



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 01:49 am BST

PDB ID : 8PKL / pdb_00008pkl
EMDB ID : EMD-17743
Title : Escherichia coli paused disome complex (leading 70S non-rotated closed PRE state)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-06-26
Resolution : 3.09 Å(reported)
Based on initial model : 7N1P

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:

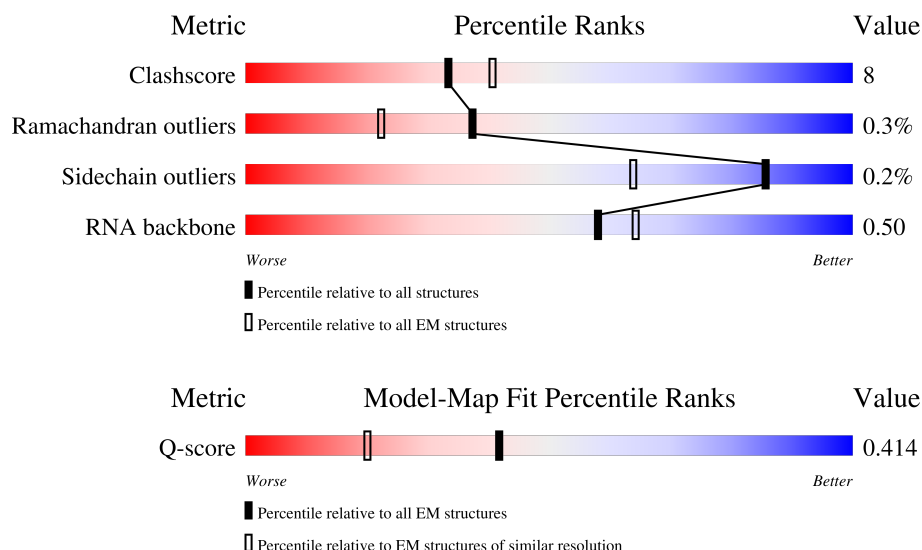
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 3.09 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	14003 (2.59 - 3.59)

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	0	38	
2	1	78	
3	2	63	

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Mol	Chain	Length	Quality of chain
4	3	59	
5	4	70	
6	5	57	
7	6	65	
8	7	2921	
9	8	120	
10	A	1535	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	G	179	
17	H	130	
18	I	130	
19	J	103	
20	K	129	
21	L	124	
22	M	118	
23	N	101	
24	O	89	
25	P	82	
26	Q	84	
27	R	75	
28	S	92	

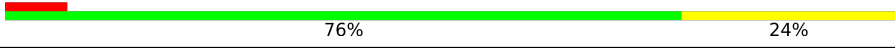
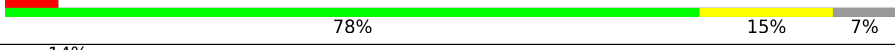
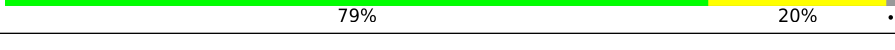
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Mol	Chain	Length	Quality of chain
29	T	87	
30	U	71	
31	V	24	
32	W	76	
33	X	77	
34	Y	76	
35	a	234	
36	b	273	
37	c	209	
38	d	201	
39	e	179	
40	f	177	
41	g	55	
42	h	136	
43	i	149	
44	j	165	
45	k	142	
46	l	46	
47	m	142	
48	n	123	
49	o	144	
50	p	36	
51	q	127	
52	r	117	
53	s	115	

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Mol	Chain	Length	Quality of chain
54	t	118	
55	u	103	
56	v	110	
57	w	100	
58	x	104	
59	y	94	
60	z	85	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 151734 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 L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	68	Total	C	N	O	S	0	0
			533	330	101	96	6		

- Molecule 6 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1535	Total	C	N	O	P	0	0
			32950	14703	6044	10668	1535		

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 24 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 25 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 30 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	24	Total	C	N	O	P	0	0
			516	231	99	162	24		

- Molecule 32 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 33 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	X	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

- Molecule 34 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	76	Total	C	N	O	P	0	0
			1628	726	293	533	76		

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 38 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 39 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 41 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	g	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 43 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 44 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 45 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 46 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 47 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 48 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 49 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 50 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	p	36	Total	C	N	O	0	0
			206	125	44	37		

- Molecule 51 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 52 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	r	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 53 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 54 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	t	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 55 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 56 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 57 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 58 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 59 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	y	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

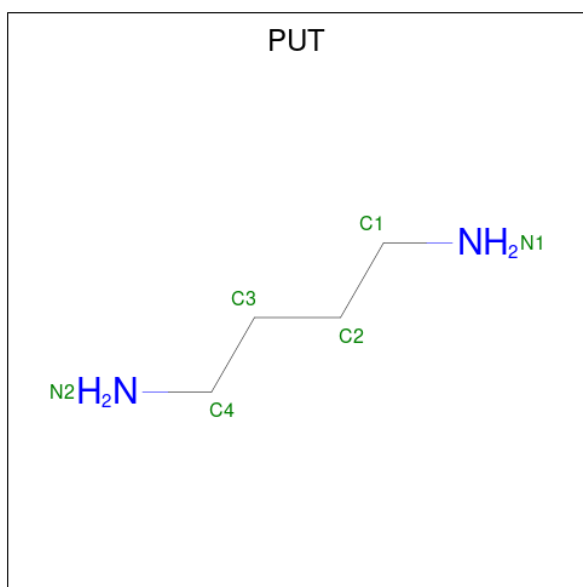
- Molecule 60 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	z	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

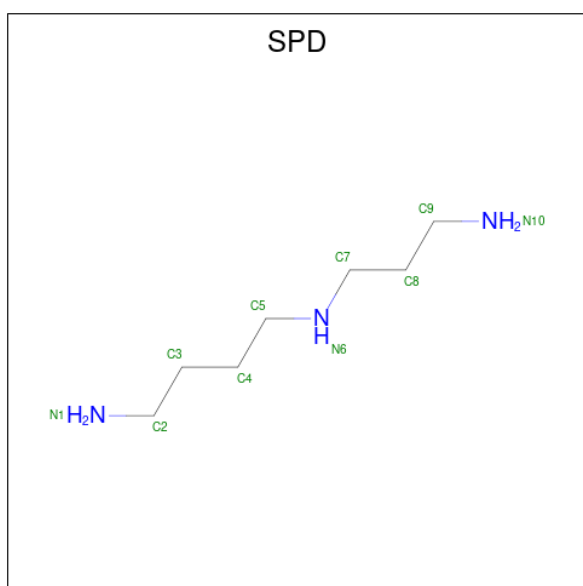
Mol	Chain	Residues	Atoms		AltConf
61	0	1	Total	Zn	0
			1	1	
61	4	1	Total	Zn	0
			1	1	

- Molecule 62 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
62	7	1	Total	C	N	0
			6	4	2	
62	7	1	Total	C	N	0
			6	4	2	

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

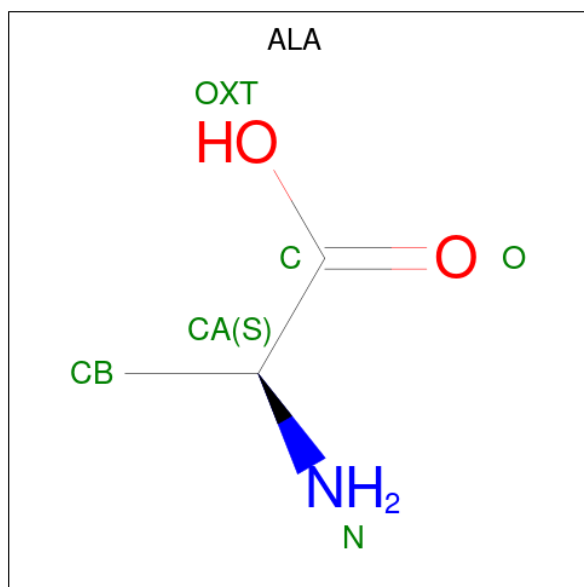


Mol	Chain	Residues	Atoms			AltConf
63	7	1	Total	C	N	0
			10	7	3	

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	7	257	Total	Mg	0
			257	257	
64	A	23	Total	Mg	0
			23	23	
64	I	1	Total	Mg	0
			1	1	
64	V	1	Total	Mg	0
			1	1	
64	X	1	Total	Mg	0
			1	1	
64	Y	1	Total	Mg	0
			1	1	
64	b	1	Total	Mg	0
			1	1	
64	q	1	Total	Mg	0
			1	1	
64	r	1	Total	Mg	0
			1	1	

- Molecule 65 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				AltConf
65	Y	1	Total	C	N	O	0
			5	3	1	1	

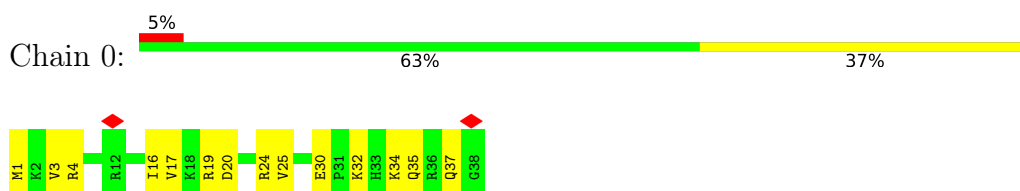
- Molecule 66 is water.

