



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 09:13 PM JST

PDB ID : 8Y5O / pdb_00008y5o
EMDB ID : EMD-38944
Title : E.coli transcription translation coupling complex in TTC-B state 3 (subclass1) containing mRNA with 30-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-01-31
Resolution : 4.20 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
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

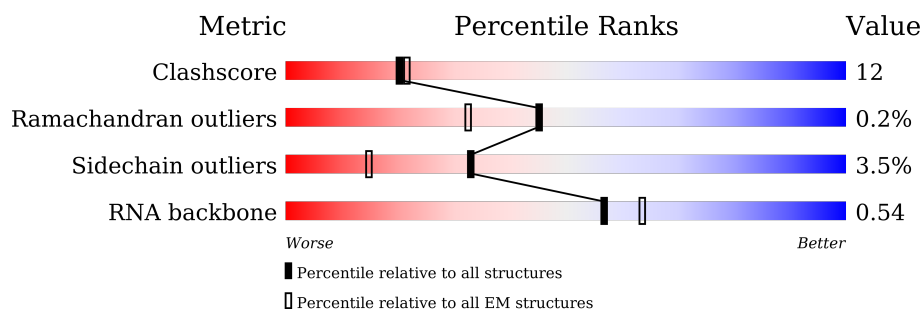
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.









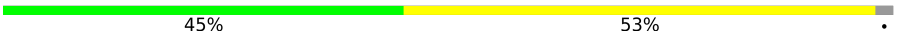


















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	 50% 16% 34%
2	B	57	 68% 28% ..
3	C	55	 53% 38% 9%
4	D	46	 59% 37% .
5	E	65	 65% 32% ..
6	F	38	 61% 39%
7	G	241	 64% 26% 10%

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

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

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Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
65	a	234	
66	0	716	
67	h	6	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 183377 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	46	Total	C	N	O	S	0	0
			355	221	62	66	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	149	Total	C	N	O	S	0	0
			1111	699	197	214	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	30	Total	C	N	O	P	0	0
			627	280	92	225	30		

- 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		

- Molecule 65 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	a	132	Total	C	N	O	S	0	0
			1013	638	183	190	2		

- Molecule 66 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	0	697	Total	C	N	O	S	0	0
			5399	3403	929	1042	25		

There are 12 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

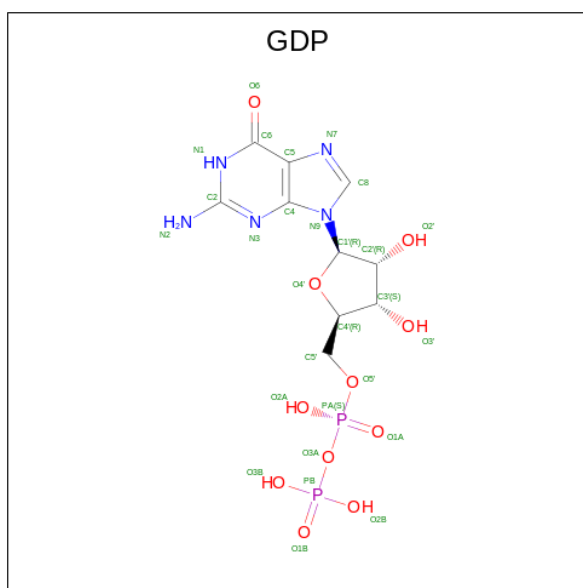
- Molecule 67 is a protein (with D amino acids) called Viomycin.

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

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

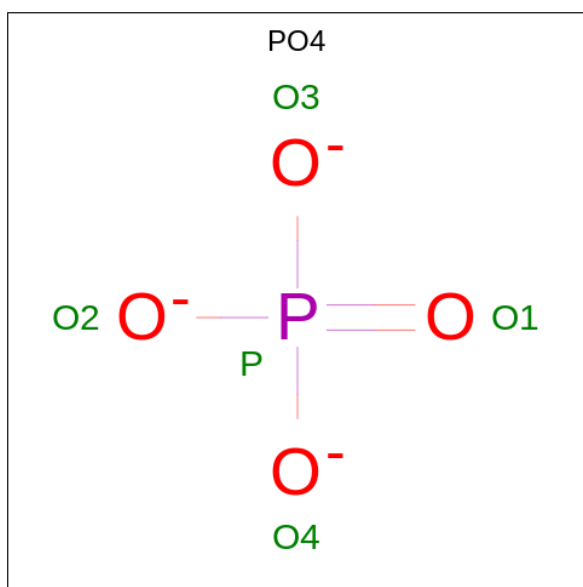
Mol	Chain	Residues	Atoms		AltConf
68	B1	1	Total	Mg	0
			1	1	

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
69	0	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 70 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

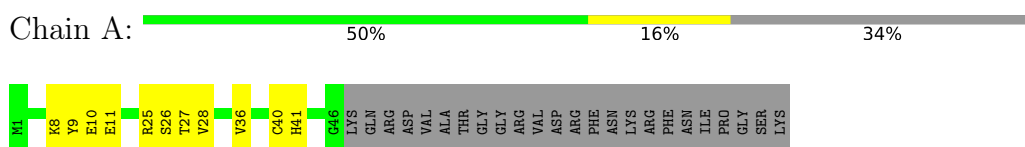


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

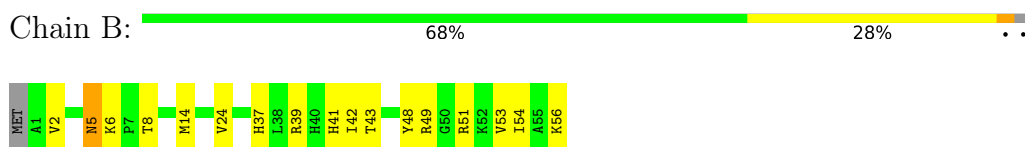
3 Residue-property plots

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

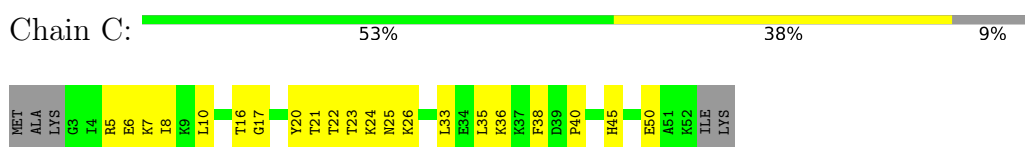
• Molecule 1: 50S ribosomal protein L31



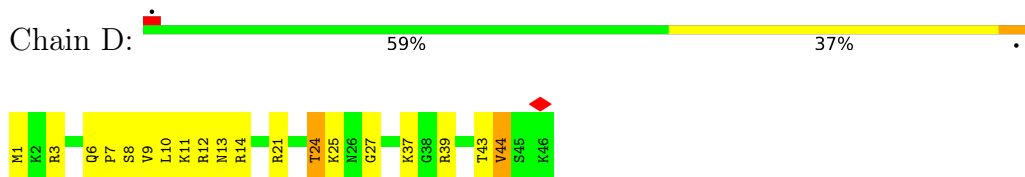
• Molecule 2: 50S ribosomal protein L32



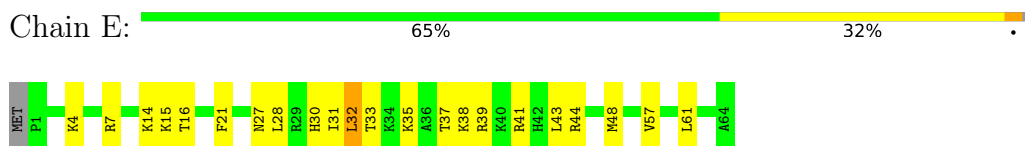
• Molecule 3: 50S ribosomal protein L33



• Molecule 4: 50S ribosomal protein L34

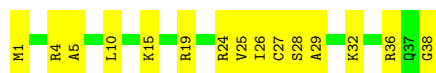


• Molecule 5: 50S ribosomal protein L35



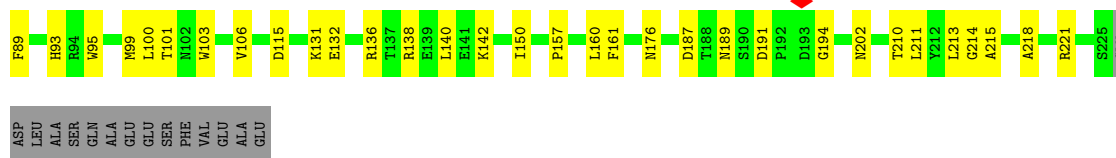
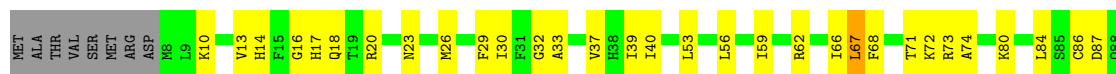
• Molecule 6: 50S ribosomal protein L36

Chain F:  61% 39%



• Molecule 7: 30S ribosomal protein S2

Chain G:  64% 26% 10%



• Molecule 8: 30S ribosomal protein S3

Chain H:  63% 24% 12%



• Molecule 9: 30S ribosomal protein S4

Chain I:  71% 27%



• Molecule 10: 30S ribosomal protein S5

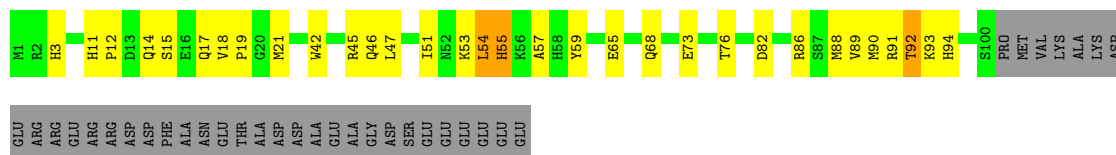
Chain J:  66% 28% 6%





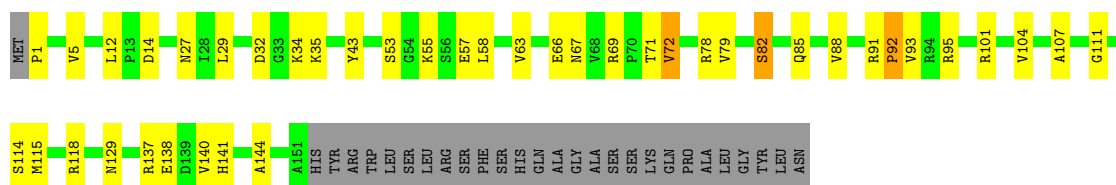
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K: 50% 21% 26%



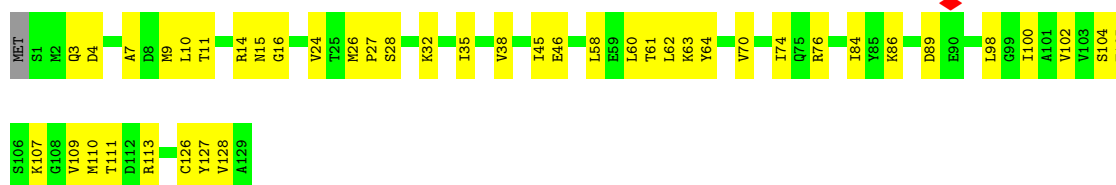
- Molecule 12: 30S ribosomal protein S7

Chain L: 61% 22% 16%



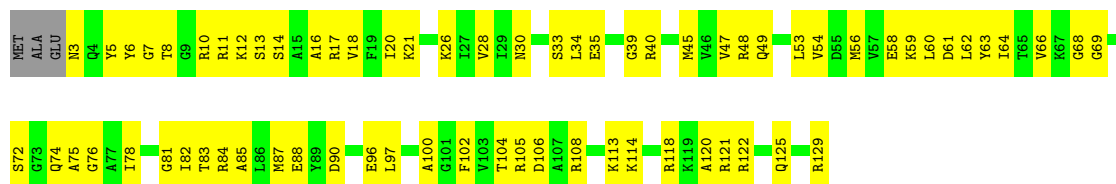
- Molecule 13: 30S ribosomal protein S8

Chain M: 66% 33% 1%



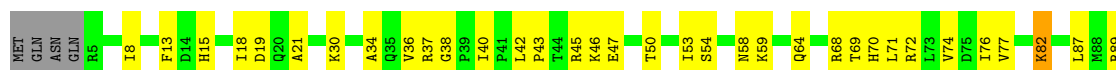
- Molecule 14: 30S ribosomal protein S9

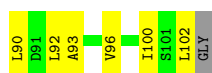
Chain N: 45% 53% 2%



- Molecule 15: 30S ribosomal protein S10

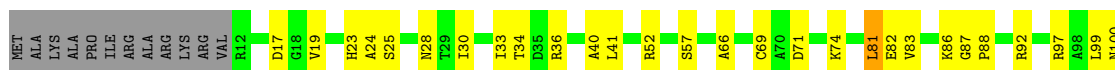
Chain O: 56% 38% 5%





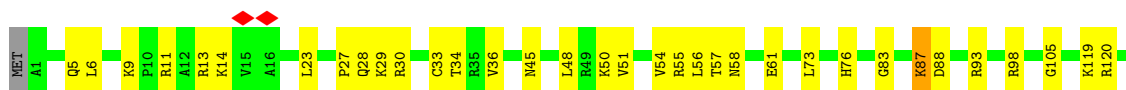
- Molecule 16: 30S ribosomal protein S11

Chain P: 61% 28% 10%



- Molecule 17: 30S ribosomal protein S12

Chain Q: 72% 27% 1%



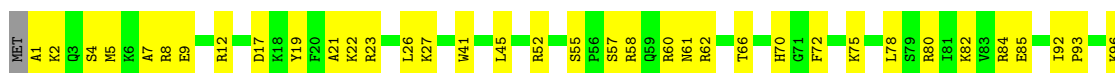
- Molecule 18: 30S ribosomal protein S13

Chain R: 69% 27% 4%



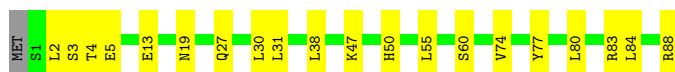
- Molecule 19: 30S ribosomal protein S14

Chain S: 60% 39% 1%



- Molecule 20: 30S ribosomal protein S15

Chain T: 76% 22% 2%



- Molecule 21: 30S ribosomal protein S16

Chain U:  72% 28%



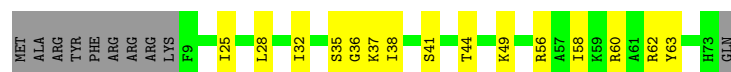
- Molecule 22: 30S ribosomal protein S17

Chain V:  67% 29% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  67% 20% 13%



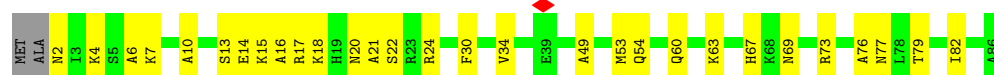
- Molecule 24: 30S ribosomal protein S19

Chain X:  64% 22% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  64% 33% 3%



