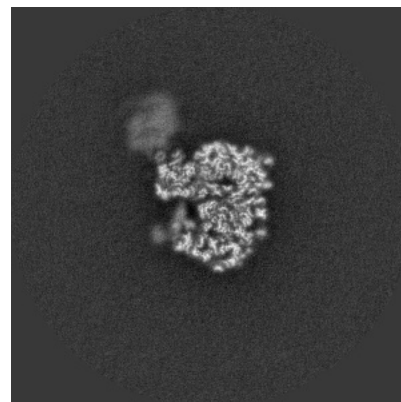
### 6.3.2 Raw map



X Index: 243



Y Index: 223

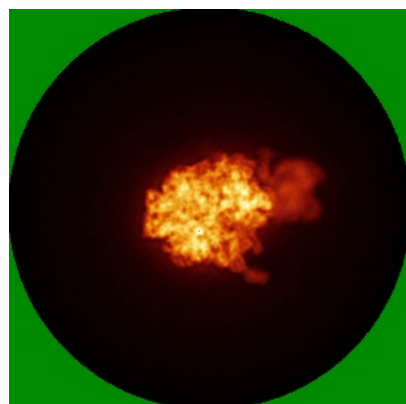


Z Index: 246

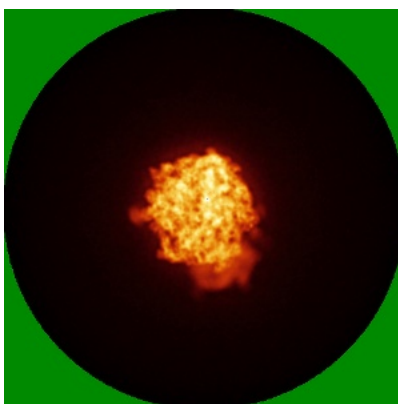
The images above show the largest variance slices of the map in three orthogonal directions.

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

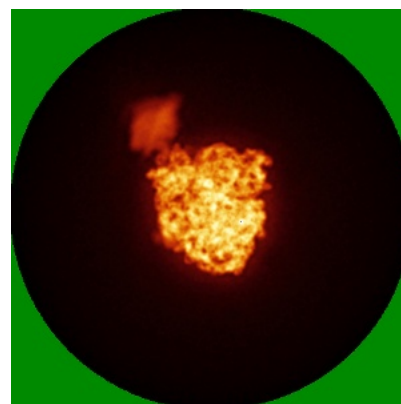
### 6.4.1 Primary map



X

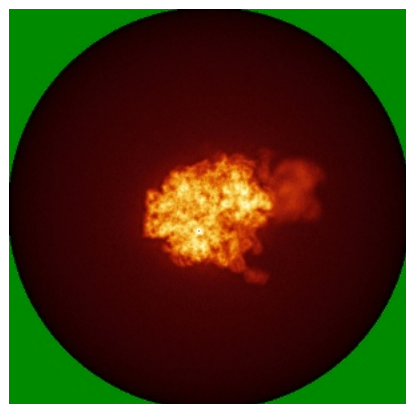


Y

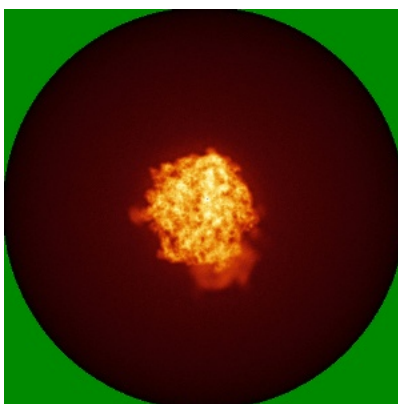


Z

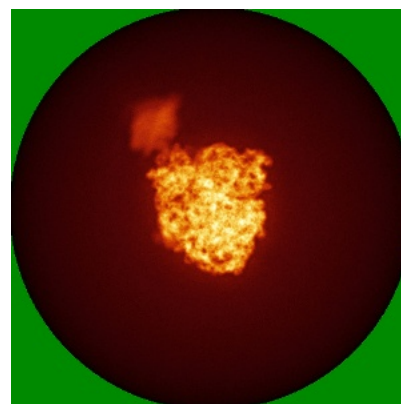
### 6.4.2 Raw map



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.