Mol	Chain	Residues	Atoms		AltConf
66	7	12	Total 12	O 12	0
66	x	1	Total 1	O 1	0

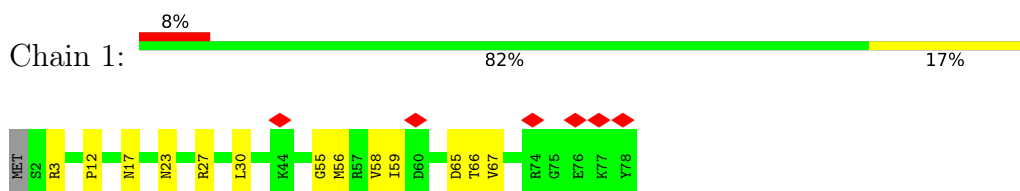
3 Residue-property plots

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.

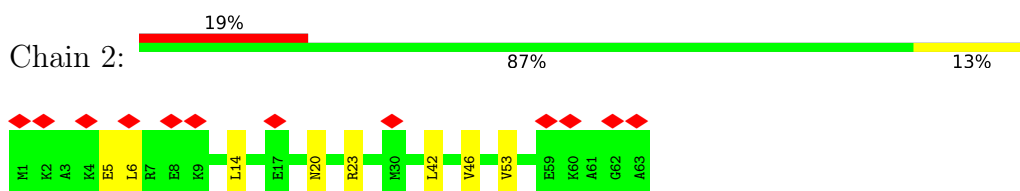
- Molecule 1: 50S ribosomal protein L36



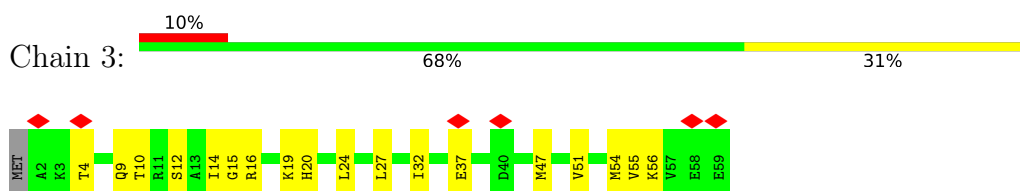
- Molecule 2: 50S ribosomal protein L28



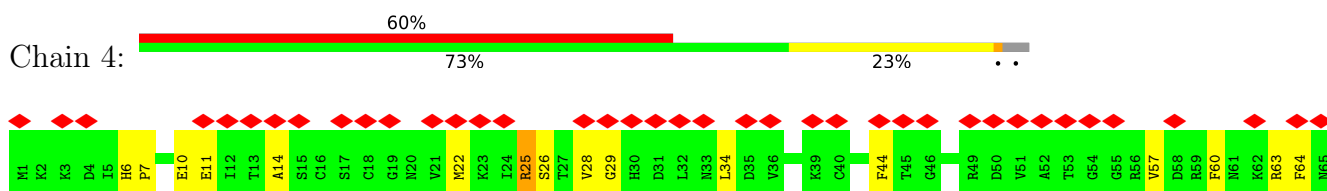
- Molecule 3: 50S ribosomal protein L29



- Molecule 4: 50S ribosomal protein L30



- Molecule 5: Large ribosomal subunit protein bL31A