- Molecule 26: 30S ribosomal protein S21

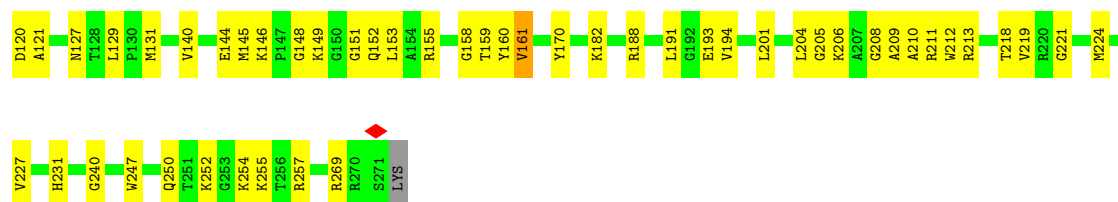
Chain Z:  61% 25% 6% 8%



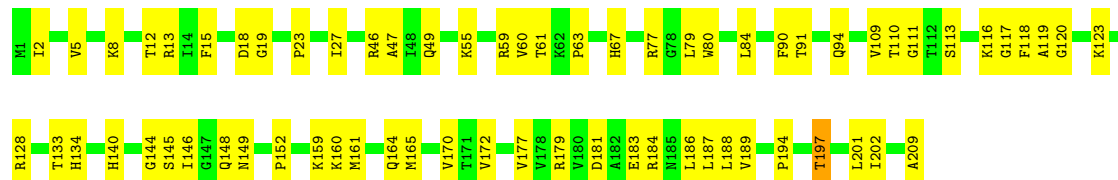
- Molecule 27: 50S ribosomal protein L2

Chain b:  70% 29% 1%

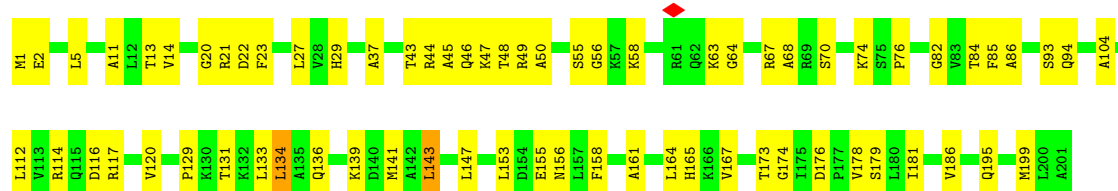




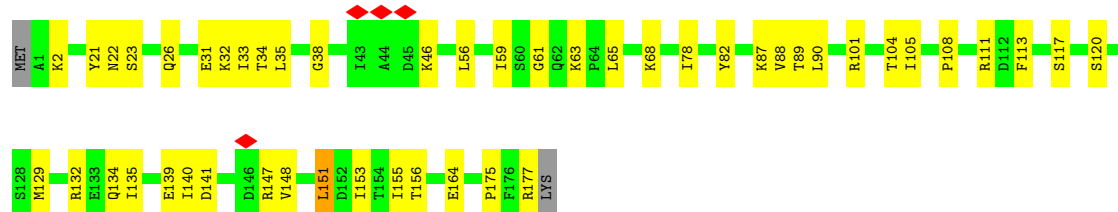
• Molecule 28: 50S ribosomal protein L3



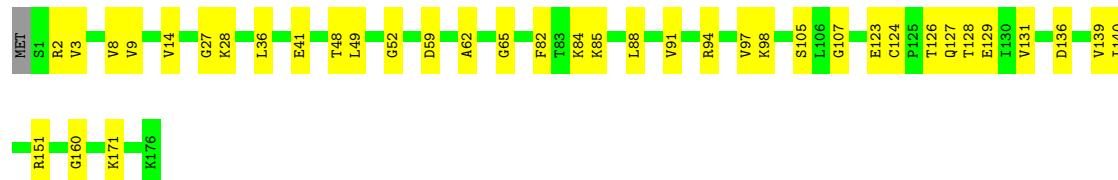
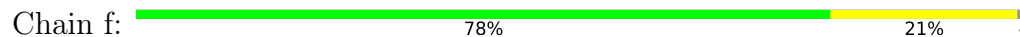
• Molecule 29: 50S ribosomal protein L4



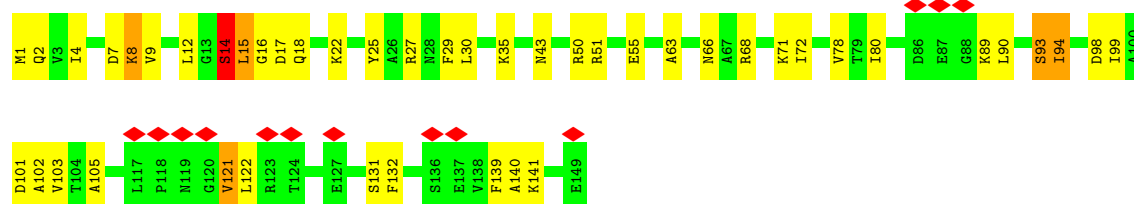
• Molecule 30: 50S ribosomal protein L5



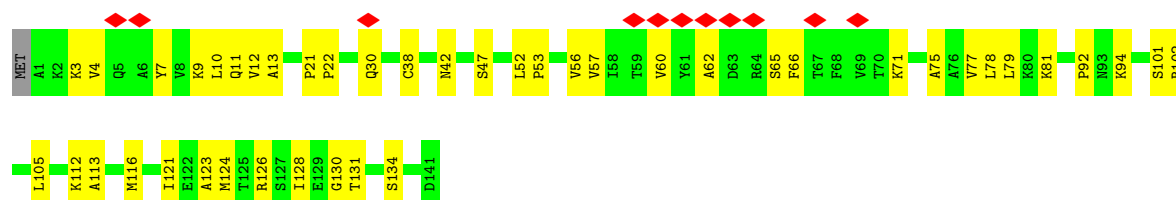
• Molecule 31: 50S ribosomal protein L6



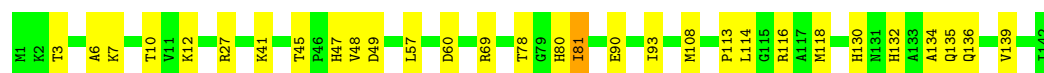
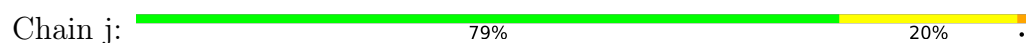
• Molecule 32: 50S ribosomal protein L9



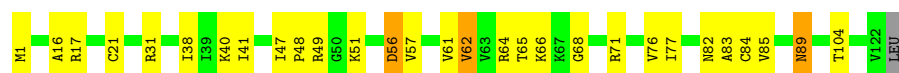
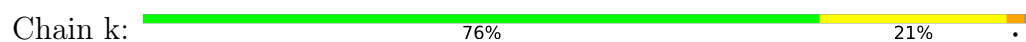
- Molecule 33: 50S ribosomal protein L11



- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



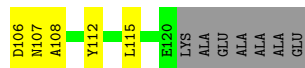
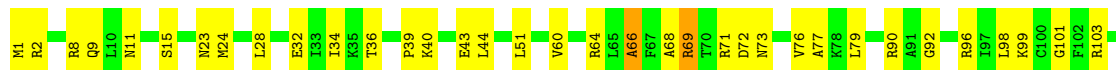
- Molecule 37: 50S ribosomal protein L16





- Molecule 38: 50S ribosomal protein L17

Chain n: 63% 30% 6%



- Molecule 39: 50S ribosomal protein L18

Chain o: 71% 28%



- Molecule 40: 50S ribosomal protein L19

Chain p: 77% 23%



- Molecule 41: 50S ribosomal protein L20

Chain q: 77% 22%



- Molecule 42: 50S ribosomal protein L21

Chain r: 70% 30%

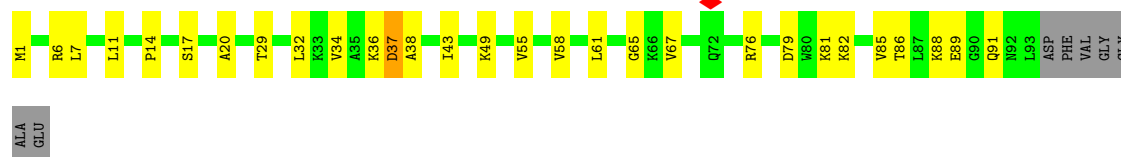


- Molecule 43: 50S ribosomal protein L22

Chain s: 72% 28%



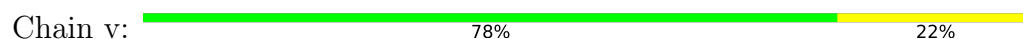
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25



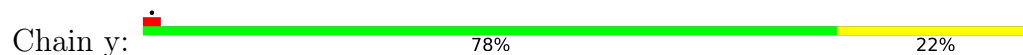
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



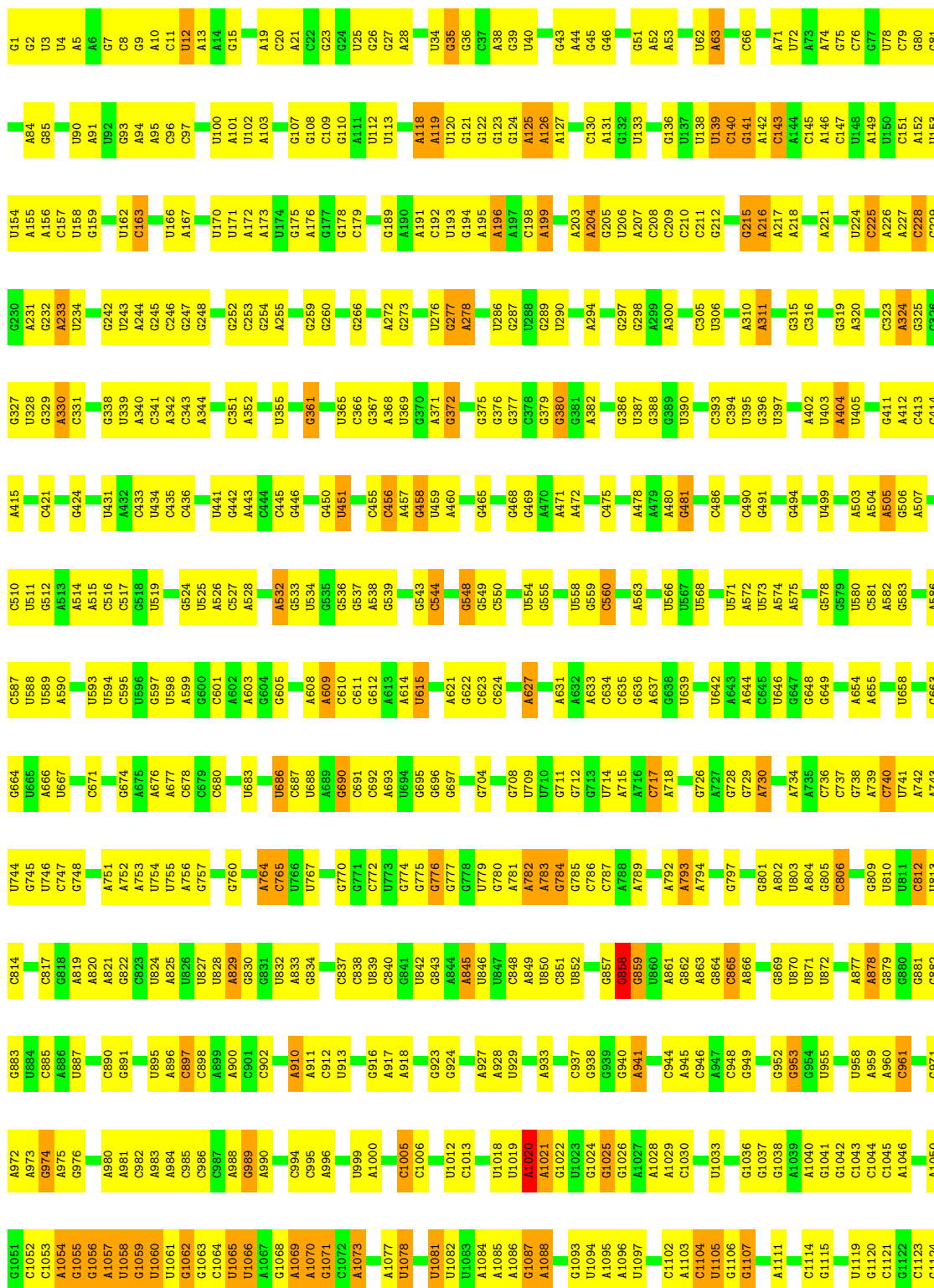
- Molecule 50: 50S ribosomal protein L30