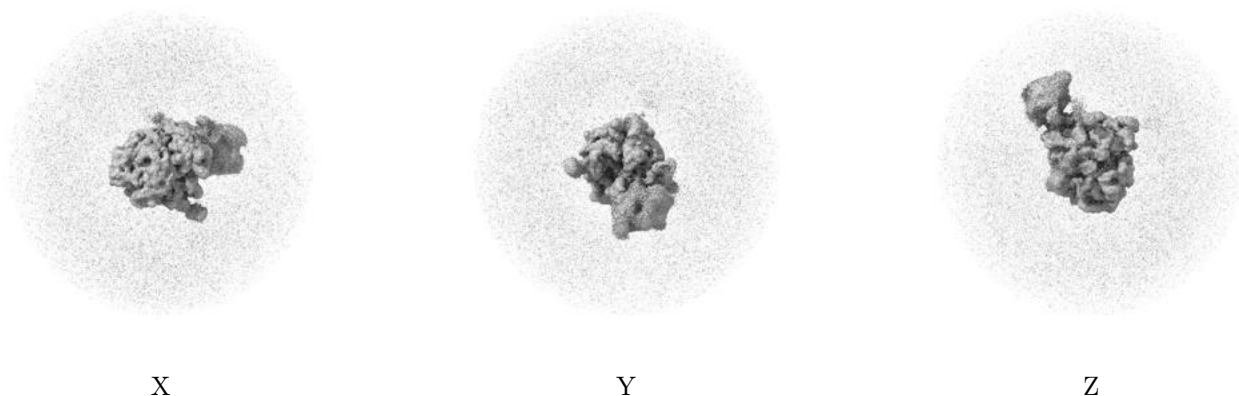
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

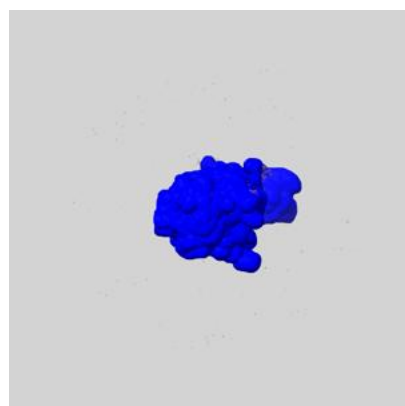
## 6.6 Mask visualisation [i](#)

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

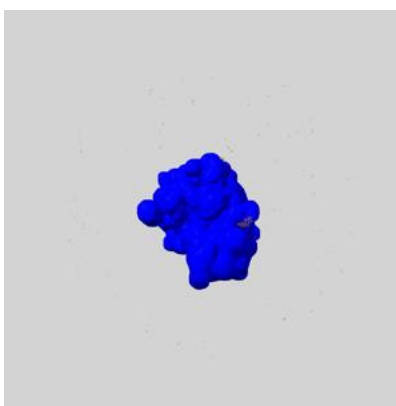
A mask typically either:

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

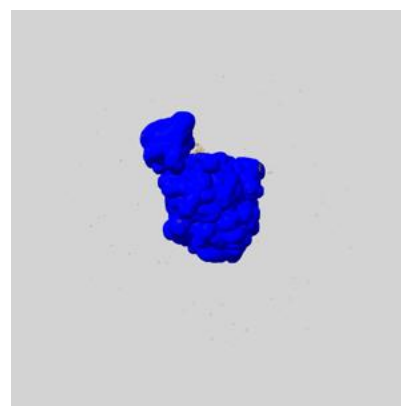
### 6.6.1 emd\_38949\_msk\_1.map [i](#)



