



wwPDB EM Validation Summary Report ⓘ

Aug 18, 2025 – 02:49 PM JST

PDB ID : 8YDF / pdb_00008ydf
EMDB ID : EMD-39169
Title : E.coli transcription translation coupling complex in TTC-B state 1 (subclass 2) containing mRNA with 39-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-02-20
Resolution : 4.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

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

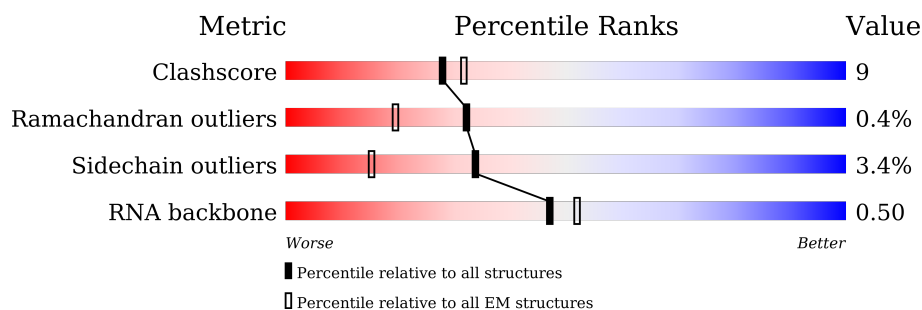
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	70	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
2	B	57	<div> <div>79%</div> <div>18%</div> <div>• •</div> </div>
3	C	55	<div> <div>•</div> <div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>
4	D	46	<div> <div>•</div> <div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>
5	E	65	<div> <div>•</div> <div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
6	F	38	<div> <div>68%</div> <div>29%</div> <div>•</div> </div>
7	G	241	<div> <div>67%</div> <div>22%</div> <div>• 10%</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
64	7	77	
65	h	6	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 178150 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	36	Total	C	N	O	P	0	0
			749	335	107	271	36		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	301	Total	C	N	O	S	0	0
			2088	1293	380	409	6		
57	A2	288	Total	C	N	O	S	0	0
			2029	1257	366	400	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
64	7	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

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

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

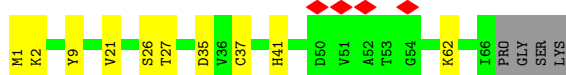
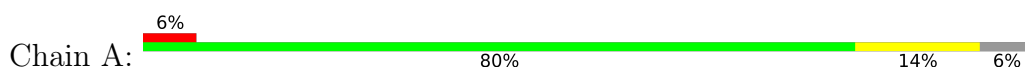
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

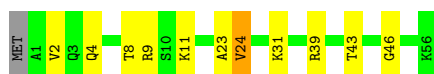
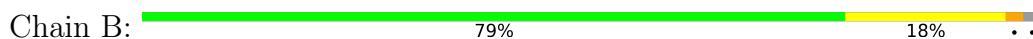
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

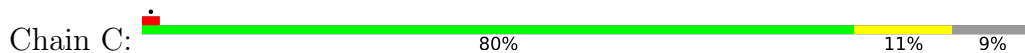
- Molecule 1: 50S ribosomal protein L31



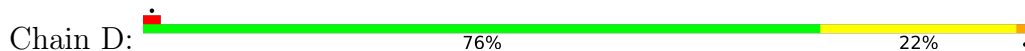
- Molecule 2: 50S ribosomal protein L32



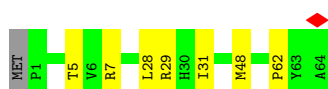
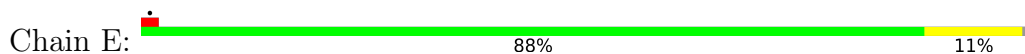
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34

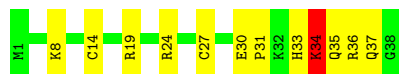


- Molecule 5: 50S ribosomal protein L35



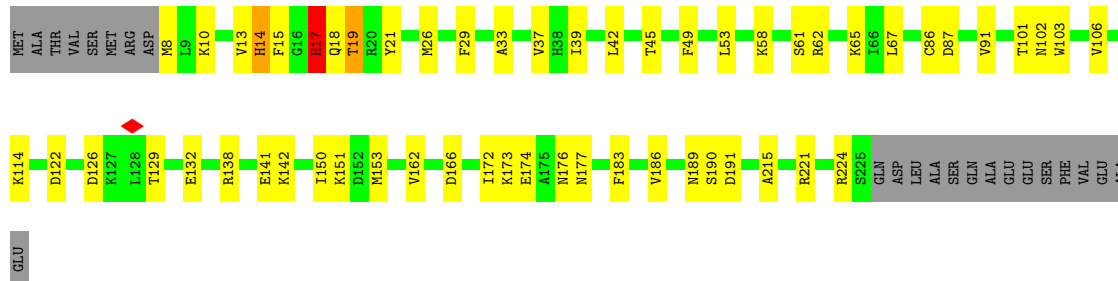
- Molecule 6: 50S ribosomal protein L36

Chain F:  68% 29%



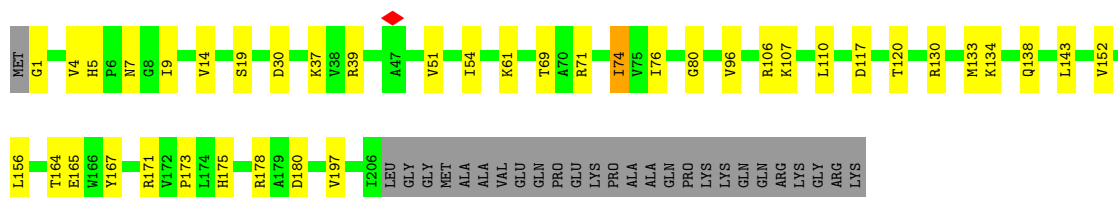
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% 10%



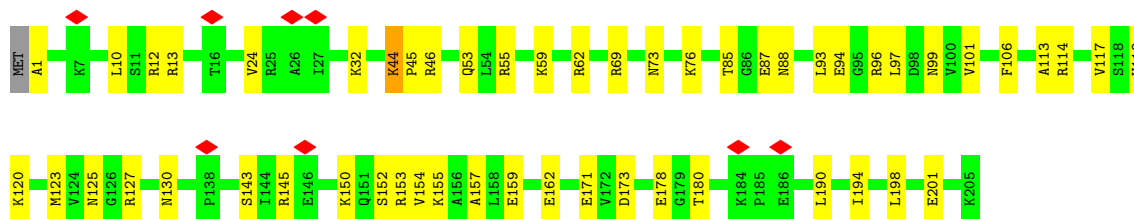
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% 12%




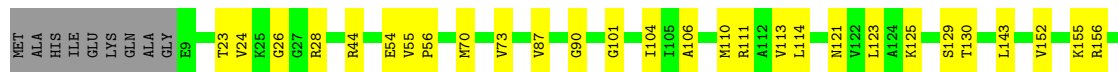
- Molecule 9: 30S ribosomal protein S4

Chain I:  74% 25%



- Molecule 10: 30S ribosomal protein S5

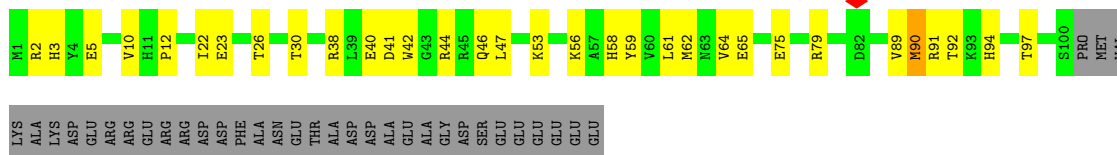
Chain J:  77% 17% 6%



Q165
LYS

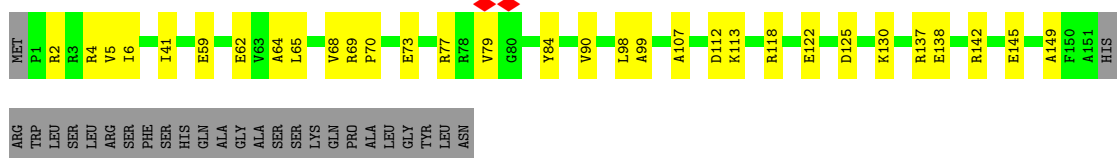
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  50% 23% 26%




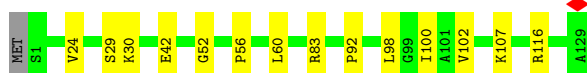
- Molecule 12: 30S ribosomal protein S7

Chain L:  67% 17% 16%



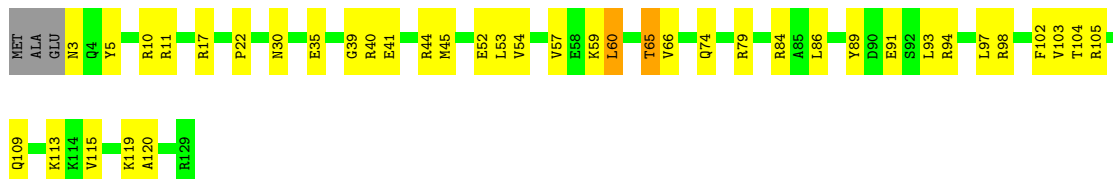
- Molecule 13: 30S ribosomal protein S8

Chain M:  88% 11%



- Molecule 14: 30S ribosomal protein S9

Chain N:  67% 29%



- Molecule 15: 30S ribosomal protein S10

Chain O:  72% 18% 5% 5%



- Molecule 16: 30S ribosomal protein S11

- Molecule 17: 30S ribosomal protein S12

- Molecule 18: 30S ribosomal protein S13


- Molecule 19: 30S ribosomal protein S14

- Molecule 20: 30S ribosomal protein S15

- Molecule 21: 30S ribosomal protein S16

WORLDWIDE
PDB
PROTEIN DATA BANK

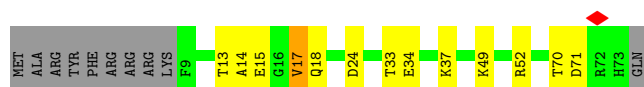
- Molecule 22: 30S ribosomal protein S17

Chain V:  76% 19% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  69% 16% 13%




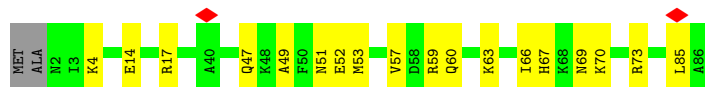
- Molecule 24: 30S ribosomal protein S19

Chain X:  74% 12% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  77% 21% 2%




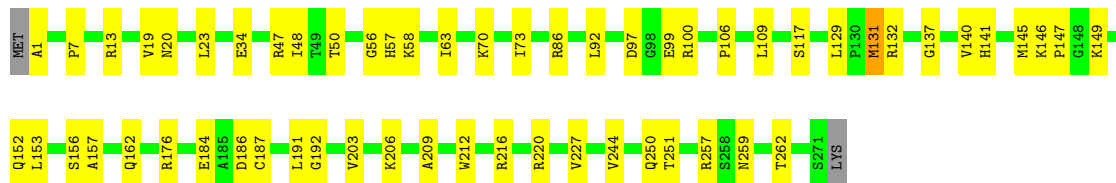
- Molecule 26: 30S ribosomal protein S21

Chain Z:  58% 30% 8%




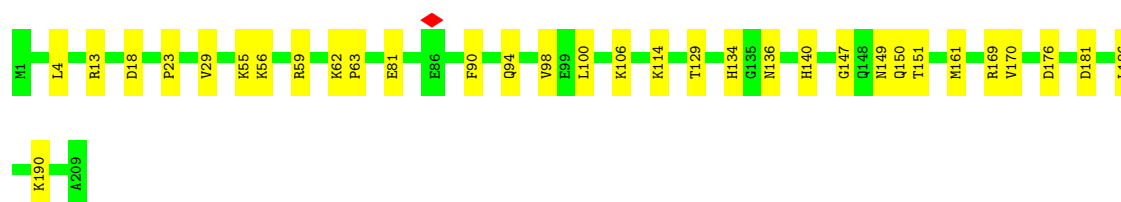
- Molecule 27: 50S ribosomal protein L2

Chain b:  78% 21% 1%



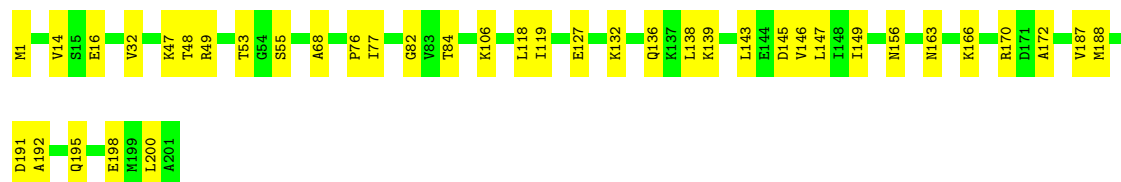
- Molecule 28: 50S ribosomal protein L3

Chain c:  85% 15%



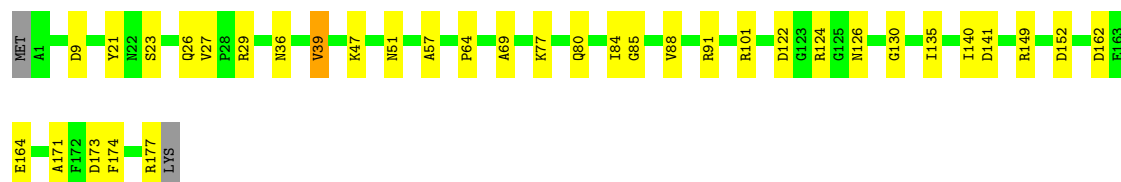
- Molecule 29: 50S ribosomal protein L4

Chain d: 81% 19%



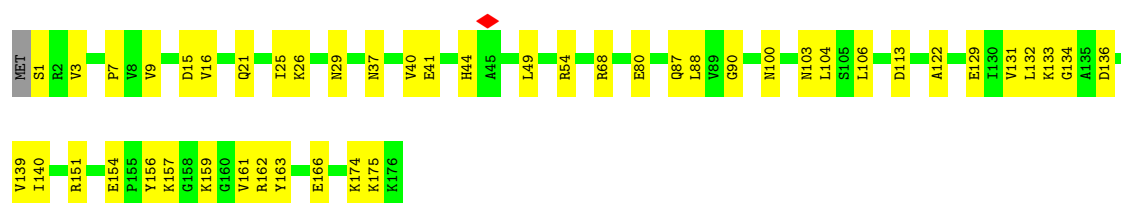
- Molecule 30: 50S ribosomal protein L5

Chain e: 79% 19% ..