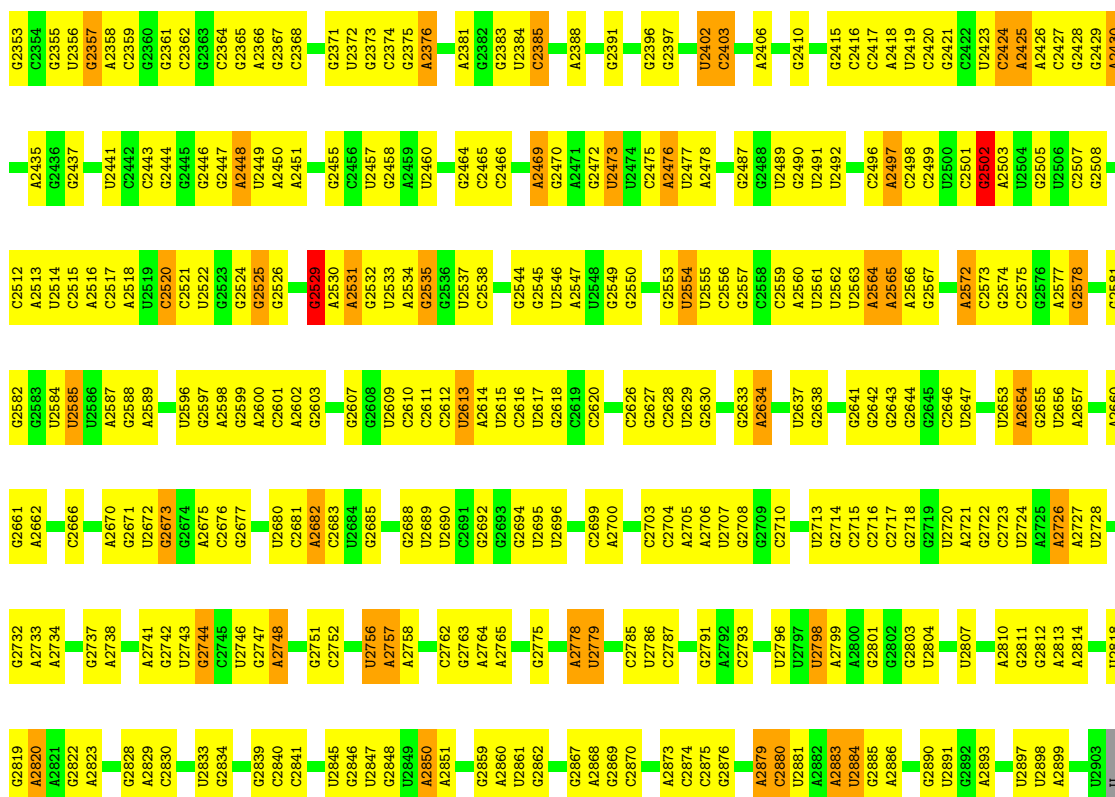


• Molecule 51: 23S rRNA

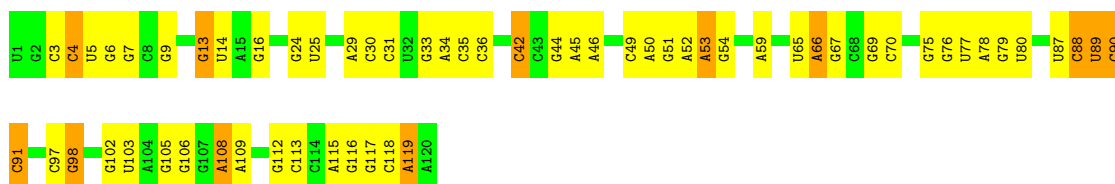
Chain 1: 44% 48% 8%



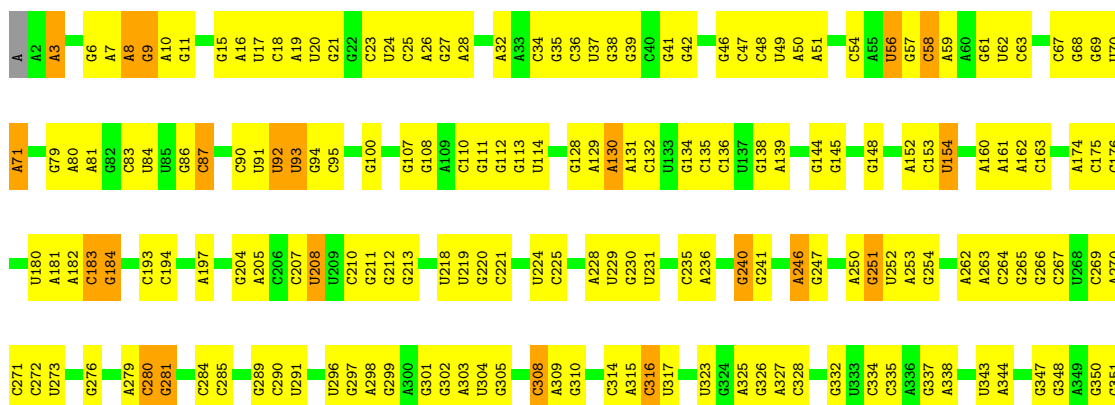
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C2196	C2197	A2198	A2199	G2200	G2201	U2202	U2203	G2204	A2205	G2206	G2207	G2208	G2209	U2210	A2211	A2212	G2213	G2214	G2215	G2216	G2221	G2222	A2225	G2226	A2227	A2228	G2230	G2234	G2235	U2236	G2237	G2238	G2239	A2247	G2248	U2249	G2250	G2251	G2255	G2256	U2257	G2258	U2262	G2263	A2267	A2268	G2269	A2270	G2271	U2272	A2273			
G2124	G2125	A2126	G2127	G2128	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	A2141	A2142	G2143	G2144	G2145	C2146	U2151	G2152	A2154	U2155	G2156	G2157	A2158	G2162	C2165	U2166	G2167	G2168	U2172	U2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2187	U2188	U2189	A2190	A2191	G2194	U2195			
G2048	G2049	A2050	A2051	A2052	C2055	G2056	A2059	G2060	A2061	A2062	C2063	G2064	C2065	G2066	G2067	U2068	G2069	A2070	A2071	C2072	C2073	U2074	A2080	U2081	A2082	G2083	U2086	G2087	U2092	G2093	A2094	U2099	G2100	A2101	G2102	C2103	U2106	U2107	A2108	U2111	G2112	U2113	A2114	G2115	U2118	U2119	A2120	G2121	U2122	G2123				
C1874	G1884	A1889	A1890	C1893	C1894	A1900	A1901	C1902	G1903	G1904	C1905	A1912	A1913	C1914	U1917	A1918	U1923	C1924	C1925	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1951	A1952	A1953	G1954	U1955	U1956	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970						
C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1803	C1804	A1805	C1806	G1807	A1808	A1809	A1810	G1811	A1815	C1816	U1817	U1818	A1819	U1820	A1821	C1822	G1823	G1824	U1825	G1826	U1827	G1828	A1829	C1830	C1832	C1833	C1836	C1837	U1841	G1842	C1843	C1844	A1853	A1854	U1855	U1856	G1857	A1858	G1863	U1864	G1867	C1868	G1869	C1870		
U1716	A1717	G1718	G1719	C1730	U1736	G1737	G1738	A1739	U1740	G1741	U1742	G1743	A1744	A1745	A1746	U1747	C1748	C1752	G1753	A1754	A1755	G1756	A1757	U1758	A1759	G1760	C1761	C1764	G1767	G1770	C1771	A1772	A1773	C1774	U1775	G1776	U1777	A1780	U1781	U1782	A1783	A1784	A1785	A1786	C1787	A1788	A1789	C1790	A1791	G1792	C1793	A1794		
C1638	C1639	G1643	A1640	A1641	G1642	G1643	C1644	G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1652	G1653	A1654	A1655	C1656	U1657	C1658	G1659	G1660	G1661	G1662	G1663	A1664	A1665	G1666	G1667	C1674	C1675	A1676	A1677	A1678	A1679	U1680	G1681	C1686	G1687	C1694	G1695	C1696	G1697	A1698	G1699	A1700	A1701	G1707	C1710	A1711	C1715		
C1550	A1551	G1555	C1558	U1559	C1564	C1565	A1566	U1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	A1580	G1581	C1582	G1587	G1588	A1591	C1592	A1593	U1594	C1595	A1596	A1597	A1598	U1599	C1600	G1601	U1602	A1603	C1607	A1608	A1609	A1614	C1615	A1616	C1617	A1618	G1619	G1620	U1621	U1622	C1625	A1626	A1630	G1631					
C1461	C1462	C1463	A1464	U1468	A1469	A1470	G1473	U1474	G1475	A1478	U1481	G1482	G1483	U1484	U1485	U1486	A1490	A1504	U1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	A1515	G1518	G1521	A1522	U1523	G1524	A1528	G1529	C1532	A1534	A1535	U1536	A1537	U1538	A1539	U1540	G1541	U1542	A1545	A1546	C1547	A1548	A1549	A1550				
G1369	C1370	G1371	U1372	A1373	C1374	A1378	U1379	G1380	A1383	A1387	G1388	G1389	U1390	U1391	U1394	A1395	U1396	U1397	A1403	C1404	U1409	G1410	U1411	U1412	A1413	G1414	U1415	G1416	C1417	G1418	A1419	A1420	G1424	G1425	C1428	G1429	G1432	A1433	A1434	A1439	U1440	G1444	G1445	G1446	A1447	G1448	A1453							
C1289	C1294	C1297	G1300	A1301	A1302	A1303	A1304	G1305	C1306	A1307	A1308	G1309	G1310	G1311	U1312	U1313	C1319	A1321	A1322	U1325	A1326	G1327	U1328	G1329	G1330	G1331	G1332	G1333	G1334	G1337	G1338	G1339	U1340	U1341	A1342	G1343	U1352	A1353	A1354	A1355	A1356	C1357	G1360	G1361	C1362	C1363	G1364	A1365	A1366	G1368	A1369			
G1197	U1198	U1203	A1204	A1205	G1206	U1209	G1210	C1211	G1212	G1216	U1219	G1220	G1221	G1225	A1226	C1229	A1230	G1236	A1246	G1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	C1257	U1258	G1259	A1262	A1265	G1266	U1267	A1268	A1269	G1270	G1271	A1272	A1275	A1276	G1277	G1278	G1279	G1287	G1288						
C1125	A1126	A1127	G1128	A1129	U1130	G1131	U1132	A1133	G1134	C1135	G1136	G1137	G1138	G1139	C1140	U1141	A1142	A1143	A1144	C1145	C1146	A1147	U1148	C1153	G1154	A1155	A1156	G1157	C1158	C1161	G1162	A1169	C1170	G1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1185	G1186	G1187	G1191	G1192	G1193	C1196



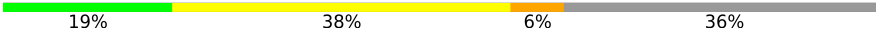
• Molecule 52: 5S rRNA



• Molecule 53: 16S rRNA



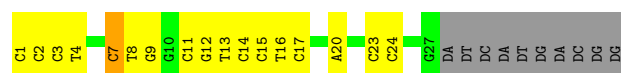
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A1492	C1402	G1253	A1179	G1099	A1022	G946	A860	C770	U684	U598	G514	U426	G354
A1493	C1403	A1254	A1180	C1100	U1023	G947	A861	G771	G685	G599	G515	U427	C355
G1494	C1404	G1255	G1181	A1102	G1024	U950	G862	U772	G690	A600	G516	G428	A356
U1495	G1405	G1331	G1182	C1103	U1025	U951	U863	G773	G691	G601	G517	U429	G357
U1496	U1406	A1257	U1183	C1104	G1026	U952	A864		G690	A602	C518	U358	U358
C1407	C1407	G1184	G1184	A1105	G1027	U953	A865	A777	G691	A607	C519	A431	G359
A1408	A1408	G1185	G1185	C1106	U1028	U954	G866	G778	U701	A608	A520	A432	G362
C1409	C1409	G1186	G1186	C1107	U1029	G954	G867	G779	U702		C528	G433	G363
A1412	C1412	A1188	A1188	G1108	U1030	U955	A872	A782	G703	C613	G529	U434	A363
A1413	A1413	C1109	C1109	C1109	G1031	U956	A873	A782	A706	C620	G530	U437	A366
U1414	G1415	A1111	A1111	A1110	G1032	U957	G874	A792	U793	A621	U531	U438	U867
		A1117	A1118	U1118	G1033	A958	U875	U793	G710	A622	A532	U439	U867
		A1117	A1118	U1118	G1034	A959	C876	U794	G710	A533	A533	C440	G369
		A1117	A1118	U1118	A1035	U960	C877	C795	G713	G624	U534	G445	C372
		A1117	A1118	U1118	A1042	U961	A878	C796	G714	U625	U535		
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		A1117	A1118	U1118	G1044	G963	G882	U804	G722	G627	G540	G377	G377
		A1117	A1118	U1118	G1047	G964	C883	C805	G723	U632	U552	G386	C386
		A1117	A1118	U1118	G1048	G965	C884	C806	G724	A635	U553	G387	C387
		A1117	A1118	U1118	G1049	G966	U884	C806	G725	A636	A554	G388	G388
		A1117	A1118	U1118	U1049	G967	U885	A807	G726	C631	C546	G454	G380
		A1117	A1118	U1118	G1050	A968	G886		G727	U632	A546	G455	
		A1117	A1118	U1118	G1051	A969			G728	G633	A547		G384
		A1117	A1118	U1118	G1052	A970	A889	G812	G729	C634	U552	U458	C385
		A1117	A1118	U1118	G1053	G971		U813	G730	A635	U553	U459	C386
		A1117	A1118	U1118	G1054	G972	G894	A814	G731	U636	A554	A460	U387
		A1117	A1118	U1118	G1055	G973	C895	A815	G732	C637	U555	A461	G388
		A1117	A1118	U1118	G1056	A974	A900	C817	G733	U638	U556	G462	A389
		A1117	A1118	U1118	G1057	A975	A901	A818	G734	C639	C556	U390	U390
		A1117	A1118	U1118	G1058	A976	A902	A819	G735	U640	G557	U467	G391
		A1117	A1118	U1118	G1059	A977	G903	U820	C736	U641	G558	A468	C392
		A1117	A1118	U1118	G1060	A978	G904	G821	G737	C642	A560	U479	A393
		A1117	A1118	U1118	G1061	A979	U905	C826	G738	C643	U561	A479	A397
		A1117	A1118	U1118	G1062	C979	A906	U827	C739	U644	U562	U480	
		A1117	A1118	U1118	G1063	C980	A907	A831	C740	G650	C564	C483	C400
		A1117	A1118	U1118	G1064	C981	A908	G832	C741	C651	C565	A493	C401
		A1117	A1118	U1118	G1065	U981	A909	U833	C742	U652	U566	G484	C402
		A1117	A1118	U1118	G1066	U982	C910	U834	G743	U653	G566	U485	
		A1117	A1118	U1118	G1067	G993	A913	U835	G744	U657	C569	U486	U405
		A1117	A1118	U1118	G1068	A994	A914	G836	A745	C658	G570	U467	G406
		A1117	A1118	U1118	G1069	A1000	G917	U837	A746	U659	U571	A408	U409
		A1117	A1118	U1118	G1070	A1001	A923	C840	G747	C660	A572	G410	G410
		A1117	A1118	U1118	G1071	A1002	C924	U841	A748	G661	A573	G411	
		A1117	A1118	U1118	G1072	A1003	C925	U842	C750	A665	A574	G412	G413
		A1117	A1118	U1118	G1073	A1004	G926	U843	G751	A666	A575	A414	A414
		A1117	A1118	U1118	G1074	A1005	G927	U844	G752	G667	C578	A415	A415
		A1117	A1118	U1118	G1075	A1006	G928	U845	G753	G668	A579	G416	G416
		A1117	A1118	U1118	G1076	A1007	G929	U846	G754	G669	C580	G417	G417
		A1117	A1118	U1118	G1077	A1008	C934	U847	G755	G670	G581	G505	C418
		A1117	A1118	U1118	G1078	A1009	A935	U848	G756	C674	C581	G506	C419
		A1117	A1118	U1118	G1079	A1010	C936	U849	G757	A673	G582	U420	U420
		A1117	A1118	U1118	G1080	A1011	A937	U850	C758	G674	C583	U421	U421
		A1117	A1118	U1118	G1081	A1012	A938	U851	G759	A675	C584	A509	A509
		A1117	A1118	U1118	G1082	A1013	A939	U852	G760	A676	C585	A510	C422
		A1117	A1118	U1118	G1083	A1014	A940	U853	G761	U677	U593	A511	G423
		A1117	A1118	U1118	G1084	A1015	A941	U854	G762	U678	U594		
		A1117	A1118	U1118	G1085	A1016	A942	U855	G763	U679	U595		
		A1117	A1118	U1118	G1086	A1017	A943	U856	G764	U680	U596		
		A1117	A1118	U1118	G1087	A1018	A944	U857	G765	U681	A597		
		A1117	A1118	U1118	G1088	A1019	A945	U858	G766	U682	A598		
		A1117	A1118	U1118	G1089	A1020	A946	U859	G767	U683	A599		
		A1117	A1118	U1118	G1090	A1021	A947	U860	G768	U684	A600		
		A1117	A1118	U1118	G1091	A1022	A948	U861	G769	U685	A601		
		A1117	A1118	U1118	G1092	A1023	A949	U862	G770	U686	A602		
		A1117	A1118	U1118	G1093	A1024	A950	U863	G771	U687	A603		
		A1117	A1118	U1118	G1094	A1025	A951	U864	G772	U688	A604		
		A1117	A1118	U1118	G1095	A1026	A952	U865	G773	U689	A605		
		A1117	A1118	U1118	G1096	A1027	A953	U866	G774	U690	A606		
		A1117	A1118	U1118	G1097	A1028	A954	U867	G775	U691	A607		
		A1117	A1118	U1118	G1098	A1029	A955	U868	G776	U692	A608		
		A1117	A1118	U1118	G1099	A1030	A956	U869	G777	U693	A609		
		A1117	A1118	U1118	G1100	A1031	A957	U870	G778	U694	A610		
		A1117	A1118	U1118	G1101	A1032	A958	U871	G779	U695	A611		
		A1117	A1118	U1118	G1102	A1033	A959	U872	G780	U696	A612		
		A1117	A1118	U1118	G1103	A1034	A960	U873	G781	U697	A613		
		A1117	A1118	U1118	G1104	A1035	A961	U874	G782	U698	A614		
		A1117	A1118	U1118	G1105	A1036	A962	U875	G783	U699	A615		
		A1117	A1118	U1118	G1106	A1037	A963	U876	G784	U700	A616		
		A1117	A1118	U1118	G1107	A1038	A964	U877	G785	U701	A617		
		A1117	A1118	U1118	G1108	A1039	A965	U878	G786	U702	A618		
		A1117	A1118	U1118	G1109	A1040	A966	U879	G787	U703	A619		
		A1117	A1118	U1118	G1110	A1041	A967	U880	G788	U704	A620		
		A1117	A1118	U1118	G1111	A1042	A968	U881	G789	U705	A621		
		A1117	A1118	U1118	G1112	A1043	A969	U882	G790	U706	A622		
		A1117	A1118	U1118	G1113	A1044	A970	U883	G791	U707	A623		
		A1117	A1118	U1118	G1114	A1045	A971	U884	G792	U708	A624		
		A1117	A1118	U1118	G1115	A1046	A972	U885	G793	U709	A625		
		A1117	A1118	U1118	G1116	A1047	A973	U886	G794	U710	A626		
		A1117	A1118	U1118	G1117	A1048	A974	U887	G795	U711	A627		
		A1117	A1118	U1118	G1118	A1049	A975	U888	G796	U712	A628		
		A1117	A1118	U1118	G1119	A1050	A976	U889	G797	U713	A629		
		A1117	A1118	U1118	G1120	A1051	A977	U890	G798	U714	A630		
		A1117	A1118	U1118	G1121	A1052	A978	U891	G799	U715	A631		
		A1117	A1118	U1118	G1122	A1053	A979	U892	G800	U716	A632		
		A1117	A1118	U1118	G1123	A1054	A980	U893	G801	U717	A633		
		A1117	A1118	U1118	G1124	A1055	A981	U894	G802	U718	A634		
		A1117	A1118	U1118	G1125	A1056	A982	U895	G803	U719	A635		
		A1117	A1118	U1118	G1126	A1057	A983	U896	G804	U720	A636		
		A1117	A1118	U1118	G1127	A1058	A984	U897	G805	U721	A637		
		A1117	A1118	U1118	G1128	A1059	A985	U898	G806	U722	A638		
		A1117	A1118	U1118	G1129	A1060	A986	U899	G807	U723	A639		
		A1117	A1118	U1118	G1130	A1061	A987	U900	G808	U724	A640		
		A1117	A1118	U1118	G1131	A1062	A988	U901	G809	U725	A641		
		A1117	A1118	U1118	G1132	A1063	A989	U902	G810	U726	A642		
		A1117	A1118	U1118	G1133	A1064	A990	U903	G811	U727	A643</		