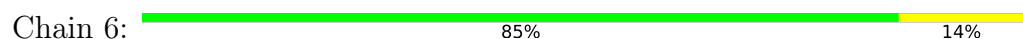




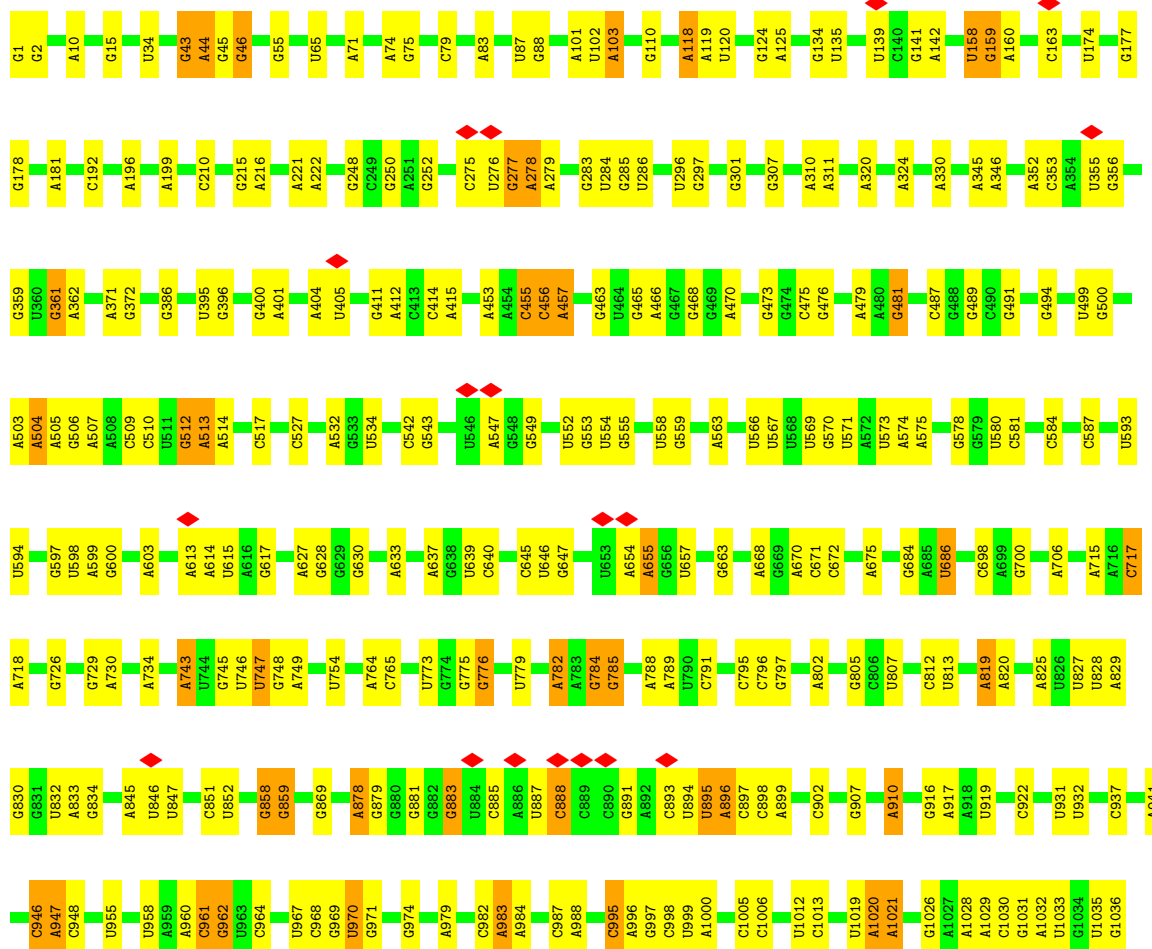
- Molecule 6: 50S ribosomal protein L32

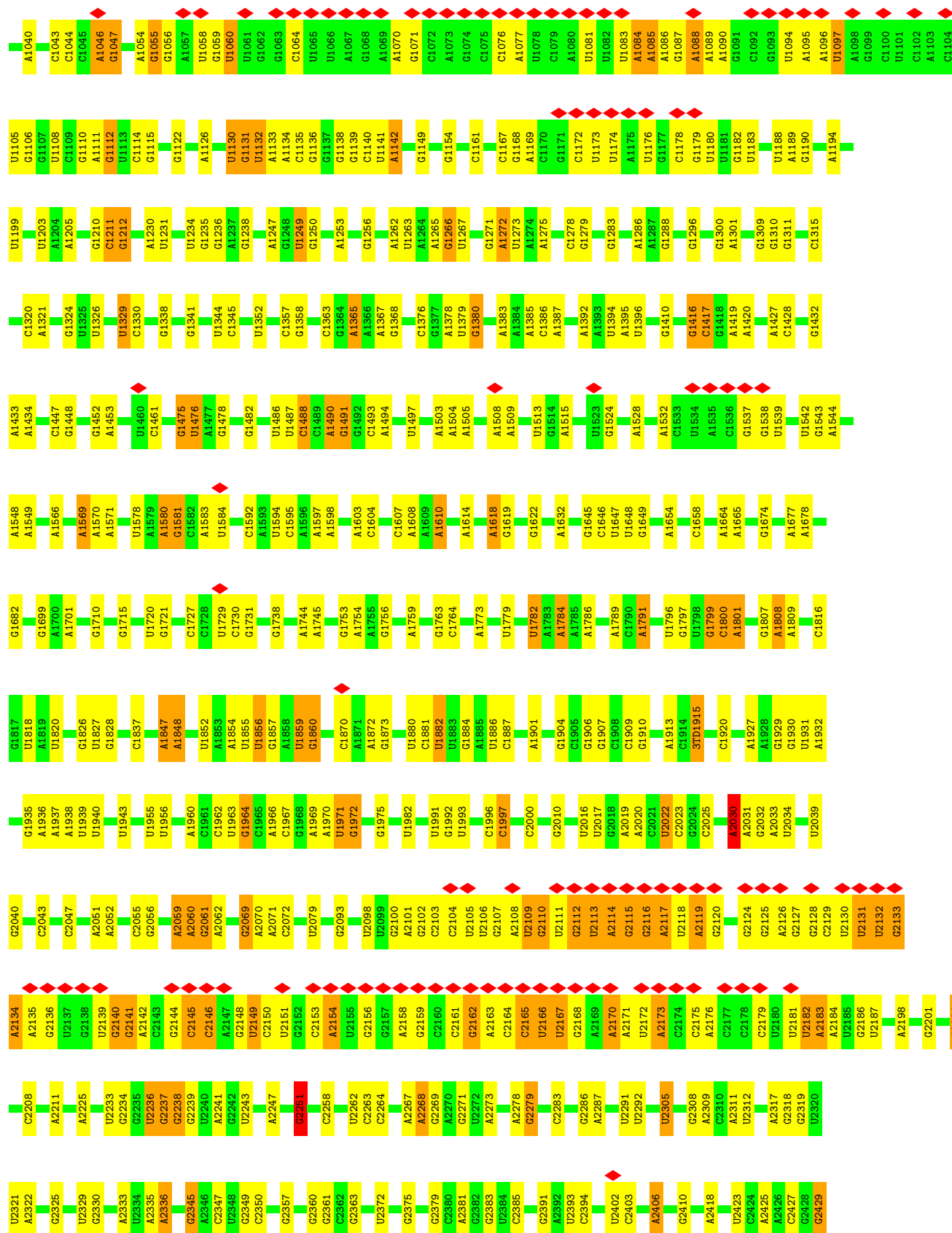


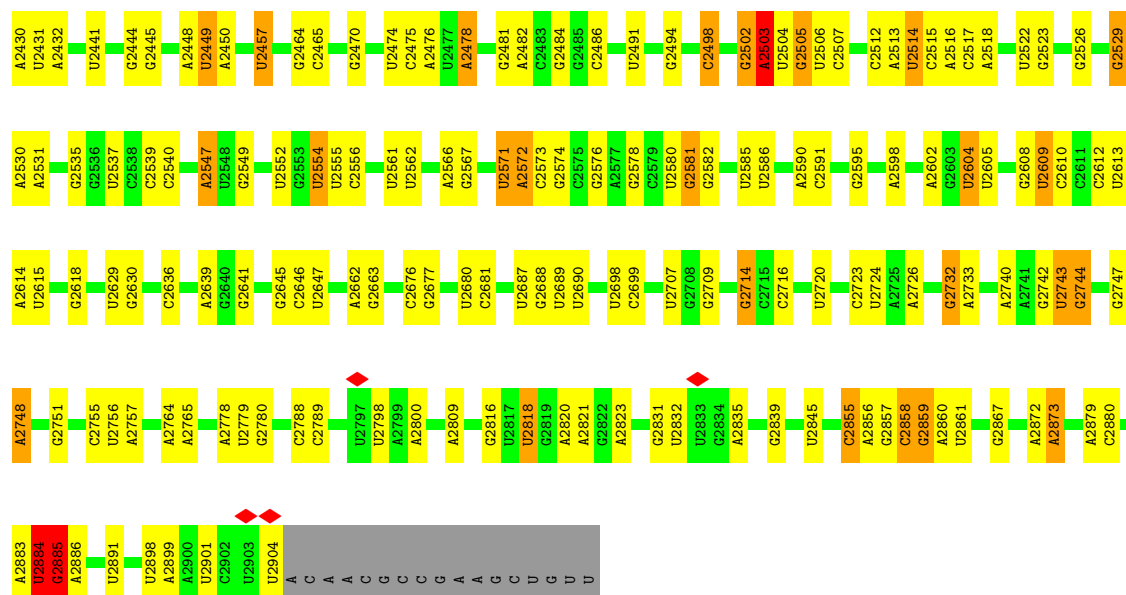
- Molecule 7: 50S ribosomal protein L35



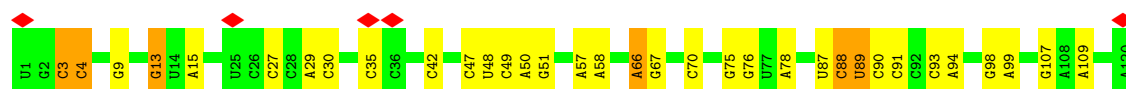
- Molecule 8: 23S ribosomal RNA



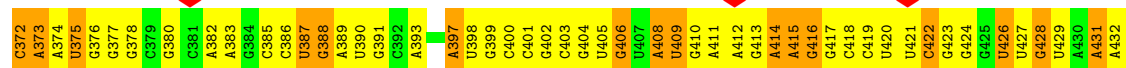
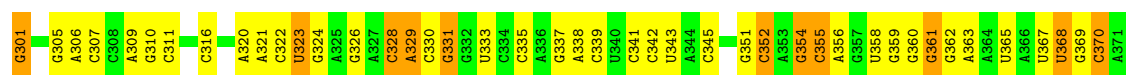
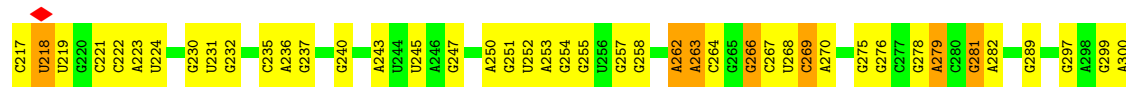
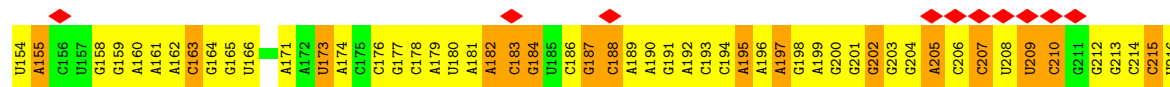
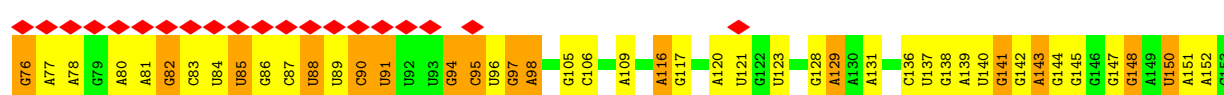
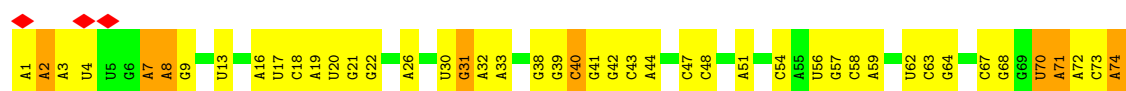