X



Y



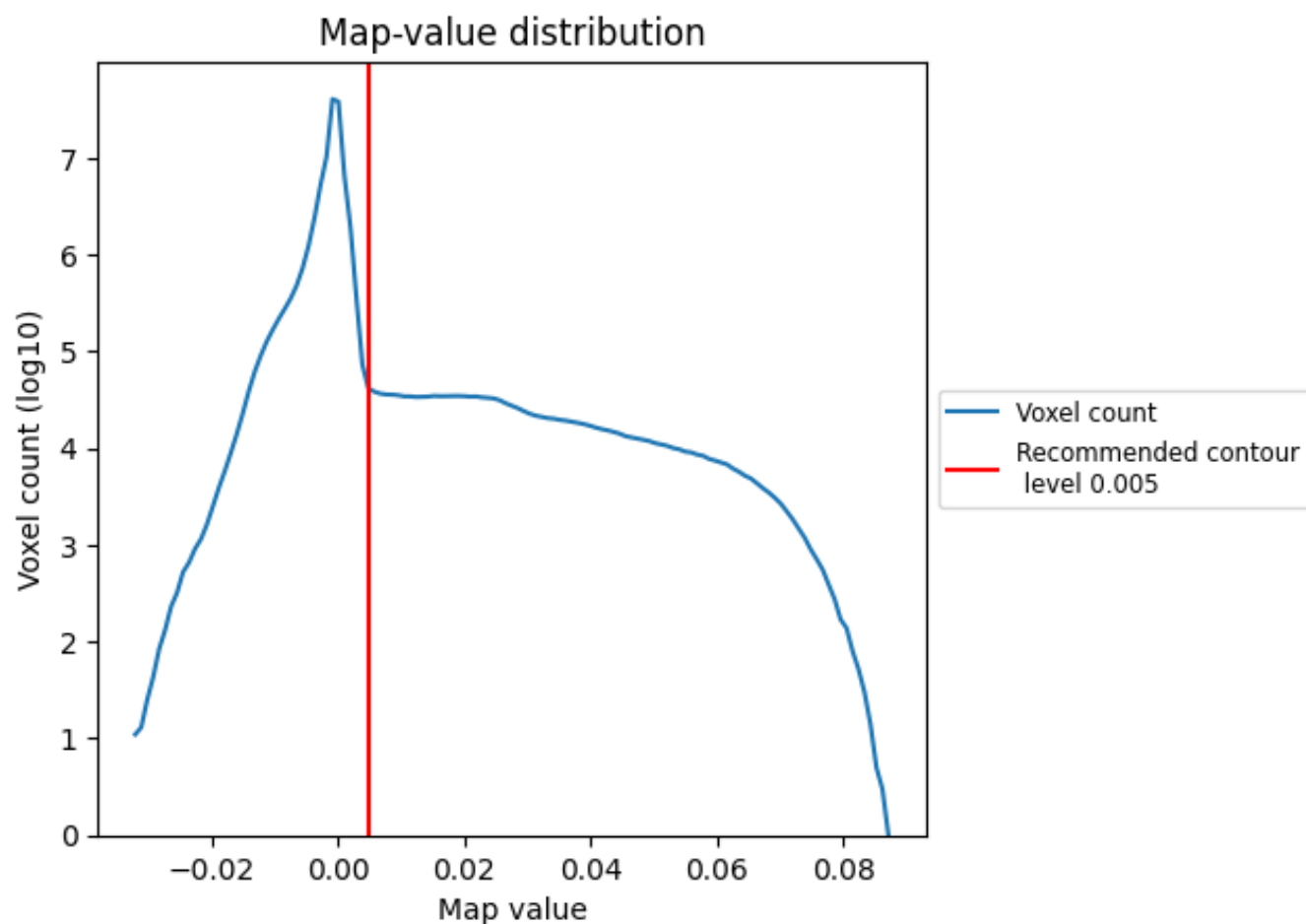
Z



## 7 Map analysis [i](#)

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