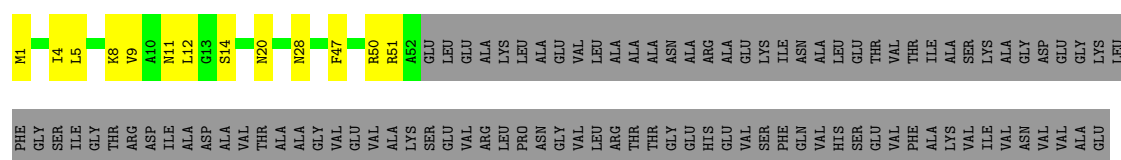
- Molecule 31: 50S ribosomal protein L6

Chain f: 73% 26% .

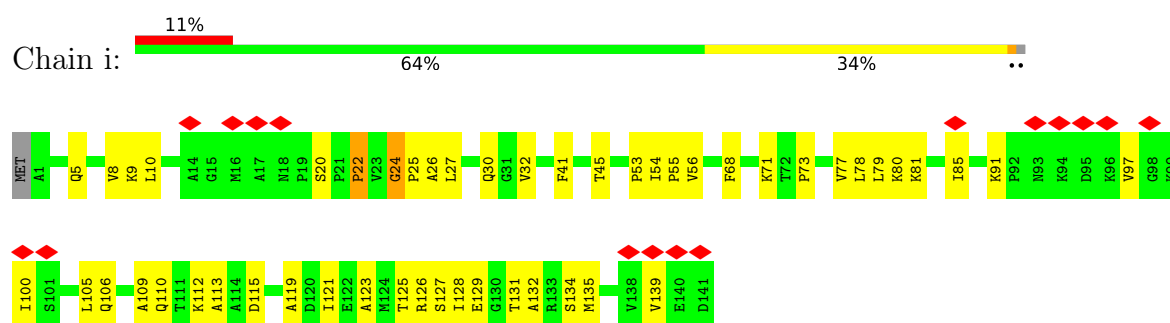


- Molecule 32: 50S ribosomal protein L9

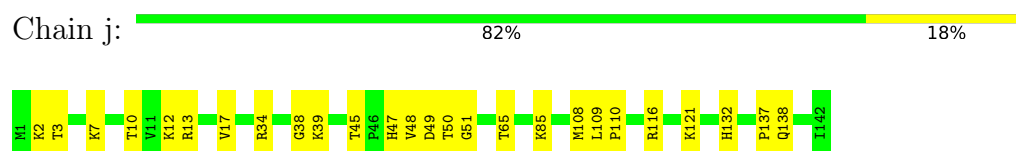
Chain g: 26% 9% 65%



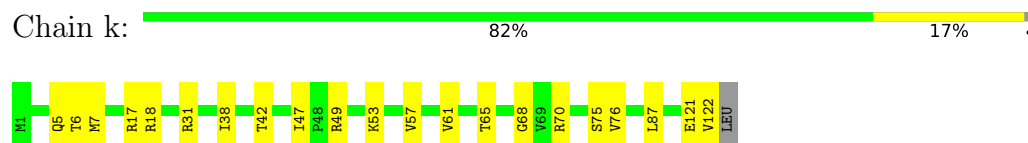
- Molecule 33: 50S ribosomal protein L11



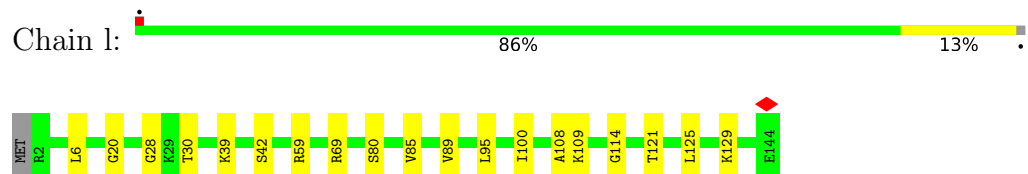
- Molecule 34: 50S ribosomal protein L13



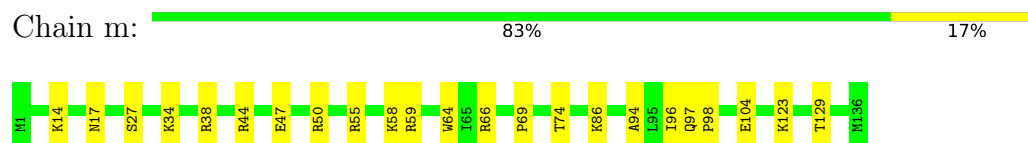
- Molecule 35: 50S ribosomal protein L14



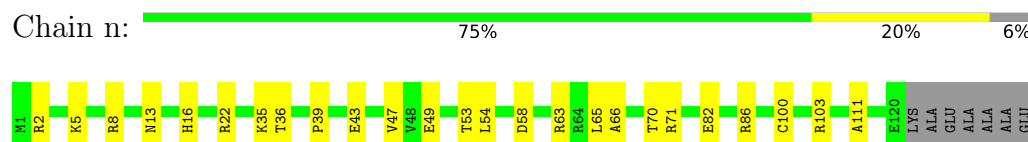
- Molecule 36: 50S ribosomal protein L15



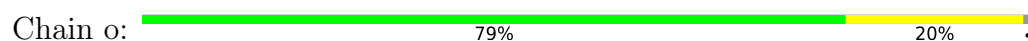
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17

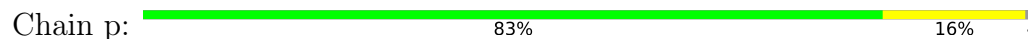


- Molecule 39: 50S ribosomal protein L18

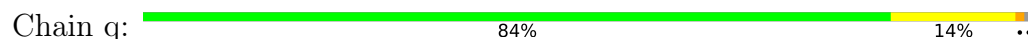




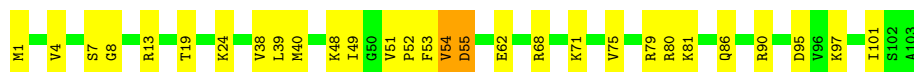
- Molecule 40: 50S ribosomal protein L19



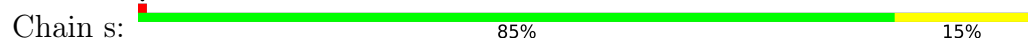
- Molecule 41: 50S ribosomal protein L20



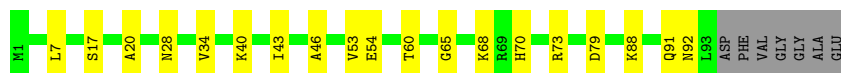
- Molecule 42: 50S ribosomal protein L21



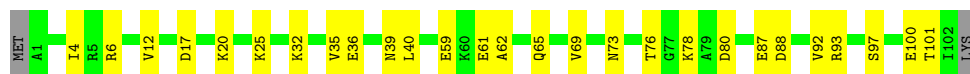
- Molecule 43: 50S ribosomal protein L22



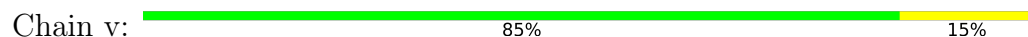
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24



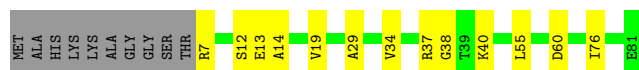
- Molecule 46: 50S ribosomal protein L25





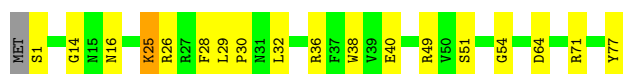
- Molecule 47: 50S ribosomal protein L27

Chain w: 73% 15% 12%



- Molecule 48: 50S ribosomal protein L28

Chain x: 76% 22% ..



- Molecule 49: 50S ribosomal protein L29

Chain y: 76% 24%



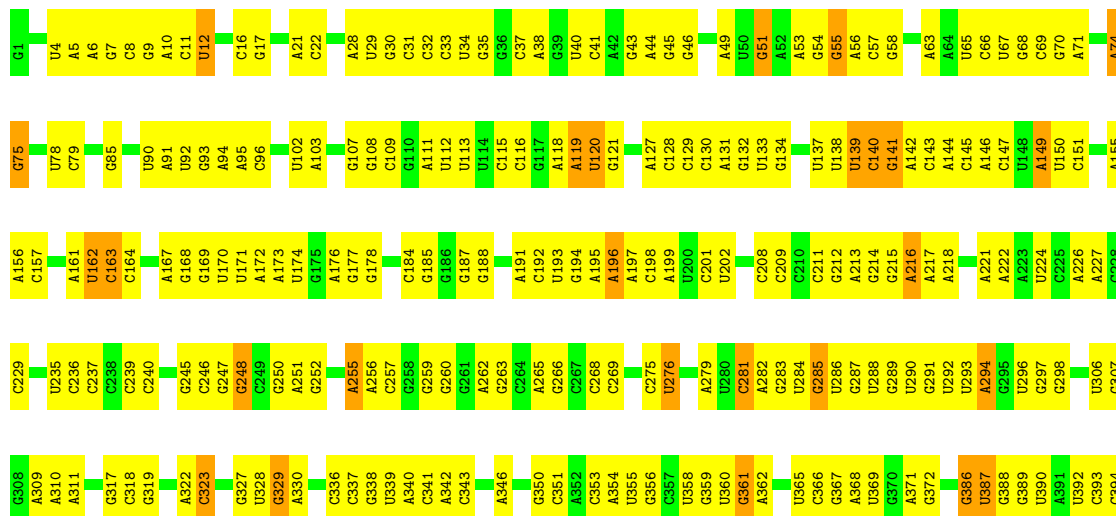
- Molecule 50: 50S ribosomal protein L30

Chain z: 76% 22% .



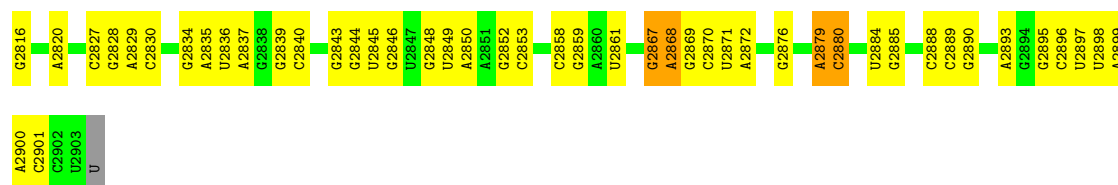
- Molecule 51: 23S rRNA

Chain 1: 43% 51% 6%



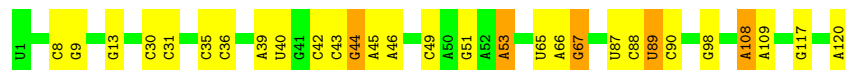
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U1181	G1182	U1183	U1184	G1185	G1186	G1187	U1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	U1198	U1199	C1200	A1204	A1205	U1209	G1210	G1211	G1212	A1213	U1219	G1220	G1225	A1230	U1231	G1232	C1233	A1237	G1238	G1239	U1240	A1246	A1247	A1253	C1254	G1255	U1256	C1257	U1258	G1259	G1266	U1267	C1270	G1271	U1272	U1273																																																																																
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C2788	C2626	U2540	U2448	G2369	U2292	C2214	G2146	G2062	U1970	A1808	A1738	U1648	U1648
U2789	U2627	G2541	G2449	U2370	G2293	C2215	A2147	G2069	G1971	A1809	G1739	G1651	G1651
G2790	C2628	U2542	U2450	G2371	G2294	C2216	U2148	C2070	U1972	U1812	G1740	U1742	U1742
U2791	U2629	A2543	A2451	U2372	C2295	G2217	C2149	C2071	G1813	C1816	G1741	G1652	G1652
C2792	A2630	G2544	G2452	G2373	U2296	U2218	U2150	U2073	A1978	C1817	G1742	G1663	G1663
U2793	G2631	U2545	C2453	U2374	A2297	G2219	G2151	U2074	G1983	U1818	G1743	G1666	G1666
G2794	U2632	G2546	U2454	G2375	C2298	C2221	C2152	U2085	G1984	C1902	A1745	G1667	G1667
A2797	C2633	U2547	G2455	U2376	G2299	C2222	U2153	U2086	U1819	A1820	A1746	U1747	U1747
U2798	U2634	G2548	U2456	G2377	U2299	G2223	G2154	C2091	G1985	A1821	C1748	A1668	A1668
C2799	A2635	U2549	A2457	U2378	C2300	A2224	G2155	U2092	C1986	C1822	A1749	C1669	C1669
G2800	G2636	G2550	G2458	U2379	U2299	A2225	G2156	G2093	G1906	G1823	G1750	A1670	A1670
U2801	U2637	U2551	U2459	G2380	A2299	C2226	U2157	C2094	G1907	C1824	U1751	U1671	U1671
G2802	C2638	U2552	G2460	A2381	U2299	A2227	G2158	A2095	U1991	U1827	C1752	A1672	A1672
U2803	G2639	G2553	C2461	G2382	U2300	G2230	C2159	U2096	U1993	G1828	G1753	G1673	G1673
C2804	U2640	A2554	U2462	U2383	C2301	U2231	G2160	C2097	C1987	A1829	A1754	G1674	G1674
U2805	G2641	U2555	A2463	C2384	G2302	C2232	G2161	A2098	U1998	C1832	C1675	A1676	A1676
G2806	U2642	G2556	U2464	C2385	G2303	A2226	G2162	C2099	G1999	C1833	U1758	G1677	G1677
U2807	C2643	U2557	G2465	A2386	G2304	A2227	G2163	U2099	G2012	U1834			
C2808	G2644	U2558	A2466	U2387	U2305	G2233	A2164	U2098					
U2809	U2645	G2559	U2467	U2388	U2306	G2234	C2165	C2099					
G2810	C2646	U2560	A2468	G2389	C2307	A2235	G2166	U2099					
C2811	U2647	G2561	A2469	U2390	U2308	G2236	U2167	G2100					
U2812	G2648	U2562	U2470	G2391	A2309	A2237	C2168	A2101					
G2813	C2649	A2563	G2471	C2392	G2310	G2238	G2169						
A2814	U2650	G2564	A2472	A2393	A2311	U2239	C2170						
C2815	U2651	U2565	U2473	U2394	U2312	G2240	C2171						
	C2652	G2566	A2474	C2395	U2313	A2241	U2172						
		U2567	A2475	G2396	G2314	U2242	U2173						
		U2568	U2476	C2397		U2243	U2174						
		G2569	A2477	G2398		U2244	U2175						
		U2570	U2478	C2399		U2245	U2176						
		G2571	A2479	G2400		U2246	U2177						
		U2572	U2480	C2401		U2247	U2178						
		A2573	A2481	A2399		U2248	U2179						
		G2574	U2482	U2399		U2249	U2180						
		C2575	C2483	C2399		U2250	U2181						
		U2576	U2484	C2399		U2251	U2182						
		G2577	G2485	C2399		U2252	U2183						
		C2578	A2486	C2399		U2253	U2184						
		U2579	U2487	C2399		U2254	U2185						
		G2580	A2488	C2399		U2255	U2186						
		C2581	U2489	C2399		U2256	U2187						
		U2582	A2490	C2399		U2257	U2188						
		G2583	U2491	C2399		U2258	U2189						
		C2584	C2492	C2399		U2259	U2190						
		U2585	A2493	C2399		U2260	U2191						
		G2586	U2494	C2399		U2261	U2192						
		C2587	A2495	C2399		U2262	U2193						
		U2588	U2496	C2399		U2263	U2194						
		G2589	A2497	C2399		U2264	U2195						
		C2590	U2498	C2399		U2265	U2196						
		U2591	A2499	C2399		U2266	U2197						
		G2592	U2500	C2399		U2267	U2198						
		C2593	A2501	C2399		U2268	U2199						
		U2594	U2502	C2399		U2269	U2200						
		G2595	C2503	C2399		U2270	U2201						
		A2596	U2504	C2399		U2271	U2202						
		C2597	A2505	C2399		U2272	U2203						
		U2598	U2506	C2399		U2273	U2204						
		G2599	C2507	C2399		U2274	U2205						
		A2600	U2508	C2399		U2275	U2206						
		C2601	U2509	C2399		U2276	U2207						
		U2602	U2510	C2399		U2277	U2208						
		A2603	G2511	C2399		U2278	U2209						
		G2604	U2512	C2399		U2279	U2210						
		C2605	A2513	C2399		U2280	U2211						
		U2606	G2514	C2399		U2281	U2212						
		G2607	U2515	C2399		U2282	U2213						
		A2608	A2516	C2399		U2283	U2214						
		C2609	U2517	C2399		U2284	U2215						
		U2610	G2518	C2399		U2285	U2216						
		G2611	A2519	C2399		U2286	U2217						
		C2612	U2520	C2399		U2287	U2218						
		U2613	G2521	C2399		U2288	U2219						
		A2614	U2522	C2399		U2289	U2220						