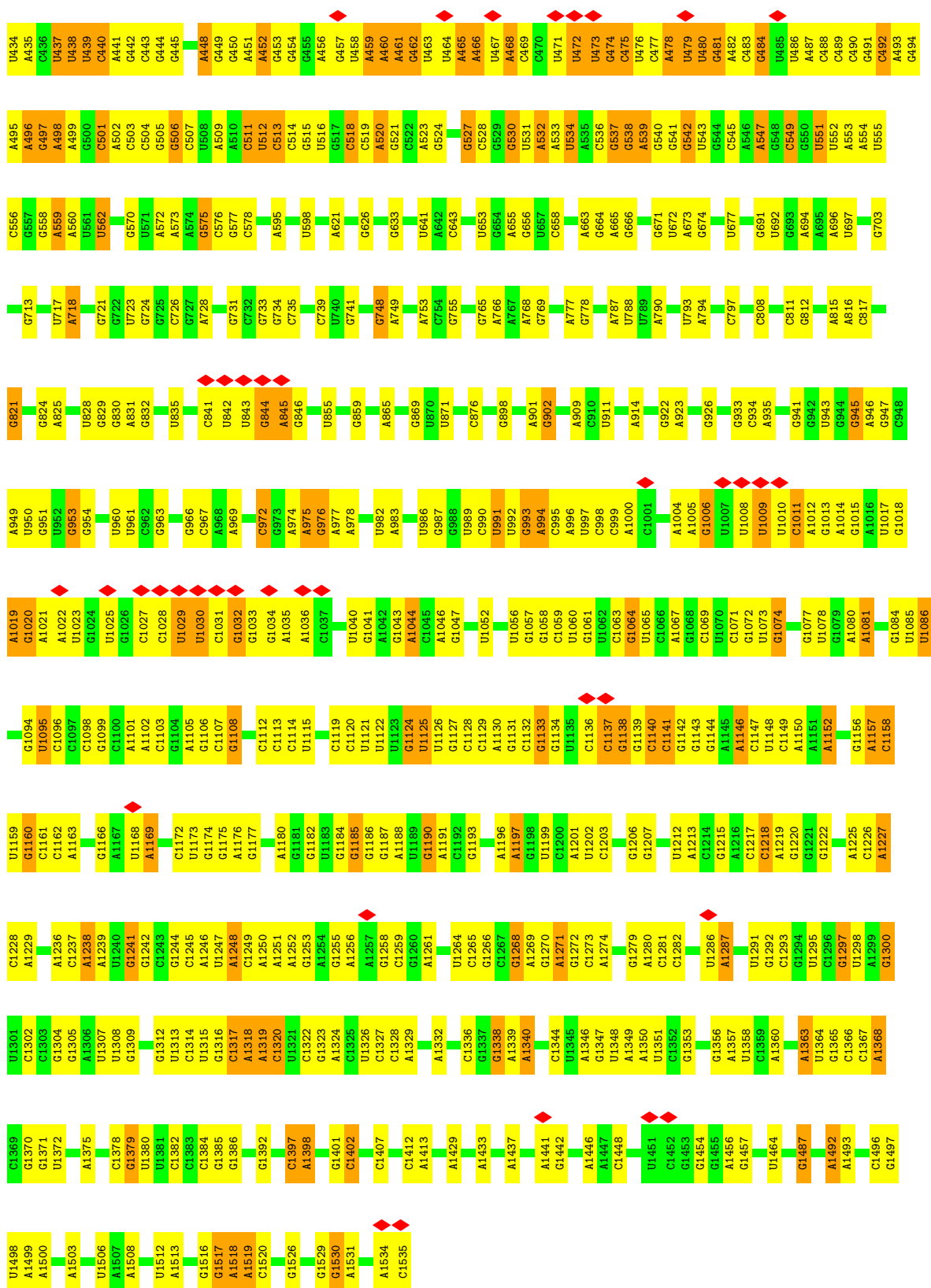


• Molecule 9: 5S ribosomal RNA



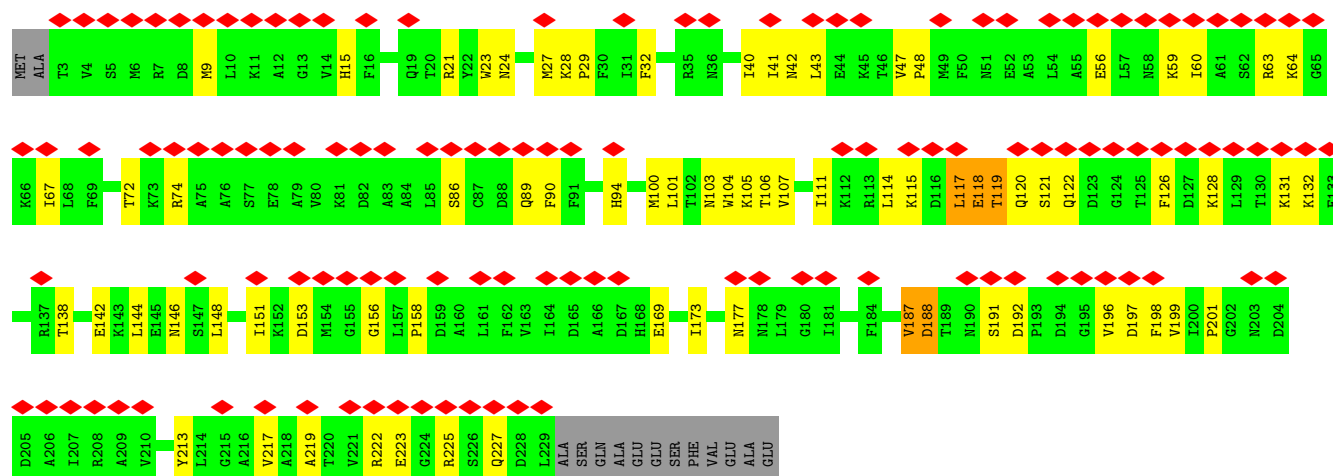
• Molecule 10: 16S ribosomal RNA



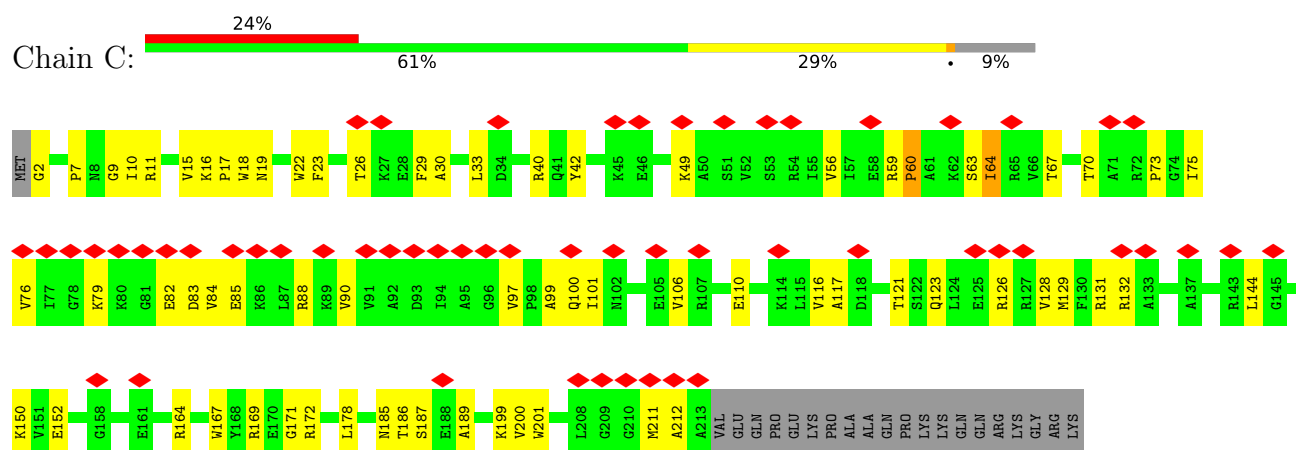


• Molecule 11: Small ribosomal subunit protein uS2

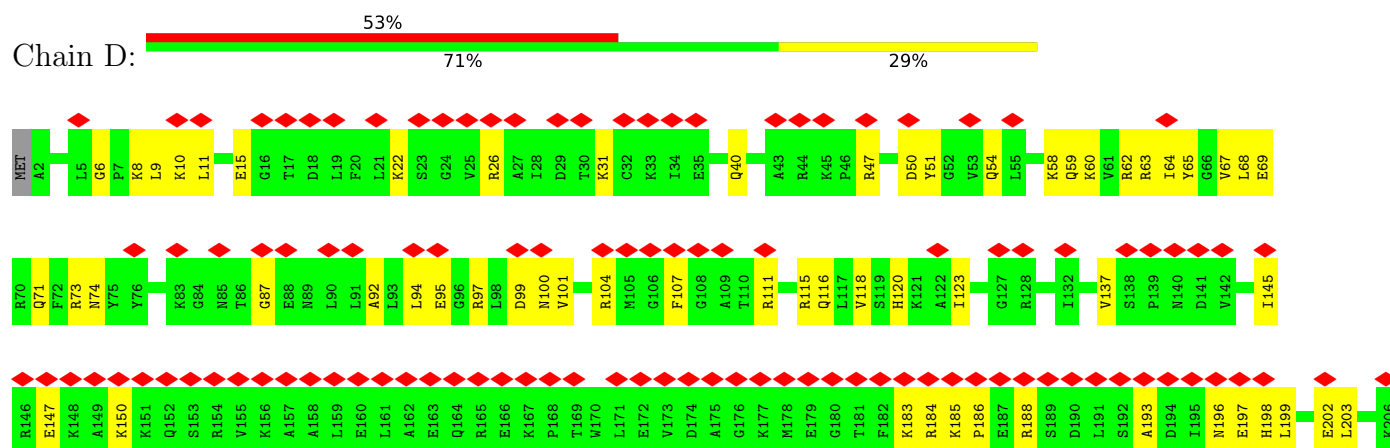




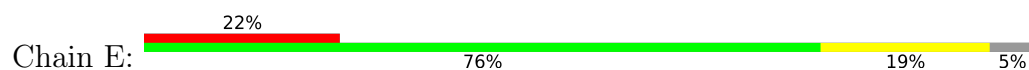
• Molecule 12: Small ribosomal subunit protein uS3

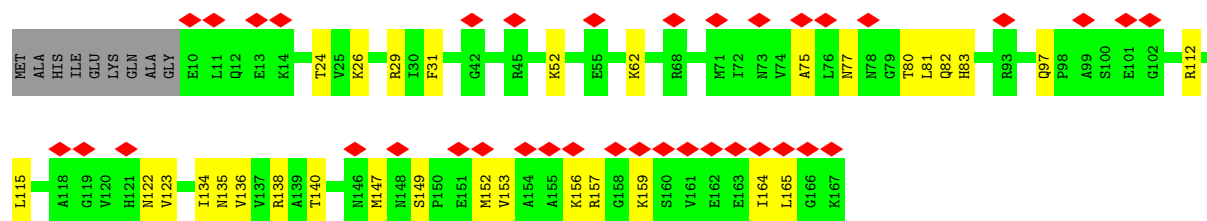


• Molecule 13: Small ribosomal subunit protein uS4

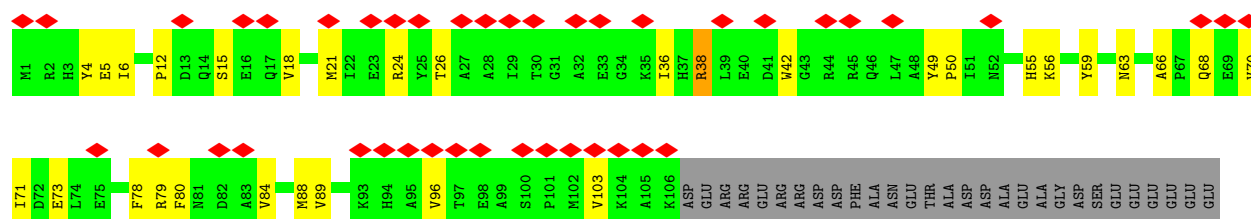


• Molecule 14: Small ribosomal subunit protein uS5