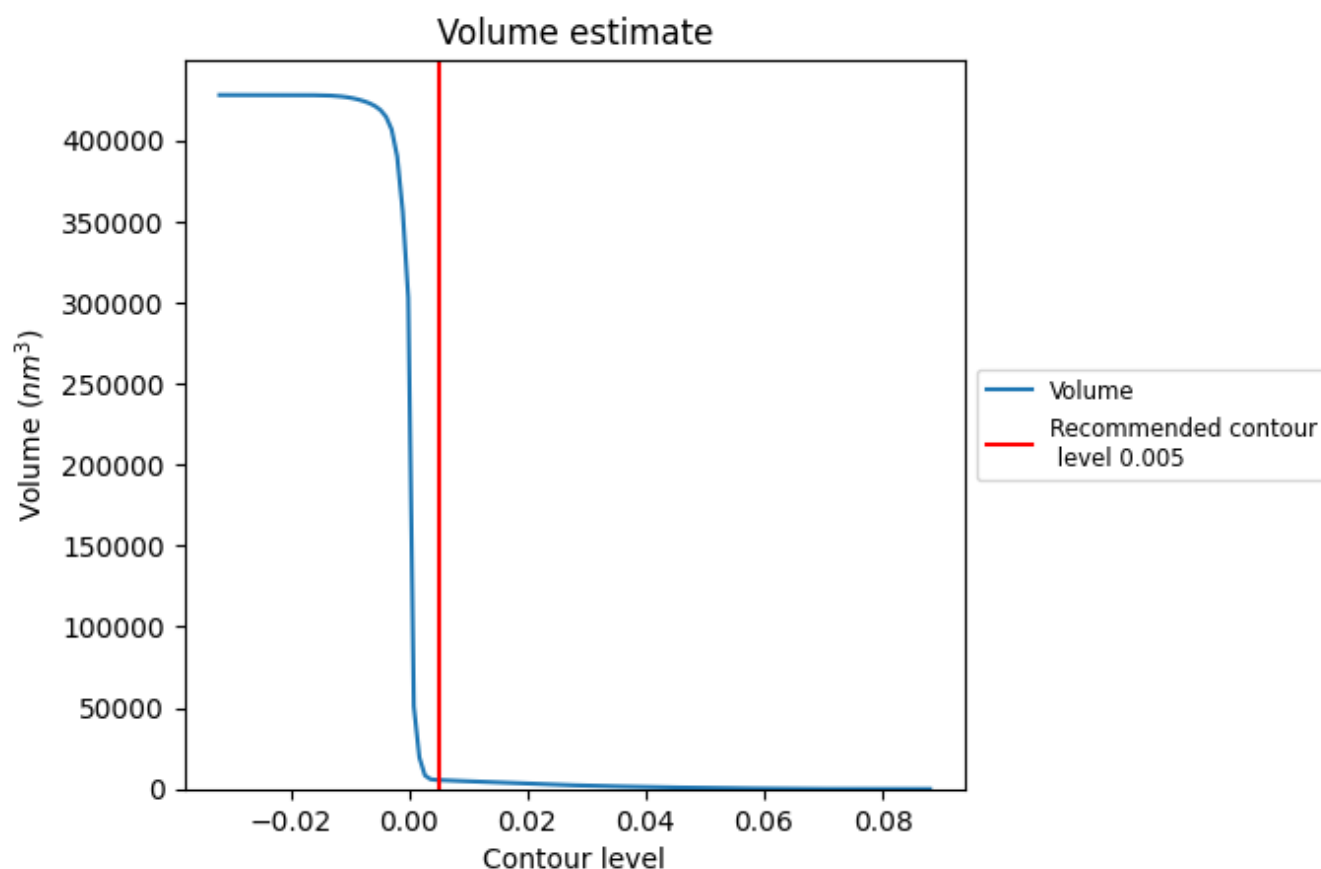
### 7.1 Map-value distribution [i](#)



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.