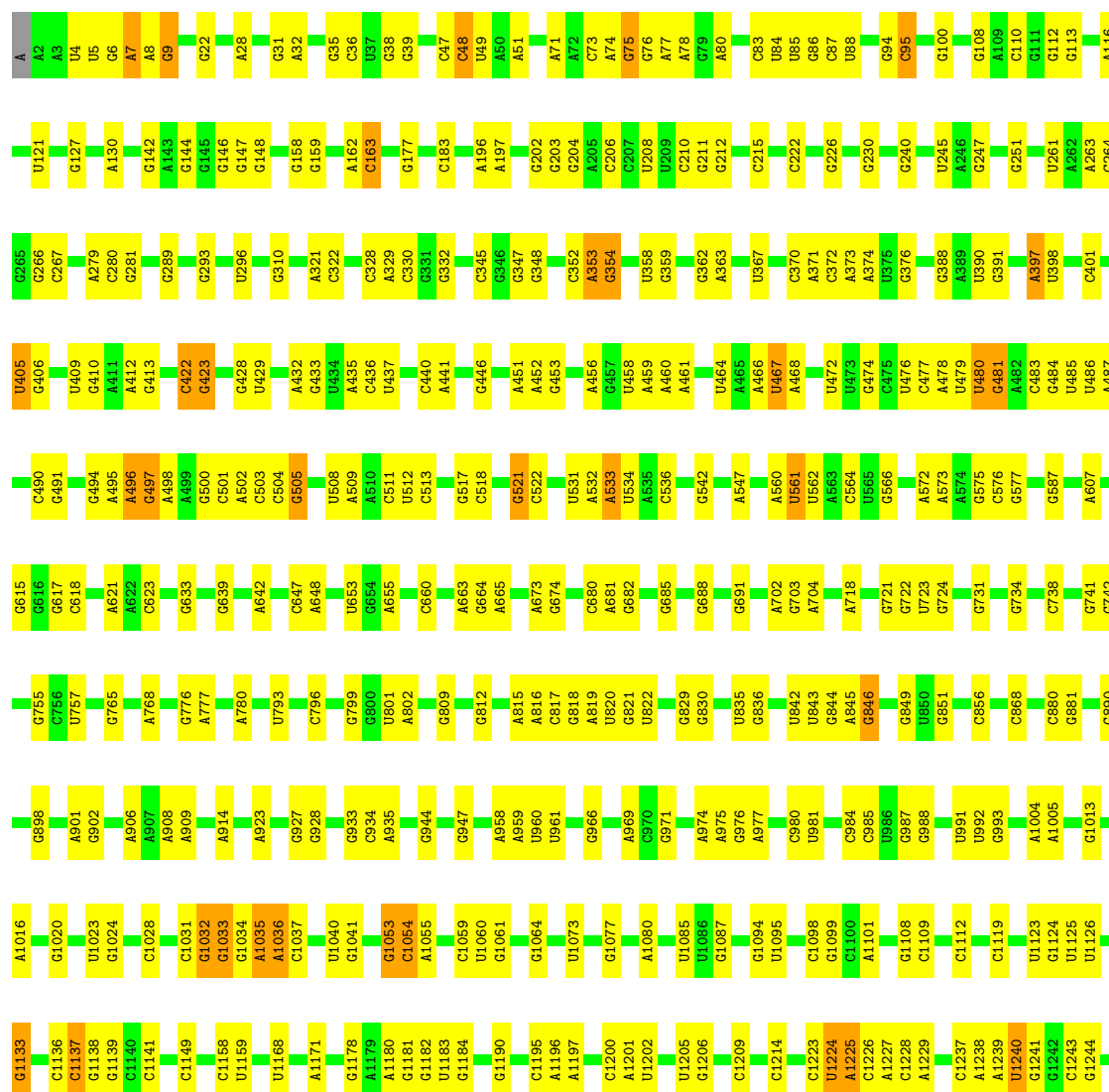
• Molecule 52: 5S rRNA

Chain 2: 76% 20%



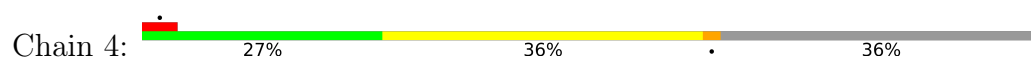
• Molecule 53: 16S rRNA

Chain 3: 69% 29%

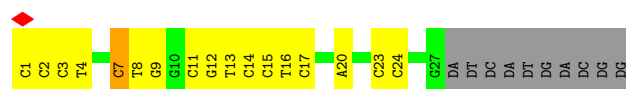




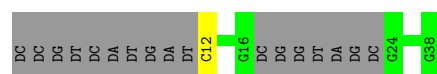
• Molecule 54: mRNA



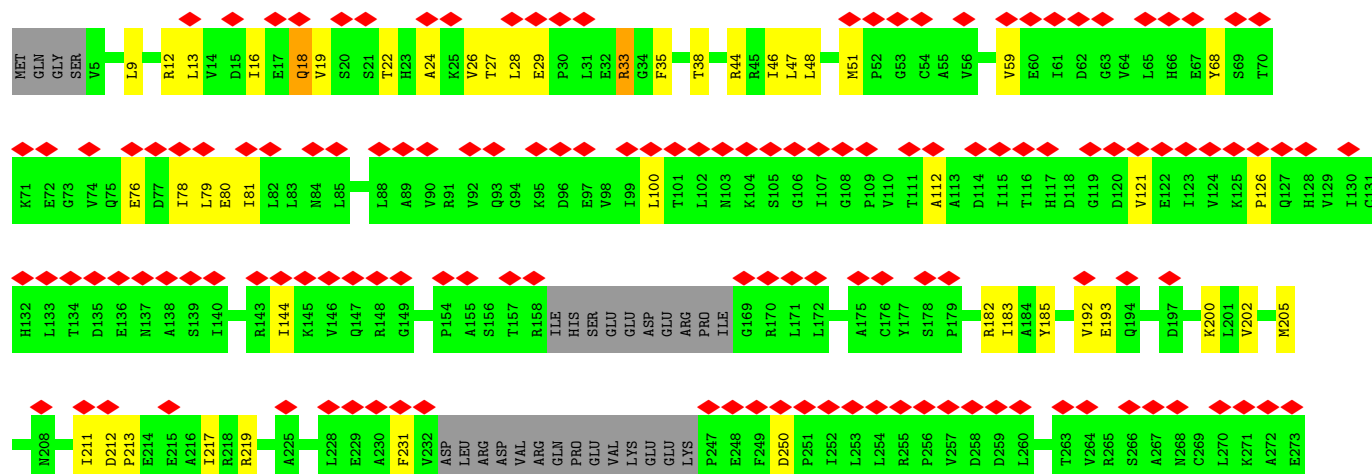
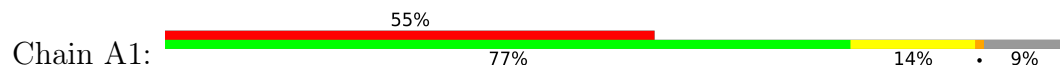
• Molecule 55: template DNA strand

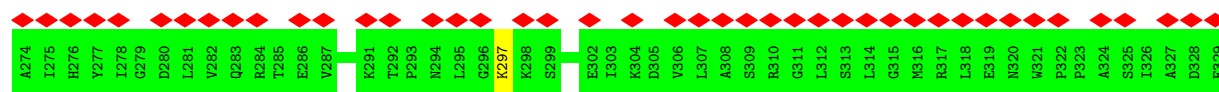


• Molecule 56: non-template DNA strand

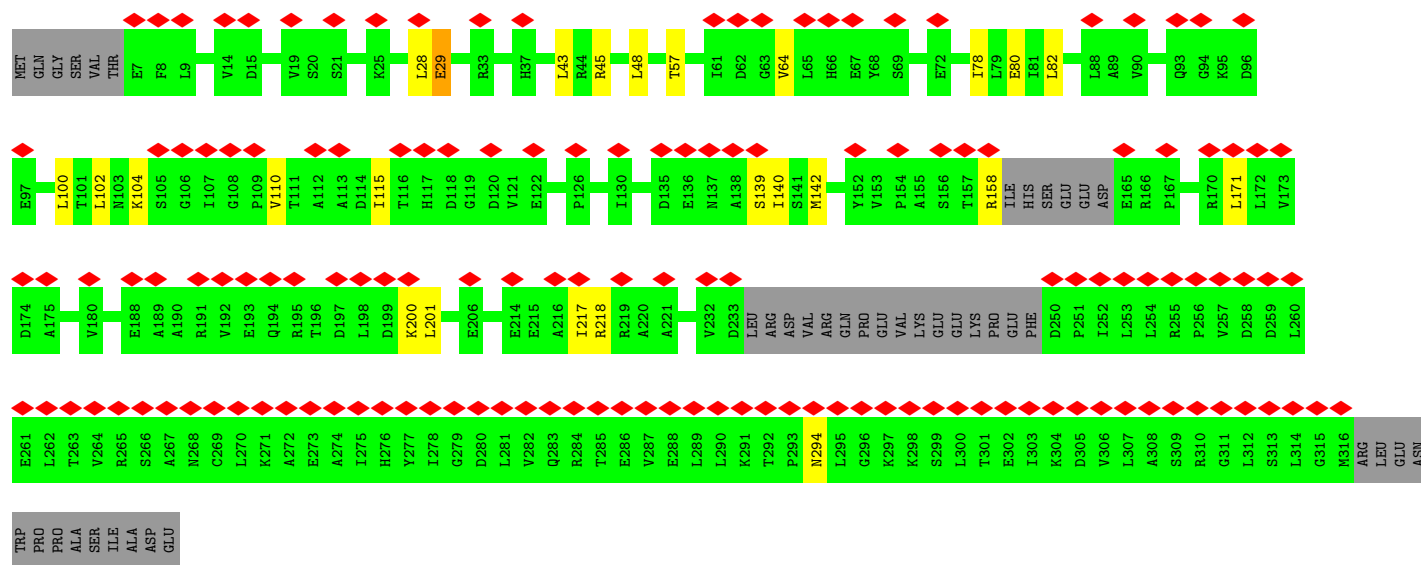
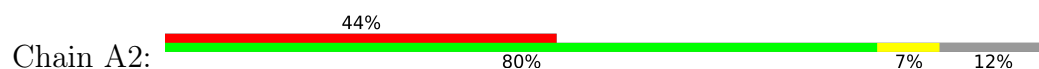