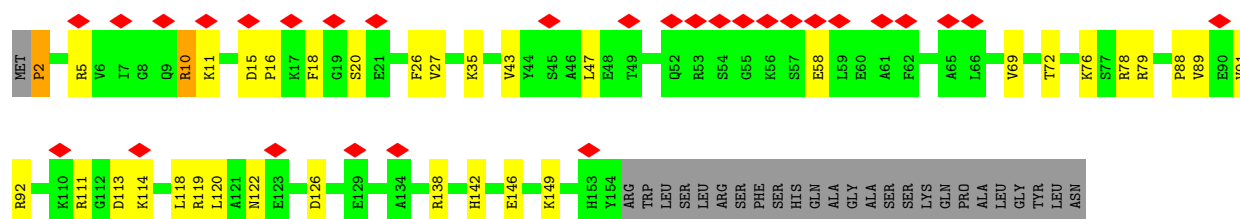




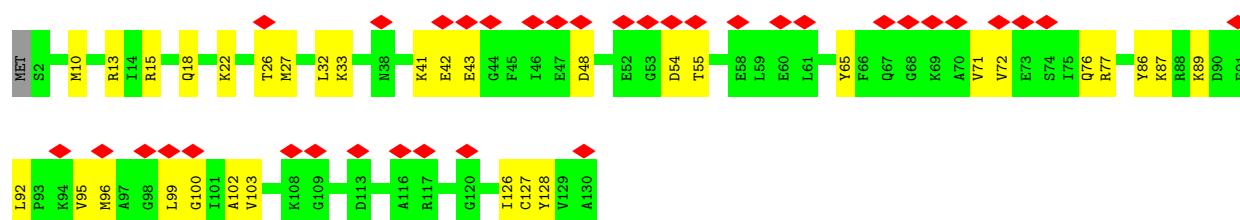
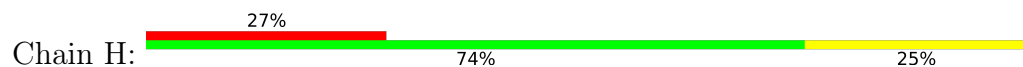
• Molecule 15: 30S ribosomal protein S6



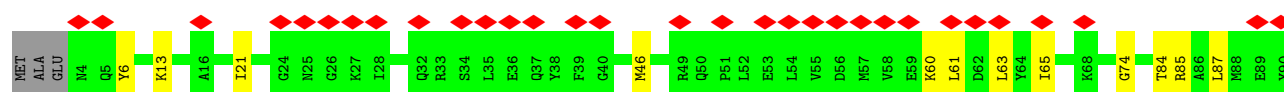
• Molecule 16: 30S ribosomal protein S7

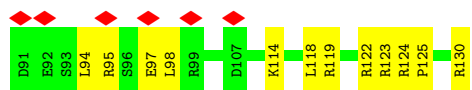


• Molecule 17: Small ribosomal subunit protein uS8

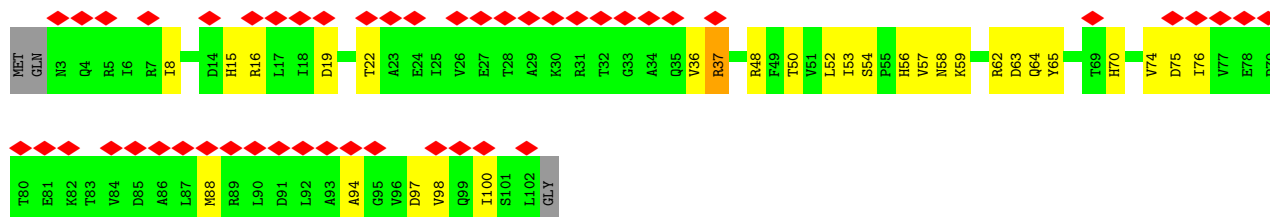


• Molecule 18: Small ribosomal subunit protein uS9

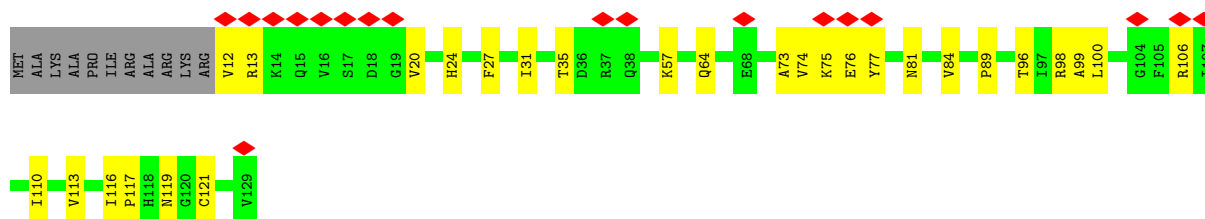




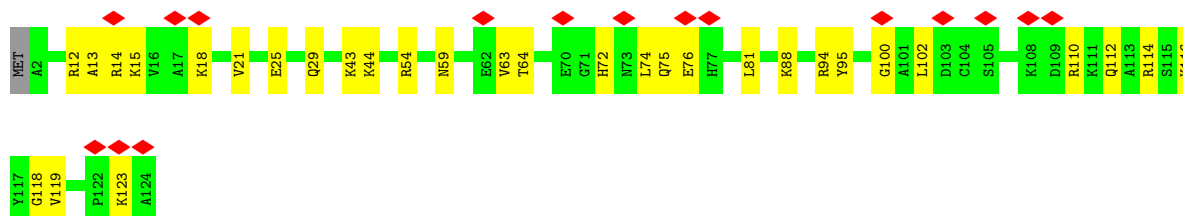
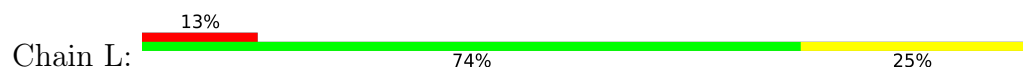
- Molecule 19: 30S ribosomal protein S10