Chain 4: 



- Molecule 55: template DNA strand

Chain 8: 




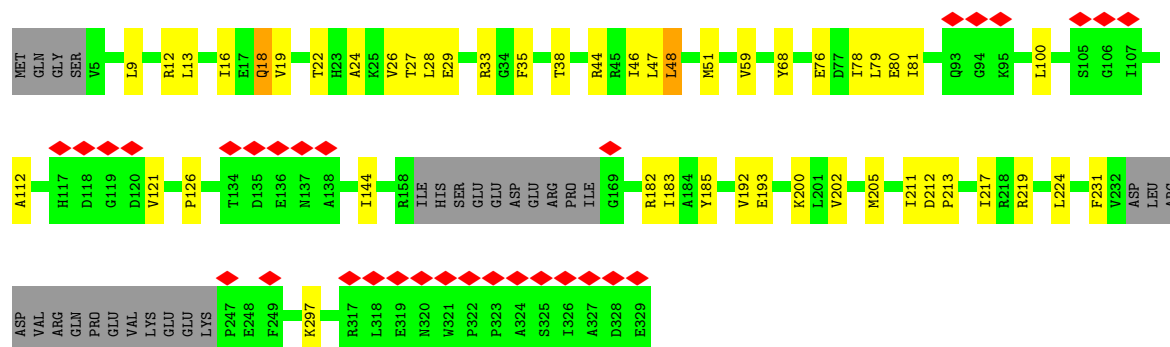
- Molecule 56: non-template DNA strand

Chain 9: 




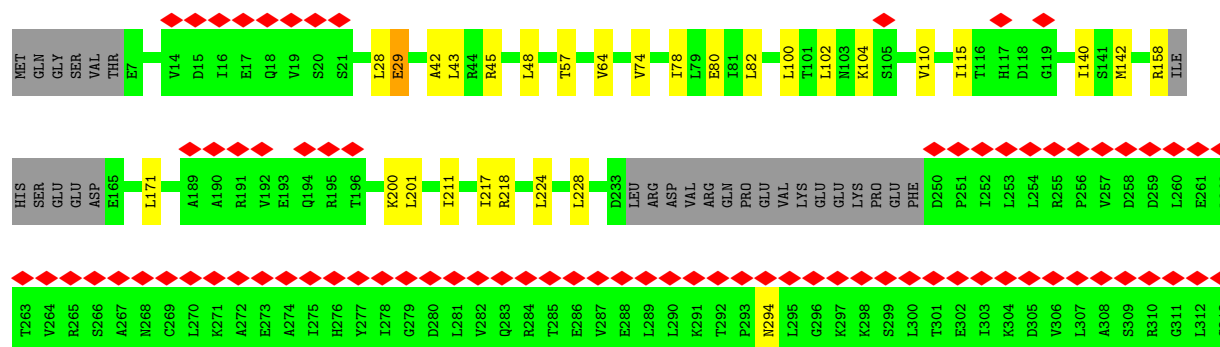
- Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain A1: 



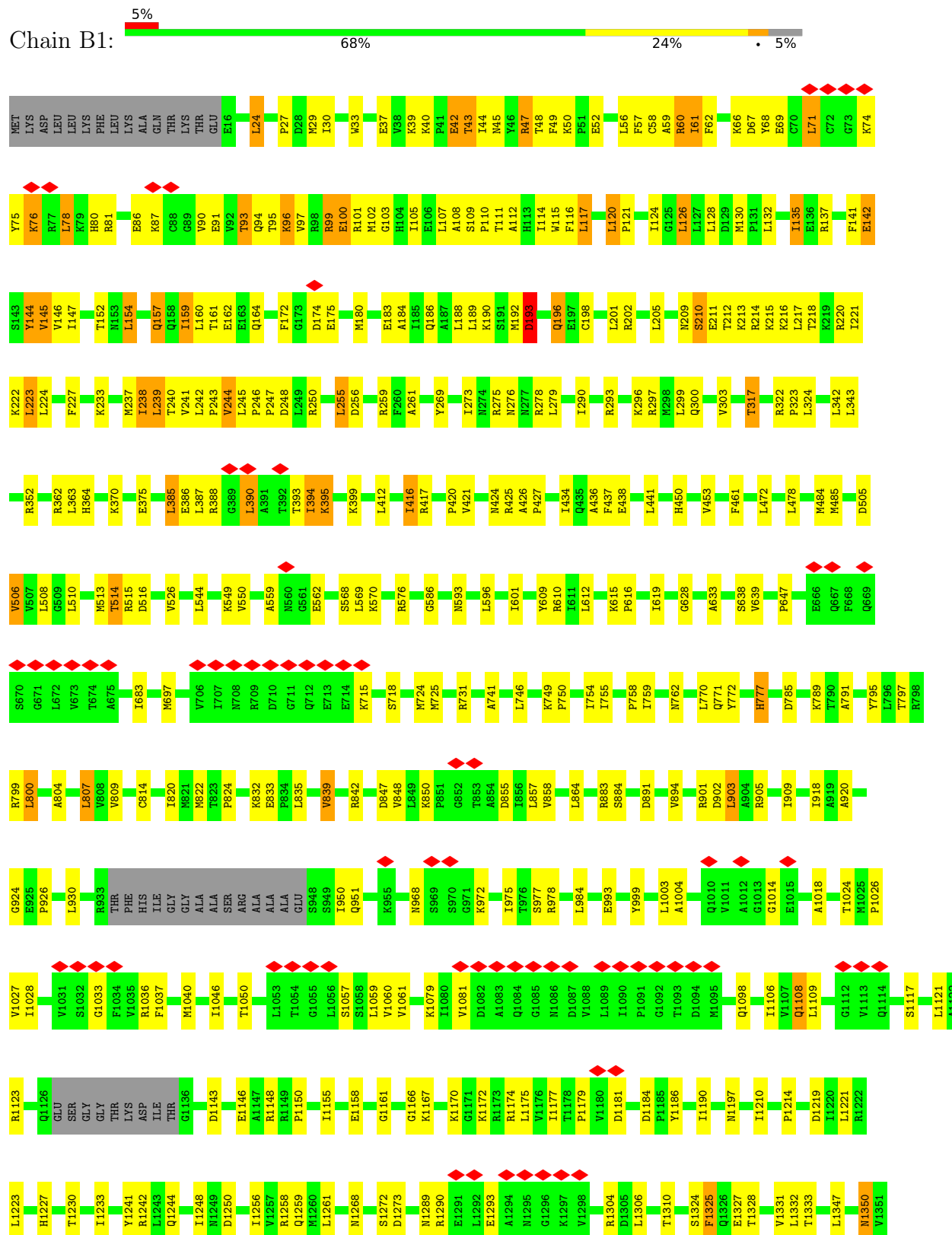
- Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain A2: 



PRO
ALA
SER
ILE
ALA
ASP
GLU

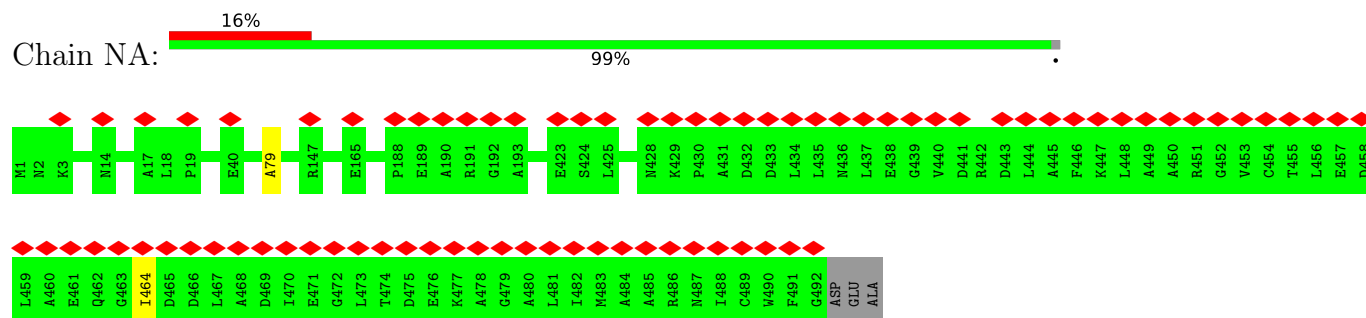
• Molecule 58: DNA-directed RNA polymerase subunit beta'



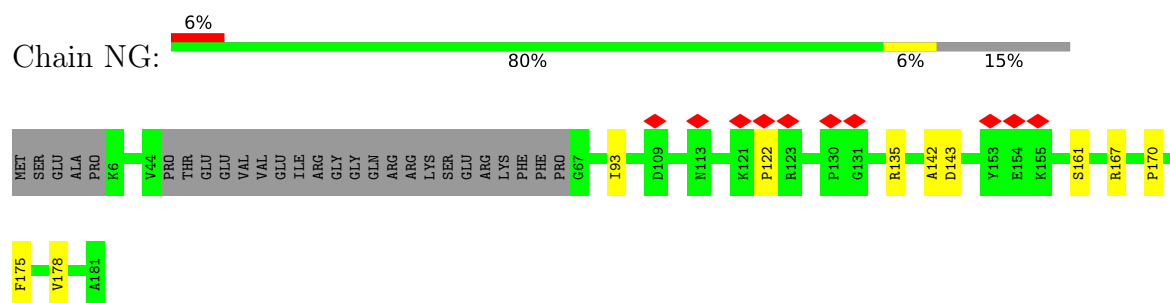


GLU
GLY
ARG
ARG

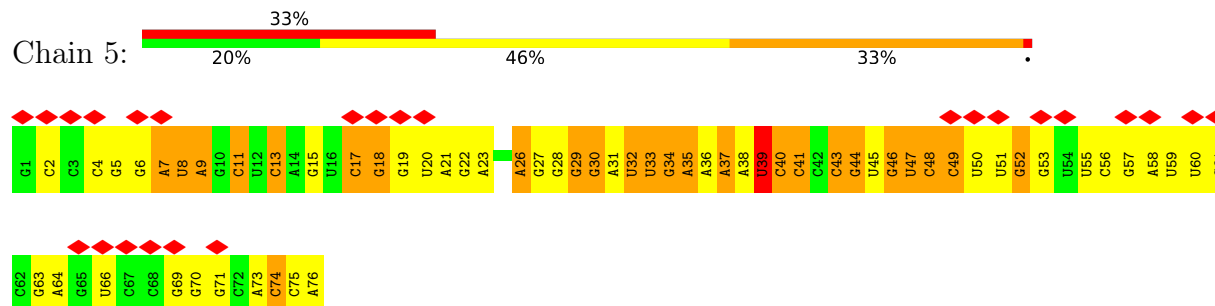
- Molecule 61: Transcription termination/antitermination protein NusA



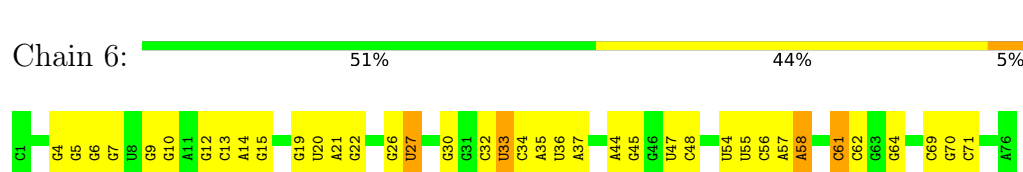
- Molecule 62: Transcription termination/antitermination protein NusG



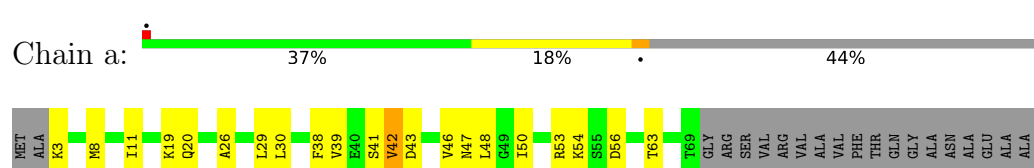
- Molecule 63: tRNA(Phe)

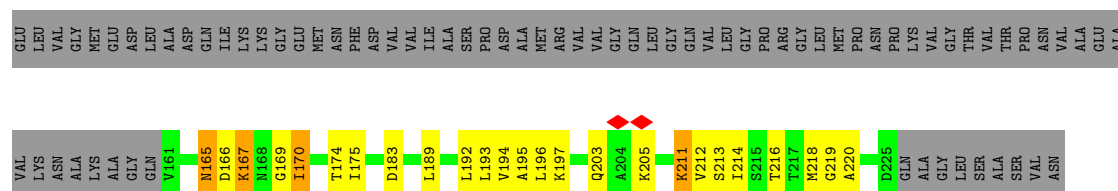


- Molecule 64: tRNA(fMet)

