



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:19 PM UTC

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:

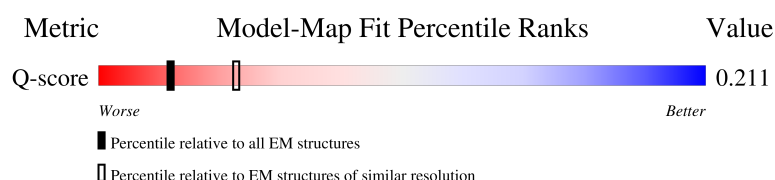
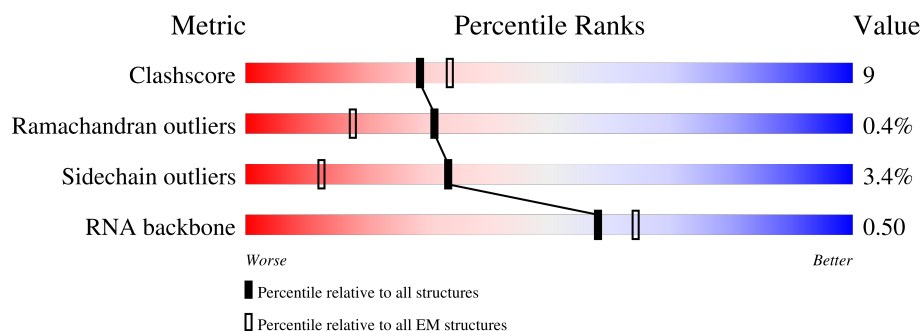
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 Å.

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



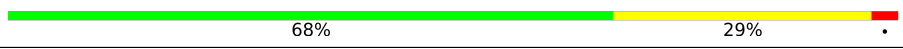
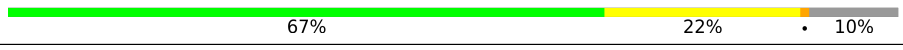
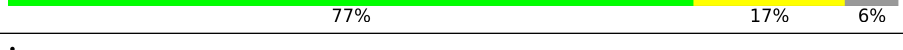
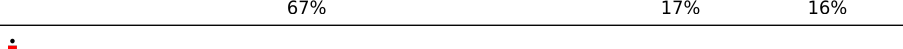
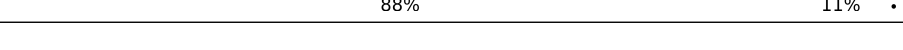
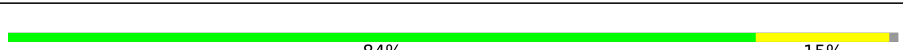
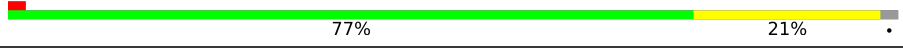
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

Mol	Chain	Length	Quality of chain
1	A	70	 6% 80% 14% 6%
2	B	57	 79% 18% . .
3	C	55	 80% 11% 9%

Continued on next page...

Continued from previous page...

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

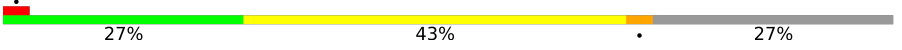
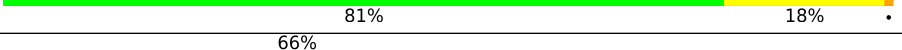
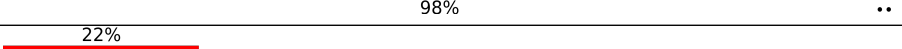
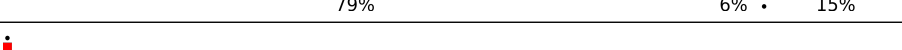
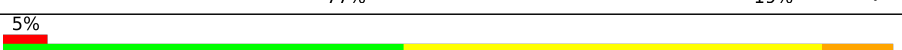
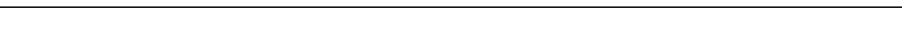
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	4	56	
55	8	37	
56	9	37	
57	A1	329	
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
64	7	77	
65	h	6	

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		

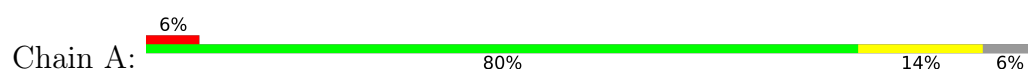
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

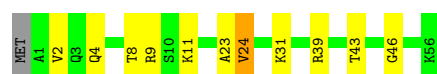
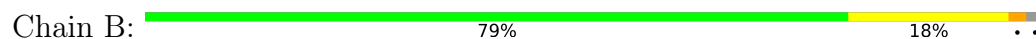
3 Residue-property plots [i](#)

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.

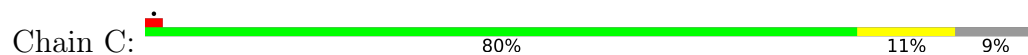
- Molecule 1: 50S ribosomal protein L31



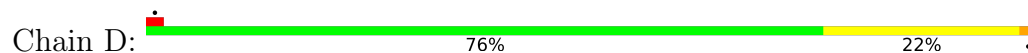
- Molecule 2: 50S ribosomal protein L32



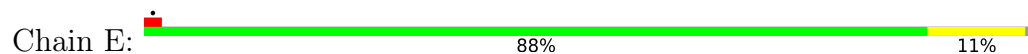
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34

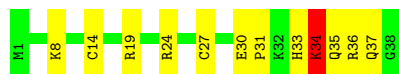


- Molecule 5: 50S ribosomal protein L35



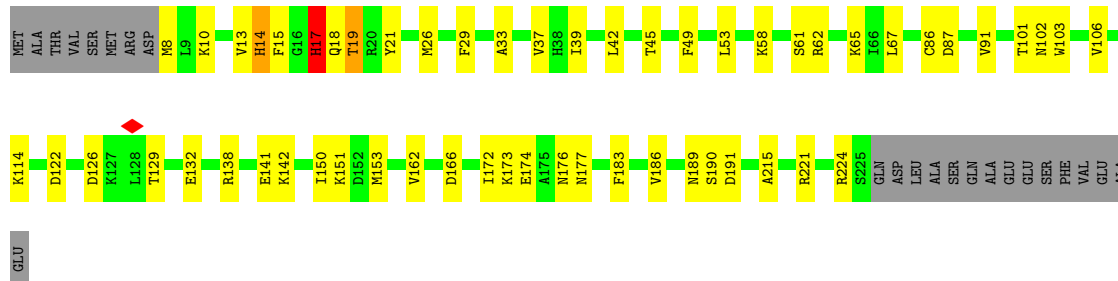
- Molecule 6: 50S ribosomal protein L36

Chain F:  68% 29%



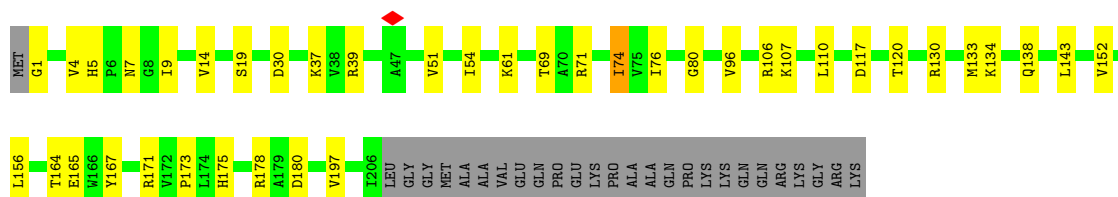
- Molecule 7: 30S ribosomal protein S2

Chain G:  67% 22% 10%



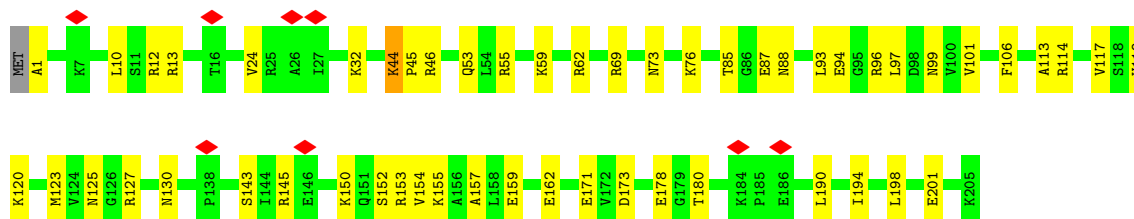
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% 12%



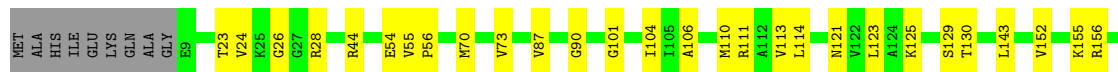
- Molecule 9: 30S ribosomal protein S4

Chain I:  74% 25%



- Molecule 10: 30S ribosomal protein S5

Chain J:  77% 17% 6%

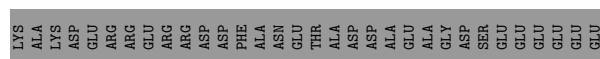


Q165
LYS

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

Chain K:  50% 23% 26%

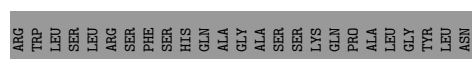




- Molecule 12: 30S ribosomal protein S7

Chain L:  67% 17% 16%





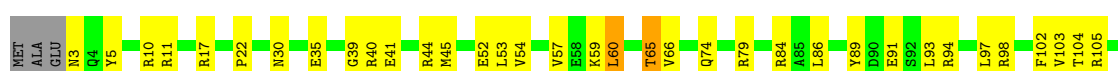
- Molecule 13: 30S ribosomal protein S8

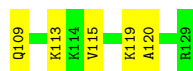
Chain M:  88% 11%



- Molecule 14: 30S ribosomal protein S9

Chain N:  67% 29%





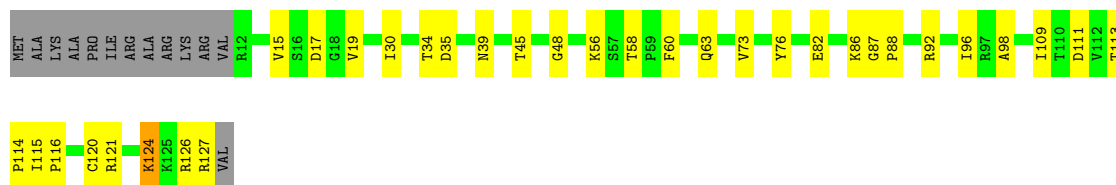
- Molecule 15: 30S ribosomal protein S10

Chain O:  72% 18% 5% 5%



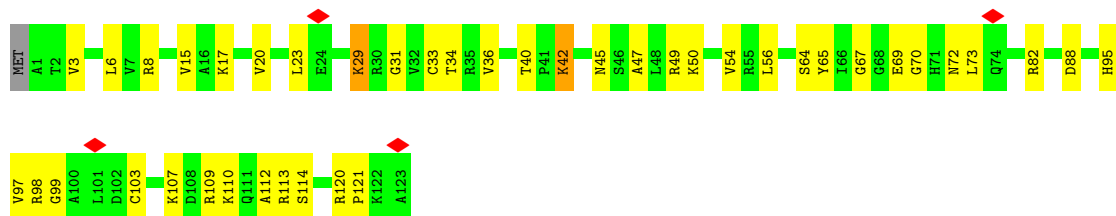
- Molecule 16: 30S ribosomal protein S11

Chain P:  64% 25% 10%



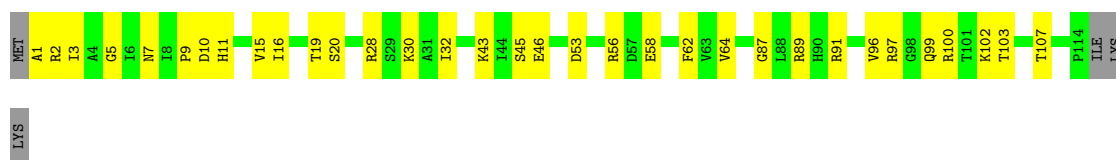
- Molecule 17: 30S ribosomal protein S12

Chain Q:  65% 32% 2%



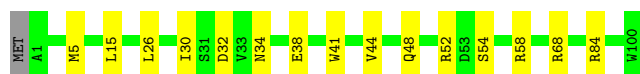
- Molecule 18: 30S ribosomal protein S13

Chain R:  69% 28% 2%



- Molecule 19: 30S ribosomal protein S14

Chain S:  84% 15% 1%



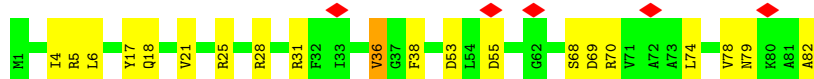
- Molecule 20: 30S ribosomal protein S15

Chain T:  85% 13% 2%



- Molecule 21: 30S ribosomal protein S16

Chain U:  6% 76% 18%



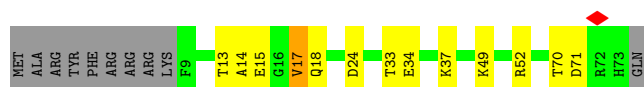
- Molecule 22: 30S ribosomal protein S17

Chain V:  76% 19% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  69% 16% 13%



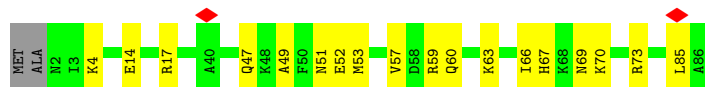
- Molecule 24: 30S ribosomal protein S19

Chain X:  74% 12% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  77% 21% 2%