• Molecule 57: DNA-directed RNA polymerase subunit alpha

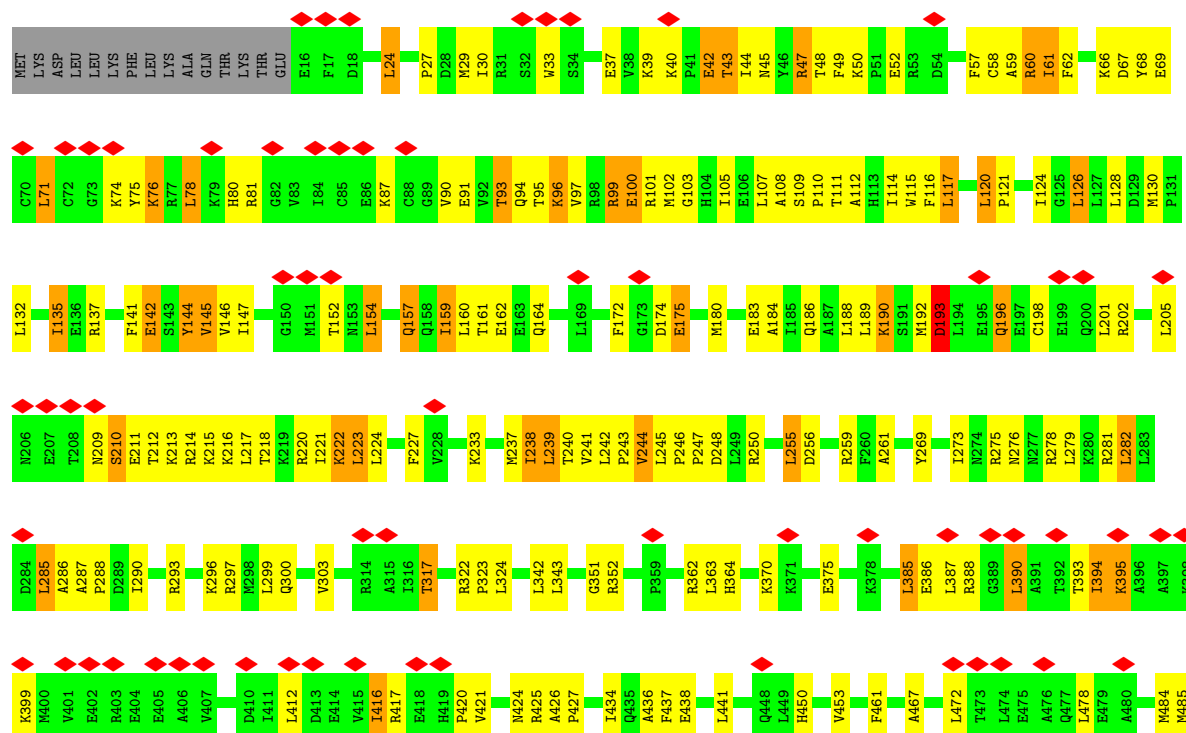


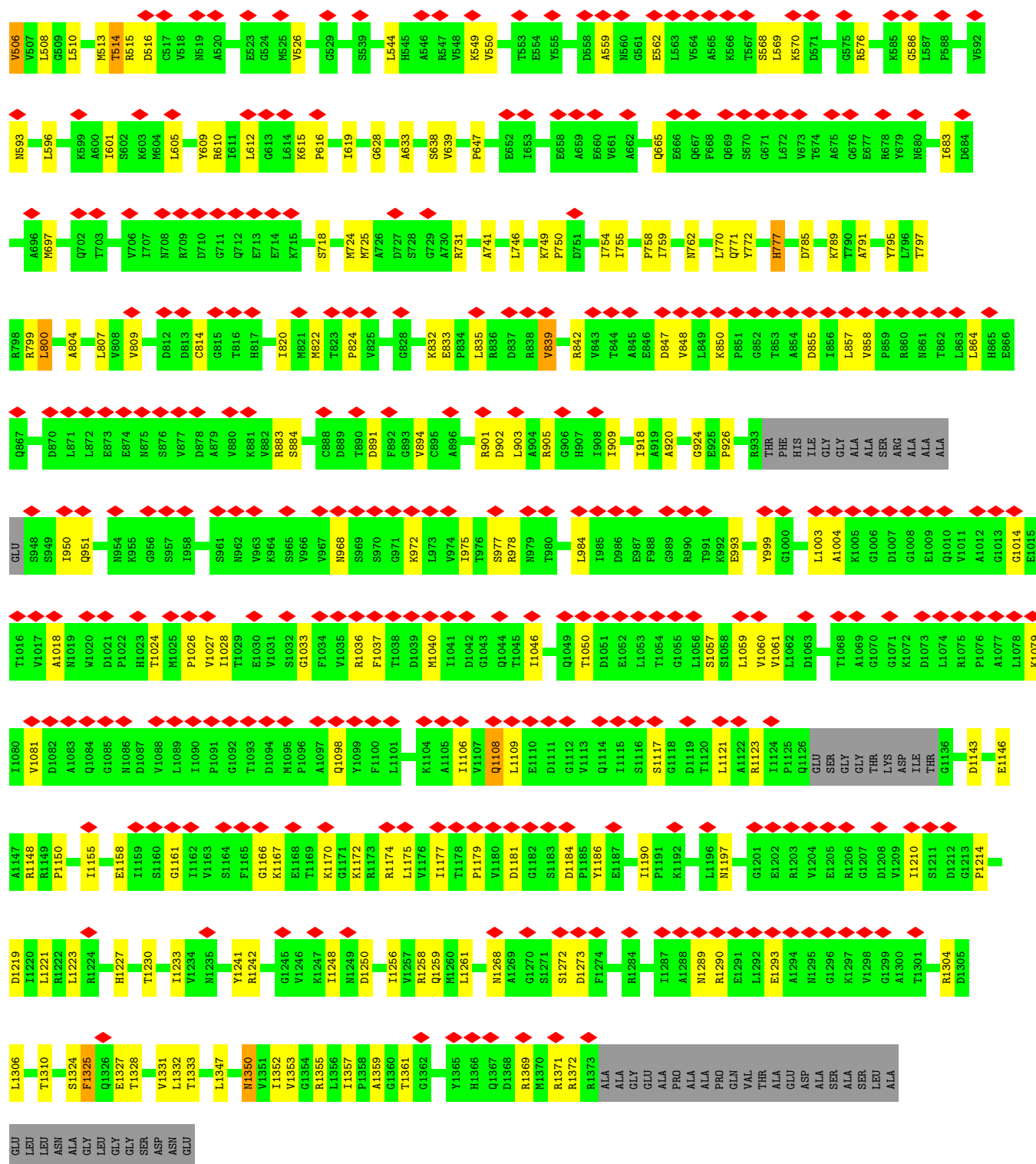


• Molecule 57: DNA-directed RNA polymerase subunit alpha

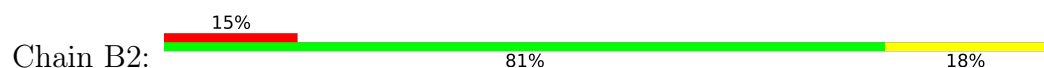


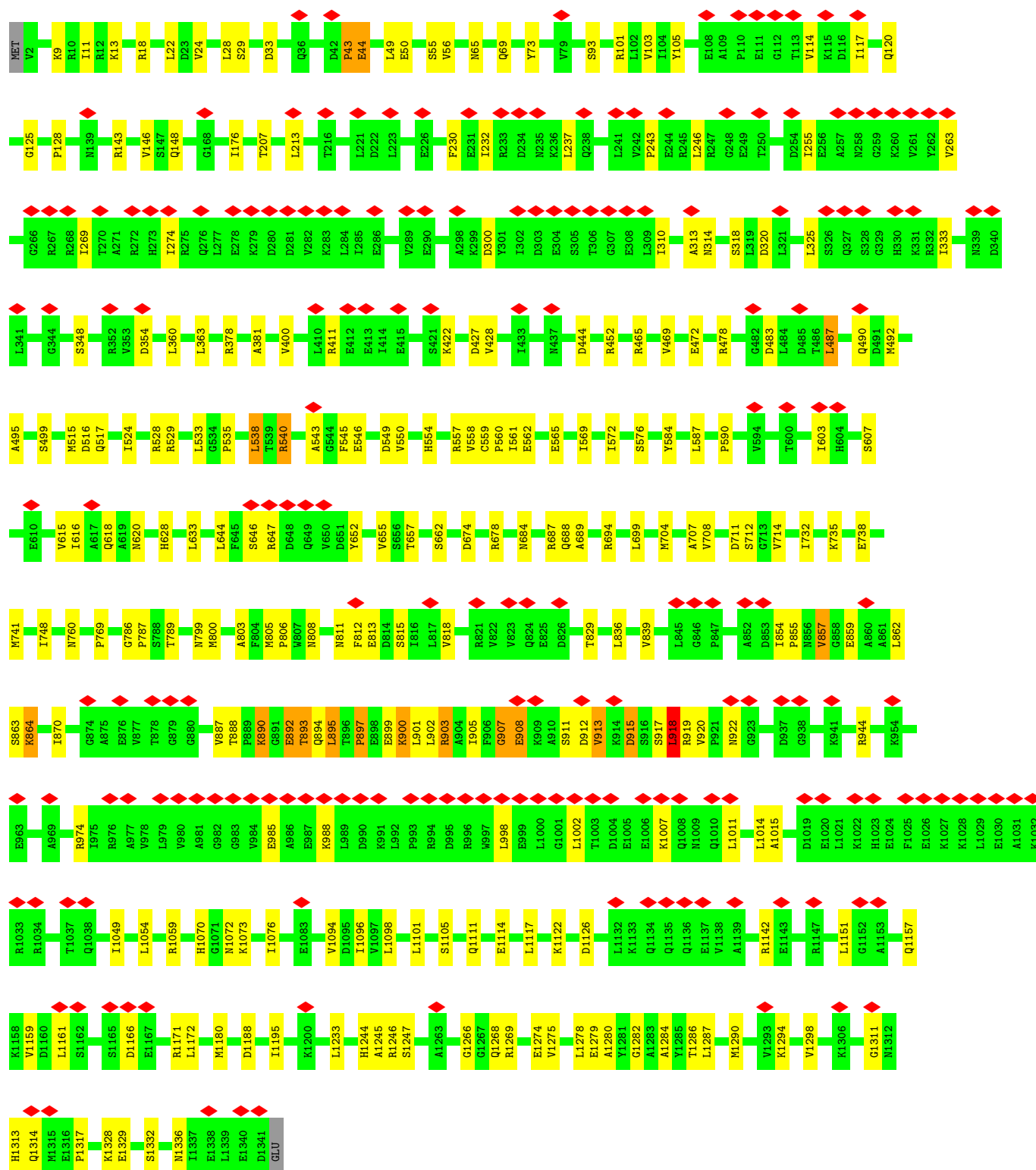
• Molecule 58: DNA-directed RNA polymerase subunit beta'



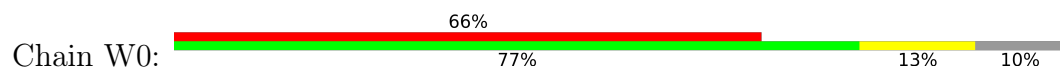


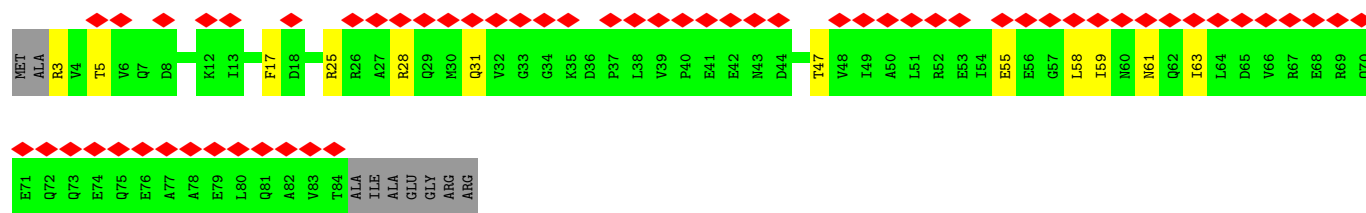
- Molecule 59: DNA-directed RNA polymerase subunit beta





- Molecule 60: DNA-directed RNA polymerase subunit omega

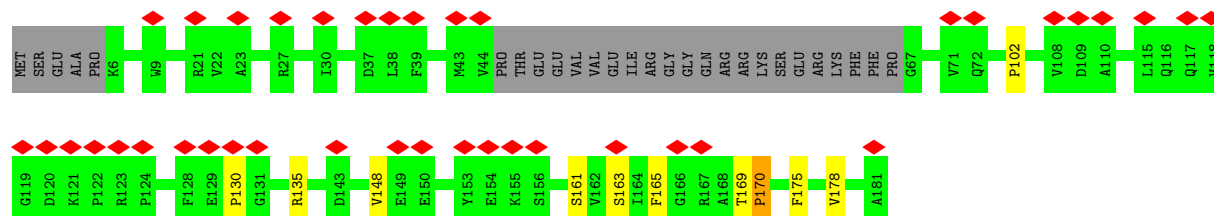
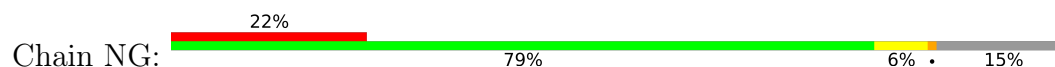




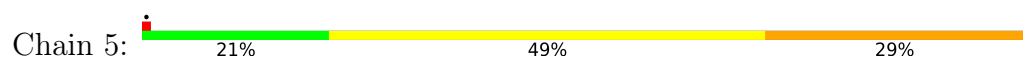
• Molecule 61: Transcription termination/antitermination protein NusA

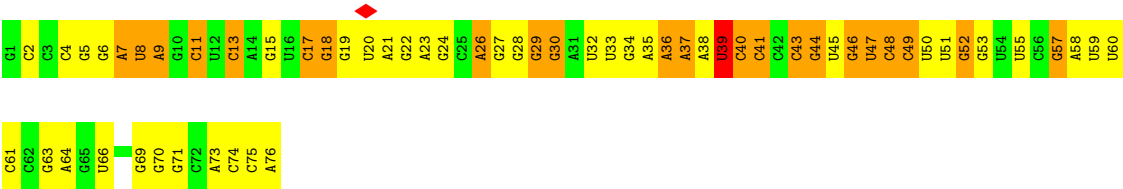


• Molecule 62: Transcription termination/antitermination protein NusG

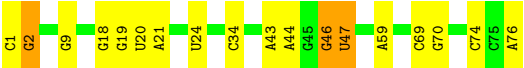


• Molecule 63: tRNA(Phe)

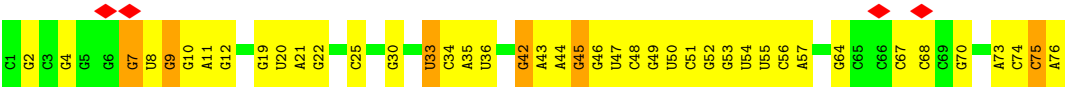




• Molecule 64: tRNA(fMet)



• Molecule 64: tRNA(fMet)