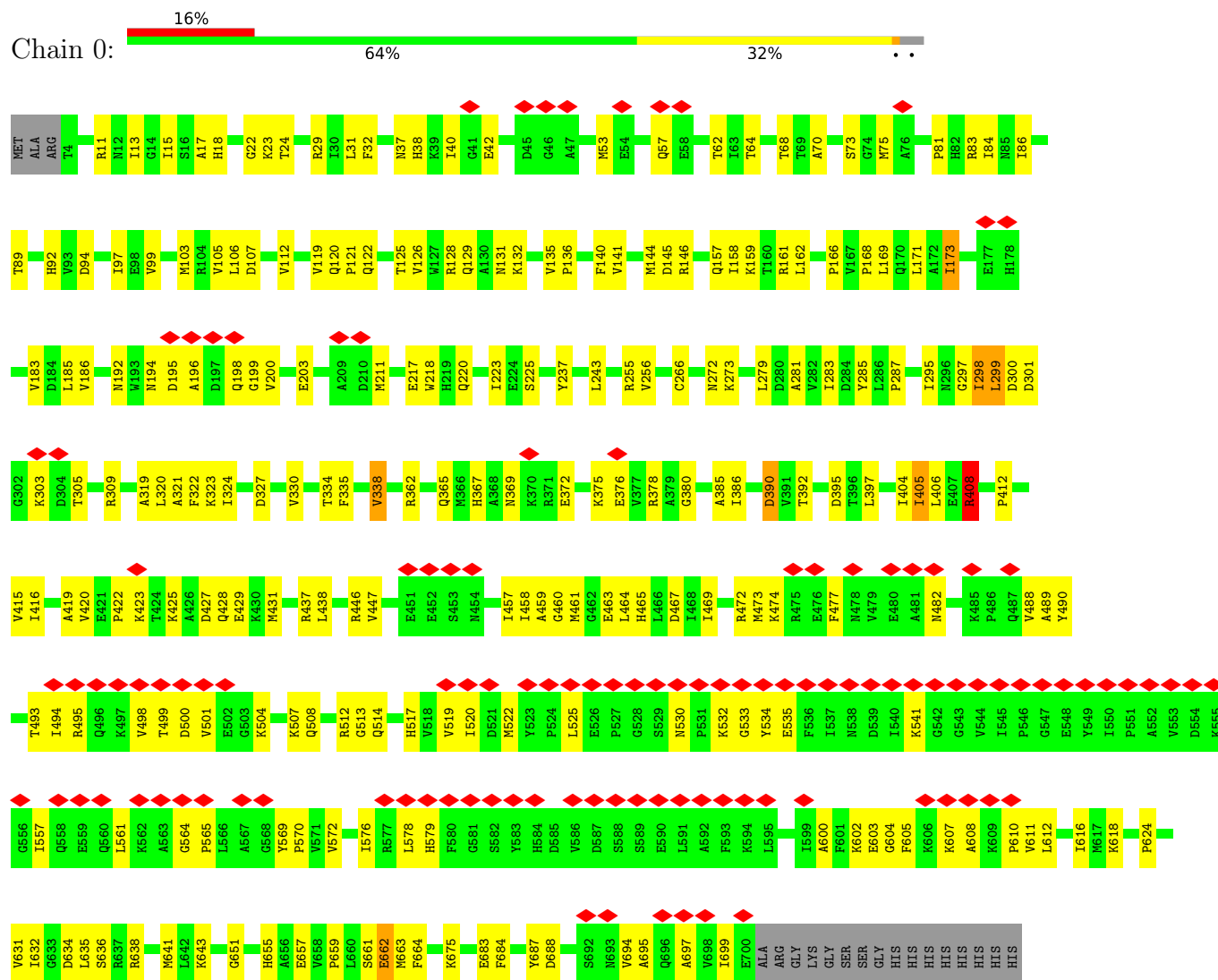


- Molecule 65: Large ribosomal subunit protein uL1





• Molecule 66: Elongation factor G



• Molecule 67: Viomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35620	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	0.082	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	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: MG, PO4, KBE, DPP, UAL, 5OH, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/362	0.73	0/485
2	B	0.37	0/450	0.80	2/599 (0.3%)
3	C	0.31	0/416	0.61	0/554
4	D	0.48	0/380	0.95	0/498
5	E	0.46	0/513	0.80	0/676
6	F	0.40	0/303	0.79	0/397
7	G	0.41	0/1735	0.83	0/2338
8	H	0.41	0/1651	0.80	0/2225
9	I	0.31	0/1665	0.77	1/2227 (0.0%)
10	J	0.47	0/1169	0.81	0/1573
11	K	0.44	0/835	0.87	0/1128
12	L	0.41	0/1195	0.82	2/1602 (0.1%)
13	M	0.31	0/989	0.75	0/1326
14	N	0.29	0/1034	0.74	0/1375
15	O	0.56	0/796	0.81	0/1077
16	P	0.47	0/885	0.78	0/1195
17	Q	0.42	0/969	0.80	0/1300
18	R	0.28	0/892	0.68	0/1193
19	S	0.28	0/817	0.68	1/1088 (0.1%)
20	T	0.37	0/722	0.74	0/964
21	U	0.29	0/659	0.63	0/884
22	V	0.33	0/657	0.72	0/881
23	W	0.28	0/544	0.69	0/731
24	X	0.28	0/652	0.65	0/877
25	Y	0.26	0/671	0.64	2/888 (0.2%)
26	Z	0.56	0/550	1.09	1/728 (0.1%)
27	b	0.49	0/2121	0.82	0/2852
28	c	0.45	0/1586	0.77	0/2134
29	d	0.40	0/1571	0.80	3/2113 (0.1%)
30	e	0.32	0/1434	0.66	0/1926
31	f	0.29	0/1343	0.61	0/1816
32	g	0.41	0/1122	0.73	1/1515 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.39	0/1046	0.80	1/1410 (0.1%)
34	j	0.46	0/1152	0.72	0/1551
35	k	0.42	0/947	0.91	1/1268 (0.1%)
36	l	0.41	1/1054 (0.1%)	0.80	2/1403 (0.1%)
37	m	0.39	0/1093	0.81	2/1460 (0.1%)
38	n	0.54	1/973 (0.1%)	0.87	0/1301
39	o	0.32	0/902	0.68	0/1209
40	p	0.39	0/929	0.72	0/1242
41	q	0.43	0/960	0.72	0/1278
42	r	0.42	0/829	0.79	0/1107
43	s	0.52	0/864	0.83	0/1156
44	t	0.48	0/744	0.81	1/994 (0.1%)
45	u	0.38	0/787	0.75	2/1051 (0.2%)
46	v	0.35	0/766	0.66	0/1025
47	w	0.40	0/582	0.80	2/769 (0.3%)
48	x	0.64	0/635	1.13	4/848 (0.5%)
49	y	0.28	0/510	0.71	0/677
50	z	0.36	0/453	0.76	1/605 (0.2%)
51	1	0.59	0/69796	0.60	12/108888 (0.0%)
52	2	0.60	0/2872	0.55	1/4479 (0.0%)
53	3	0.60	0/36963	0.57	4/57662 (0.0%)
54	4	0.61	0/695	0.77	0/1076
55	8	0.56	0/599	0.70	1/919 (0.1%)
56	9	0.49	0/468	0.53	0/719
57	A1	0.56	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.56	4/10510 (0.0%)	0.74	8/14196 (0.1%)
59	B2	0.45	0/10714	0.66	0/14459
60	W0	0.30	0/652	0.61	0/879
61	NA	0.76	0/2431	1.22	0/3385
62	NG	1.16	0/756	1.03	0/1048
63	5	0.59	0/1812	0.90	3/2823 (0.1%)
64	6	0.59	0/1832	0.59	0/2855
65	a	0.49	0/1020	0.81	0/1370
66	0	0.40	0/5501	0.72	3/7446 (0.0%)
67	h	3.21	2/11 (18.2%)	0.75	0/13
All	All	0.54	8/196700 (0.0%)	0.67	61/289390 (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
66	0	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	3	SER	CA-C	-6.73	1.38	1.52
67	h	4	SER	CA-C	-6.31	1.39	1.52
38	n	66	ALA	CA-C	-5.95	1.44	1.52
58	B1	1350	ASN	CG-ND2	-5.26	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.16	1.33	1.23

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	PRO	N-CA-C	-10.48	98.48	113.47
51	1	1020	A	C2'-C3'-O3'	7.36	120.54	109.50
48	x	11	PRO	N-CA-C	-7.35	99.50	111.77
12	L	82	SER	N-CA-C	6.91	116.43	108.49
58	B1	450	HIS	CB-CG-CD2	-6.57	122.66	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	0	408	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	355	0	353	10	0
2	B	444	0	461	14	0
3	C	409	0	440	17	0
4	D	377	0	418	17	0
5	E	504	0	574	16	0
6	F	302	0	341	14	0
7	G	1704	0	1732	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1624	0	1699	43	0
9	I	1643	0	1710	47	0
10	J	1156	0	1199	38	0
11	K	817	0	808	23	0
12	L	1181	0	1240	44	0
13	M	979	0	1034	32	0
14	N	1022	0	1070	56	0
15	O	786	0	828	32	0
16	P	869	0	878	27	0
17	Q	955	0	1019	34	0
18	R	883	0	944	23	0
19	S	805	0	847	33	0
20	T	714	0	737	18	0
21	U	649	0	666	21	0
22	V	648	0	691	17	0
23	W	535	0	552	15	0
24	X	637	0	665	17	0
25	Y	665	0	714	21	0
26	Z	544	0	579	16	0
27	b	2082	0	2157	73	0
28	c	1565	0	1616	57	0
29	d	1552	0	1619	50	0
30	e	1410	0	1447	40	0
31	f	1323	0	1374	30	0
32	g	1111	0	1148	33	0
33	i	1032	0	1088	34	0
34	j	1129	0	1162	31	0
35	k	938	0	1012	21	0
36	l	1045	0	1117	30	0
37	m	1074	0	1157	29	0
38	n	960	0	1000	34	0
39	o	892	0	923	21	0
40	p	917	0	965	23	0
41	q	947	0	1022	23	0
42	r	816	0	839	24	0
43	s	857	0	922	19	0
44	t	738	0	807	15	0
45	u	779	0	834	23	0
46	v	753	0	780	14	0
47	w	575	0	592	21	0
48	x	625	0	655	23	0
49	y	509	0	543	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	z	449	0	491	10	0
51	1	62317	0	31346	1363	0
52	2	2568	0	1303	59	0
53	3	33012	0	16618	723	0
54	4	627	0	313	8	0
55	8	539	0	305	28	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	27	0
57	A2	2029	0	1864	20	0
58	B1	10353	0	10548	321	0
59	B2	10546	0	10550	171	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	3	0
62	NG	758	0	334	9	0
63	5	1622	0	821	31	0
64	6	1640	0	837	24	0
65	a	1013	0	1081	35	0
66	0	5399	0	5363	154	0
67	h	48	0	40	6	0
68	B1	1	0	0	0	0
69	0	28	0	12	1	0
70	0	5	0	0	0	0
All	All	183377	0	132752	3780	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 12.

The worst 5 of 3780 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)
12:L:92:PRO:HA	12:L:95:ARG:HE	1.12	1.13
51:1:1060:U:H4'	51:1:1061:U:H5'	1.32	1.10
53:3:112:G:H21	53:3:354:G:H5'	1.16	1.10
51:1:2061:G:H2'	51:1:2501:C:O2'	1.52	1.08
50:z:37:ARG:HH12	51:1:929:U:H5'	1.12	1.07

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	44/70 (63%)	38 (86%)	6 (14%)	0	100	100
2	B	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
3	C	48/55 (87%)	37 (77%)	11 (23%)	0	100	100
4	D	44/46 (96%)	35 (80%)	9 (20%)	0	100	100
5	E	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	8	38
6	F	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
7	G	216/241 (90%)	181 (84%)	35 (16%)	0	100	100
8	H	204/233 (88%)	187 (92%)	17 (8%)	0	100	100
9	I	203/206 (98%)	169 (83%)	33 (16%)	1 (0%)	25	62
10	J	155/167 (93%)	129 (83%)	26 (17%)	0	100	100
11	K	98/135 (73%)	79 (81%)	19 (19%)	0	100	100
12	L	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
13	M	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
14	N	125/130 (96%)	110 (88%)	15 (12%)	0	100	100
15	O	96/103 (93%)	82 (85%)	14 (15%)	0	100	100
16	P	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
17	Q	121/124 (98%)	97 (80%)	23 (19%)	1 (1%)	16	54
18	R	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
19	S	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
20	T	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
21	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
22	V	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
23	W	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
24	X	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
25	Y	83/87 (95%)	77 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	63/71 (89%)	47 (75%)	16 (25%)	0	100	100
27	b	269/273 (98%)	227 (84%)	42 (16%)	0	100	100
28	c	207/209 (99%)	177 (86%)	30 (14%)	0	100	100
29	d	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
30	e	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
31	f	174/177 (98%)	157 (90%)	17 (10%)	0	100	100
32	g	147/149 (99%)	125 (85%)	20 (14%)	2 (1%)	9	40
33	i	139/142 (98%)	124 (89%)	15 (11%)	0	100	100
34	j	140/142 (99%)	120 (86%)	20 (14%)	0	100	100
35	k	120/123 (98%)	98 (82%)	22 (18%)	0	100	100
36	l	141/144 (98%)	117 (83%)	24 (17%)	0	100	100
37	m	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
38	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
39	o	114/117 (97%)	103 (90%)	11 (10%)	0	100	100
40	p	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
41	q	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
42	r	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
43	s	108/110 (98%)	92 (85%)	16 (15%)	0	100	100
44	t	91/100 (91%)	77 (85%)	14 (15%)	0	100	100
45	u	100/104 (96%)	82 (82%)	18 (18%)	0	100	100
46	v	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
47	w	73/85 (86%)	63 (86%)	10 (14%)	0	100	100
48	x	75/78 (96%)	65 (87%)	10 (13%)	0	100	100
49	y	61/63 (97%)	61 (100%)	0	0	100	100
50	z	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	22 (8%)	0	100	100
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1207 (91%)	118 (9%)	4 (0%)	37	71
59	B2	1338/1342 (100%)	1205 (90%)	129 (10%)	4 (0%)	37	71
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	476 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	NG	150/181 (83%)	137 (91%)	12 (8%)	1 (1%)	19	56
65	a	128/234 (55%)	105 (82%)	23 (18%)	0	100	100
66	0	695/716 (97%)	617 (89%)	73 (10%)	5 (1%)	19	56
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10486/11185 (94%)	9322 (89%)	1145 (11%)	19 (0%)	45	77

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	15	LEU
58	B1	121	PRO
32	g	14	SER
59	B2	43	PRO
59	B2	918	LEU

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	42/62 (68%)	42 (100%)	0	100	100
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%)	35 (92%)	3 (8%)	10	32
5	E	51/52 (98%)	46 (90%)	5 (10%)	6	23
6	F	34/34 (100%)	33 (97%)	1 (3%)	37	58
7	G	180/199 (90%)	172 (96%)	8 (4%)	24	47
8	H	170/190 (90%)	162 (95%)	8 (5%)	22	46
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	64
10	J	119/126 (94%)	113 (95%)	6 (5%)	20	44
11	K	87/116 (75%)	82 (94%)	5 (6%)	17	41
12	L	124/147 (84%)	121 (98%)	3 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	104/105 (99%)	102 (98%)	2 (2%)	52	69
14	N	105/107 (98%)	105 (100%)	0	100	100
15	O	86/90 (96%)	78 (91%)	8 (9%)	7	25
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	53
17	Q	103/104 (99%)	101 (98%)	2 (2%)	52	69
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	79
19	S	83/84 (99%)	82 (99%)	1 (1%)	67	78
20	T	76/77 (99%)	76 (100%)	0	100	100
21	U	65/65 (100%)	65 (100%)	0	100	100
22	V	74/78 (95%)	74 (100%)	0	100	100
23	W	56/65 (86%)	56 (100%)	0	100	100
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	46 (84%)	9 (16%)	2	11
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	163 (99%)	1 (1%)	84	88
29	d	165/165 (100%)	160 (97%)	5 (3%)	36	57
30	e	148/150 (99%)	145 (98%)	3 (2%)	50	68
31	f	137/138 (99%)	136 (99%)	1 (1%)	81	86
32	g	114/114 (100%)	107 (94%)	7 (6%)	15	39
33	i	109/110 (99%)	109 (100%)	0	100	100
34	j	116/116 (100%)	113 (97%)	3 (3%)	41	61
35	k	103/104 (99%)	100 (97%)	3 (3%)	37	58
36	l	102/103 (99%)	100 (98%)	2 (2%)	50	68
37	m	109/109 (100%)	108 (99%)	1 (1%)	75	83
38	n	100/103 (97%)	98 (98%)	2 (2%)	50	68
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%)	89 (100%)	0	100	100
42	r	84/84 (100%)	83 (99%)	1 (1%)	67	78
43	s	93/93 (100%)	87 (94%)	6 (6%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	t	80/84 (95%)	77 (96%)	3 (4%)	28	50
45	u	83/85 (98%)	80 (96%)	3 (4%)	30	52
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	76
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	65 (97%)	2 (3%)	36	57
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	47 (98%)	1 (2%)	48	66
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	40
57	A2	186/286 (65%)	184 (99%)	2 (1%)	70	79
58	B1	1110/1168 (95%)	1021 (92%)	89 (8%)	10	31
59	B2	1150/1157 (99%)	1119 (97%)	31 (3%)	40	60
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	a	109/181 (60%)	98 (90%)	11 (10%)	6	22
66	0	574/588 (98%)	550 (96%)	24 (4%)	25	48
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8120/8683 (94%)	7832 (96%)	288 (4%)	33	53