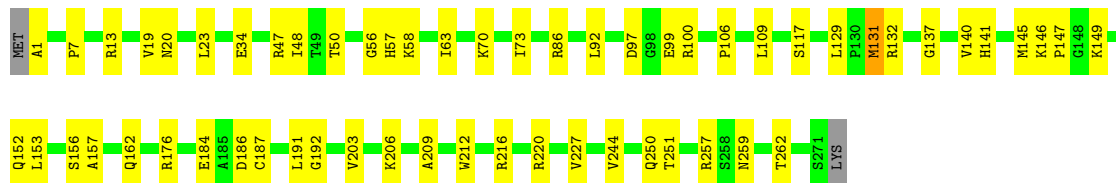
- Molecule 26: 30S ribosomal protein S21

Chain Z:  58% 30% 8%



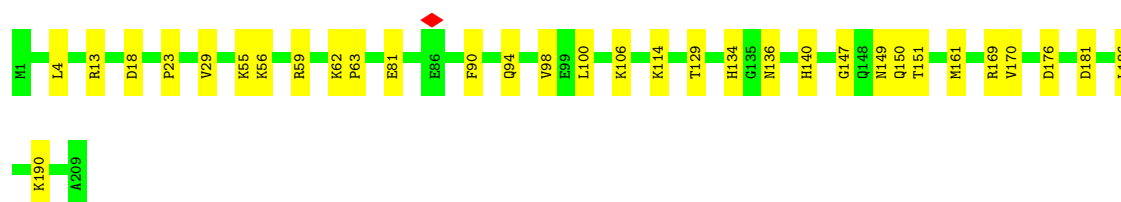
- Molecule 27: 50S ribosomal protein L2

Chain b:  78% 21% 1%



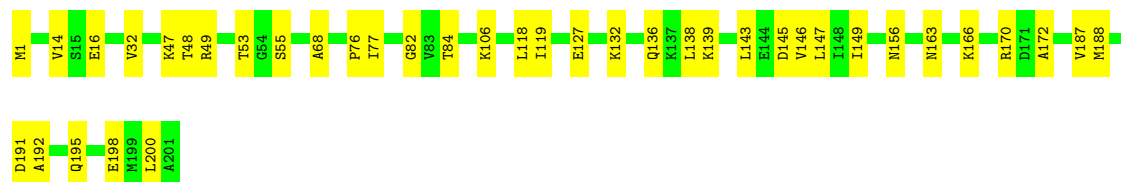
- Molecule 28: 50S ribosomal protein L3

Chain c:  85% 15% 0%



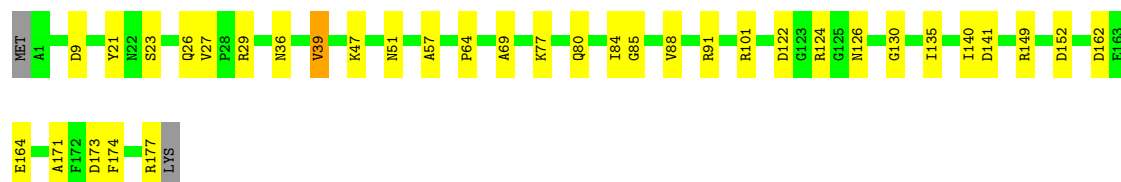
- Molecule 29: 50S ribosomal protein L4

Chain d: 81% 19%



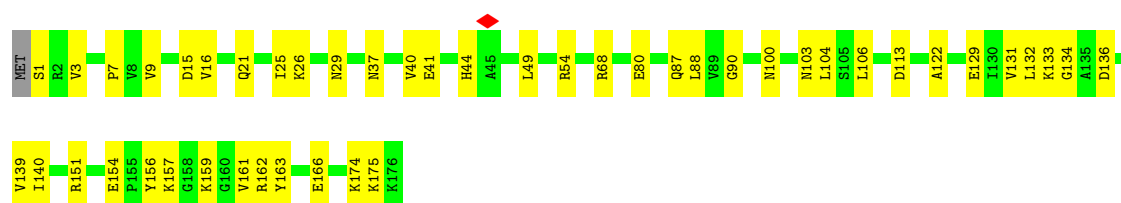
- Molecule 30: 50S ribosomal protein L5

Chain e: 79% 19% ..



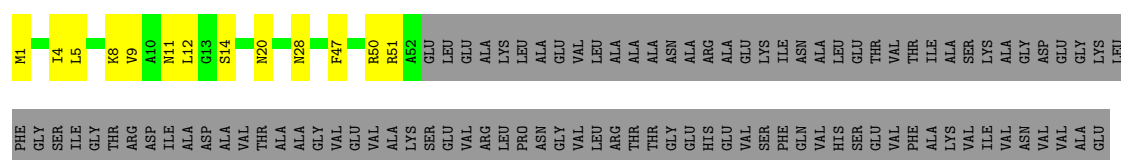
- Molecule 31: 50S ribosomal protein L6

Chain f: 73% 26% .

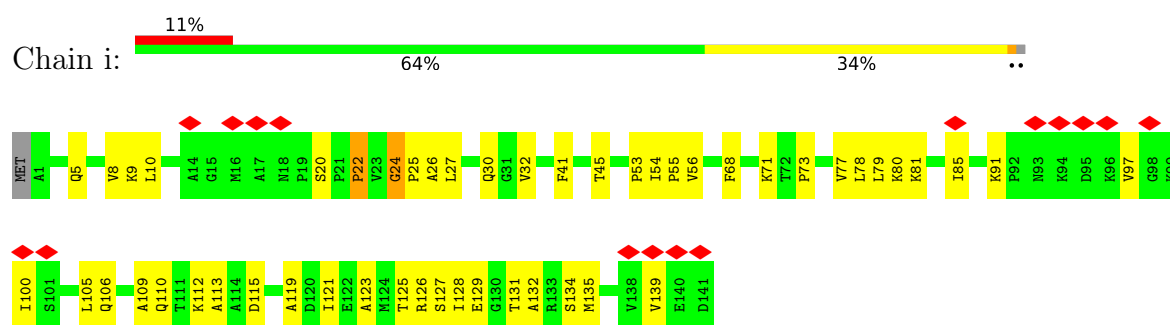


- Molecule 32: 50S ribosomal protein L9

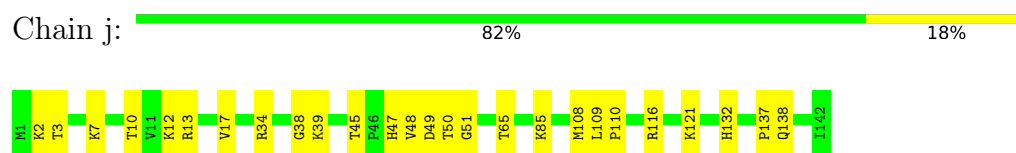
Chain g: 26% 9% 65%



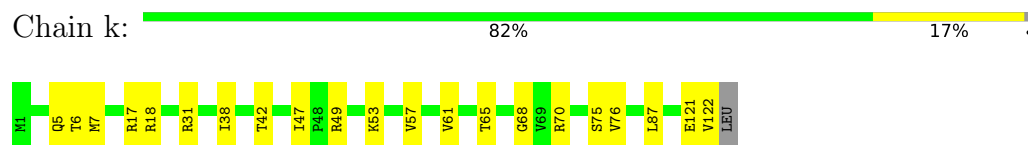
- Molecule 33: 50S ribosomal protein L11



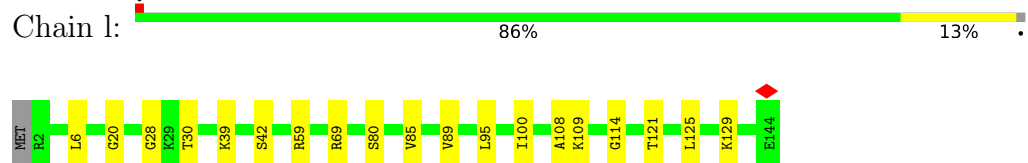
- Molecule 34: 50S ribosomal protein L13



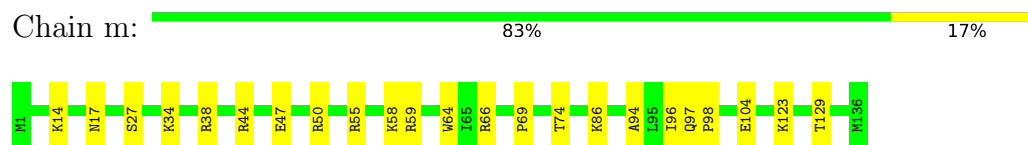
- Molecule 35: 50S ribosomal protein L14



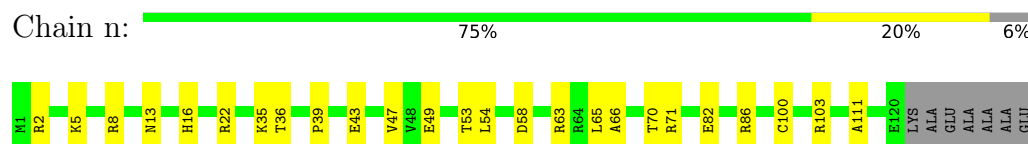
- Molecule 36: 50S ribosomal protein L15



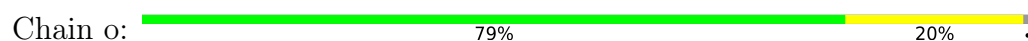
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17

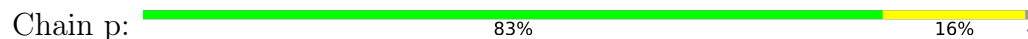


- Molecule 39: 50S ribosomal protein L18

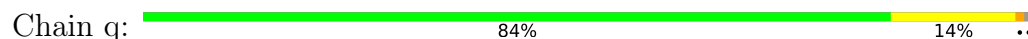




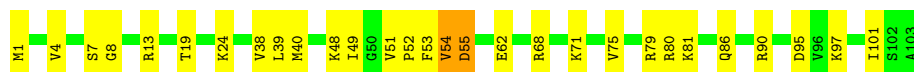
- Molecule 40: 50S ribosomal protein L19



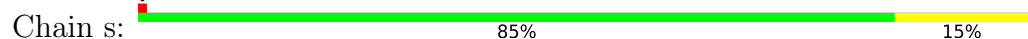
- Molecule 41: 50S ribosomal protein L20



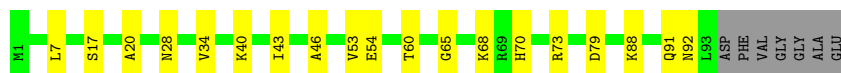
- Molecule 42: 50S ribosomal protein L21



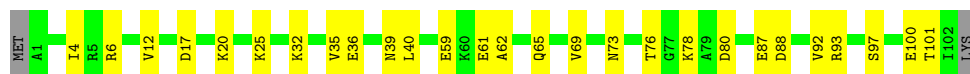
- Molecule 43: 50S ribosomal protein L22



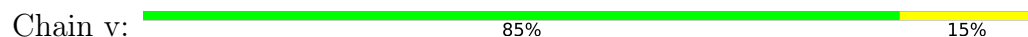
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24



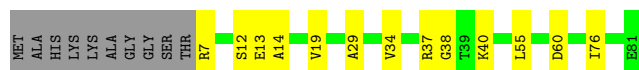
- Molecule 46: 50S ribosomal protein L25





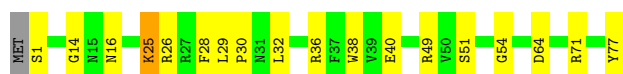
- Molecule 47: 50S ribosomal protein L27

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%



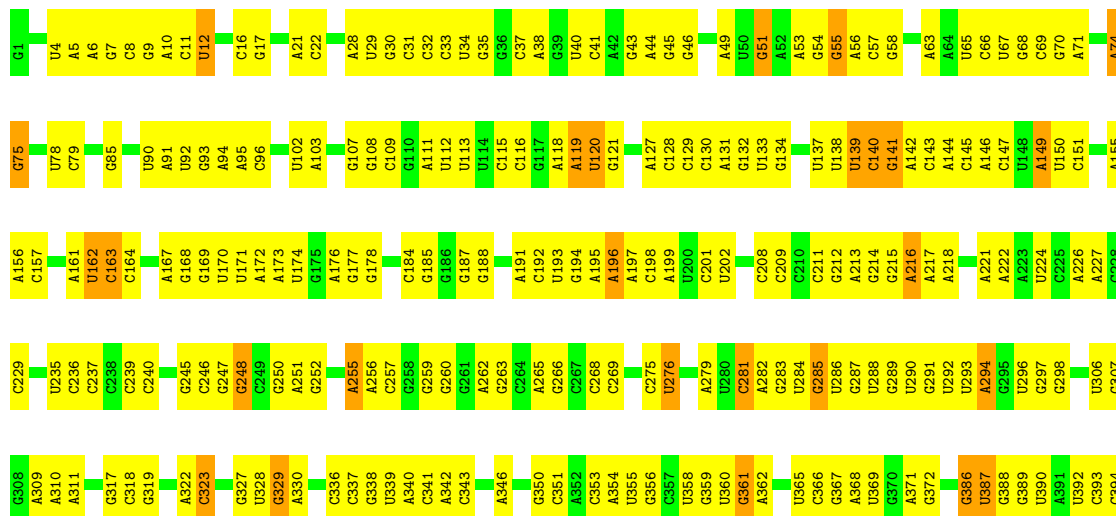
- Molecule 50: 50S ribosomal protein L30

Chain z: 76% 22% .