• Molecule 65: Viomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32000	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	0.179	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.012	Depositor
Map size (\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 (\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: DPP, UAL, MG, 5OH, KBE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/531	0.54	0/709
2	B	0.41	0/450	0.60	2/599 (0.3%)
3	C	0.28	0/416	0.52	0/554
4	D	0.47	0/380	0.76	2/498 (0.4%)
5	E	0.53	0/513	0.60	0/676
6	F	0.57	0/303	0.65	0/397
7	G	0.37	0/1735	0.64	0/2338
8	H	0.34	0/1651	0.55	0/2225
9	I	0.35	0/1665	0.71	0/2227
10	J	0.38	0/1169	0.68	2/1573 (0.1%)
11	K	0.46	0/835	0.77	0/1128
12	L	0.31	0/1195	0.66	3/1602 (0.2%)
13	M	0.35	0/989	0.52	0/1326
14	N	0.41	0/1034	0.77	0/1375
15	O	0.50	0/796	0.78	2/1077 (0.2%)
16	P	0.45	0/885	0.64	1/1195 (0.1%)
17	Q	0.50	0/969	0.85	2/1300 (0.2%)
18	R	0.33	0/892	0.72	2/1193 (0.2%)
19	S	0.33	0/817	0.61	0/1088
20	T	0.49	0/722	0.64	0/964
21	U	0.30	0/659	0.71	2/884 (0.2%)
22	V	0.44	0/657	0.71	0/881
23	W	0.54	0/544	0.74	1/731 (0.1%)
24	X	0.28	0/652	0.55	0/877
25	Y	0.28	0/671	0.52	0/888
26	Z	0.66	0/550	1.01	2/728 (0.3%)
27	b	0.49	0/2121	0.65	0/2852
28	c	0.42	0/1586	0.59	2/2134 (0.1%)
29	d	0.43	0/1571	0.62	0/2113
30	e	0.38	0/1434	0.60	2/1926 (0.1%)
31	f	0.29	0/1343	0.54	0/1816
32	g	0.32	0/405	0.74	0/544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.31	0/1046	0.77	3/1410 (0.2%)
34	j	0.42	0/1152	0.55	1/1551 (0.1%)
35	k	0.45	0/947	0.66	0/1268
36	l	0.40	0/1054	0.63	0/1403
37	m	0.56	0/1093	0.74	0/1460
38	n	0.46	0/973	0.72	1/1301 (0.1%)
39	o	0.32	0/902	0.51	0/1209
40	p	0.42	0/929	0.61	0/1242
41	q	0.52	0/960	0.63	1/1278 (0.1%)
42	r	0.44	0/829	0.69	0/1107
43	s	0.43	0/864	0.58	0/1156
44	t	0.33	0/744	0.52	0/994
45	u	0.46	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	0.63	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	0.52	0/830	0.65	0/1285
55	8	0.56	0/599	0.71	1/919 (0.1%)
56	9	0.49	0/468	0.53	0/719
57	A1	0.55	0/2106	0.82	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.57	5/10510 (0.0%)	0.75	8/14196 (0.1%)
59	B2	0.47	0/10714	0.68	2/14459 (0.0%)
60	W0	0.30	0/652	0.61	0/879
61	NA	0.78	0/2431	1.21	0/3385
62	NG	1.12	0/756	1.07	0/1048
63	5	0.57	0/1812	0.86	3/2823 (0.1%)
64	6	0.40	0/1832	0.48	0/2855
64	7	0.39	0/1832	0.57	1/2855 (0.0%)
65	h	3.17	2/11 (18.2%)	0.75	0/13
All	All	0.48	7/191598 (0.0%)	0.62	68/282891 (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
59	B2	0	1

The worst 5 of 7 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	-6.14	1.40	1.52
58	B1	1350	ASN	CG-ND2	-5.25	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.17	1.33	1.23
58	B1	424	ASN	CG-ND2	-5.09	1.22	1.33

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	73	VAL	N-CA-C	-9.06	104.50	113.20
41	q	33	VAL	N-CA-C	-8.80	104.73	112.12
12	L	64	ALA	N-CA-C	-7.67	105.09	114.75
51	1	1130	U	C2'-C3'-O3'	7.58	120.86	109.50
64	7	33	U	C2'-C3'-O3'	7.22	120.33	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
59	B2	903	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	8	0
2	B	444	0	461	9	0
3	C	409	0	440	4	0
4	D	377	0	418	9	0
5	E	504	0	574	4	0
6	F	302	0	343	6	0
7	G	1704	0	1732	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1624	0	1699	26	0
9	I	1643	0	1710	34	0
10	J	1156	0	1199	18	0
11	K	817	0	808	18	0
12	L	1181	0	1240	19	0
13	M	979	0	1034	9	0
14	N	1022	0	1070	23	0
15	O	786	0	828	15	0
16	P	869	0	878	22	0
17	Q	955	0	1019	30	0
18	R	883	0	944	19	0
19	S	805	0	847	10	0
20	T	714	0	737	5	0
21	U	649	0	666	15	0
22	V	648	0	691	8	0
23	W	535	0	552	7	0
24	X	637	0	665	7	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	28	0
29	d	1552	0	1619	28	0
30	e	1410	0	1447	22	0
31	f	1323	0	1374	31	0
32	g	400	0	423	7	0
33	i	1032	0	1088	41	0
34	j	1129	0	1162	22	0
35	k	938	0	1012	17	0
36	l	1045	0	1117	16	0
37	m	1074	0	1157	13	0
38	n	960	0	1000	18	0
39	o	892	0	923	16	0
40	p	917	0	965	17	0
41	q	947	0	1022	9	0
42	r	816	0	839	19	0
43	s	857	0	922	11	0
44	t	738	0	807	10	0
45	u	779	0	834	13	0
46	v	753	0	780	9	0
47	w	575	0	592	9	0
48	x	625	0	655	11	0
49	y	509	0	543	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	z	449	0	491	9	0
51	1	62317	0	31346	1456	0
52	2	2568	0	1303	15	0
53	3	33012	0	16618	185	0
54	4	749	0	374	6	0
55	8	539	0	305	29	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	25	0
57	A2	2029	0	1864	18	0
58	B1	10353	0	10548	321	0
59	B2	10546	0	10550	172	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	6	0
62	NG	758	0	334	10	0
63	5	1622	0	821	27	0
64	6	1640	0	837	7	0
64	7	1640	0	837	19	0
65	h	48	0	40	8	0
66	B1	1	0	0	0	0
All	All	178150	0	126642	2807	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 2807 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:p:52:ARG:HH21	51:1:2720:U:H5''	0.95	1.09
51:1:275:C:H2'	51:1:276:U:H4'	1.37	1.06
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
3	C	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
4	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
5	E	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
6	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	51
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	25	64
10	J	155/167 (93%)	138 (89%)	17 (11%)	0	100	100
11	K	98/135 (73%)	84 (86%)	14 (14%)	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	48
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	51
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	8	37
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
31	f	174/177 (98%)	159 (91%)	15 (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
34	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
35	k	120/123 (98%)	106 (88%)	14 (12%)	0	100	100
36	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
37	m	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
38	n	118/127 (93%)	103 (87%)	15 (13%)	0	100	100
39	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	p	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
41	q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	36
42	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	48
43	s	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
44	t	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
45	u	100/104 (96%)	84 (84%)	15 (15%)	1 (1%)	13	48
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	10	42
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	21 (7%)	1 (0%)	37	72
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1202 (90%)	123 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1204 (90%)	129 (10%)	5 (0%)	30	68
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	472 (96%)	15 (3%)	3 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	NG	150/181 (83%)	136 (91%)	10 (7%)	4 (3%)	4	26
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9586/10235 (94%)	8668 (90%)	882 (9%)	36 (0%)	32	68

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	r	54	VAL
48	x	25	LYS
58	B1	121	PRO
61	NA	187	ARG
61	NA	188	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/62 (95%)	58 (98%)	1 (2%)	56	72
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	47	65
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	60
5	E	51/52 (98%)	49 (96%)	2 (4%)	27	49
6	F	34/34 (100%)	30 (88%)	4 (12%)	4	17
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	54
8	H	170/190 (90%)	167 (98%)	3 (2%)	54	71
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	64
10	J	119/126 (94%)	117 (98%)	2 (2%)	56	72
11	K	87/116 (75%)	82 (94%)	5 (6%)	17	39
12	L	124/147 (84%)	124 (100%)	0	100	100
13	M	104/105 (99%)	103 (99%)	1 (1%)	73	81
14	N	105/107 (98%)	98 (93%)	7 (7%)	13	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	86/90 (96%)	78 (91%)	8 (9%)	7	23
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	53
17	Q	103/104 (99%)	98 (95%)	5 (5%)	21	42
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	83 (100%)	0	100	100
20	T	76/77 (99%)	73 (96%)	3 (4%)	27	49
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	72 (97%)	2 (3%)	40	59
23	W	56/65 (86%)	52 (93%)	4 (7%)	12	32
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	64 (98%)	1 (2%)	60	75
26	Z	55/61 (90%)	47 (86%)	8 (14%)	2	13
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	54	71
30	e	148/150 (99%)	145 (98%)	3 (2%)	50	68
31	f	137/138 (99%)	135 (98%)	2 (2%)	60	75
32	g	41/114 (36%)	38 (93%)	3 (7%)	11	31
33	i	109/110 (99%)	108 (99%)	1 (1%)	75	83
34	j	116/116 (100%)	116 (100%)	0	100	100
35	k	103/104 (99%)	103 (100%)	0	100	100
36	l	102/103 (99%)	101 (99%)	1 (1%)	73	81
37	m	109/109 (100%)	103 (94%)	6 (6%)	18	40
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	81
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	99 (100%)	0	100	100
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
42	r	84/84 (100%)	82 (98%)	2 (2%)	44	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	70	80
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	25	47
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	38
57	A2	186/286 (65%)	185 (100%)	1 (0%)	86	89
58	B1	1110/1168 (95%)	1017 (92%)	93 (8%)	9	28
59	B2	1150/1157 (99%)	1117 (97%)	33 (3%)	37	57
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7132 (97%)	249 (3%)	34	53

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

Mol	Chain	Res	Type
57	A1	22	THR
59	B2	516	ASP
58	B1	96	LYS
59	B2	483	ASP
59	B2	899	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
59	B2	330	HIS
59	B2	580	GLN
27	b	142	ASN
27	b	89	ASN
59	B2	762	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%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1542 (99%)	253 (16%)	4 (0%)
54	4	34/56 (60%)	17 (50%)	2 (5%)
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	4820/4852 (99%)	764 (15%)	32 (0%)

5 of 764 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 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	0.08	0
65	5OH	h	6	65	8,12,13	0.76	0	3,16,18	1.52	1 (33%)
65	KBE	h	1	65	8,8,9	0.60	0	7,8,10	1.20	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	UAL	h	5	65	7,8,9	2.29	3 (42%)	5,9,11	2.92	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	DPP	h	2	65	-	0/2/4/6	-
65	5OH	h	6	65	-	0/2/18/20	0/1/1/1
65	KBE	h	1	65	-	0/7/7/8	-
65	UAL	h	5	65	-	0/3/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	5	UAL	C1-N1	-4.85	1.32	1.40
65	h	5	UAL	C-CA	-2.88	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	-5.30	115.59	125.60
65	h	5	UAL	O-C-CA	-3.24	121.27	125.39
65	h	6	5OH	CR-CB-CA	-2.37	110.06	112.61
65	h	1	KBE	CB-CA-C	-2.07	109.20	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

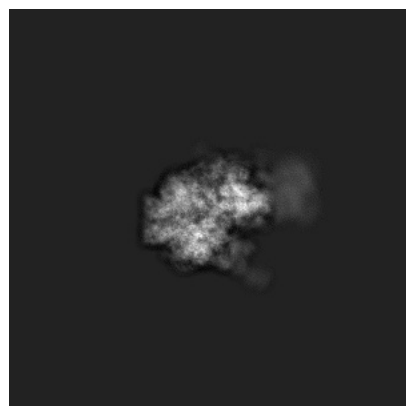
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39169. These allow visual inspection of the internal detail of the map and identification of artifacts.

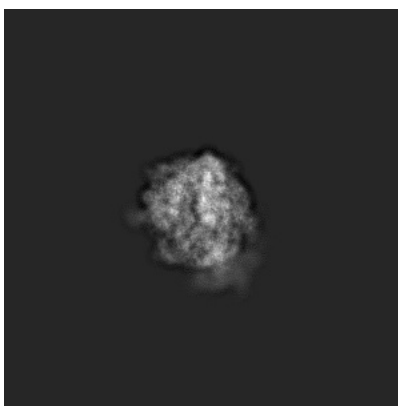
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

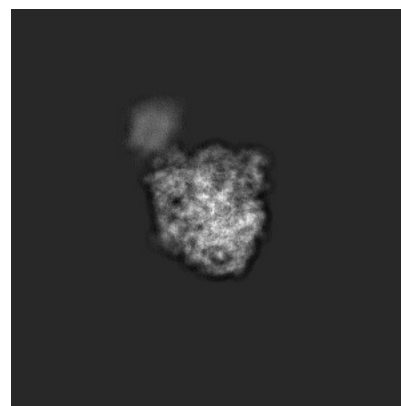
6.1.1 Primary map



X

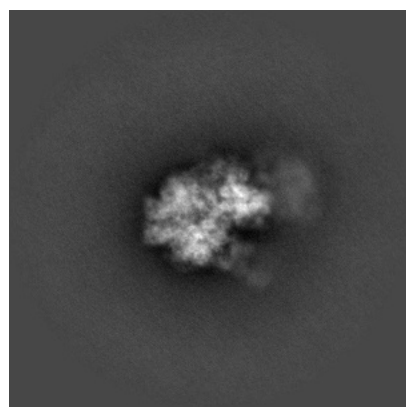


Y

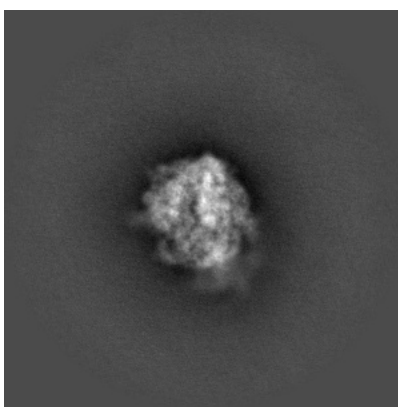


Z

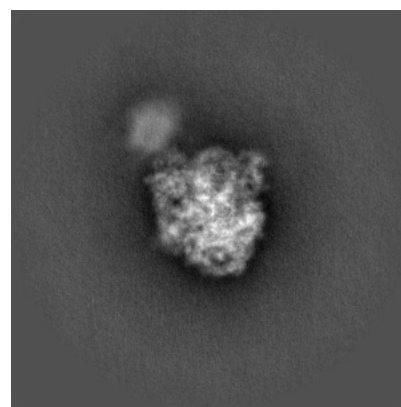
6.1.2 Raw map



X



Y

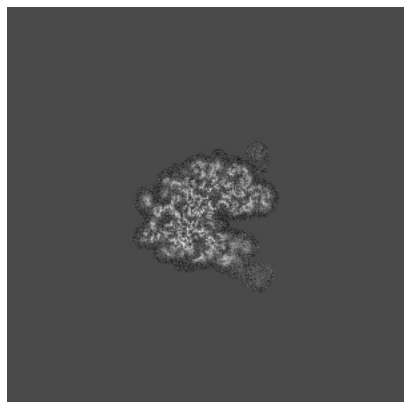


Z

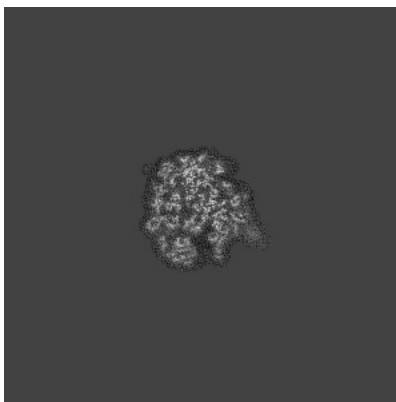
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