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	B2	546	GLU
66	0	662	GLU
59	B2	894	GLN
65	a	211	LYS
36	l	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
58	B1	771	GLN
66	0	276	GLN
58	B1	1238	GLN
59	B2	1237	HIS
21	U	79	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	442 (15%)	8 (0%)
52	2	119/120 (99%)	18 (15%)	0
53	3	1538/1542 (99%)	193 (12%)	1 (0%)
54	4	29/47 (61%)	15 (51%)	5 (17%)
63	5	75/76 (98%)	45 (60%)	11 (14%)
64	6	76/77 (98%)	14 (18%)	0
All	All	4739/4766 (99%)	727 (15%)	25 (0%)

5 of 727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	23	G
51	1	34	U
51	1	35	G

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
63	5	7	A
63	5	34	G
63	5	75	C
63	5	32	U
63	5	35	A

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	$\# Z > 2$
67	DPP	h	2	67	3,5,6	0.56	0	1,5,7	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	UAL	h	5	67	7,8,9	2.28	3 (42%)	5,9,11	2.92	2 (40%)
67	5OH	h	6	67	8,12,13	0.83	0	3,16,18	1.49	1 (33%)
67	KBE	h	1	67	8,8,9	0.63	0	7,8,10	1.21	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	DPP	h	2	67	-	0/2/4/6	-
67	UAL	h	5	67	-	0/3/7/9	-
67	5OH	h	6	67	-	0/2/18/20	0/1/1/1
67	KBE	h	1	67	-	0/7/7/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	5	UAL	C1-N1	-4.76	1.32	1.40
67	h	5	UAL	C-CA	-2.88	1.40	1.45
67	h	5	UAL	CA-N	2.07	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	h	5	UAL	CA-CB-N1	-5.30	115.60	125.60
67	h	5	UAL	O-C-CA	-3.28	121.21	125.39
67	h	6	5OH	CR-CB-CA	-2.33	110.09	112.61
67	h	1	KBE	CB-CA-C	-2.09	109.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	h	2	DPP	1	0
67	h	5	UAL	2	0
67	h	6	5OH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
69	GDP	0	801	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
70	PO4	0	802	-	4,4,4	0.95	0	6,6,6	0.47	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
69	GDP	0	801	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	0	801	GDP	C6-N1	-2.58	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	0	801	GDP	PA-O3A-PB	-3.55	120.64	132.83
69	0	801	GDP	C5-C6-N1	2.53	118.43	113.95
69	0	801	GDP	C3'-C2'-C1'	2.53	104.79	100.98
69	0	801	GDP	C8-N7-C5	2.52	107.79	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

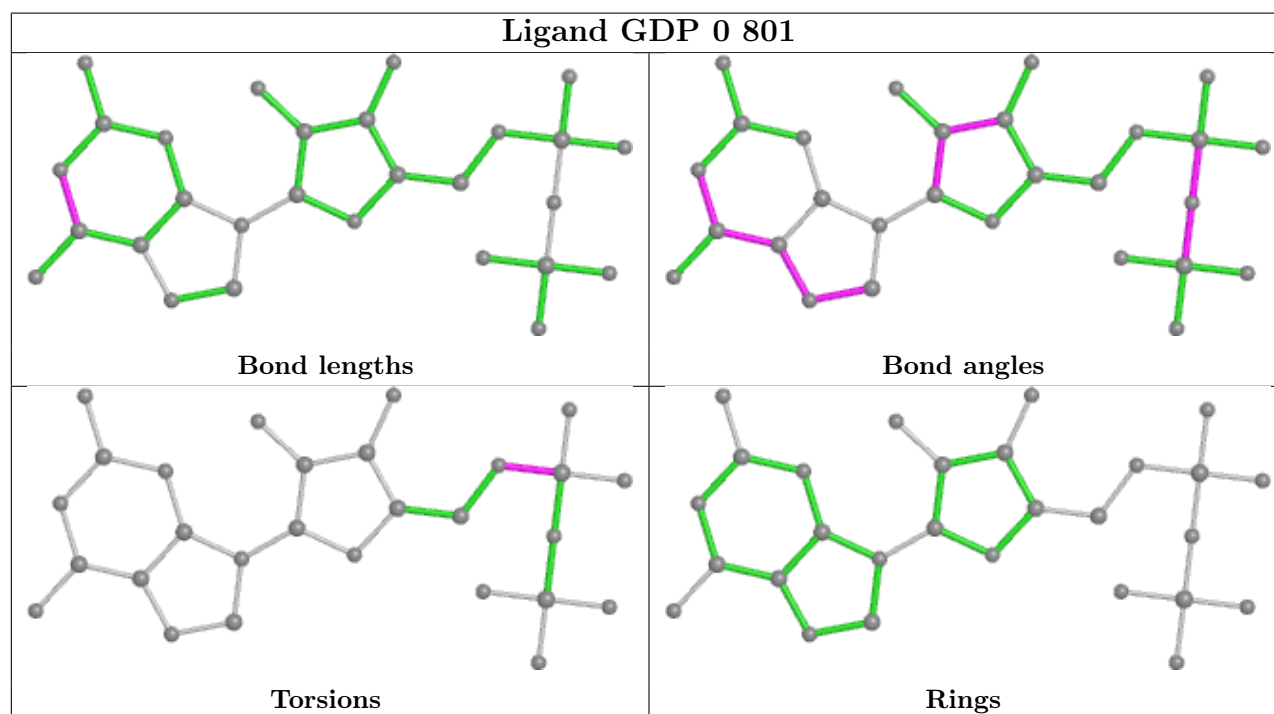
Mol	Chain	Res	Type	Atoms
69	0	801	GDP	C5'-O5'-PA-O3A
69	0	801	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	0	801	GDP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

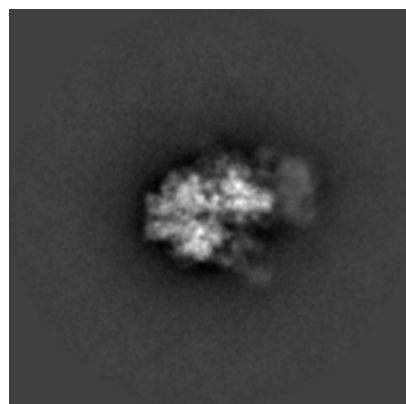
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38944. These allow visual inspection of the internal detail of the map and identification of artifacts.

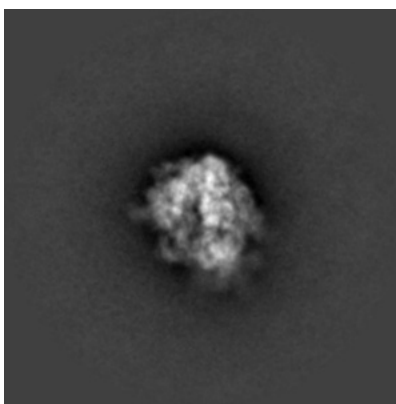
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

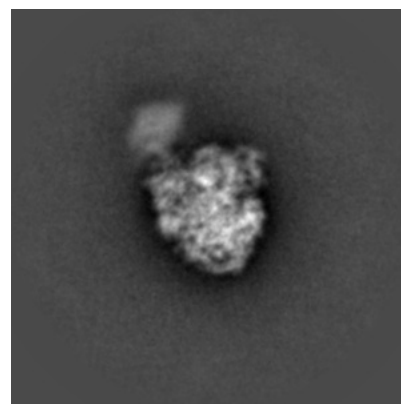
6.1.1 Primary map



X

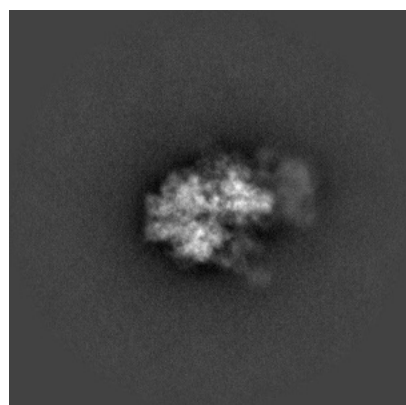


Y

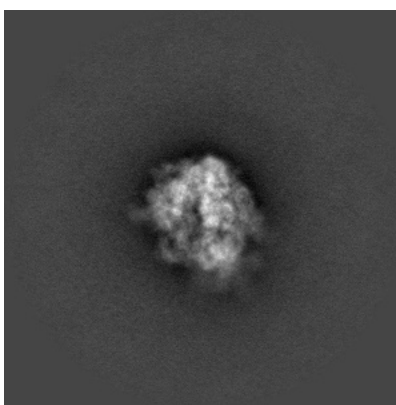


Z

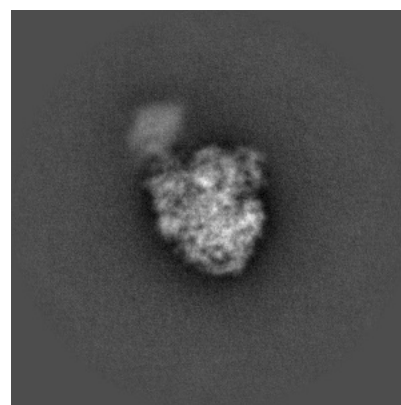
6.1.2 Raw map



X



Y

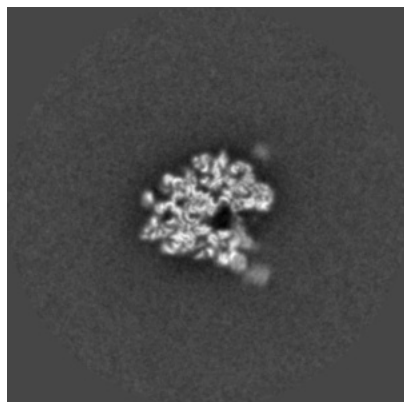


Z

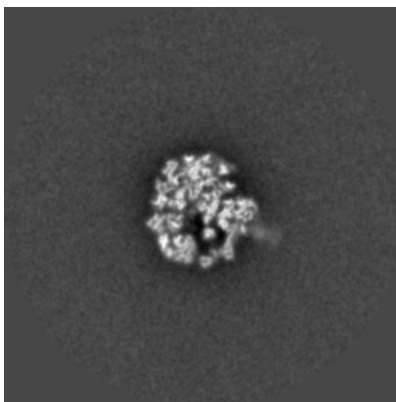
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

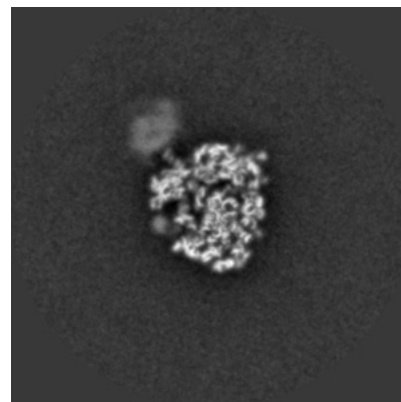
6.2.1 Primary map



X Index: 240

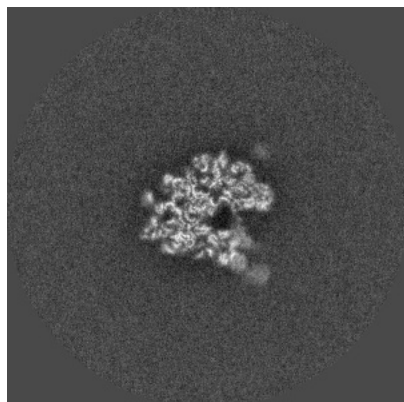


Y Index: 240

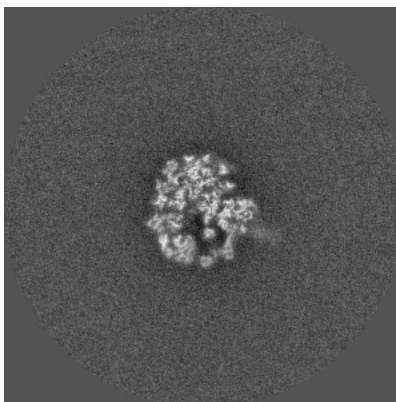


Z Index: 240

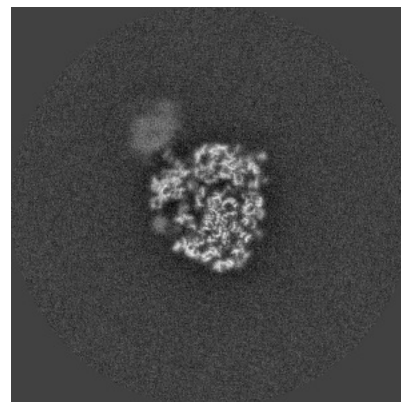
6.2.2 Raw map



X Index: 240



Y Index: 240

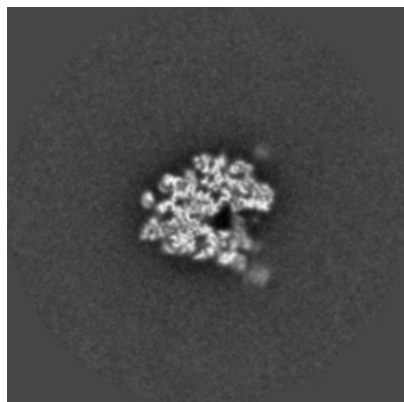


Z Index: 240

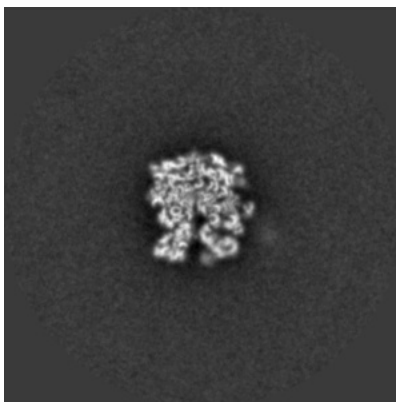
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

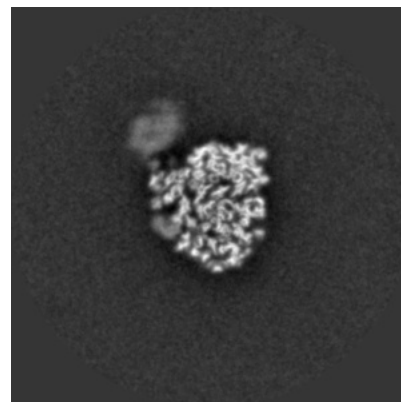
6.3.1 Primary map



X Index: 242

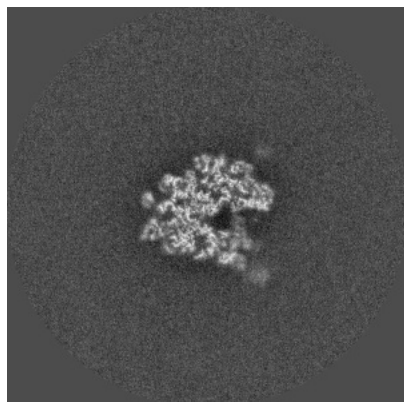


Y Index: 225

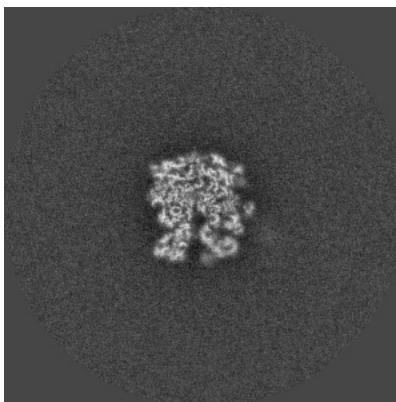


Z Index: 245

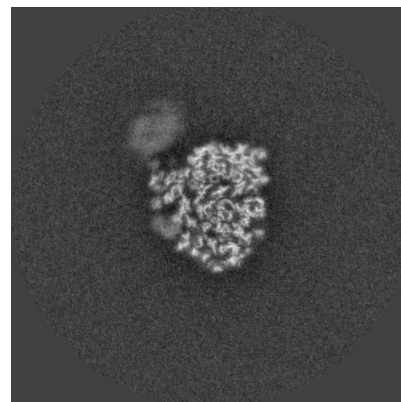
6.3.2 Raw map



X Index: 242



Y Index: 225



Z Index: 245

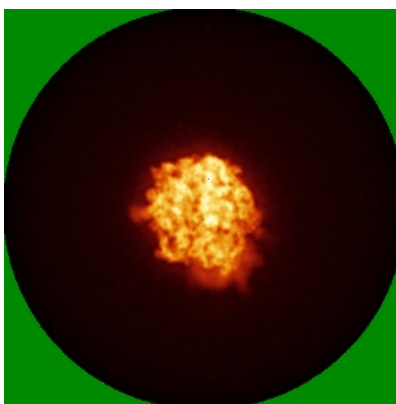
The images above show the largest variance slices of the map in three orthogonal directions.