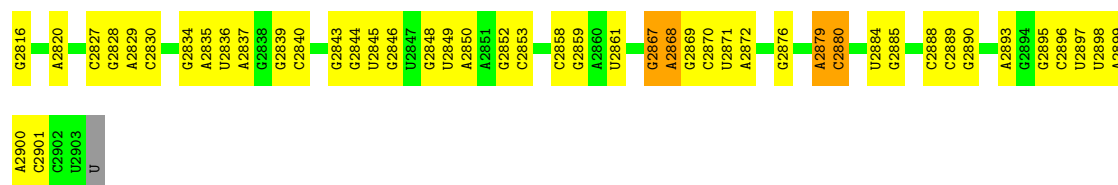
- Molecule 51: 23S rRNA

Chain 1: 43% 51% 6%



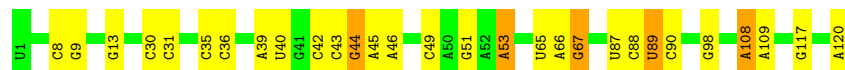


A2741	G2576	U2489	G2396	G2315	G2237	A2170	G2102	A2013	U1917	G1845	C1761	A1679	C1582
G2742	A2577	G2490	U2402	G2316	G2238	A2171	C2103	A2014	A1918	G1846	A1762	U1680	A1583
U2743	C2578	U2491	C2403	U2321	G2239	A2172	C2104	U2016	A1919	A1847	G1763	G1681	G1588
G2744	U2580	U2492	U2404	U2322	A2241	C2174	U2106	G2020	G1920	A1848	U1765	G1695	G1589
G2747	G2581	C2496	G2405	G2325	G2242	U2180	G2107	A2020	G1922	U1851	G1766	G1696	A1590
U2748	G2582	A2497	A2406	C2326	U2243	U2181	G2110	C2021	U1923	U1852	G1772	G1697	A1591
G2749	G2583	C2498	A2407	A2327	A2247	U2182	U2111	U2022	C1924	A1853	G1773	A1698	C1592
U2750	U2584	U2499	U2411	A2328	C2248	A2183	G2112	G2024	A1927	A1854	A1772	G1702	U1594
G2751	U2585	G2502	A2412	G2330	U2249	U2184	G2113	G2025	A1928	U1855	C1774	G1703	C1595
G2752	U2586	G2503	C2420	A2333	G2250	A2185	G2114	U2026	G1929	U1856	G1775	U1758	A1596
U2753	C2593	U2504	G2421	A2334	U2257	G2186	G2115	G2027	U1931	G1857	G1776	G1710	A1597
C2755	G2595	C2507	G2422	U2335	U2258	U2187	U2118	A2030	G1935	A1858	A1780	A1711	A1598
U2756	A2598	G2509	U2423	A2336	U2259	U2188	A2119	A2031	G1936	G1863	A1781	G1715	C1600
A2758	G2599	C2510	C2424	G2337	C2260	U2189	U2122	G2032	A1937	U1864	U1782	U1716	U1602
G2759	A2600	U2511	A2425	C2338	A2267	A2191	G2123	A2033	A1938	A1865	A1783	A1717	A1603
C2760	C2601	G2512	A2426	C2339	A2268	U2192	G2124	U2034	U1939	A1866	A1784	G1718	G1604
A2761	A2602	G2513	G2427	A2340	A2269	G2193	G2125	G2035	C1942	G1867	A1785	G1719	C1605
C2762	U2609	A2514	G2428	G2345	G2271	U2194	G2126	A2037	C1943	G1868	A1786	U1720	C1606
G2763	C2610	A2515	A2430	A2346	C2272	U2195	G2127	G2038	U1943	G1870	A1787	G1721	C1607
A2765	G2611	G2516	U2431	A2347	C2273	U2196	G2128	U2039	G1948	A1871	C1788	A1722	A1608
U2768	U2612	G2517	G2432	G2348	A2278	U2197	C2129	C2043	C1949	A1872	A1789	G1723	A1614
G2769	C2613	C2518	A2433	G2349	A2279	A2198	U2130	G2044	A1952	G1873	C1790	U1725	C1615
U2770	A2614	G2519	U2434	C2350	G2280	A2199	U2131	C2047	A1953	A1794	A1794	G1726	A1616
C2771	U2615	U2520	A2435	G2351	G2281	C2200	G2133	G2048	G1954	C1795	C1796	C1727	C1625
A2772	G2616	A2521	G2436	A2352	G2282	U2202	A2134	G2049	U1955	G1878	G1797	U1729	C1626
U2773	U2617	G2522	G2437	G2360	C2283	U2203	U2137	C2050	U1956	C1879	U1798	C1730	U1629
G2774	C2618	A2523	C2440	G2361	A2284	A2204	U2138	A2051	U1963	U1882	U1799	G1731	A1634
U2775	G2619	U2524	U2441	C2362	G2285	A2205	G2139	A2052	G1964	U1883	C1800	G1732	C1642
G2776	C2620	G2525	G2442	G2363	A2286	C2208	G2141	A2053	G1965	U1884	A1801	G1733	G1643
U2777	G2621	U2526	A2443	C2364	A2287	G2209	G2142	A2054	A1966	A1885	A1802	G1734	C1644
A2778	U2622	G2527	G2444	G2365	G2288	U2210	C2143	C2055	C1967	U1886	G1807	U1735	G1645
U2779	A2623	A2528	A2445	G2366	G2289	A2211	C2144	G2056	G1968	C1887	U1736	U1737	G1646
G2780	G2624	U2529	G2446	C2367	G2290	U2212	C2145	A2060	A1969	G1888	A1808	G1738	U1647
U2781	U2625	G2530	U2447	G2368	U2291	A2213	A2147	G2061	U1970	A1889	A1809	U1740	U1648
C2782	C2626	U2531	C2448	G2371	U2292	C2214	G2148	G2069	G1971	A1890	G1812	C1741	G1651
G2783	G2627	G2532	G2449	U2372	G2293	C2215	U2149	C2073	U1972	C1893	G1813	U1742	U1662
U2784	C2628	U2533	A2450	G2373	G2294	C2216	C2150	U2074	A1978	C1894	C1816	G1743	G1663
A2785	U2629	A2534	G2451	G2374	U2295	G2217	U2151	U2085	G1983	A1901	G1817	U1745	G1666
U2786	G2630	G2535	U2452	C2375	A2297	G2218	G2152	U2086	G1984	C1902	U1818	A1746	G1667
C2787	C2631	U2536	C2453	G2376	U2298	G2219	C2153	C2091	G1985	G1905	U1820	U1747	A1668
U2788	G2632	G2537	G2454	U2377	G2299	C2222	U2155	U2092	C1986	G1906	A1821	C1748	A1669
G2789	U2633	U2538	U2455	G2378	U2300	G2223	G2156	G2093	G1987	G1907	C1822	A1749	C1670
A2790	C2634	G2539	G2456	U2379	G2301	A2224	G2157	A2094	U1991	C1908	G1823	G1750	U1671
U2791	A2635	U2540	U2457	G2380	G2302	G2225	G2158	A2095	U1992	G1909	C1824	U1751	C1672
C2792	G2636	G2541	G2458	A2381	U2303	A2226	C2159	U2096	U1993	G1910	U1827	G1752	A1672
U2793	U2637	U2542	A2459	G2382	G2304	G2227	G2160	C2097	C1987	U1911	G1828	G1753	G1673
G2794	C2638	G2543	U2460	G2383	G2305	A2228	C2161	A2097	C1988	A1912	A1829	A1754	G1674
U2795	G2639	U2544	G2461	U2384	U2306	G2230	G2162	C2098	U1998	A1913	C1832	C1675	U1677
C2796	U2640	G2545	U2462	C2385	G2307	G2231	A2163	U2099	G2012	C1914	C1833	U1758	A1678
U2797	G2641	U2546	C2463	G2386	G2308	U2232	C2164	G2100		U1915	U1834		
A2798	C2642	U2547	G2464	A2387	G2309	G2233	G2165						
G2799	G2643	G2548	U2465	G2388	A2310	G2234	G2166						
U2800	U2644	A2549	A2466	U2389	A2311	A2225	C2167						
C2801	G2645	U2550	G2467	A2390	U2312	G2226	G2168						
U2802	C2646	G2551	U2468	G2391	G2313	A2227	G2169						
G2803	U2647	U2552	A2469	G2392	A2314	G2228	C2170						
U2804	G2648	G2553	U2470	G2393	G2315	G2229	G2171						
C2805	C2649	U2554	A2471	A2394	U2316	G2230	G2172						
U2806	U2650	G2555	U2472	A2395	G2317	G2231	G2173						
G2807	G2651	U2556	G2473	A2396	U2318	G2232	G2174						
A2808	C2652	A2557	U2474	G2397	G2319	G2233	G2175						
U2809	U2653	G2558	A2475	A2398	A2320	G2234	G2176						
C2810	G2654	U2559	U2476	G2399	A2321	A2225	C2177						
G2811	C2655	G2560	G2477	G2400	A2322	G2226	G2178						
U2812	U2656	A2561	A2478	A2323	U2323	G2227	G2179						
C2813	G2657	G2562	U2479	A2324	G2324	G2228	G2180						
A2814	U2658	U2563	A2480	A2325	U2325	G2229	G2181						
G2815	C2659	G2564	U2481	G2326	G2326	G2230	G2182						
	U2660	A2565	U2482	A2327	G2327	G2231	G2183						
	G2661	U2566	A2483	A2328	G2328	G2232	G2184						
	C2662	G2567	U2484	A2329	U2329	G2233	C2185						
	U2663	U2568	A2485	A2330	G2330	G2234	G2186						
	G2664	G2569	U2486	G2331	U2331	G2235	G2187						
	C2665	A2570	A2487	A2332	U2332	G2236	G2188						
	U2666	G2571	U2488	A2333	G2333	G2237	G2189						
	G2667	U2572	G2489	A2334	U2334	G2238	G2190						
	C2668	A2573	U2490	G2335	G2335	G2239	G2191						
	U2669	G2574	A2491	A2336	U2336	G2240	G2192						
	G2670	U2575	U2492	G2337	A2241	U2180	G2193						
	C2671	G2576	A2493	A2338	U2242	U2181	G2194						
	U2672	U2577	U2494	G2339	U2243	U2182	U2195						
	G2673	A2578	G2495	C2340	G2244	U2183	U2196						
	C2674	G2579	U2496	A2341	A2245	U2184	G2197						
	U2675	U2580	A2497	G2342	U2246	U2185	U2198						
	G2676	G2581	U2498	A2343	U2247	U2186	U2199						
	C2677	A2582	U2499	G2344	U2248	U2187	U2200						
	U2678	U2583	U2500	A2345	U2249	U2188	U2201						
	G2679	G2584	G2501	G2346	A2250	U2189	U2202						
	C2680	U2585	U2502	A2347	A2251	U2190	U2203						
	U2681	A2586	G2503	G2348	A2252	U2191	U2204						
	G2682	G2587	U2504	C2349	A2253	U2192	U2205						
	A2683	U2588	G2505	A2350	A2254	U2193	U2206						
	C2684	G2589	U2506	G2351	A2255	U2194	U2207						
	U2685	U2590	C2507	A2352	A2256	U2195	U2208						
	G2686	G2591	G2508	A2353	A2257	U2196	U2209						
	C2687	A2592	U2509	G2354	A2258	U2197	U2210						
	U2688	U2593	U2510	A2355	A2259	U2198	U2211						
	G2689	G2594	G2511	G2356	A2260	U2199	U2212						
	A2690	U2595	U2512	A2357	A2261	U2200	U2213						
	C2691	G2596	C2513	G2358	A2262	U2201	U2214						
	U2692	A2597	U2514	A2359	A2263	U2202	U2215						
	G2693	U2598	G2515	G2360	A2264	U2203	U2216						
	C2694	G2599	U2516	A2361	A2265	U2204	U2217						
	U2695	U2600	A2517	G2362	A2266	U2205	U2218						
	G2696	G2601	G2518	G2363	A2267	U2206	G2219						
	A2697	U2602	U2519	A2364	A2268	U2207	U2220						
	C2698	A2603	G2520										