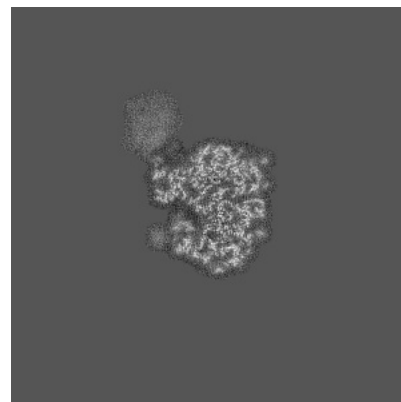
6.2.1 Primary map



X Index: 240

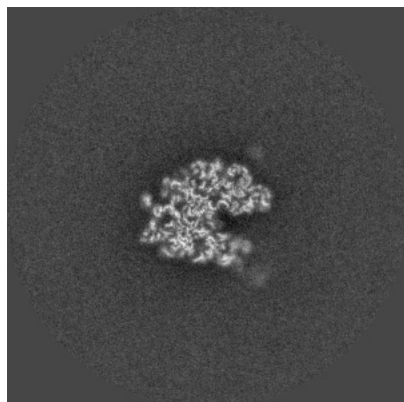


Y Index: 240

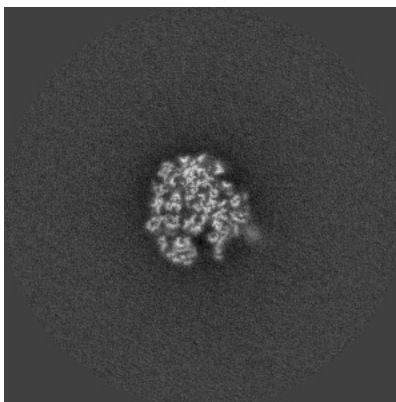


Z Index: 240

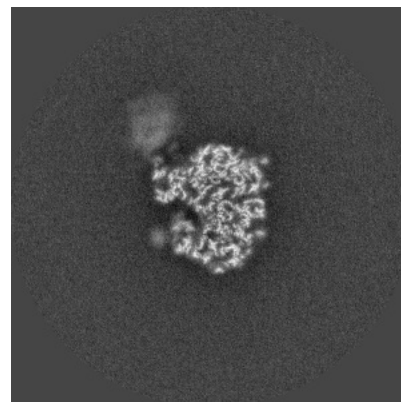
6.2.2 Raw map



X Index: 240



Y Index: 240

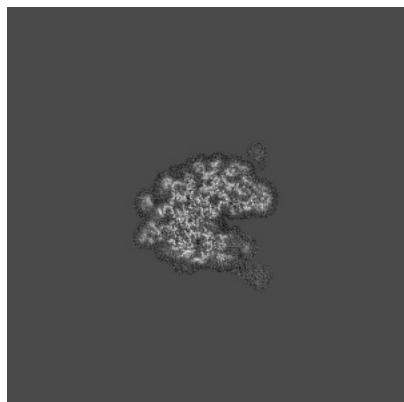


Z Index: 240

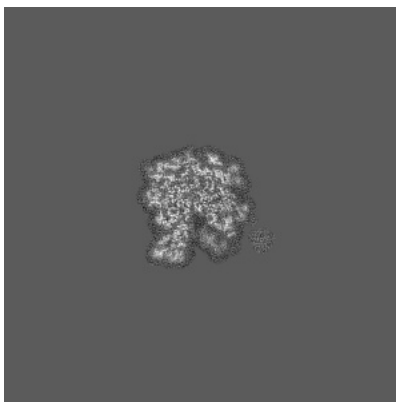
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

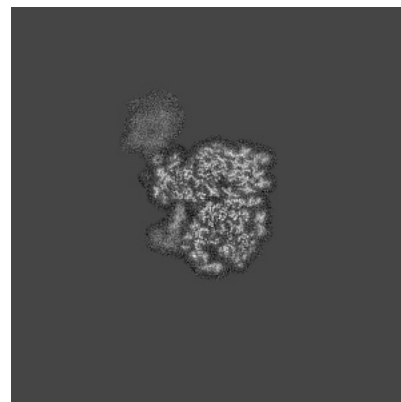
6.3.1 Primary map



X Index: 243

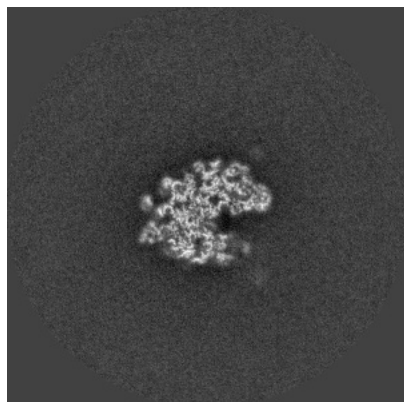


Y Index: 223

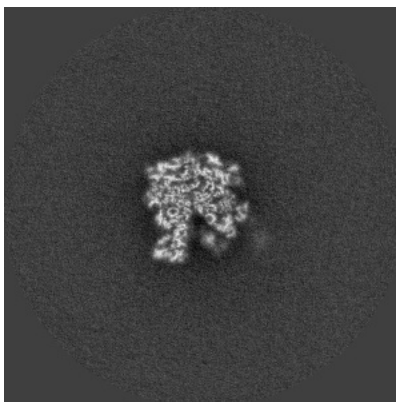


Z Index: 246

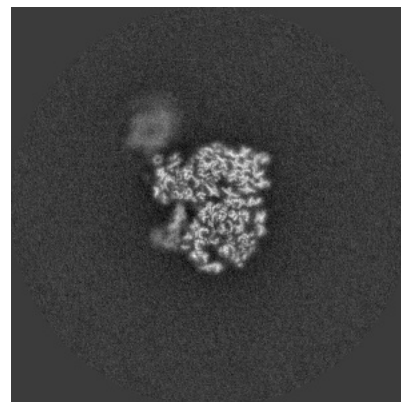
6.3.2 Raw map



X Index: 243



Y Index: 224

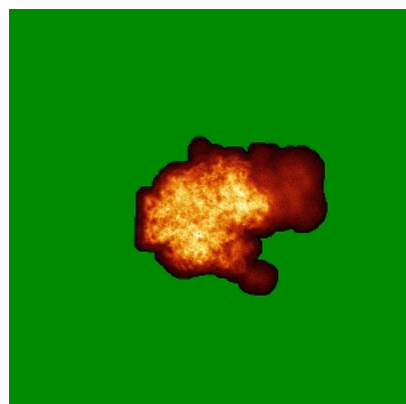


Z Index: 246

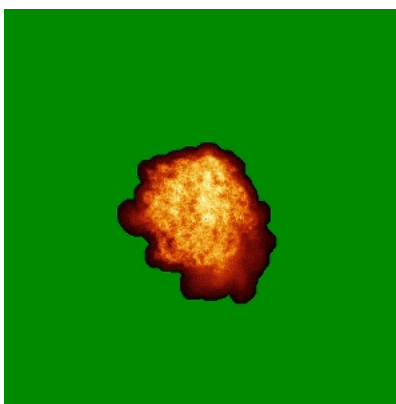
The images above show the largest variance slices of the map in three orthogonal directions.

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

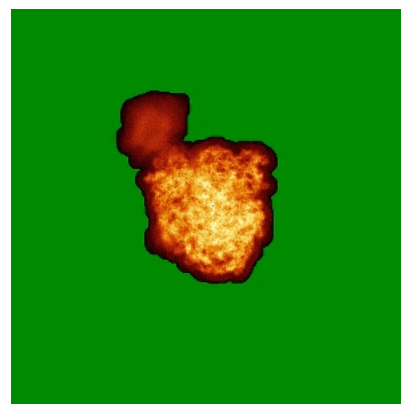
6.4.1 Primary map



X

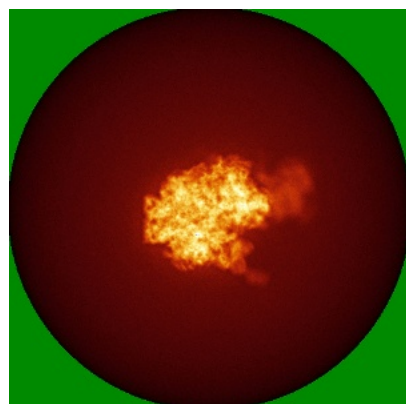


Y

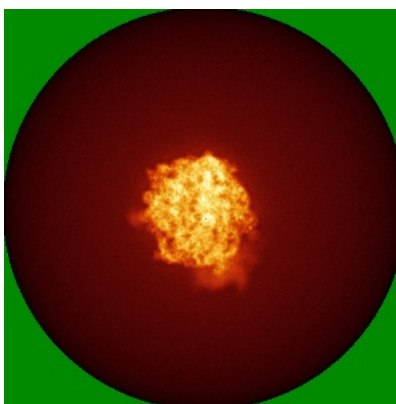


Z

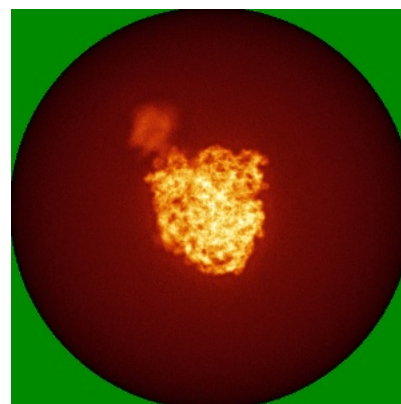
6.4.2 Raw map



X



Y

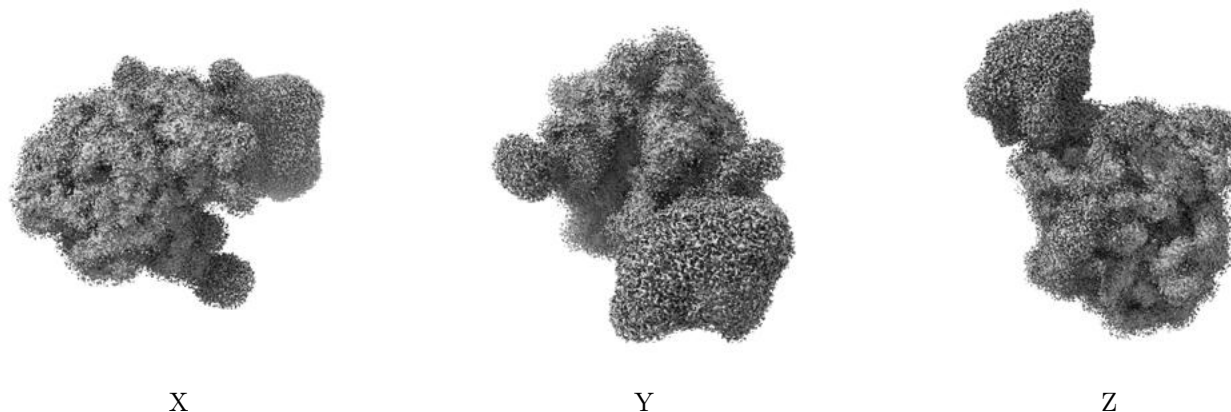


Z

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.