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

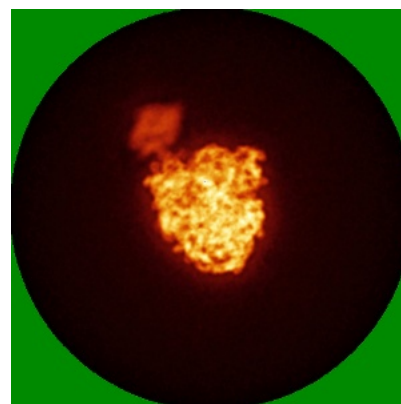
6.4.1 Primary map



X

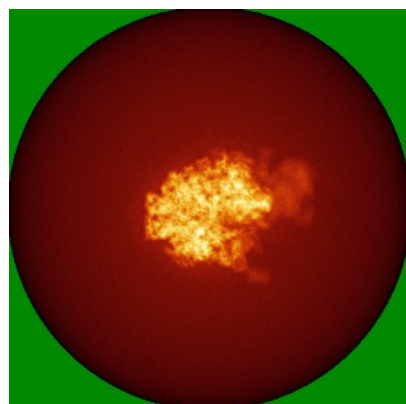


Y

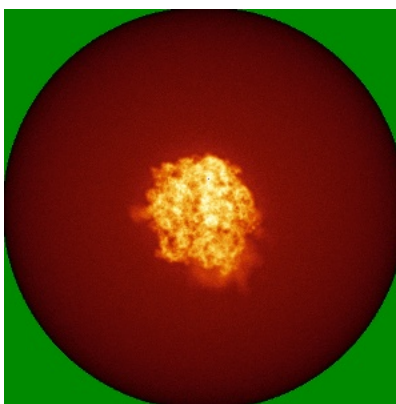


Z

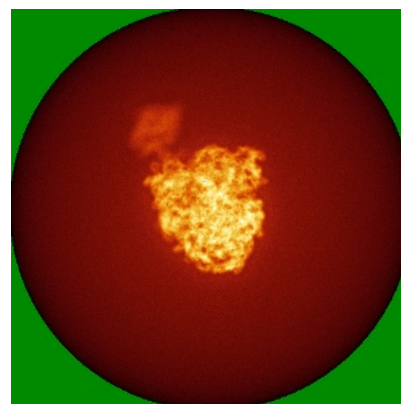
6.4.2 Raw map



X



Y



Z

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

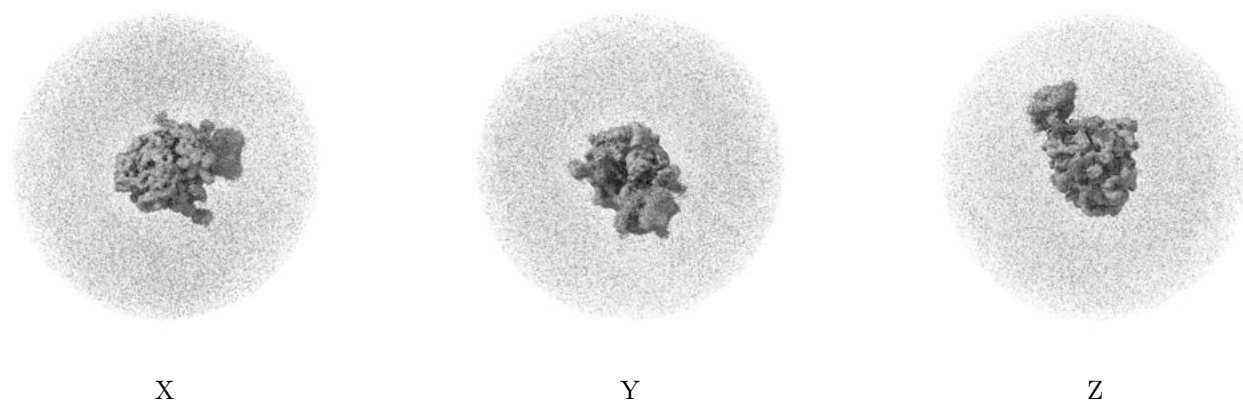
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

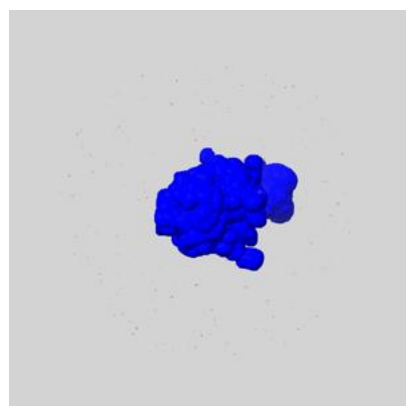
6.6 Mask visualisation [i](#)

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

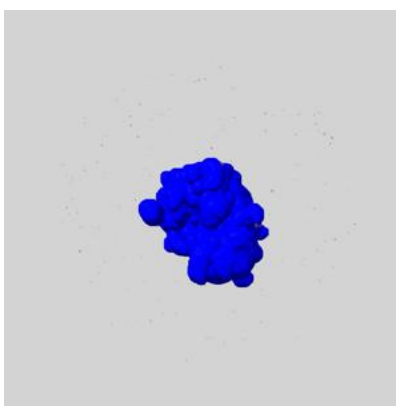
A mask typically either:

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

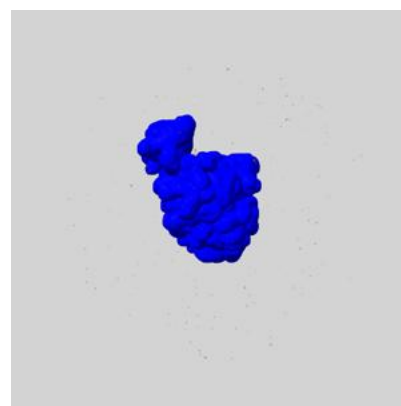
6.6.1 emd_38944_msk_1.map [i](#)



X



Y

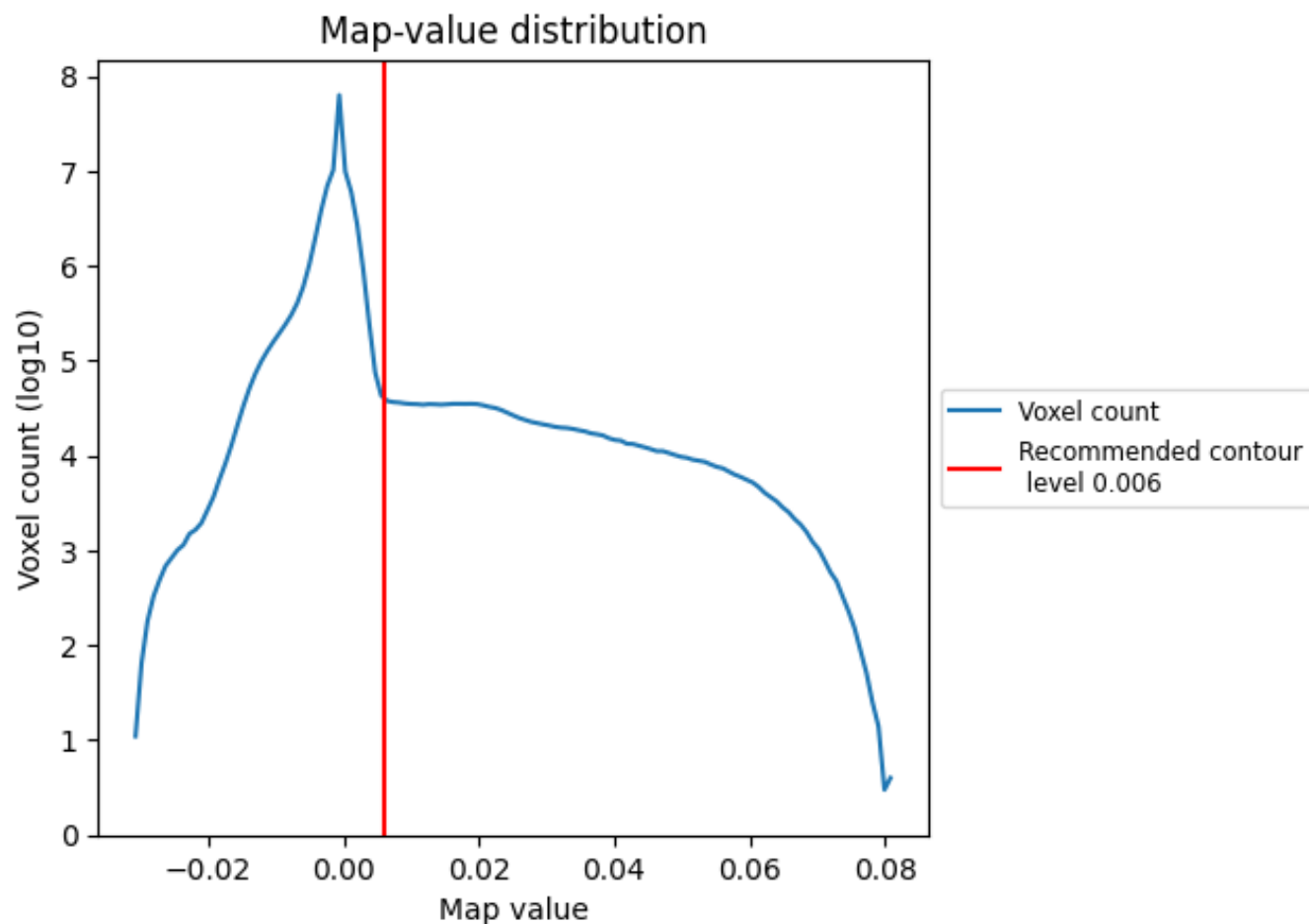


Z

7 Map analysis [i](#)

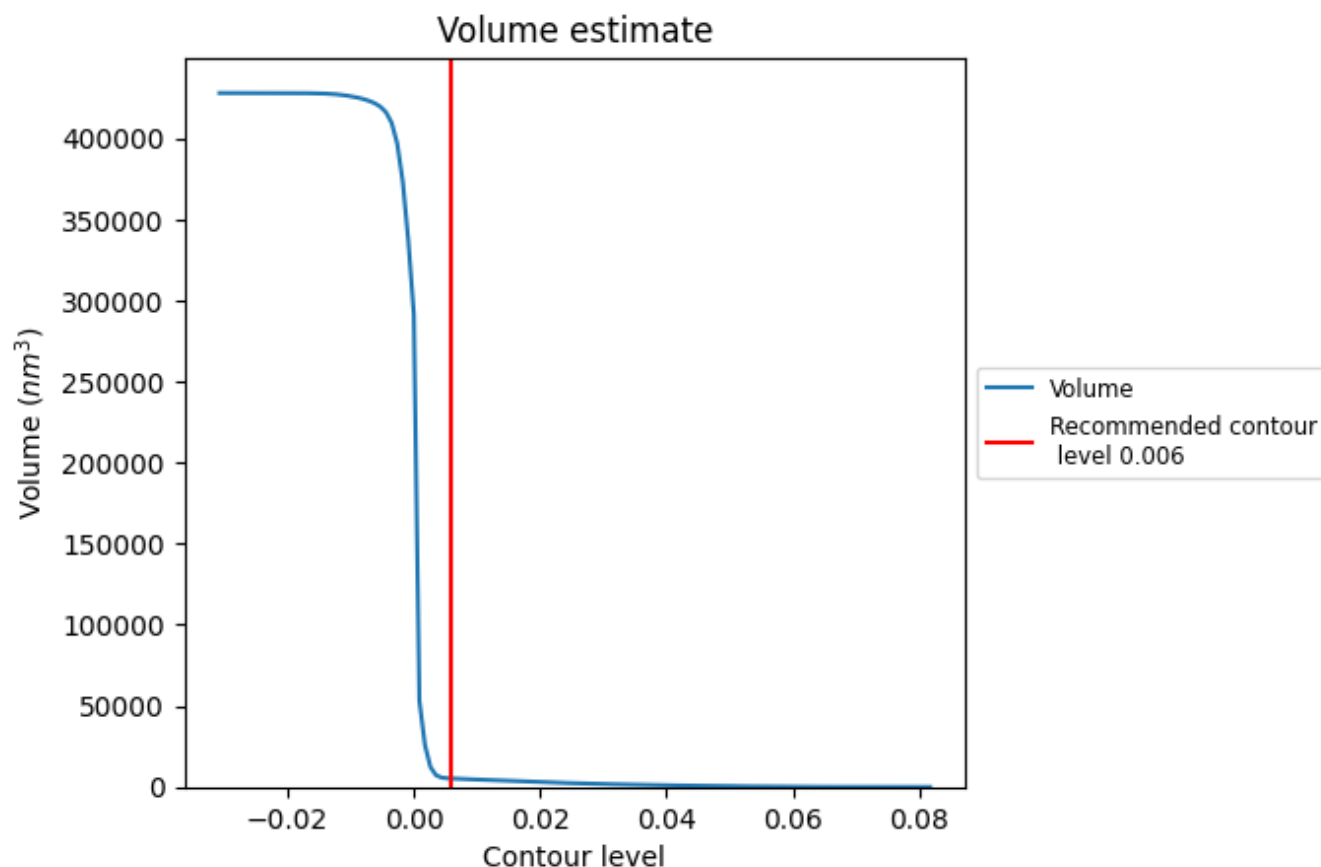
This section contains the results of statistical analysis of the map.

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.