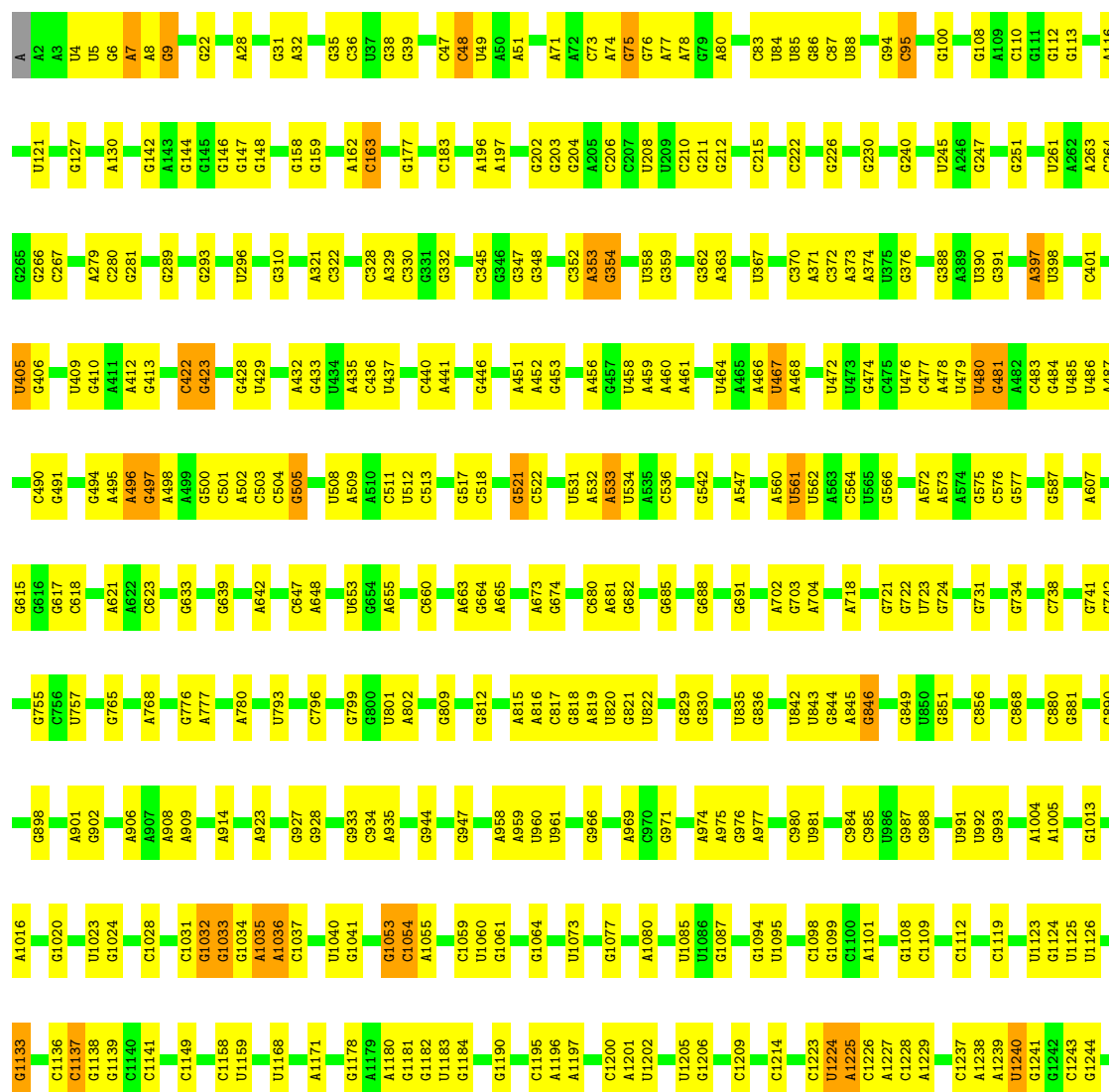
- Molecule 52: 5S rRNA

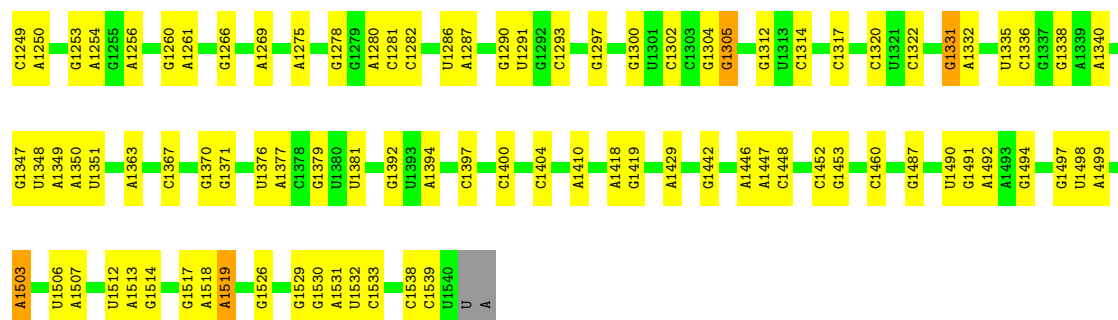
Chain 2: 76% 20%



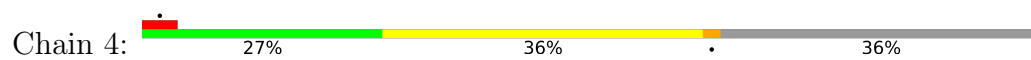
- Molecule 53: 16S rRNA

Chain 3: 69% 29%

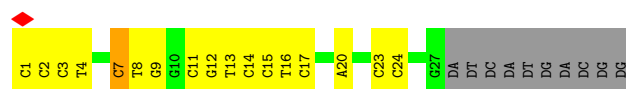




• Molecule 54: mRNA



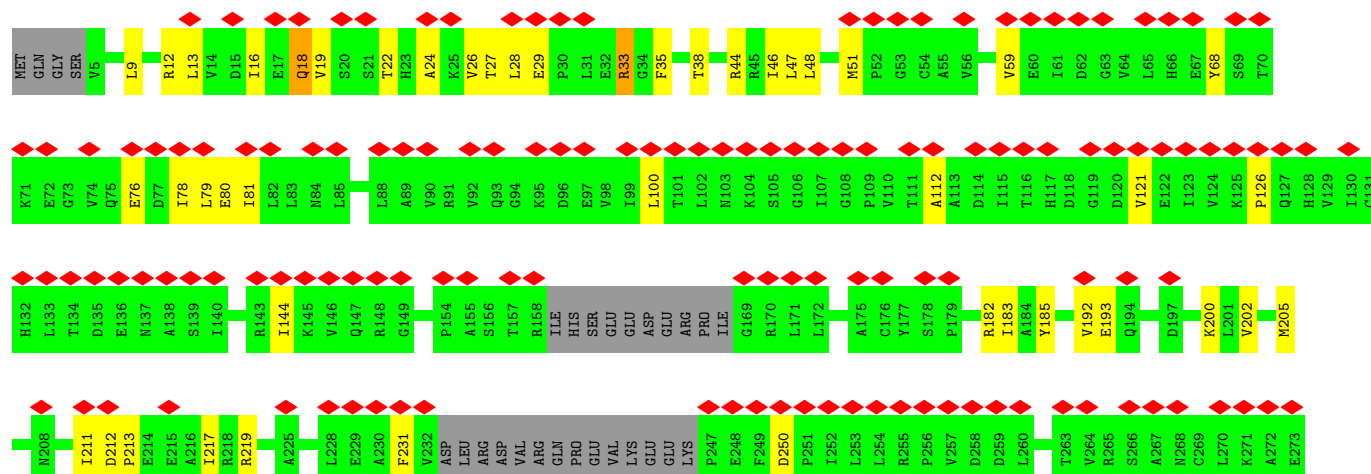
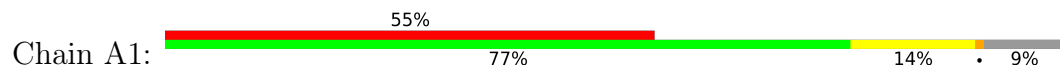
• Molecule 55: template DNA strand

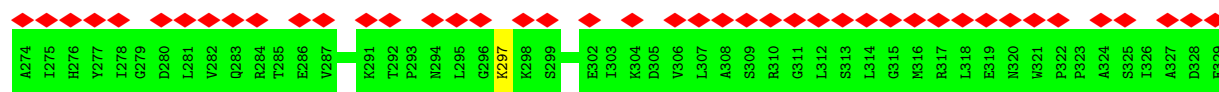


• Molecule 56: non-template DNA strand

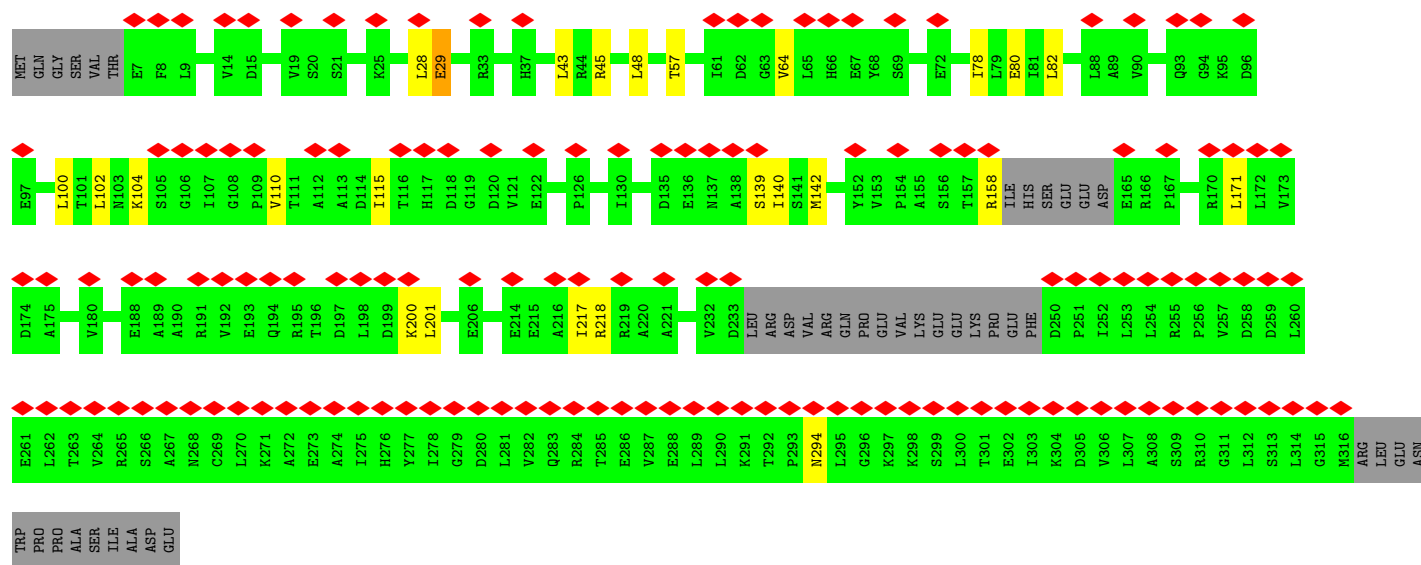
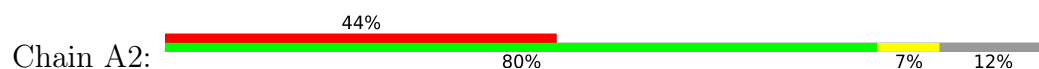


• Molecule 57: DNA-directed RNA polymerase subunit alpha

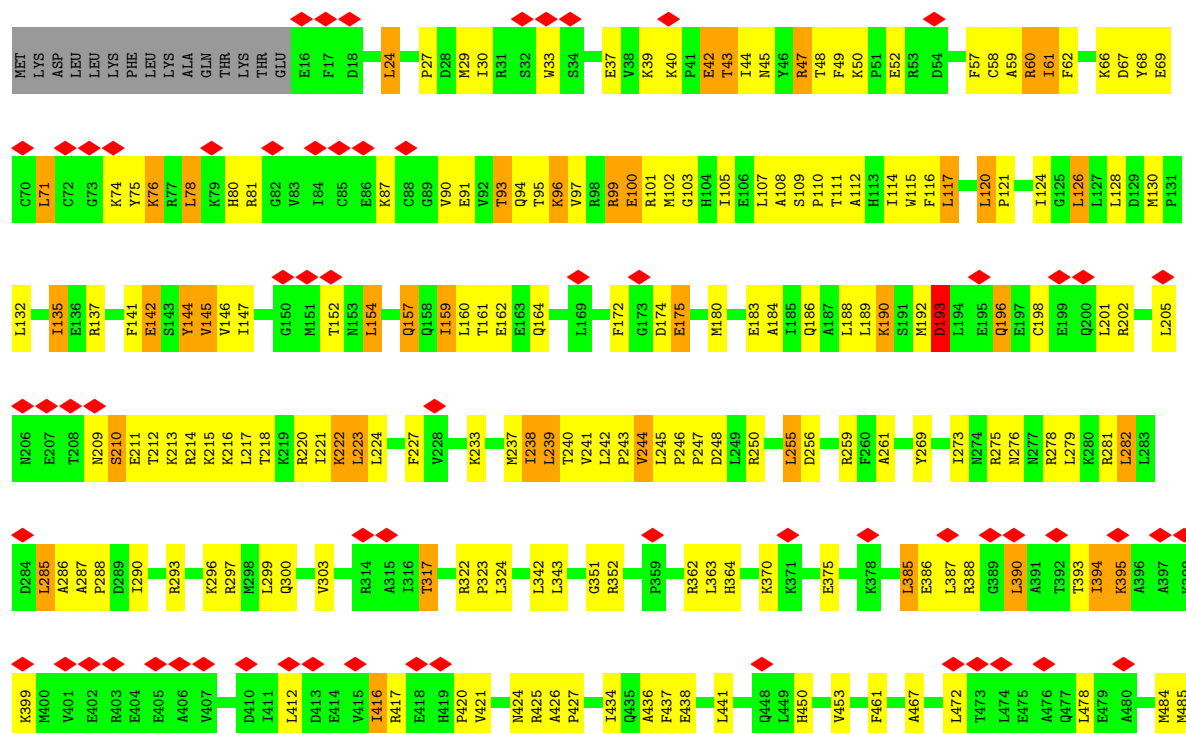




• Molecule 57: DNA-directed RNA polymerase subunit alpha

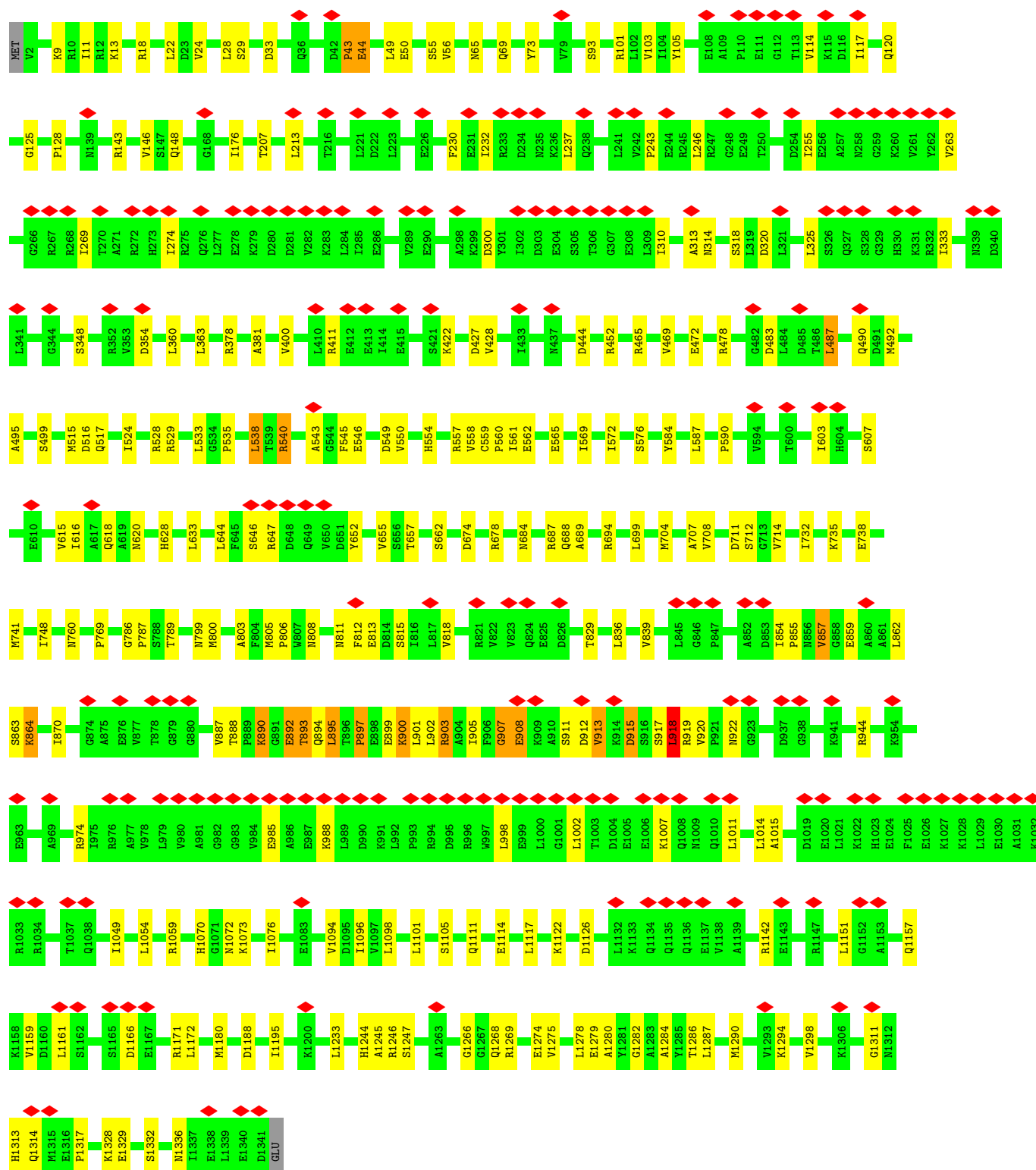


• Molecule 58: DNA-directed RNA polymerase subunit beta'