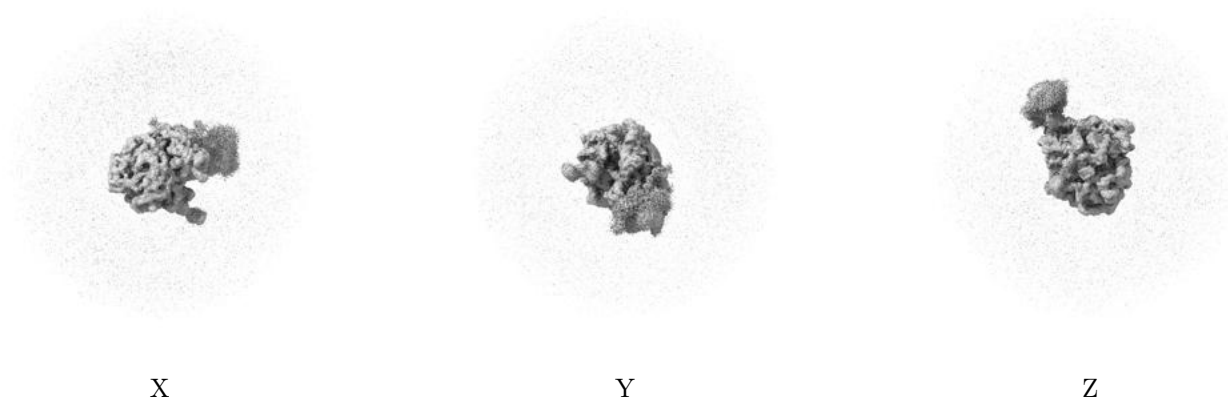
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

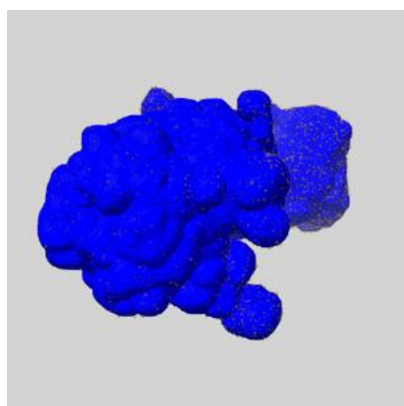
6.6 Mask visualisation [i](#)

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

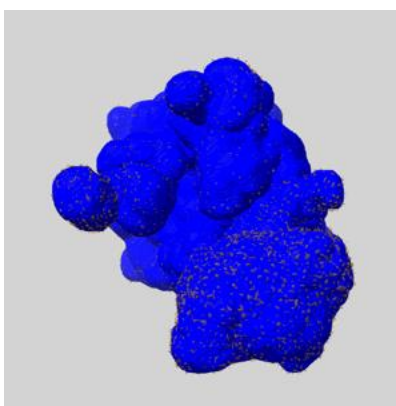
A mask typically either:

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

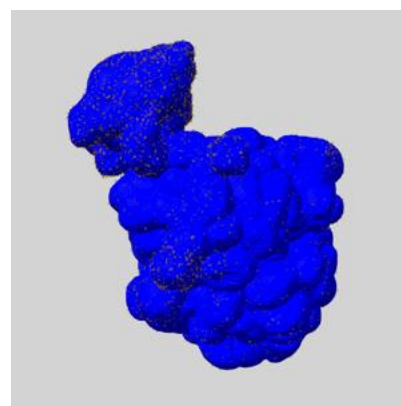
6.6.1 emd_39169_msk_1.map [i](#)



X



Y

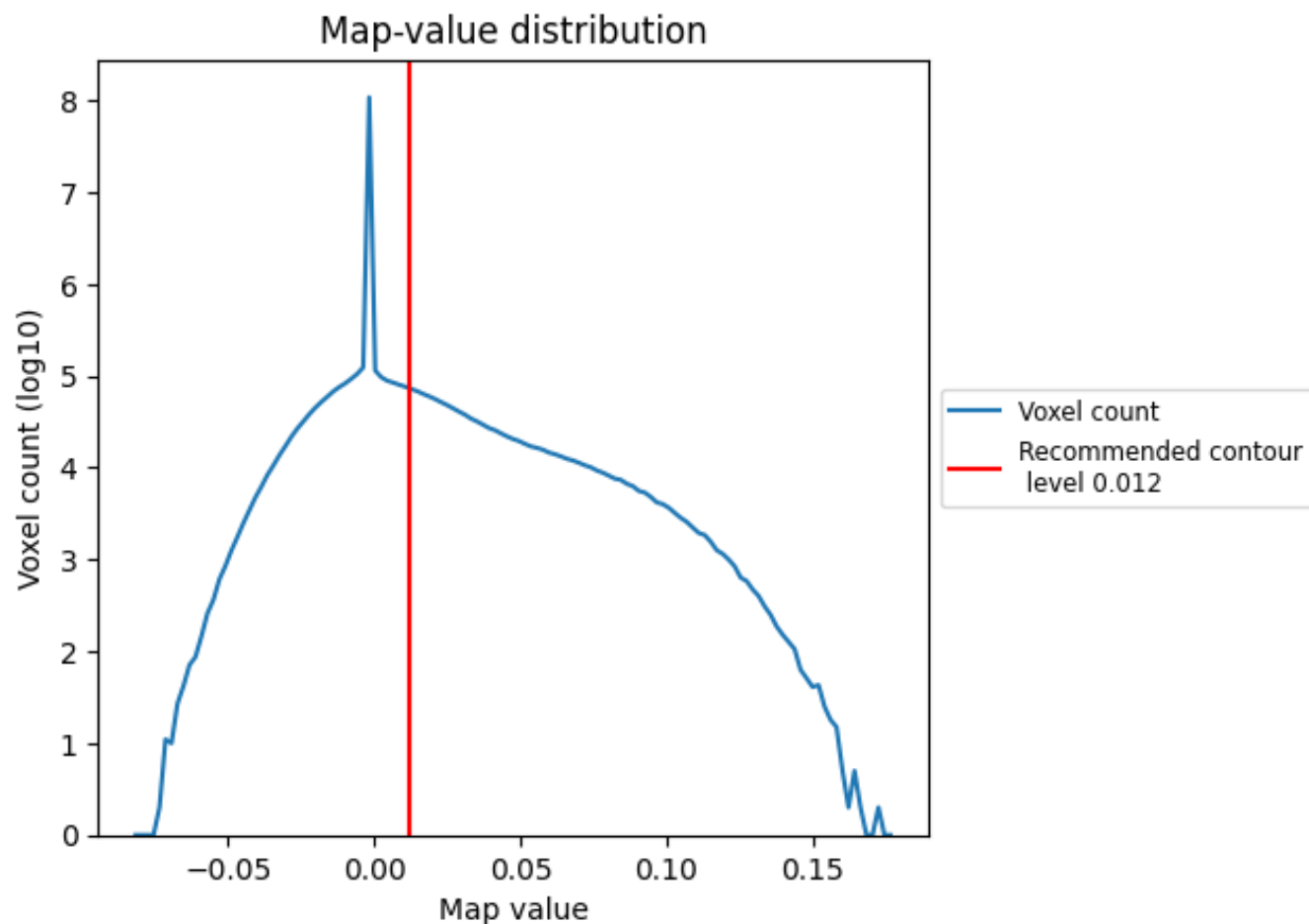


Z

7 Map analysis [i](#)

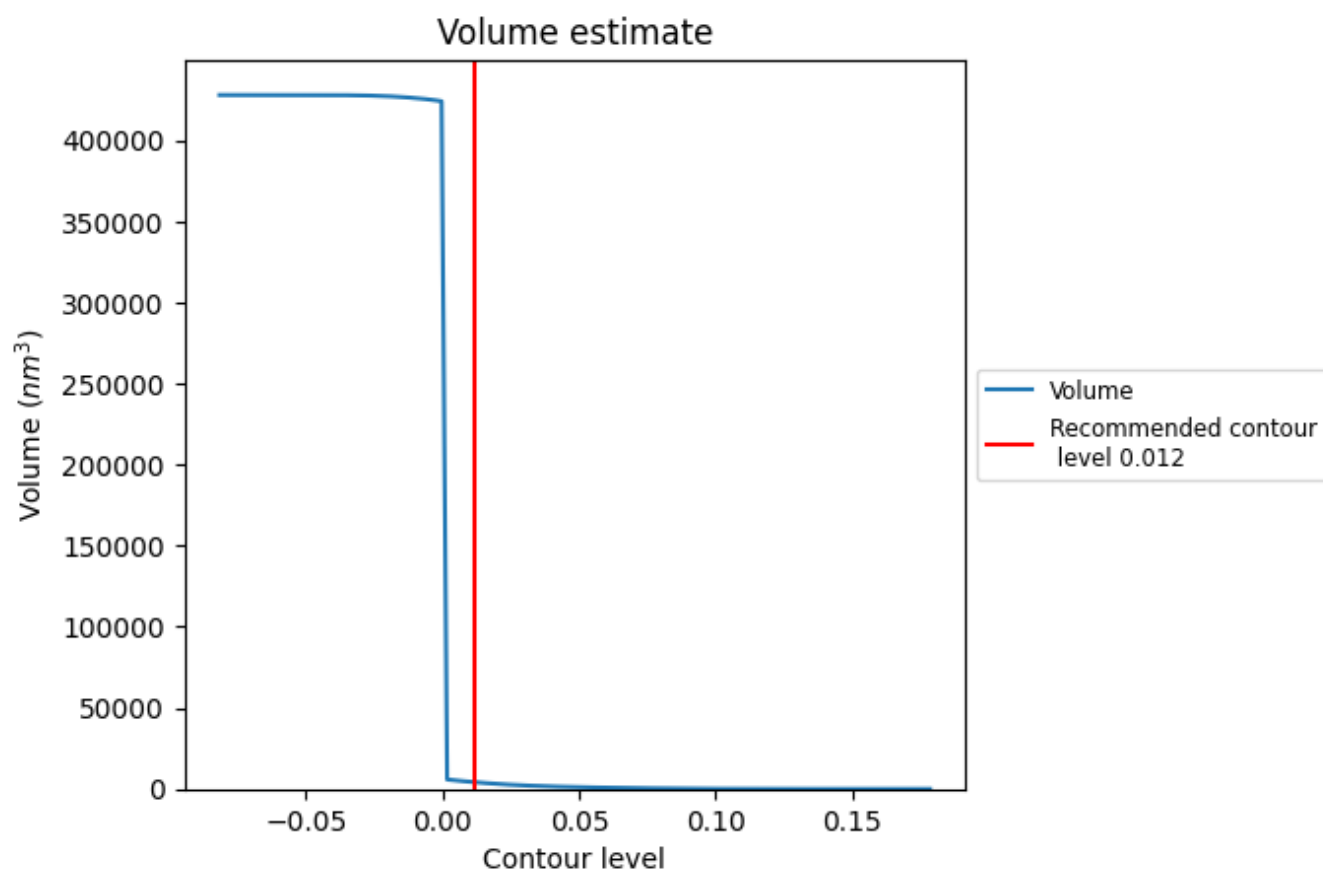
This section contains the results of statistical analysis of the map.

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.

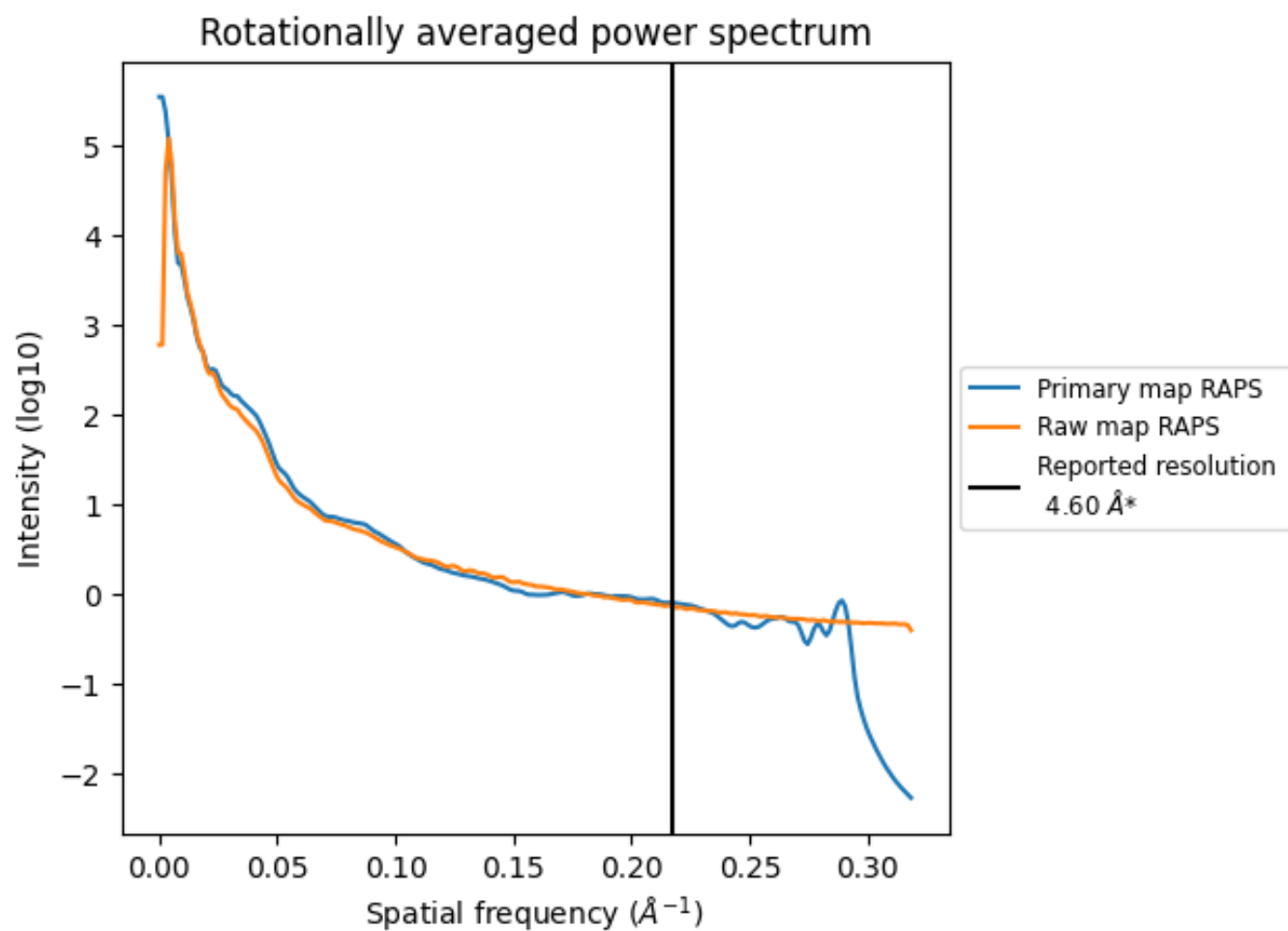
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4147 nm³; this corresponds to an approximate mass of 3746 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