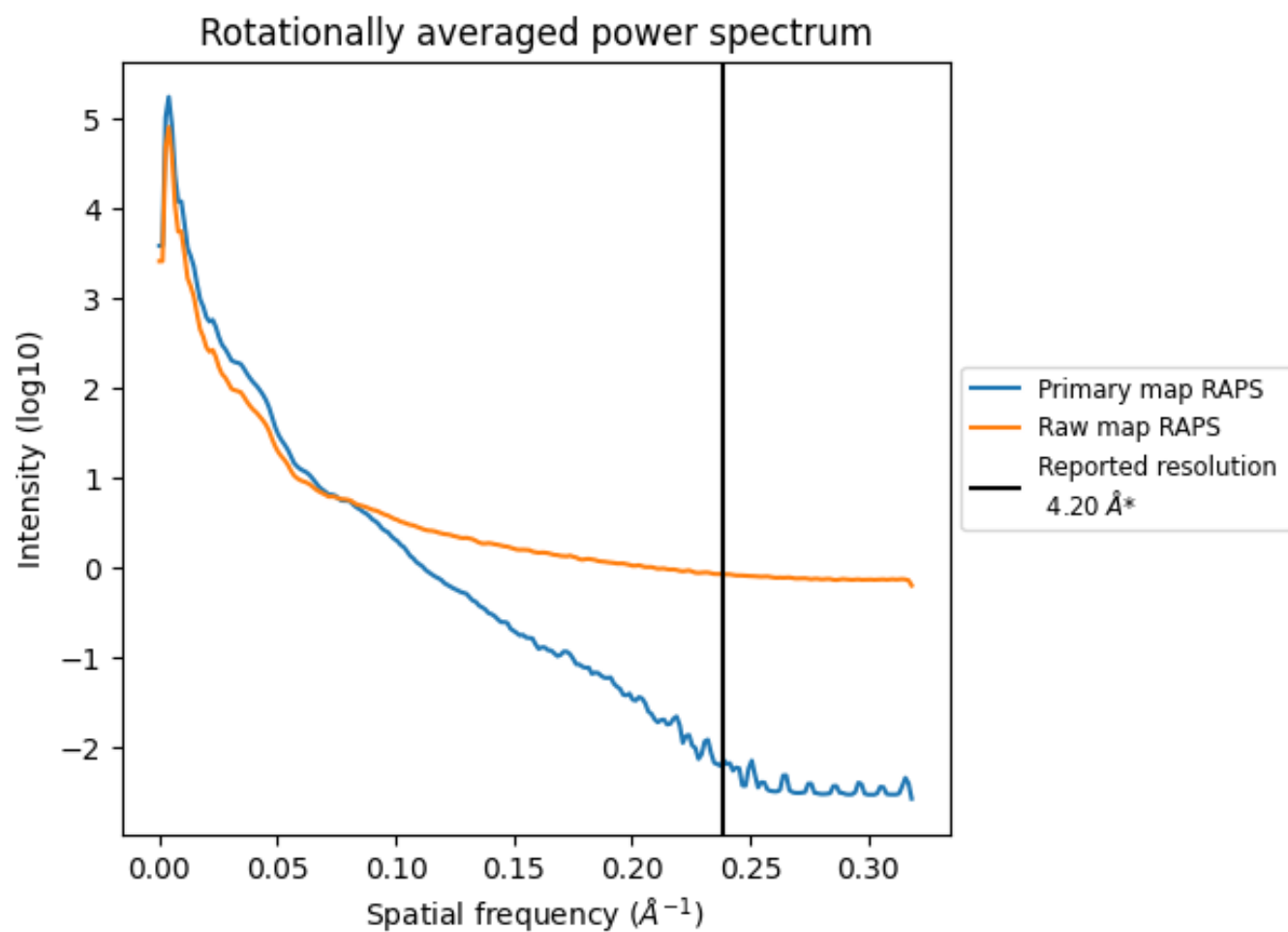
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5225 nm^3 ; this corresponds to an approximate mass of 4720 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 ⓘ

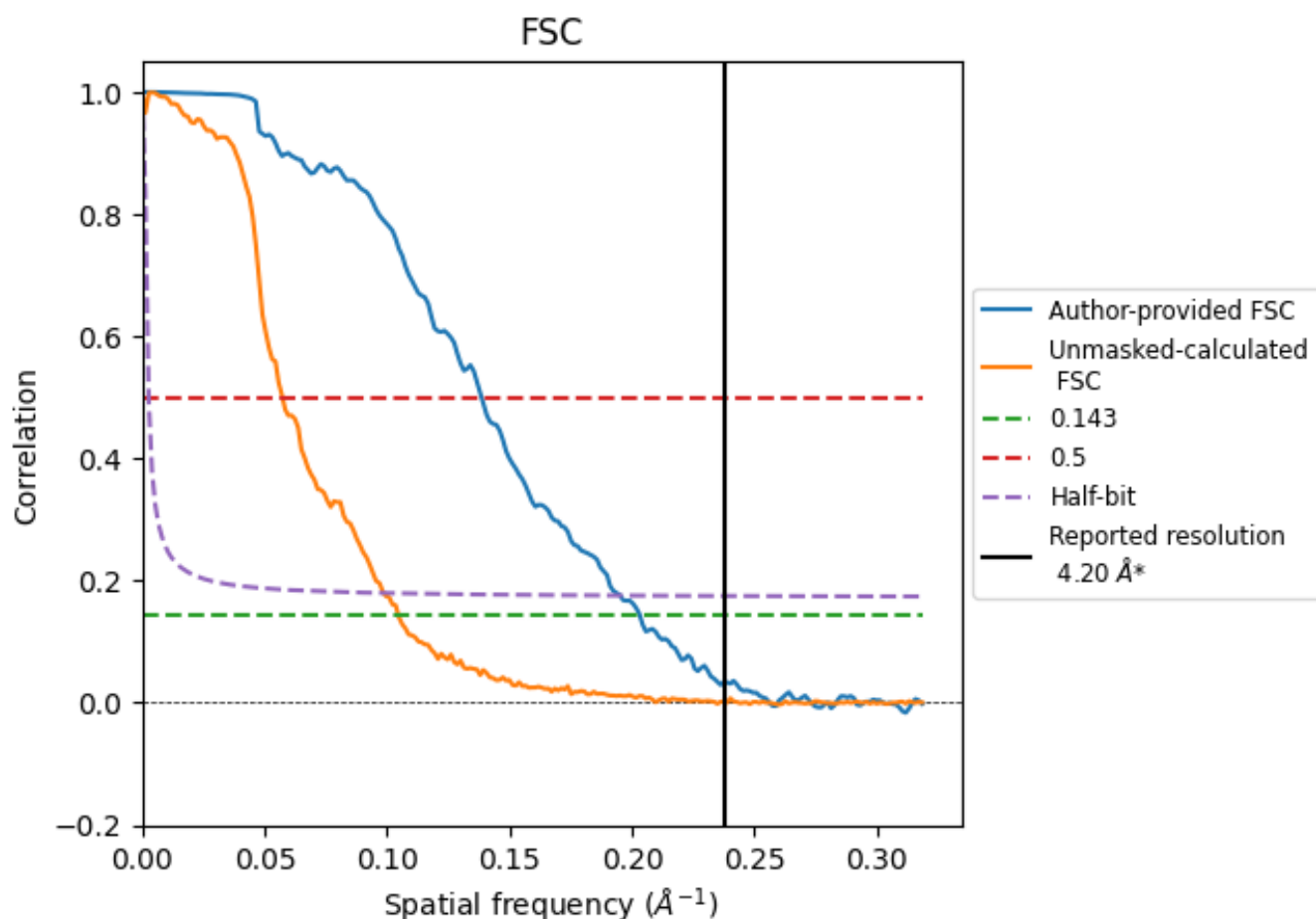


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.92	7.22	5.12
Unmasked-calculated*	9.56	17.48	10.13

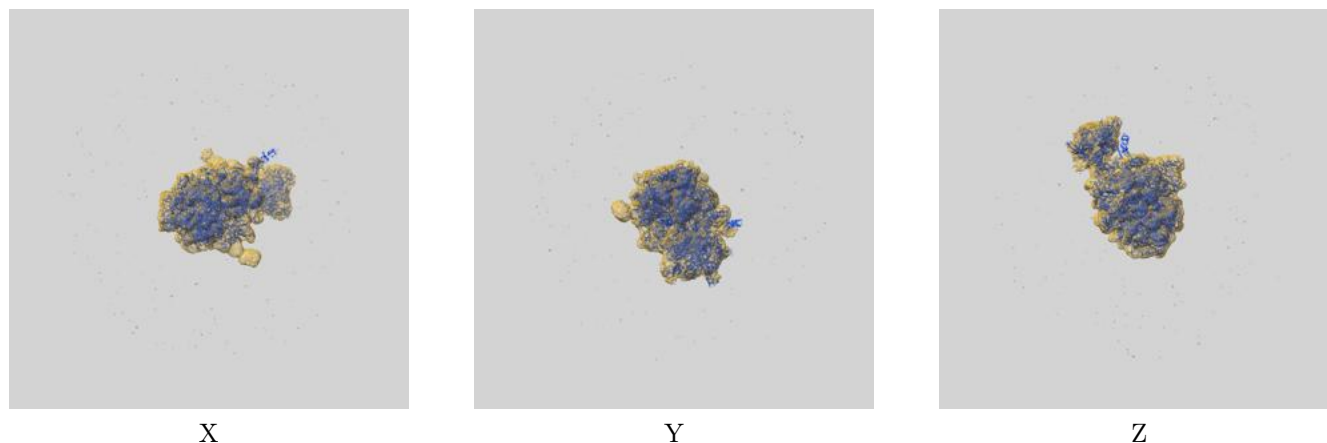
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.92 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.56 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38944 and PDB model 8Y5O. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



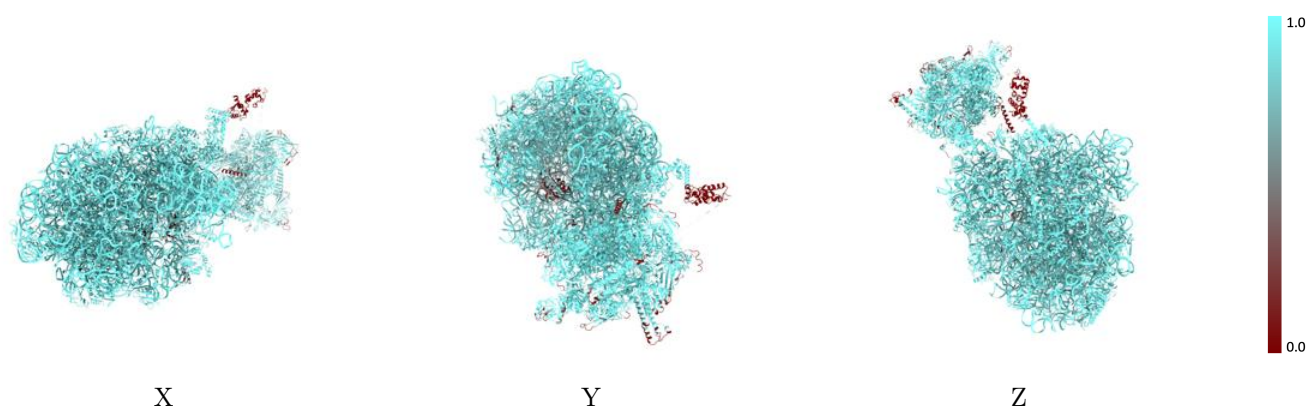
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



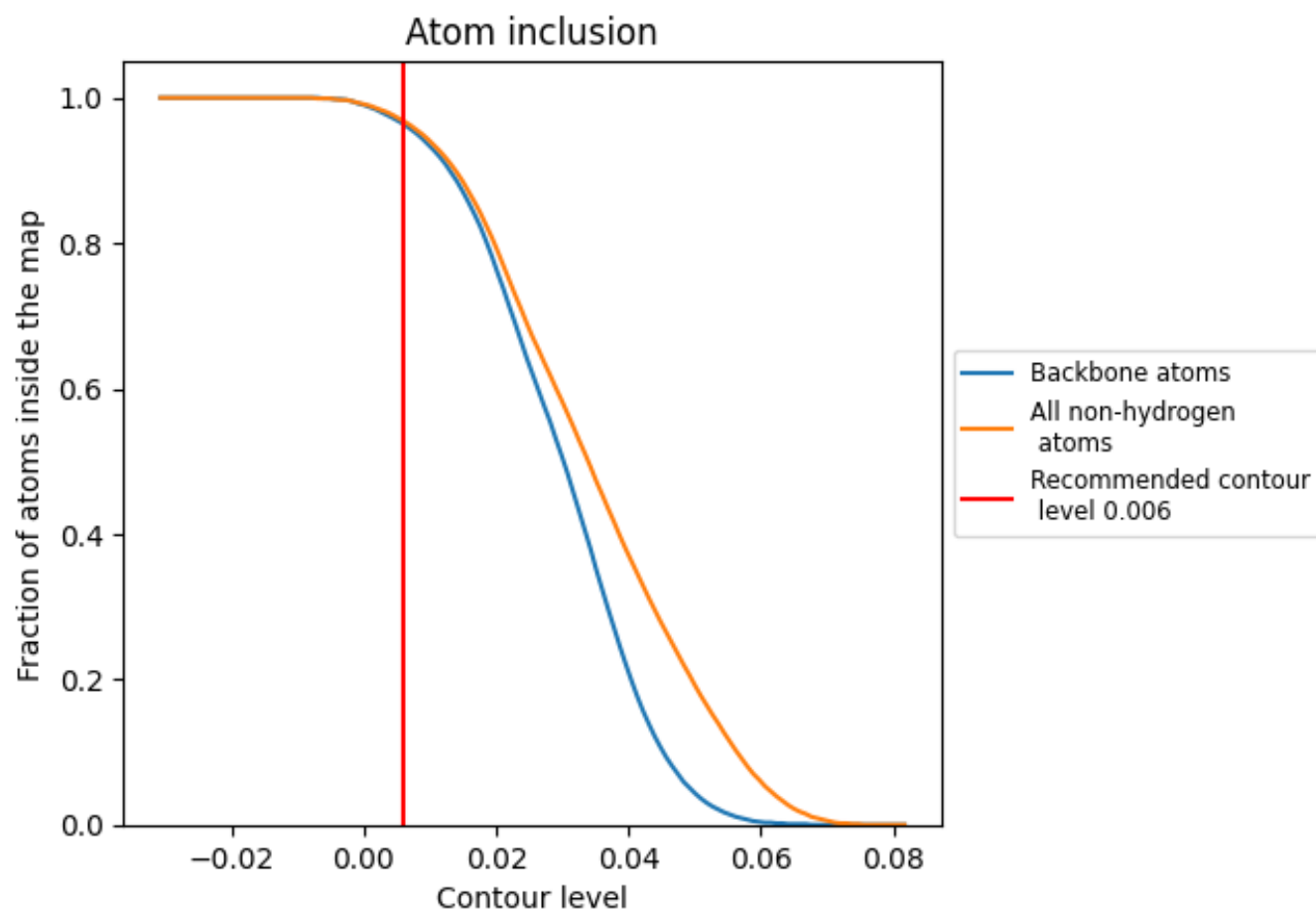
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.1480
0	 0.7960	 0.0940
1	 0.9980	 0.1980
2	 1.0000	 0.1570
3	 0.9990	 0.1790
4	 0.9680	 0.1100
5	 0.6240	 0.0980
6	 0.9930	 0.1720
8	 1.0000	 0.0200
9	 1.0000	 0.0670
A	 0.9970	 0.1130
A1	 0.8930	 0.0340
A2	 0.7520	 0.0430
B	 0.9860	 0.1430
B1	 0.9350	 0.0230
B2	 0.9170	 0.0360
C	 0.9550	 0.1350
D	 0.9750	 0.1360
E	 0.9980	 0.1230
F	 0.9930	 0.1030
G	 0.9800	 0.1360
H	 0.9880	 0.1440
I	 0.9920	 0.1270
J	 0.9900	 0.1410
K	 0.9850	 0.1510
L	 0.9730	 0.1380
M	 0.9760	 0.1110
N	 0.9810	 0.1040
NA	 0.8340	 0.1340
NG	 0.9350	 0.0530
O	 0.9950	 0.1140
P	 0.9870	 0.1500
Q	 0.9450	 0.1460
R	 0.9740	 0.1410
S	 0.9970	 0.1150



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Chain	Atom inclusion	Q-score
T	 0.9960	 0.1360
U	 1.0000	 0.1100
V	 0.9890	 0.1100
W	 0.9980	 0.1440
W0	 0.5380	 0.0170
X	 1.0000	 0.1160
Y	 0.9790	 0.1170
Z	 0.9340	 0.1470
a	 0.9770	 0.0990
b	 0.9810	 0.1670
c	 0.9940	 0.1550
d	 0.9890	 0.1430
e	 0.9500	 0.1060
f	 0.9880	 0.1370
g	 0.8680	 0.1230
h	 1.0000	 0.1790
i	 0.8950	 0.0460
j	 0.9940	 0.1560
k	 0.9580	 0.1810
l	 0.9940	 0.1200
m	 0.9630	 0.1320
n	 0.9990	 0.1550
o	 1.0000	 0.0960
p	 0.9930	 0.1790
q	 0.9970	 0.1290
r	 0.9940	 0.1370
s	 0.9880	 0.1620
t	 0.9850	 0.1470
u	 0.9840	 0.1410
v	 0.9920	 0.1410
w	 0.9890	 0.1050
x	 0.9970	 0.1580
y	 0.9900	 0.1450
z	 0.9820	 0.1480