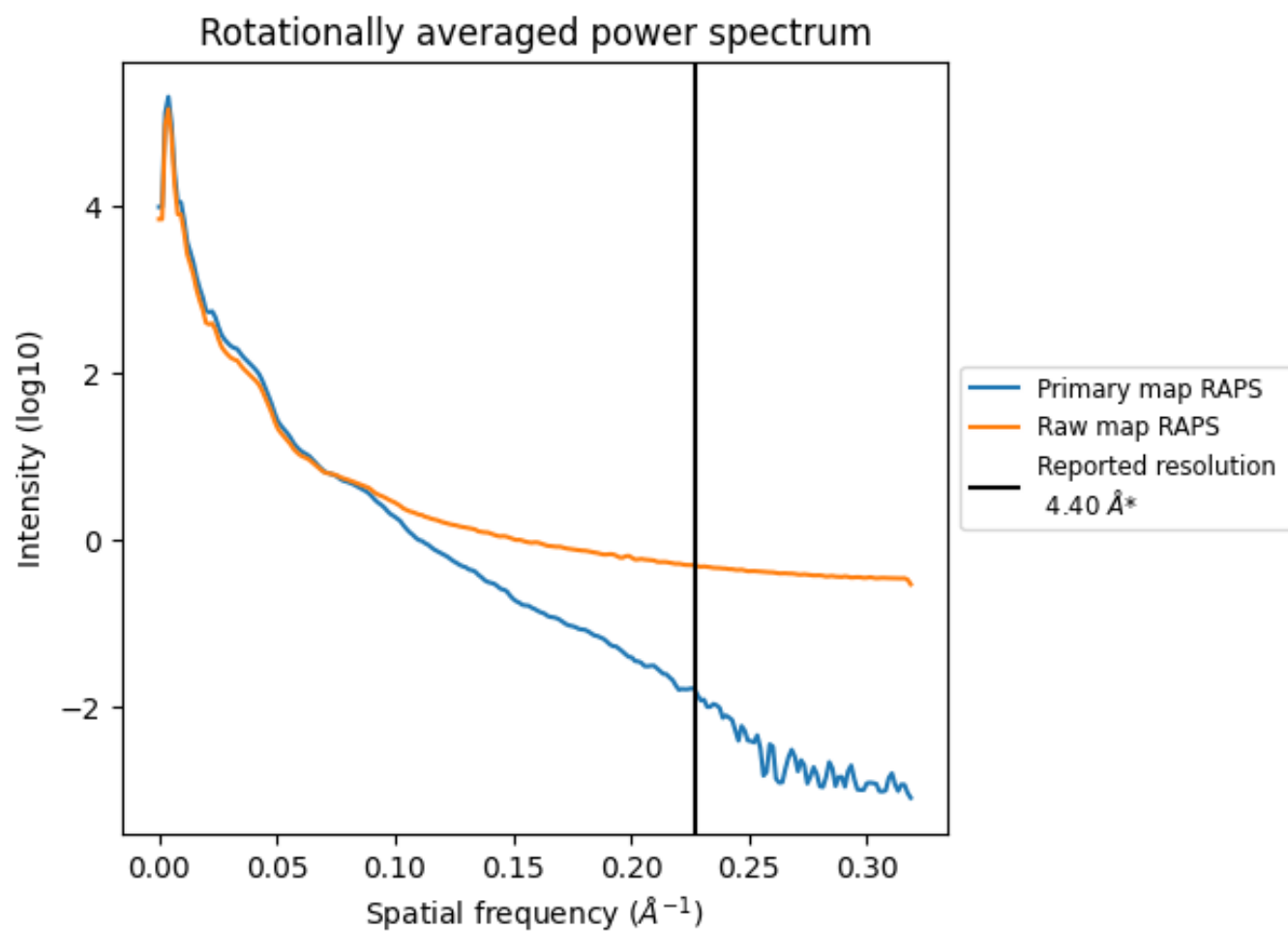
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5501  $\text{nm}^3$ ; this corresponds to an approximate mass of 4969 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 ⓘ