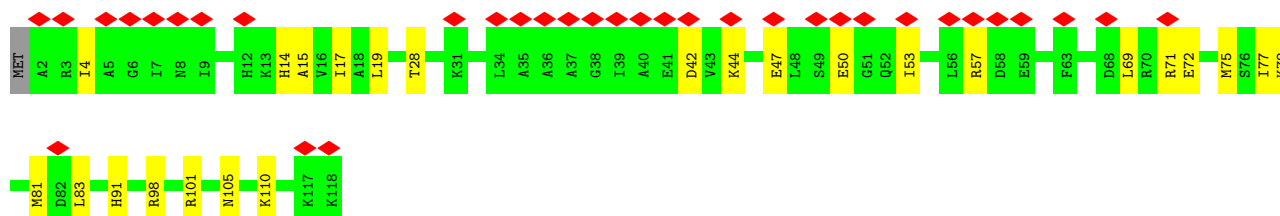
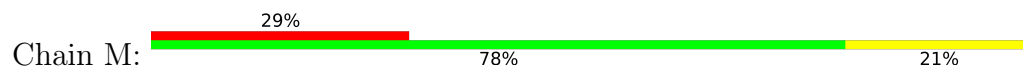
- Molecule 20: Small ribosomal subunit protein uS11



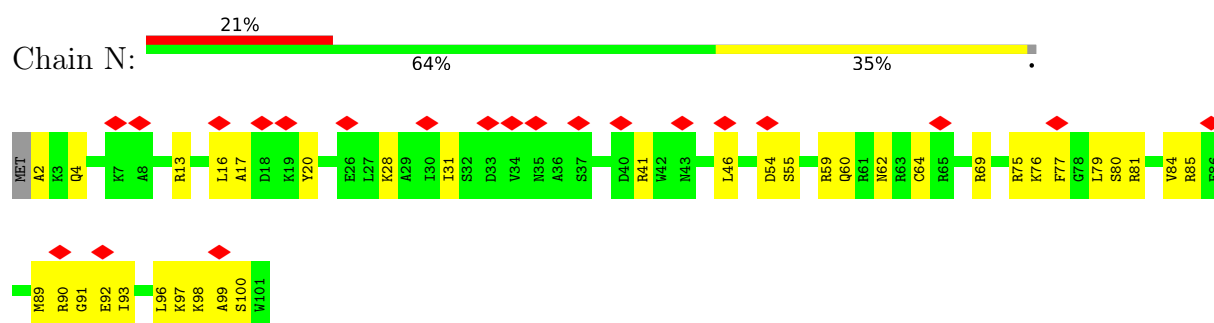
- Molecule 21: Small ribosomal subunit protein uS12



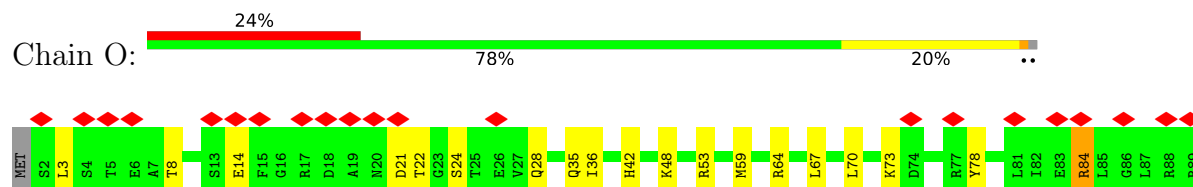
- Molecule 22: Small ribosomal subunit protein uS13



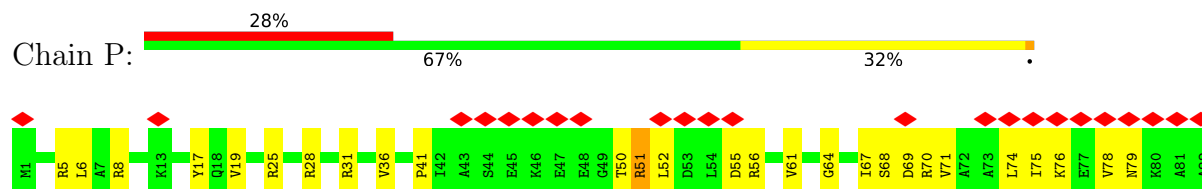
- Molecule 23: Small ribosomal subunit protein uS14



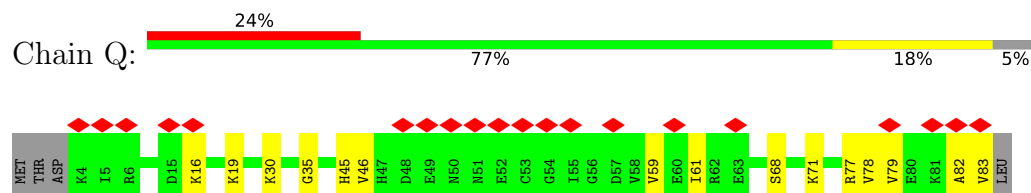
- Molecule 24: 30S ribosomal protein S15



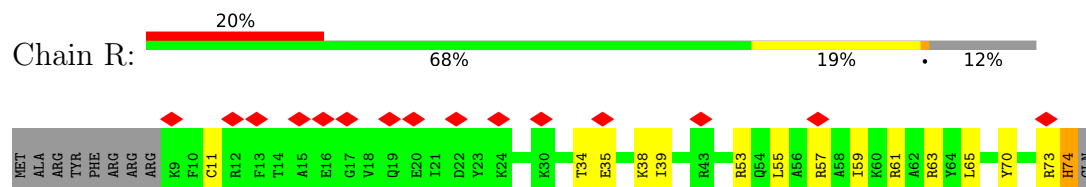
- Molecule 25: 30S ribosomal protein S16



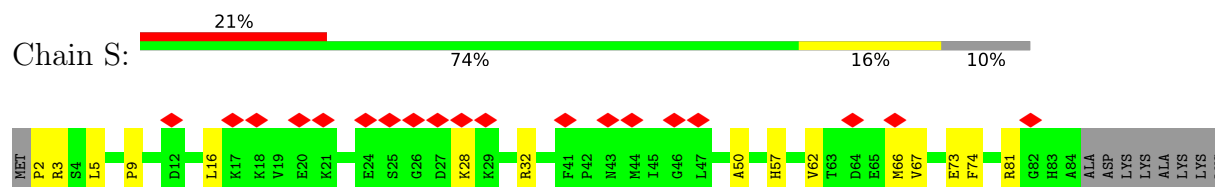
- Molecule 26: Small ribosomal subunit protein uS17



- Molecule 27: Small ribosomal subunit protein bS18

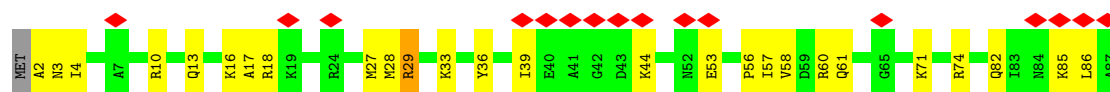


- Molecule 28: Small ribosomal subunit protein uS19

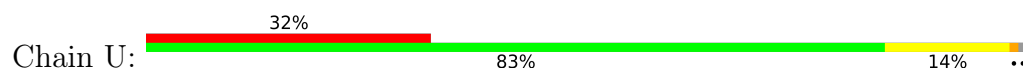


- Molecule 29: Small ribosomal subunit protein bS20

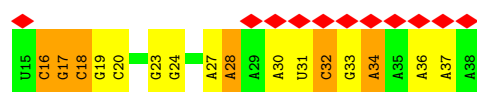




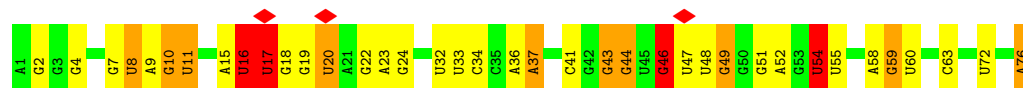
- Molecule 30: 30S ribosomal protein S21