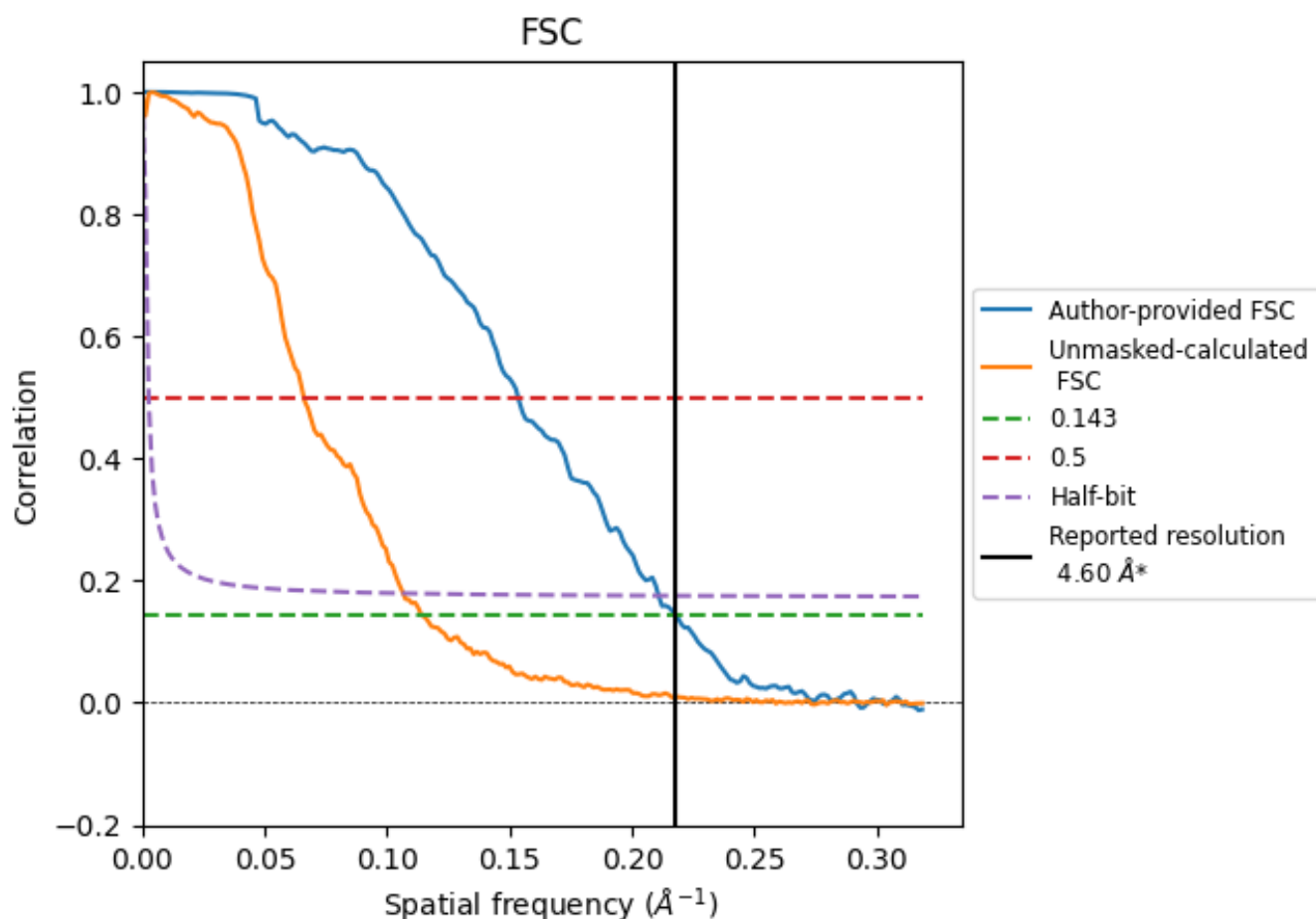


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

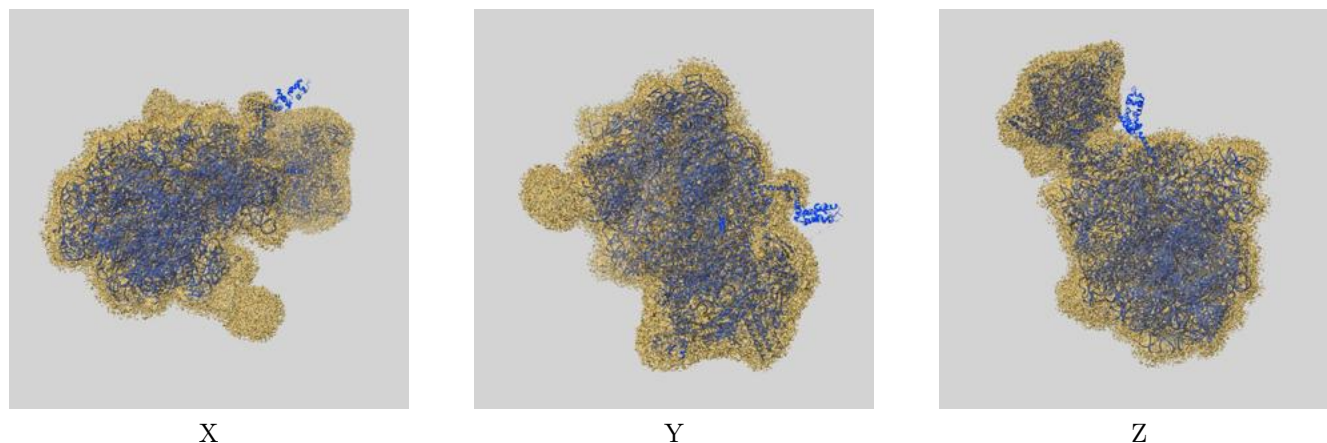
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	6.51	4.74
Unmasked-calculated*	8.76	15.15	9.39

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

9 Map-model fit [i](#)

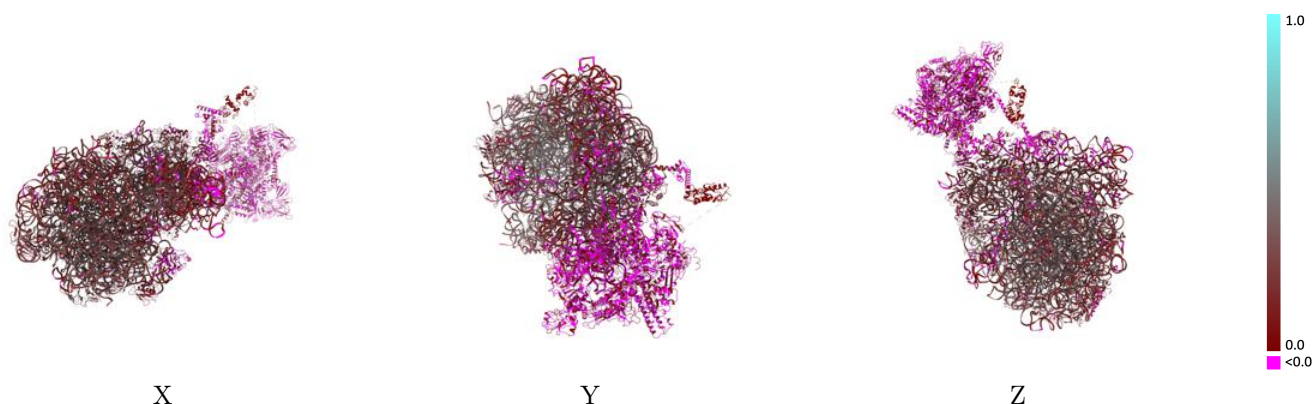
This section contains information regarding the fit between EMDB map EMD-39169 and PDB model 8YDF. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



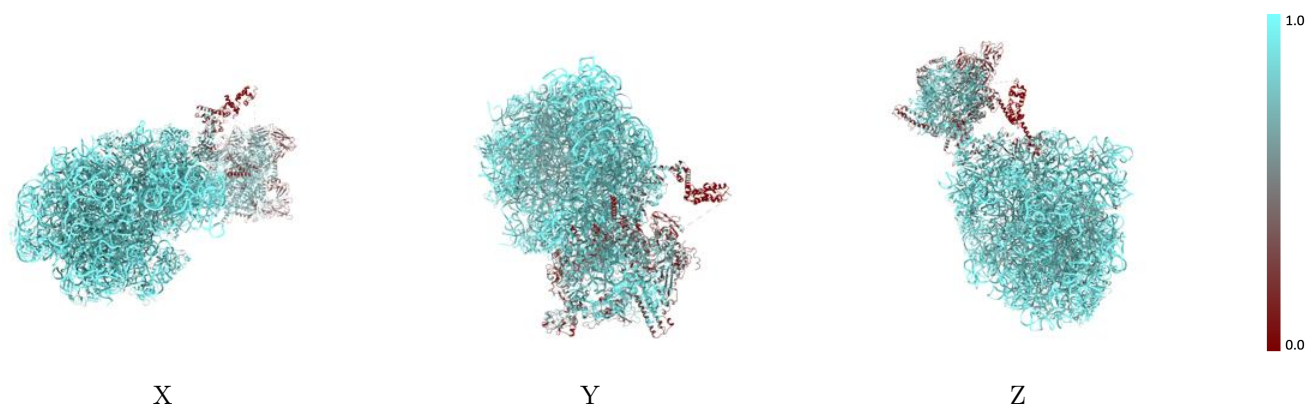
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



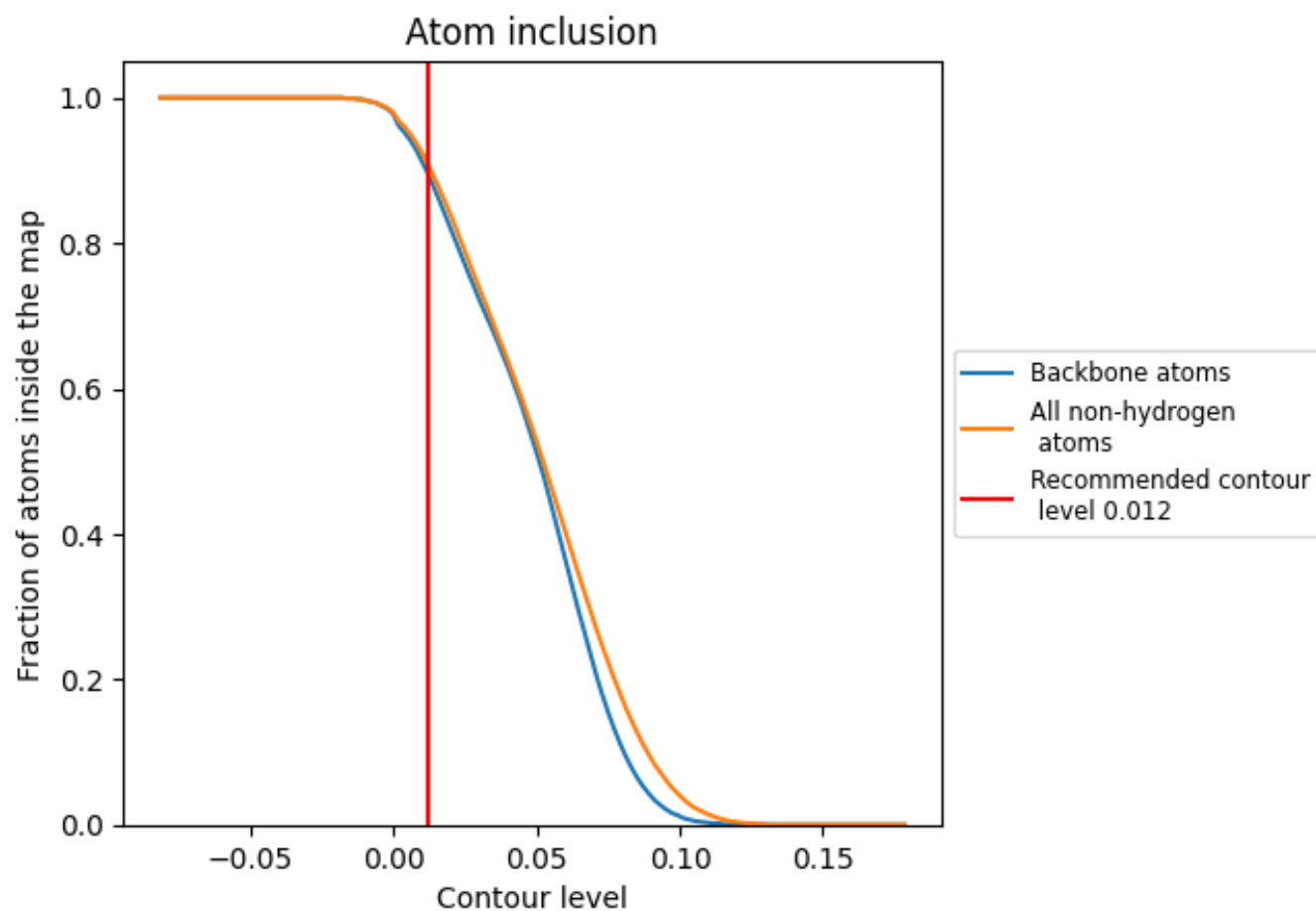
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.2110
1	 0.9890	 0.2930
2	 0.9930	 0.2710
3	 0.9840	 0.2400
4	 0.7740	 0.0340
5	 0.9130	 0.1040
6	 0.9880	 0.3000
7	 0.7790	 0.0520
8	 0.8130	 -0.0050
9	 0.8300	 0.0090
A	 0.8920	 0.1740
A1	 0.3840	 0.0040
A2	 0.4300	 -0.0030
B	 0.9510	 0.2980
B1	 0.6240	 0.0030
B2	 0.7360	 0.0050
C	 0.9150	 0.2680
D	 0.9240	 0.3050
E	 0.9590	 0.3610
F	 0.9350	 0.2540
G	 0.9190	 0.1720
H	 0.9130	 0.2450
I	 0.8410	 0.0670
J	 0.9300	 0.2740
K	 0.9090	 0.1550
L	 0.9080	 0.1780
M	 0.9280	 0.2450
N	 0.9550	 0.1830
NA	 0.4790	 0.0200
NG	 0.7110	 0.0220
O	 0.9110	 0.1580
P	 0.9370	 0.1970
Q	 0.8900	 0.1870
R	 0.9310	 0.1930
S	 0.9520	 0.1930



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Chain	Atom inclusion	Q-score
T	 0.9490	 0.2410
U	 0.8600	 0.1250
V	 0.8810	 0.1110
W	 0.9380	 0.2100
W0	 0.2620	 -0.0060
X	 0.9420	 0.1920
Y	 0.9110	 0.1620
Z	 0.8320	 0.1350
b	 0.9290	 0.3070
c	 0.9430	 0.2610
d	 0.9580	 0.2550
e	 0.9480	 0.2340
f	 0.9550	 0.1790
g	 0.9360	 0.1830
h	 0.8540	 0.2030
i	 0.8420	 0.0110
j	 0.9490	 0.2870
k	 0.8840	 0.2450
l	 0.9560	 0.2830
m	 0.9430	 0.3280
n	 0.9590	 0.2430
o	 0.9780	 0.2200
p	 0.9010	 0.1870
q	 0.9670	 0.3360
r	 0.9660	 0.3010
s	 0.9220	 0.2510
t	 0.9060	 0.1790
u	 0.9540	 0.2000
v	 0.9570	 0.2360
w	 0.9540	 0.3110
x	 0.9320	 0.2850
y	 0.9170	 0.1220
z	 0.9570	 0.3170