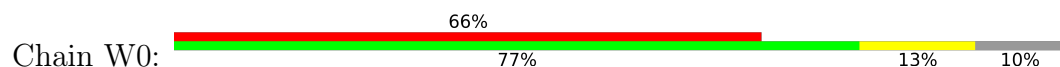


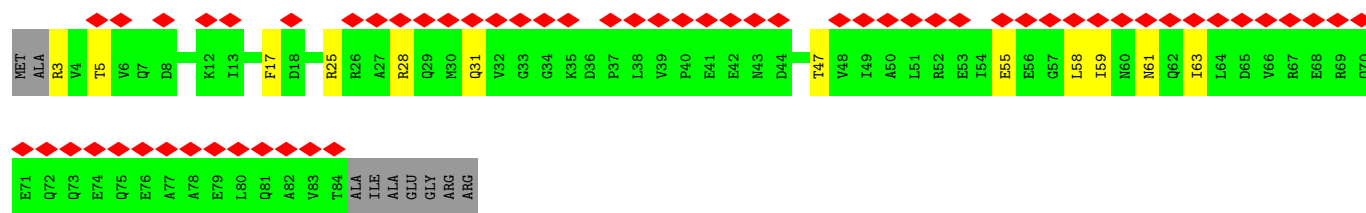


Chain B2: 



- Molecule 60: DNA-directed RNA polymerase subunit omega

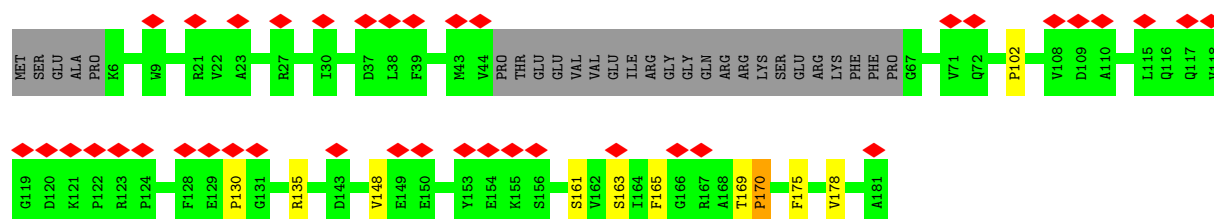
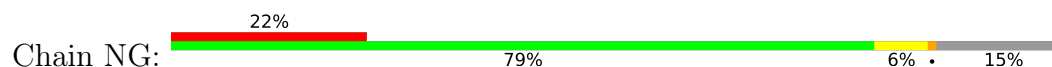




• Molecule 61: Transcription termination/antitermination protein NusA

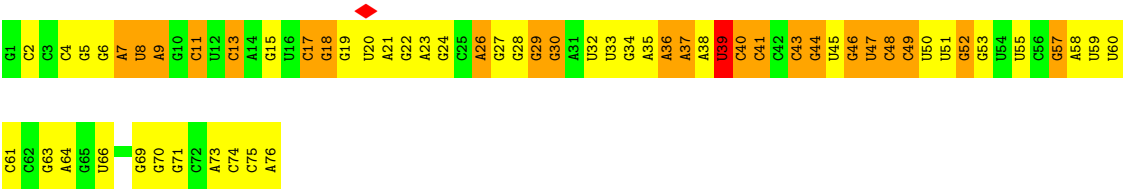


• Molecule 62: Transcription termination/antitermination protein NusG

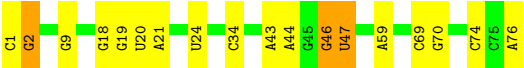


• Molecule 63: tRNA(Phe)

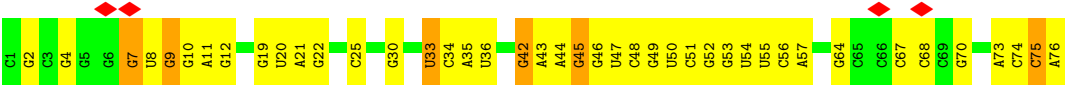




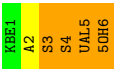
• Molecule 64: tRNA(fMet)



• 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 ($\text{\AA}$)	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: DPP, MG, 5OH, KBE, UAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/531	0.54	0/709
2	B	0.41	0/450	0.60	2/599 (0.3%)
3	C	0.28	0/416	0.52	0/554
4	D	0.47	0/380	0.76	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	19
3	C	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
4	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
5	E	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
6	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	49
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	24	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%)	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%)	12	47
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	49
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	98 (88%)	13 (12%)	1 (1%)	14	49
19	S	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
20	T	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
21	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
22	V	78/84 (93%)	69 (88%)	8 (10%)	1 (1%)	9	41
23	W	63/75 (84%)	56 (89%)	5 (8%)	2 (3%)	3	21
24	X	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
25	Y	83/87 (95%)	78 (94%)	5 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	7	37
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
31	f	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
32	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	6	31
33	i	139/142 (98%)	116 (84%)	23 (16%)	0	100	100
34	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
35	k	120/123 (98%)	106 (88%)	14 (12%)	0	100	100
36	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
37	m	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
38	n	118/127 (93%)	103 (87%)	15 (13%)	0	100	100
39	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	p	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
41	q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	35
42	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	12	47
43	s	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
44	t	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
45	u	100/104 (96%)	84 (84%)	15 (15%)	1 (1%)	12	47
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	9	41
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	21 (7%)	1 (0%)	36	71
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1202 (90%)	123 (9%)	4 (0%)	36	71
59	B2	1338/1342 (100%)	1204 (90%)	129 (10%)	5 (0%)	30	67
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	472 (96%)	15 (3%)	3 (1%)	21	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	NG	150/181 (83%)	136 (91%)	10 (7%)	4 (3%)	4	25
65	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9586/10235 (94%)	8668 (90%)	882 (9%)	36 (0%)	31	67

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%)	53	67
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	45	64
4	D	38/38 (100%)	37 (97%)	1 (3%)	40	60
5	E	51/52 (98%)	49 (96%)	2 (4%)	28	49
6	F	34/34 (100%)	30 (88%)	4 (12%)	5	19
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	55
8	H	170/190 (90%)	167 (98%)	3 (2%)	51	67
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	63
10	J	119/126 (94%)	117 (98%)	2 (2%)	53	67
11	K	87/116 (75%)	82 (94%)	5 (6%)	18	40
12	L	124/147 (84%)	124 (100%)	0	100	100
13	M	104/105 (99%)	103 (99%)	1 (1%)	68	76
14	N	105/107 (98%)	98 (93%)	7 (7%)	15	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	86/90 (96%)	78 (91%)	8 (9%)	8	26
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	54
17	Q	103/104 (99%)	98 (95%)	5 (5%)	22	44
18	R	92/96 (96%)	91 (99%)	1 (1%)	65	74
19	S	83/84 (99%)	83 (100%)	0	100	100
20	T	76/77 (99%)	73 (96%)	3 (4%)	28	49
21	U	65/65 (100%)	64 (98%)	1 (2%)	57	70
22	V	74/78 (95%)	72 (97%)	2 (3%)	39	59
23	W	56/65 (86%)	52 (93%)	4 (7%)	13	35
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	64 (98%)	1 (2%)	57	70
26	Z	55/61 (90%)	47 (86%)	8 (14%)	3	14
27	b	216/218 (99%)	212 (98%)	4 (2%)	50	66
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	51	67
30	e	148/150 (99%)	145 (98%)	3 (2%)	48	65
31	f	137/138 (99%)	135 (98%)	2 (2%)	57	70
32	g	41/114 (36%)	38 (93%)	3 (7%)	13	34
33	i	109/110 (99%)	108 (99%)	1 (1%)	70	76
34	j	116/116 (100%)	116 (100%)	0	100	100
35	k	103/104 (99%)	103 (100%)	0	100	100
36	l	102/103 (99%)	101 (99%)	1 (1%)	68	76
37	m	109/109 (100%)	103 (94%)	6 (6%)	19	42
38	n	100/103 (97%)	99 (99%)	1 (1%)	68	76
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	99 (100%)	0	100	100
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	54
42	r	84/84 (100%)	82 (98%)	2 (2%)	43	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	65	74
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	23	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	v	78/78 (100%)	77 (99%)	1 (1%)	61	72
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	26	48
57	A1	185/286 (65%)	174 (94%)	11 (6%)	18	40
57	A2	186/286 (65%)	185 (100%)	1 (0%)	81	81
58	B1	1110/1168 (95%)	1017 (92%)	93 (8%)	10	30
59	B2	1150/1157 (99%)	1117 (97%)	33 (3%)	37	57
60	W0	70/75 (93%)	69 (99%)	1 (1%)	59	71
65	h	2/2 (100%)	2 (100%)	0	100	100
All	All	7381/7914 (93%)	7132 (97%)	249 (3%)	33	54

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%)

Continued on next page...

Continued from previous page...

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 ⓘ

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	5OH	h	6	65	7,12,13	0.70	0	4,16,18	1.34	1 (25%)
65	UAL	h	5	65	6,8,9	2.36	2 (33%)	4,9,11	1.87	1 (25%)
65	KBE	h	1	65	8,8,9	0.57	0	6,8,10	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	DPP	h	2	65	4,5,6	0.50	0	1,5,7	0.07	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	h	5	UAL	C1-N1	-4.96	1.32	1.40
65	h	5	UAL	C-CA	-2.81	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	h	5	UAL	O-C-CA	-3.29	121.27	125.39
65	h	6	5OH	CR-CB-CA	-2.41	110.06	112.61

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	6	5OH	5	0
65	h	5	UAL	1	0
65	h	2	DPP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

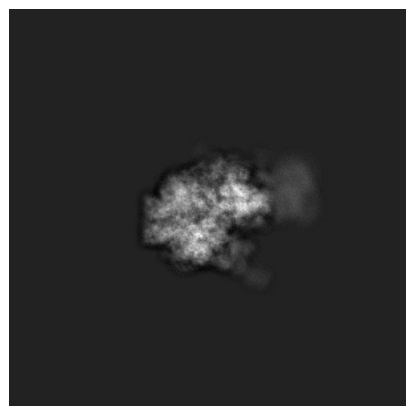
6 Map visualisation [i](#)

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

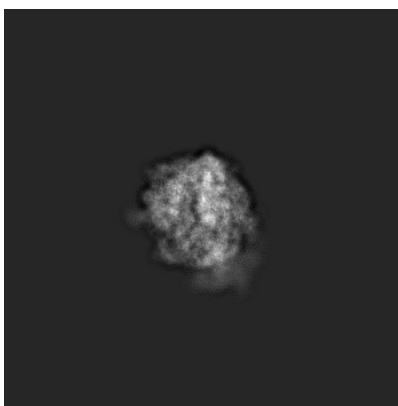
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