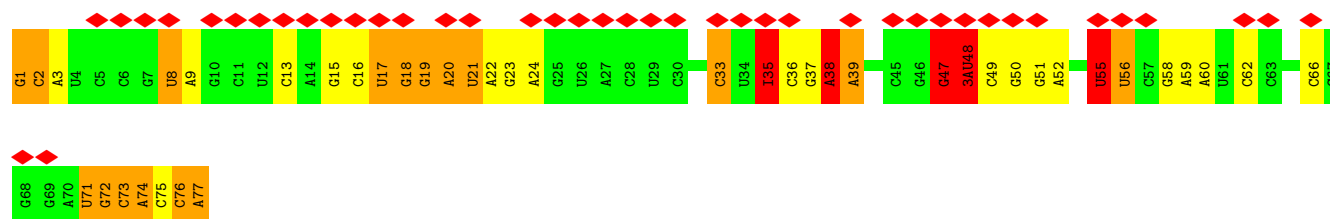
- Molecule 31: mRNA



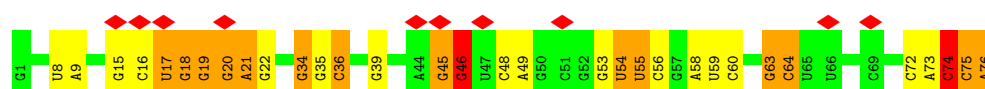
- Molecule 32: tRNA-Trp (P-site)



- Molecule 33: tRNA-Arg (E-site)

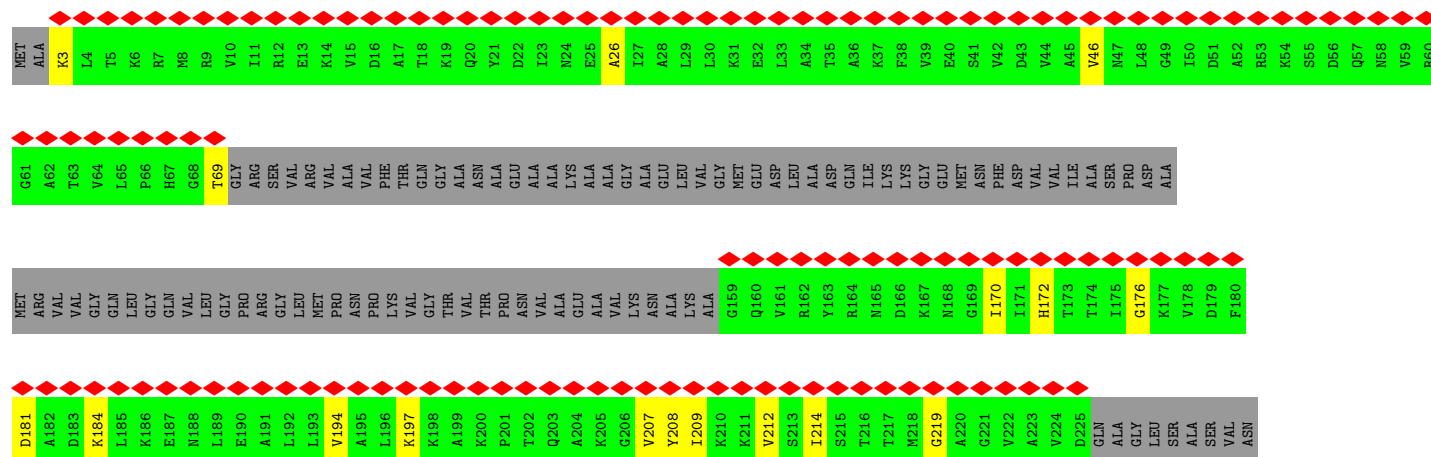


- Molecule 34: tRNA-Ala (A-site)



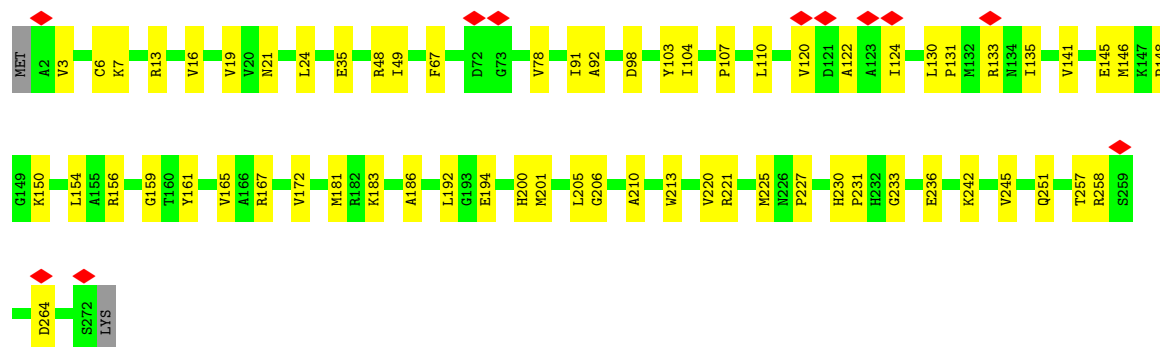
- Molecule 35: Large ribosomal subunit protein uL1