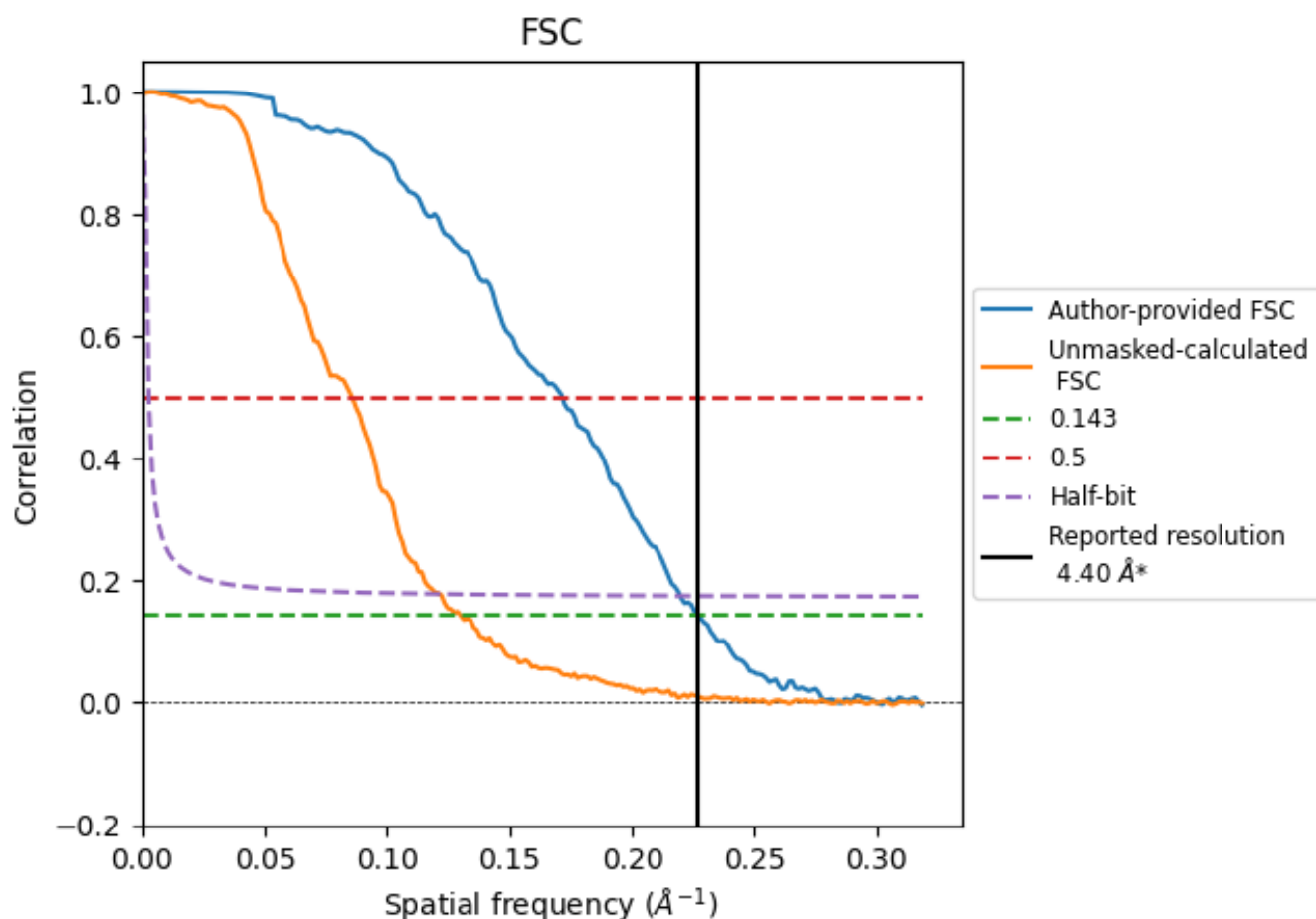


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 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 0.227 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

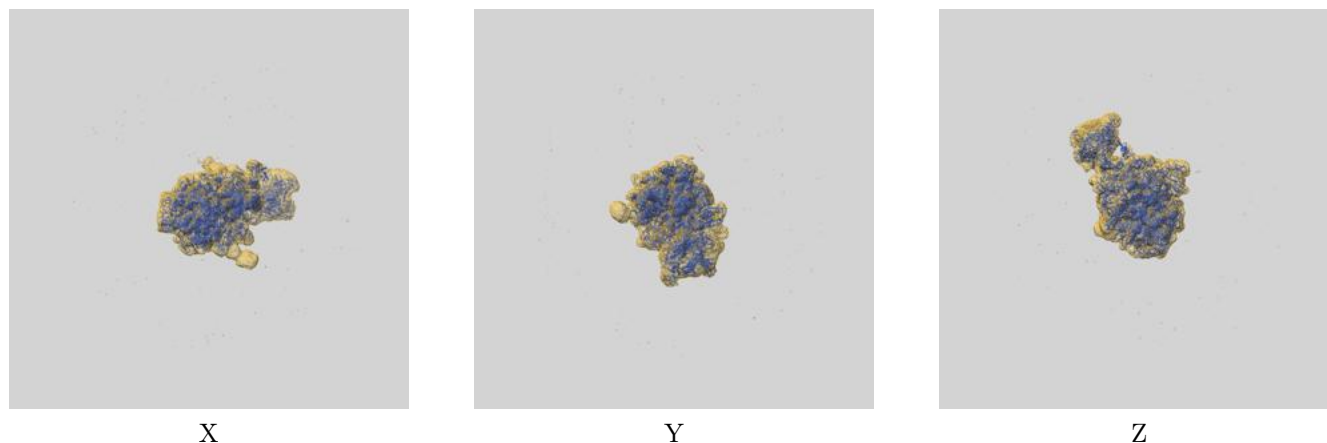
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.41	5.83	4.55
Unmasked-calculated*	7.70	11.67	8.24