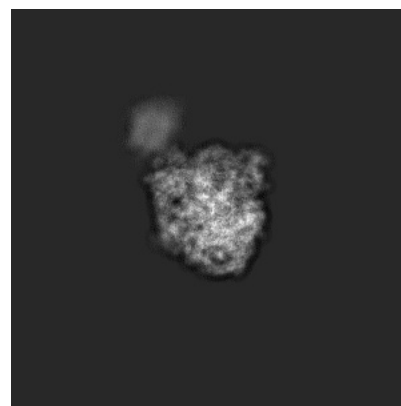
6.1.1 Primary map



X

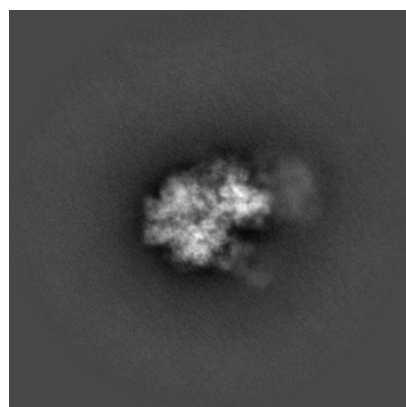


Y

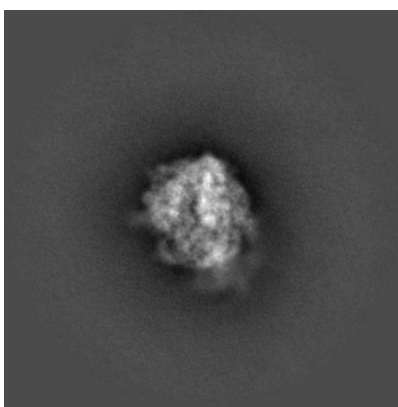


Z

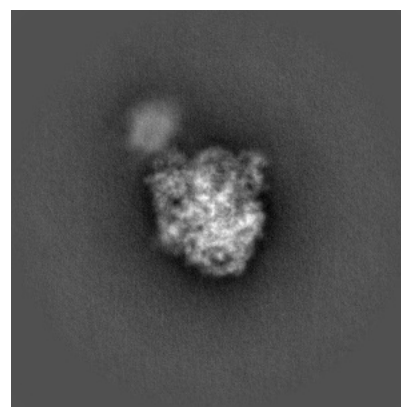
6.1.2 Raw map



X



Y

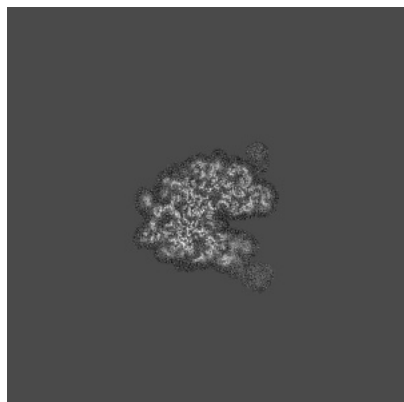


Z

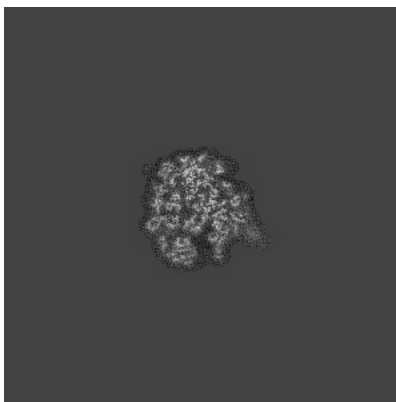
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

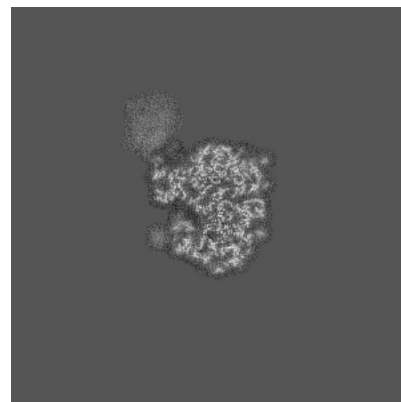
6.2.1 Primary map



X Index: 240

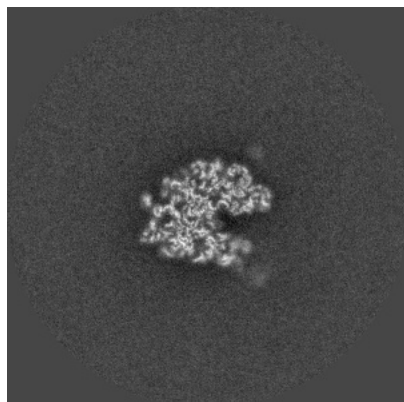


Y Index: 240

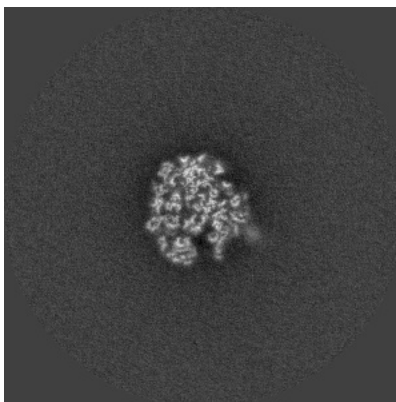


Z Index: 240

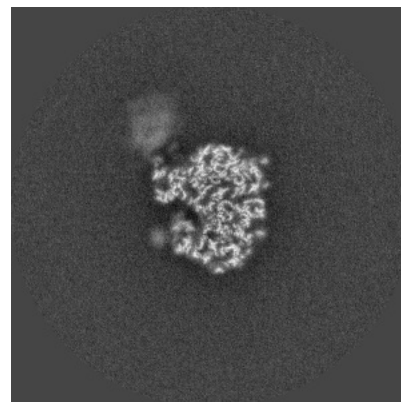
6.2.2 Raw map



X Index: 240



Y Index: 240

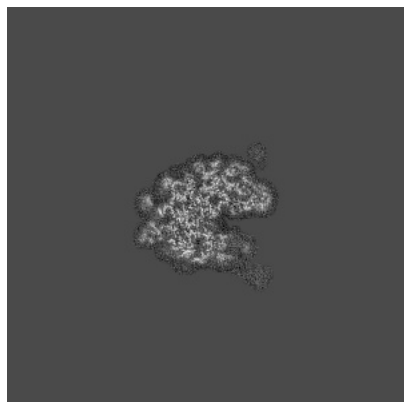


Z Index: 240

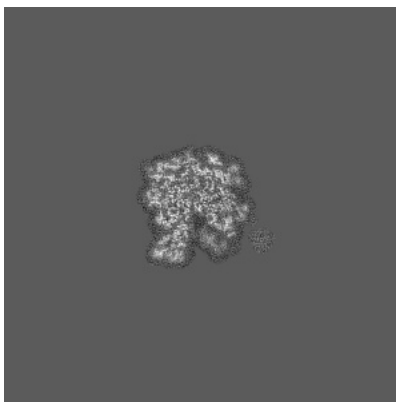
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

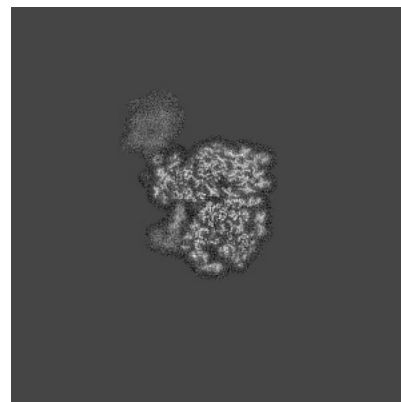
6.3.1 Primary map



X Index: 243

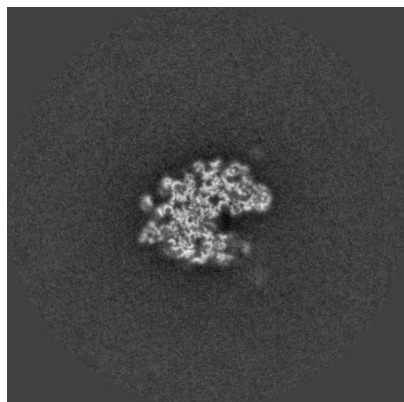


Y Index: 223

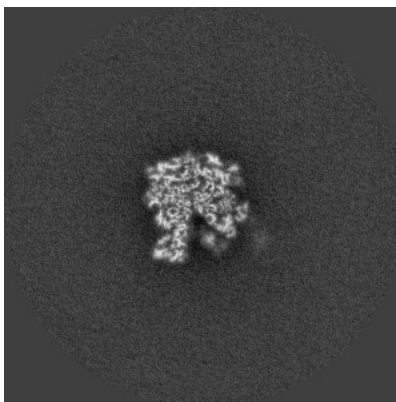


Z Index: 246

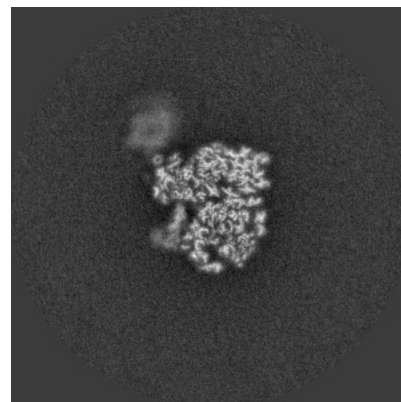
6.3.2 Raw map



X Index: 243



Y Index: 224

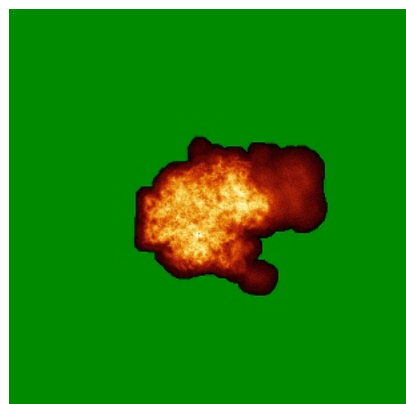


Z Index: 246

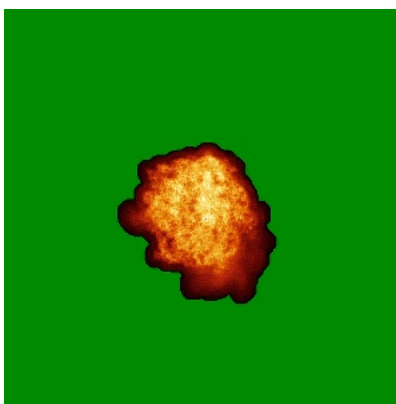
The images above show the largest variance slices of the map in three orthogonal directions.

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

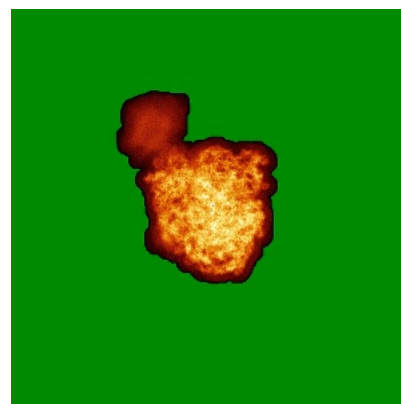
6.4.1 Primary map



X

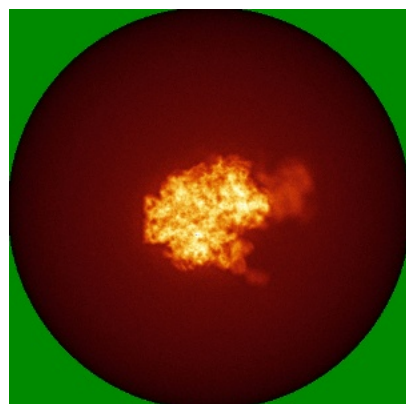


Y

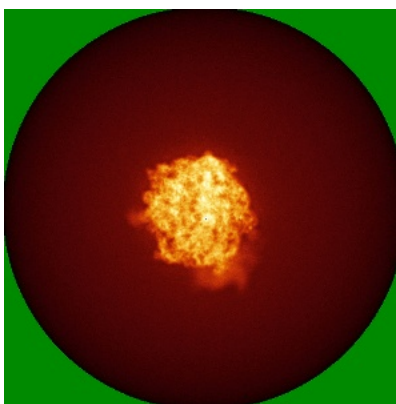


Z

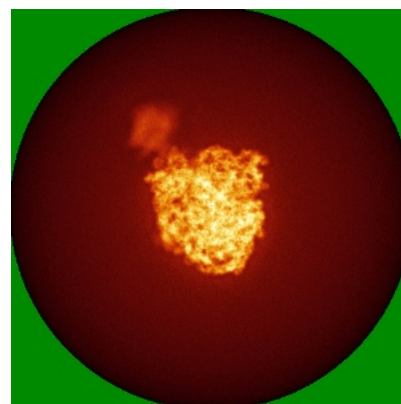
6.4.2 Raw map



X



Y

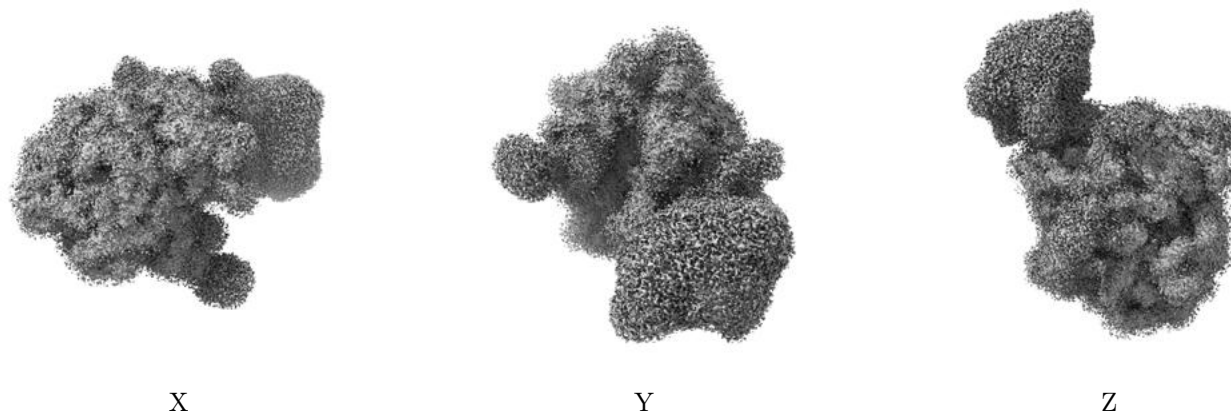


Z

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.