\*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 7.70 differs from the reported value 4.4 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-38949 and PDB model 8Y5T. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

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



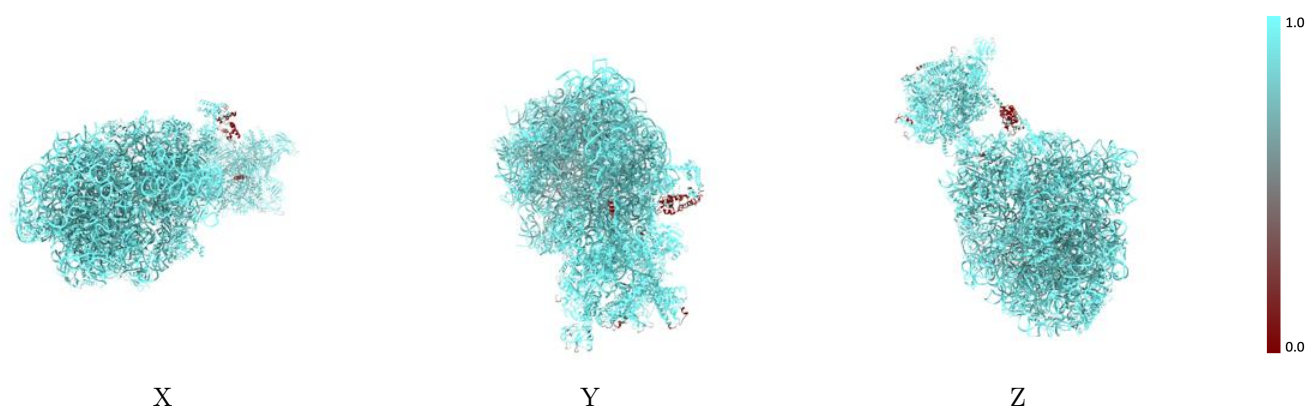
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



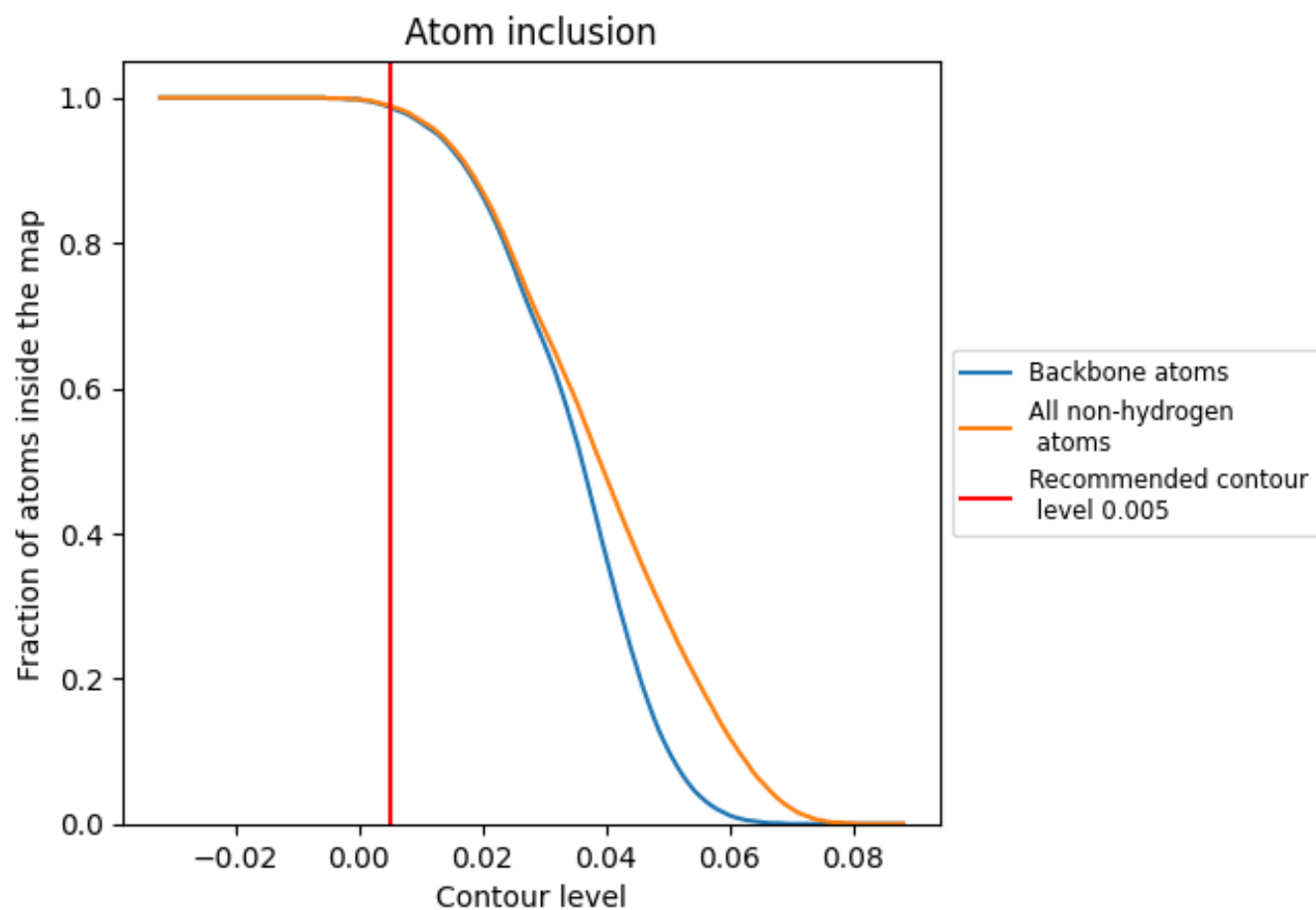
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

































































Chain	Atom inclusion	Q-score
All	 0.9890	 0.1850
0	 0.9740	 0.1590
1	 1.0000	 0.2360
2	 1.0000	 0.2150
3	 1.0000	 0.2190
4	 0.9840	 0.0830
5	 0.9820	 0.1420
6	 0.8620	 0.0790
8	 1.0000	 0.0490
9	 1.0000	 0.0490
A	 0.9860	 0.1380
A1	 0.9930	 0.0330
A2	 0.0450	 -0.0080
B	 0.9980	 0.1920
B1	 0.9840	 0.0470
B2	 0.9610	 0.0480
C	 0.9880	 0.1780
D	 0.9890	 0.1770
E	 1.0000	 0.1730
F	 1.0000	 0.1450
G	 0.9940	 0.1840
H	 0.9840	 0.1650
I	 0.9980	 0.1470
J	 0.9980	 0.1930
K	 0.9990	 0.1940
L	 0.9940	 0.1900
M	 0.9920	 0.1900
N	 1.0000	 0.1590
NA	 0.8890	 0.1530
NG	 0.9710	 0.0880
O	 1.0000	 0.1460
P	 1.0000	 0.2020
Q	 0.9630	 0.1470
R	 1.0000	 0.1630
S	 0.9990	 0.1260



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
T	 0.9960	 0.1680
U	 1.0000	 0.1560
V	 0.9970	 0.1850
W	 0.9980	 0.1540
W0	 0.7820	 0.0280
X	 0.9920	 0.0970
Y	 0.9950	 0.1700
Z	 0.9880	 0.1450
b	 0.9960	 0.2200
c	 0.9990	 0.1880
d	 0.9980	 0.1950
e	 0.9960	 0.1700
f	 0.9850	 0.1790
g	 1.0000	 0.1830
i	 0.9630	 0.0930
j	 0.9990	 0.1910
k	 0.9890	 0.2170
l	 1.0000	 0.1900
m	 0.9950	 0.1980
n	 1.0000	 0.1810
o	 1.0000	 0.1660
p	 0.9880	 0.2090
q	 0.9990	 0.1670
r	 0.9990	 0.1880
s	 0.9960	 0.1940
t	 0.9960	 0.1940
u	 0.9970	 0.1720
v	 1.0000	 0.1760
w	 1.0000	 0.1700
x	 1.0000	 0.1920
y	 1.0000	 0.1750
z	 1.0000	 0.1970