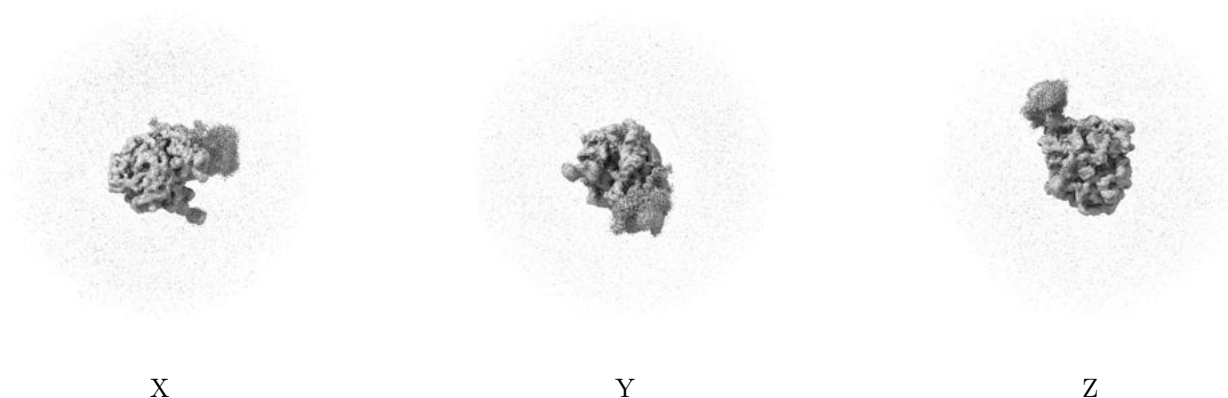
6.5 Orthogonal surface views [i](#)

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.

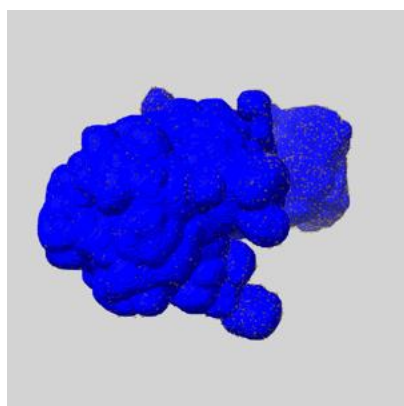
6.6 Mask visualisation [i](#)

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

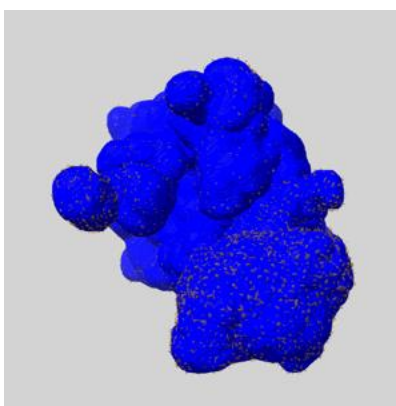
A mask typically either:

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

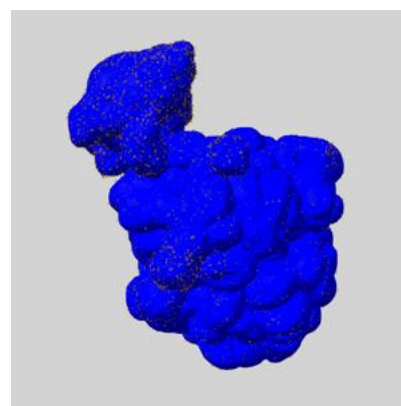
6.6.1 emd_39169_msk_1.map [i](#)



X



Y

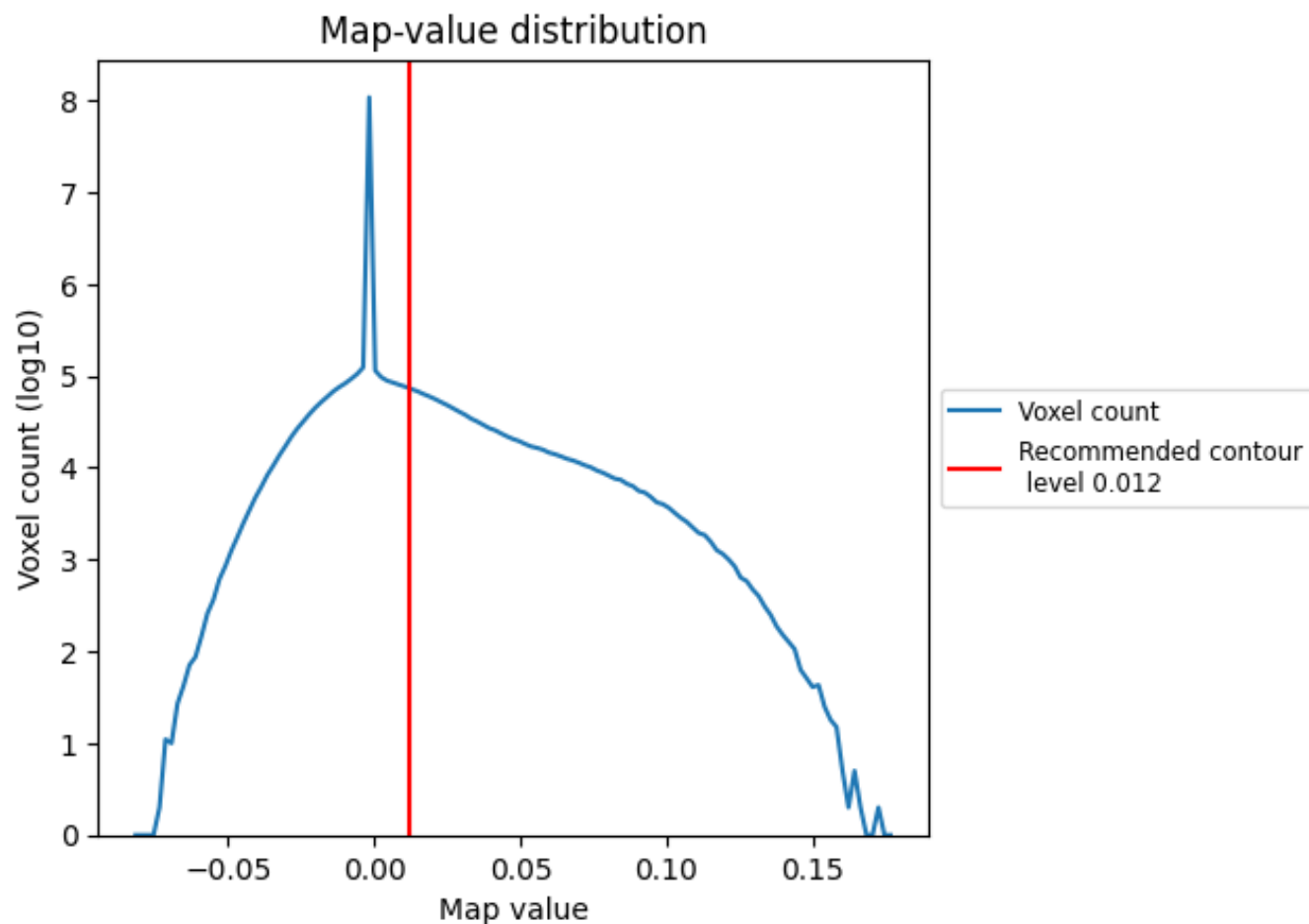


Z

7 Map analysis [i](#)

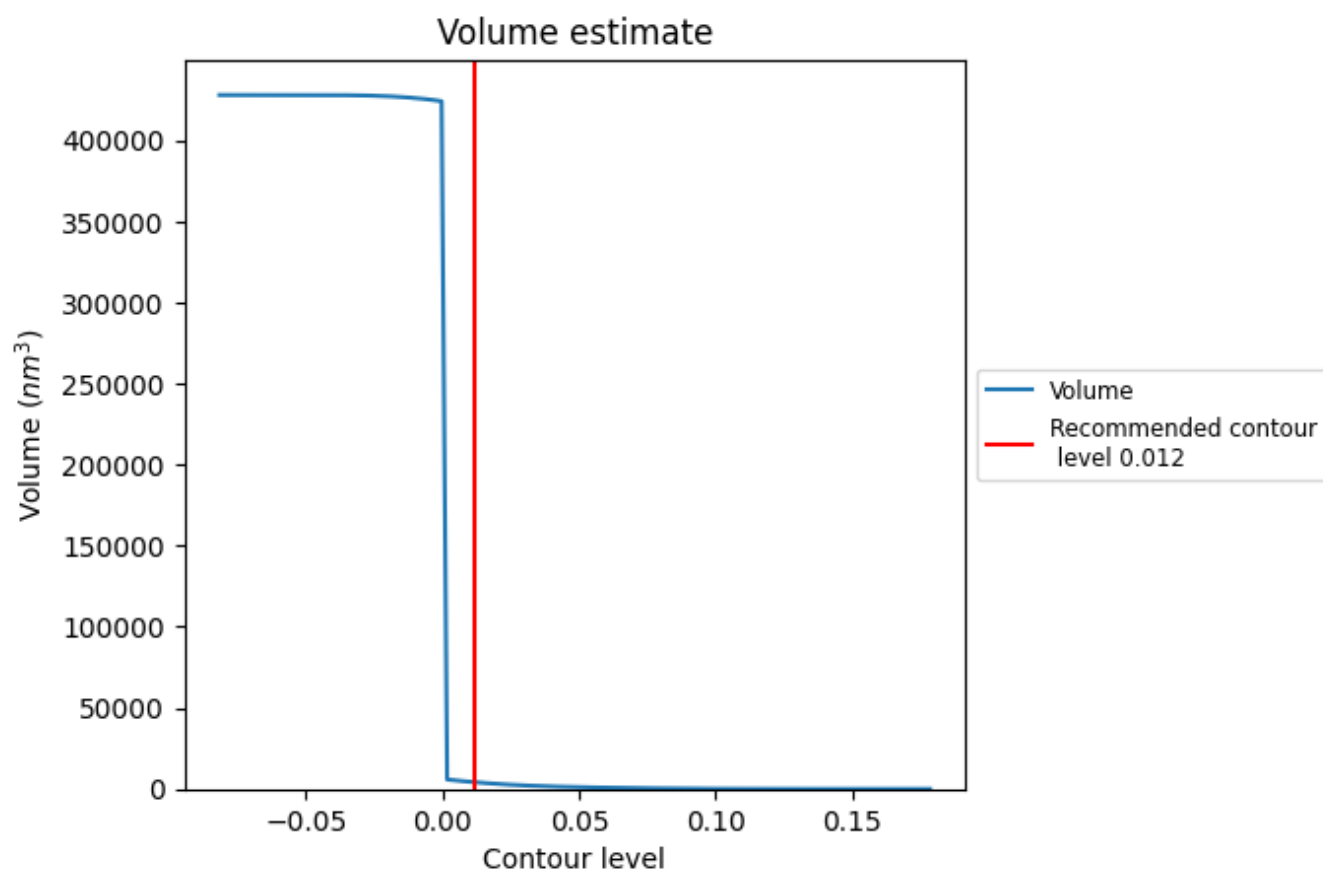
This section contains the results of statistical analysis of the map.

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.

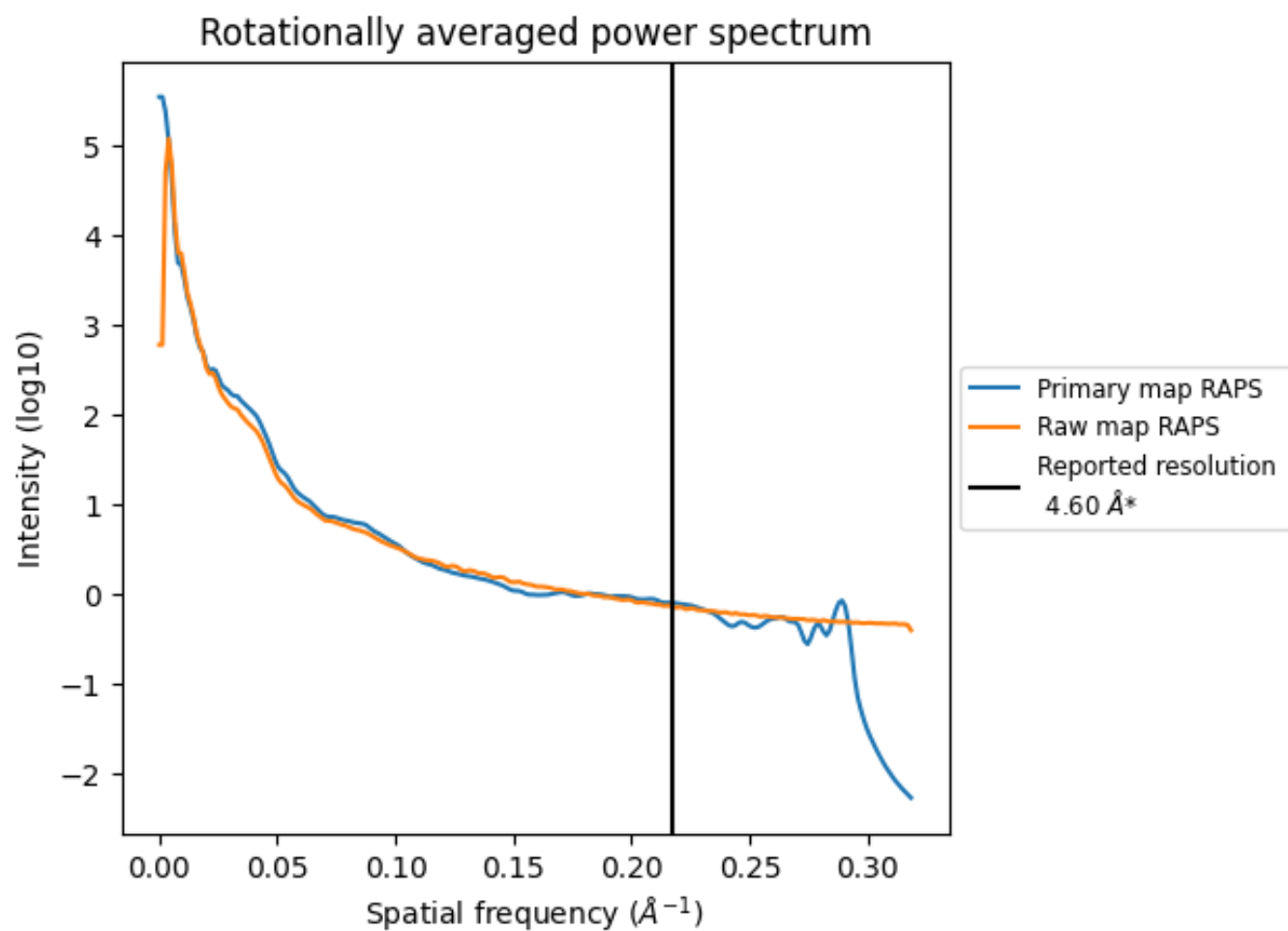
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4147 nm^3 ; 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 ⓘ

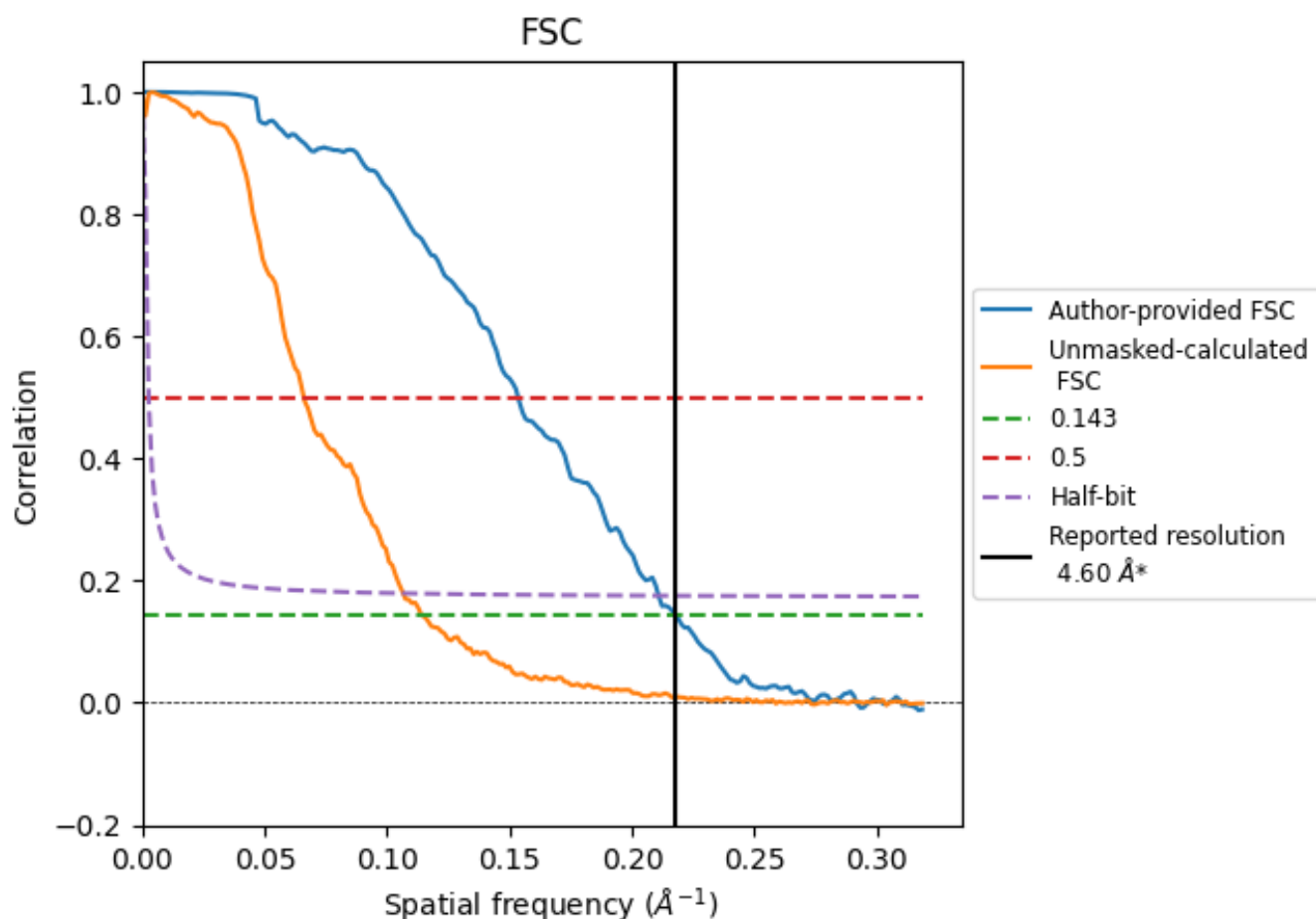


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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

8.2 Resolution estimates [i](#)

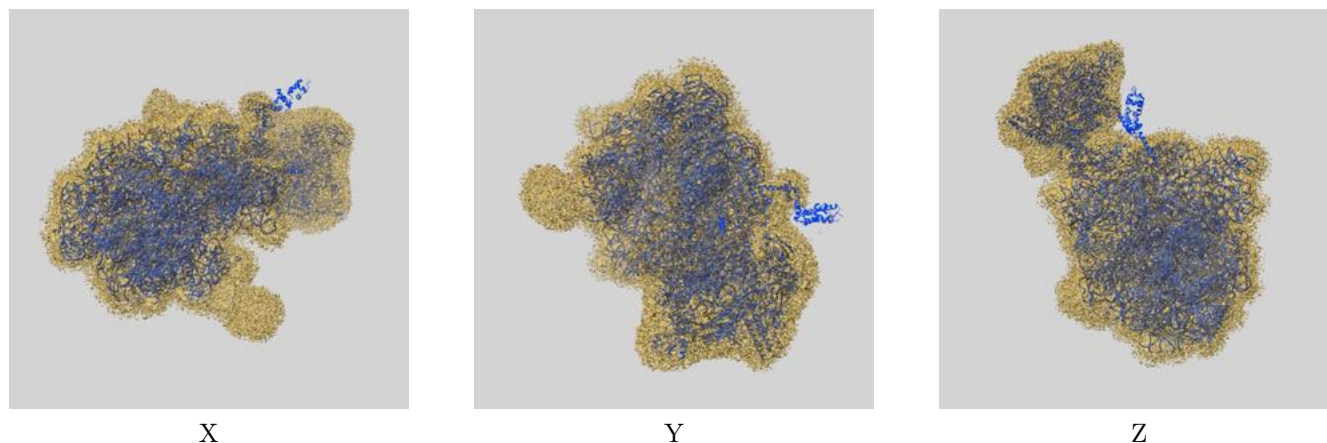
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	6.51	4.74
Unmasked-calculated*	8.76	15.15	9.39

*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](#)

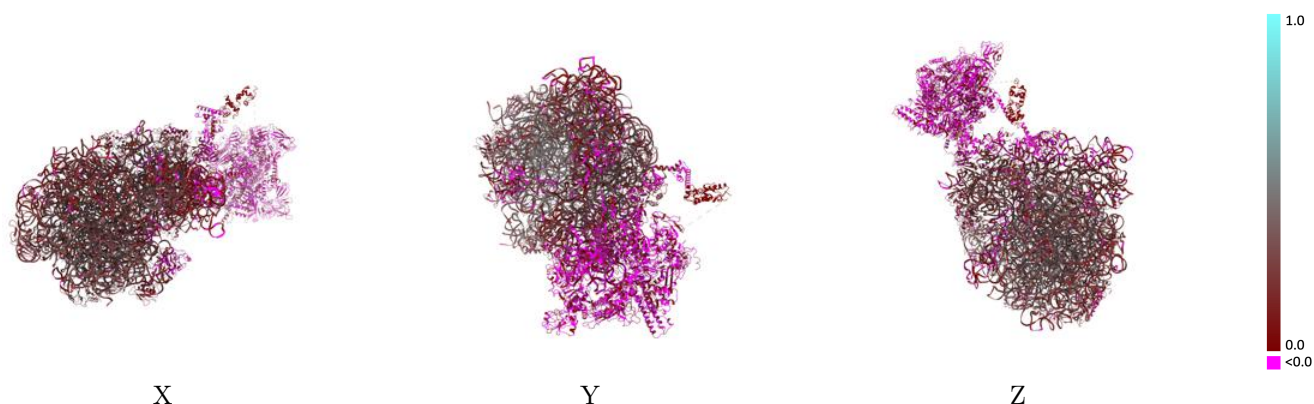
This section contains information regarding the fit between EMDB map EMD-39169 and PDB model 8YDF. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



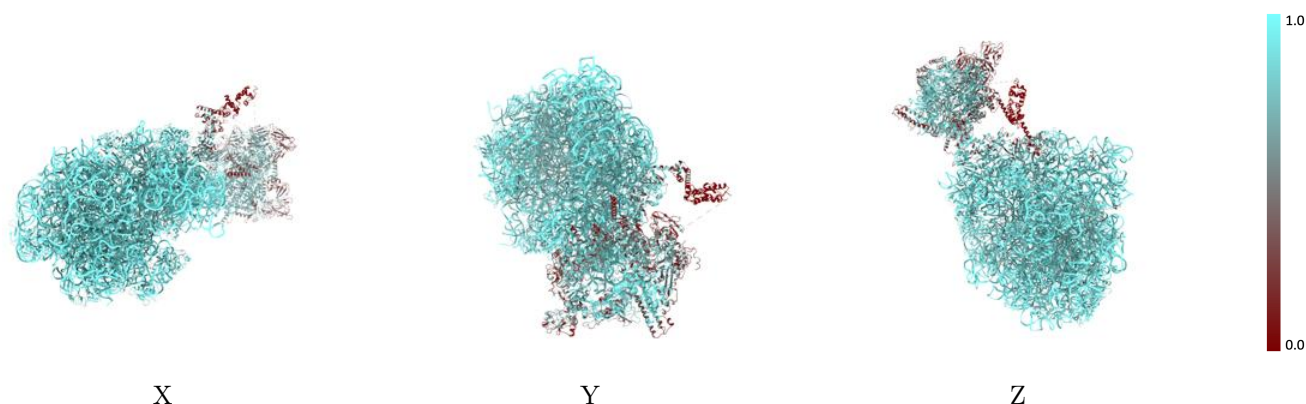
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



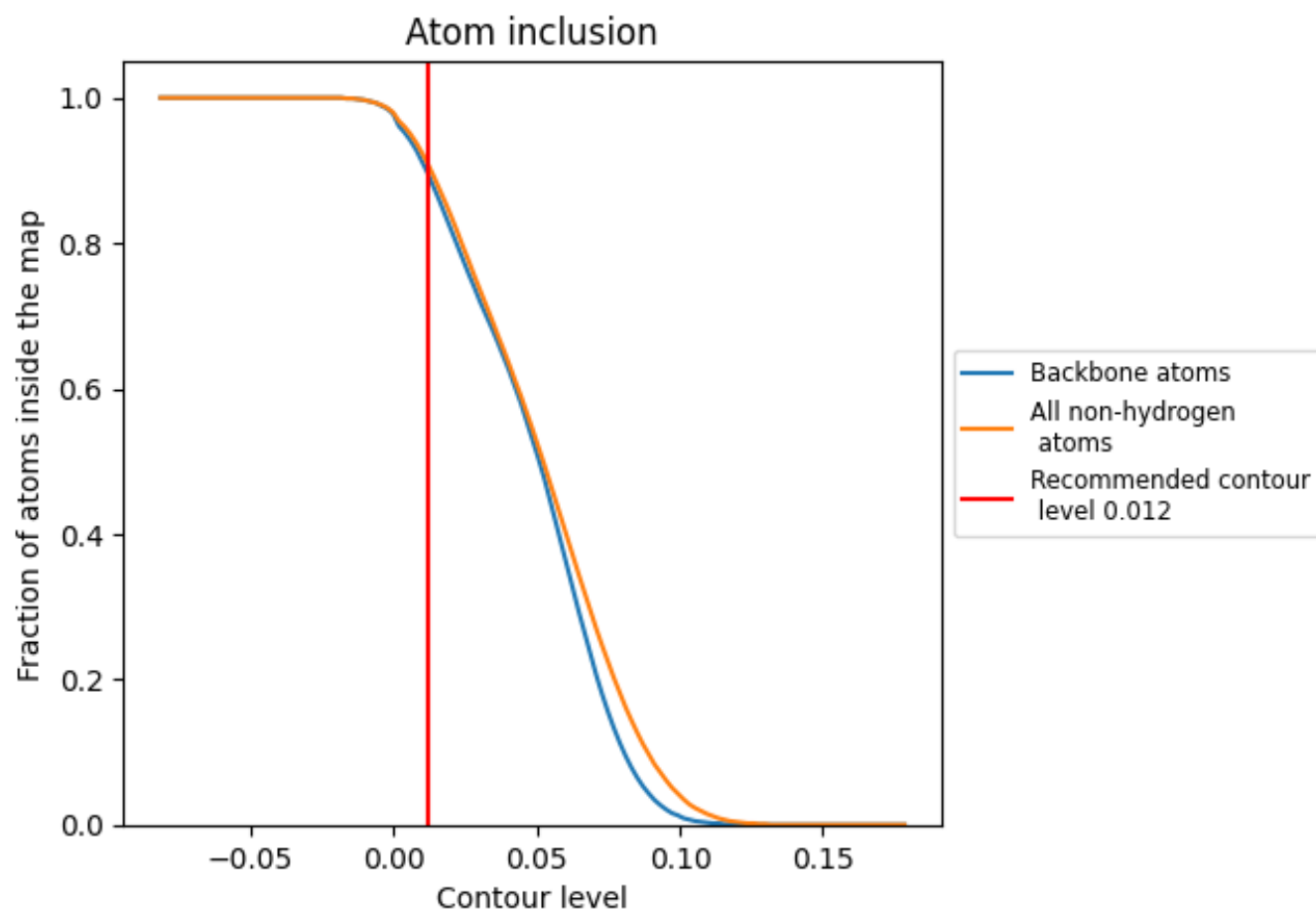
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

Continued from previous page...

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