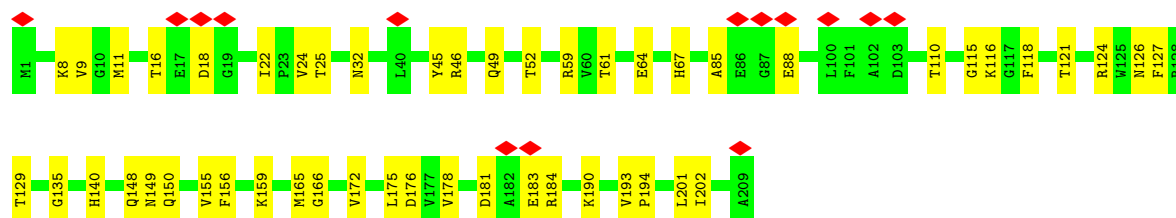
• Molecule 36: 50S ribosomal protein L2

Chain b: 76% 23%



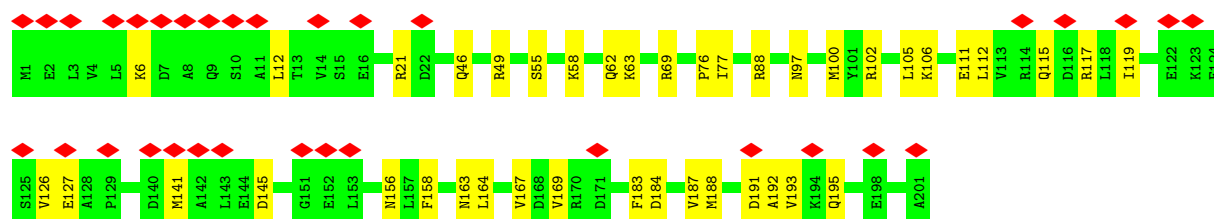
• Molecule 37: 50S ribosomal protein L3

Chain c: 7% 76% 24%

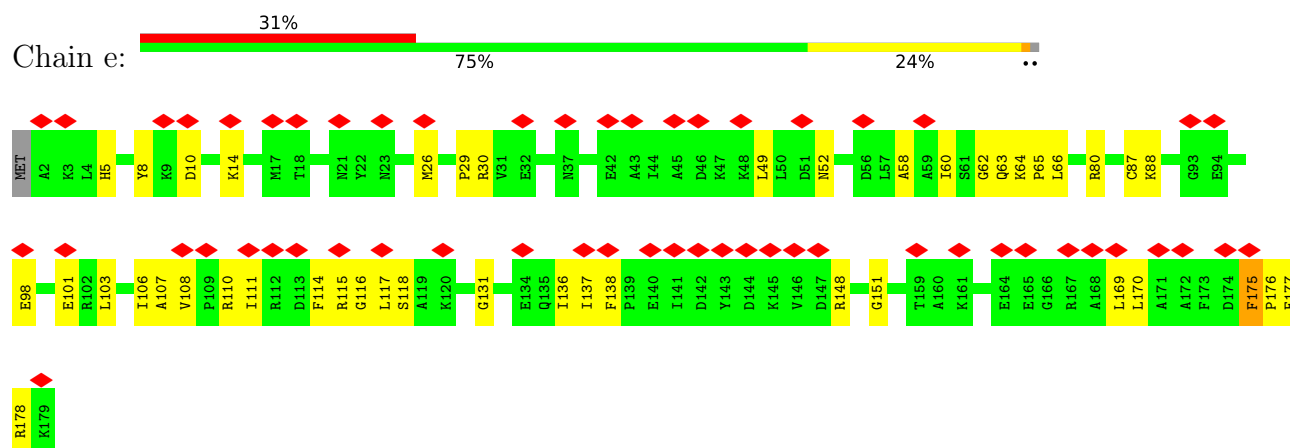


• Molecule 38: 50S ribosomal protein L4

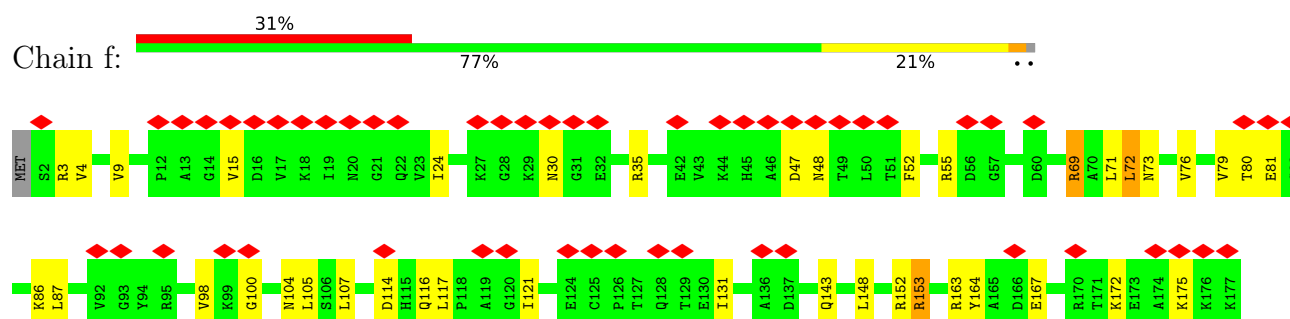
Chain d: 16% 80% 20%



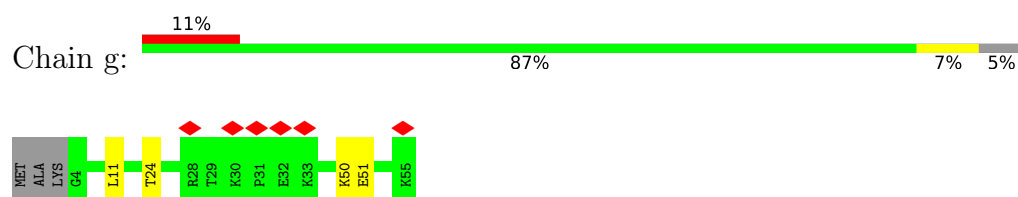
- Molecule 39: 50S ribosomal protein L5



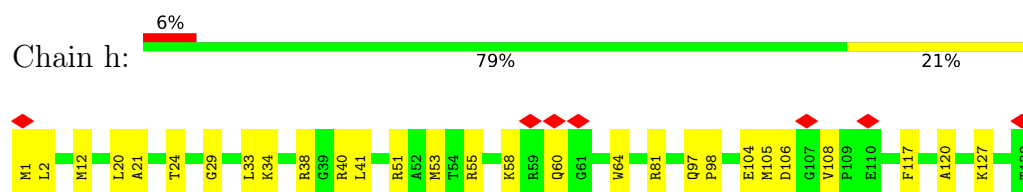
- Molecule 40: 50S ribosomal protein L6



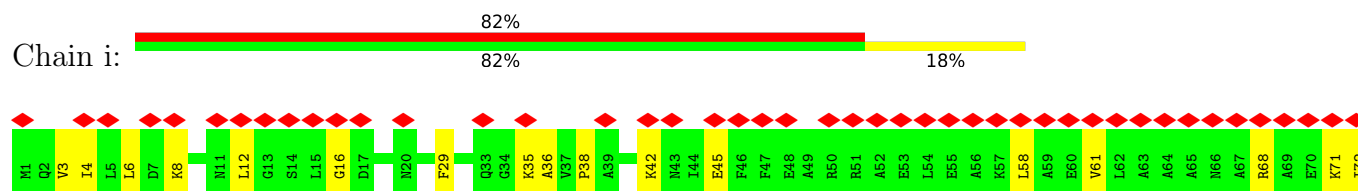
- Molecule 41: 50S ribosomal protein L33



- Molecule 42: 50S ribosomal protein L16

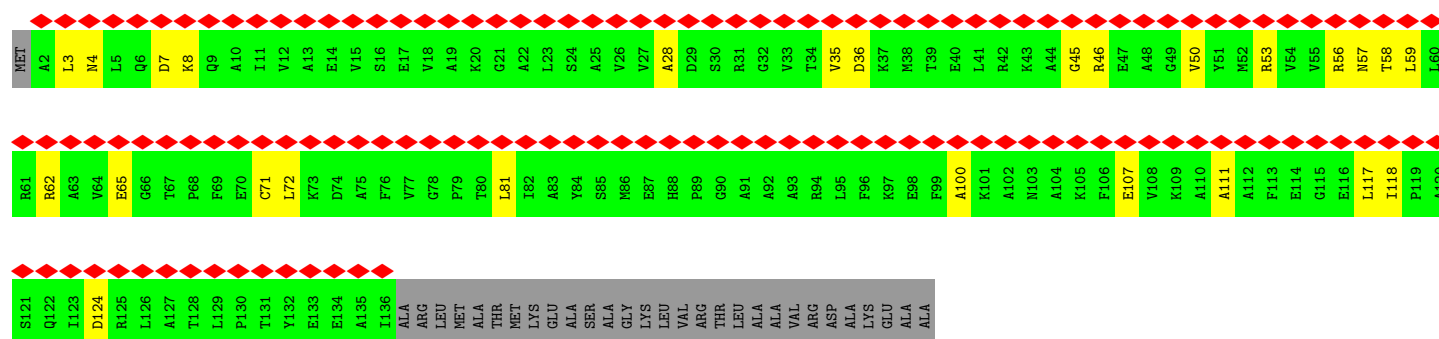
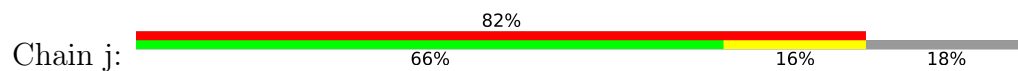


- Molecule 43: 50S ribosomal protein L9

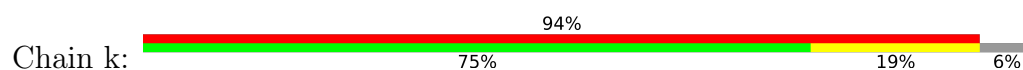




• Molecule 44: Large ribosomal subunit protein uL10



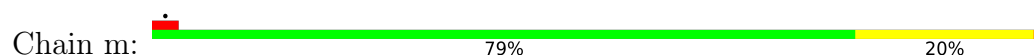
• Molecule 45: 50S ribosomal protein L11

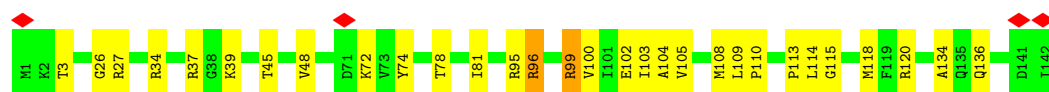


• Molecule 46: 50S ribosomal protein L34

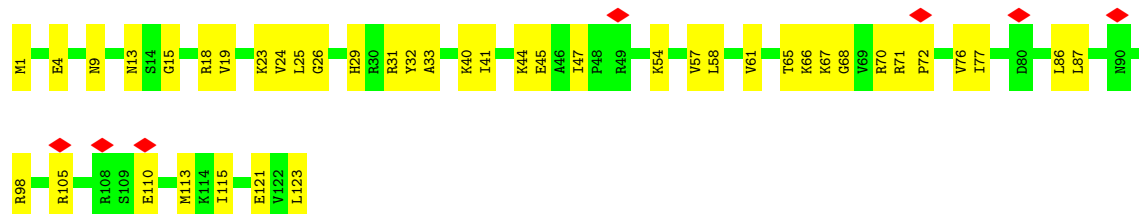


• Molecule 47: 50S ribosomal protein L13

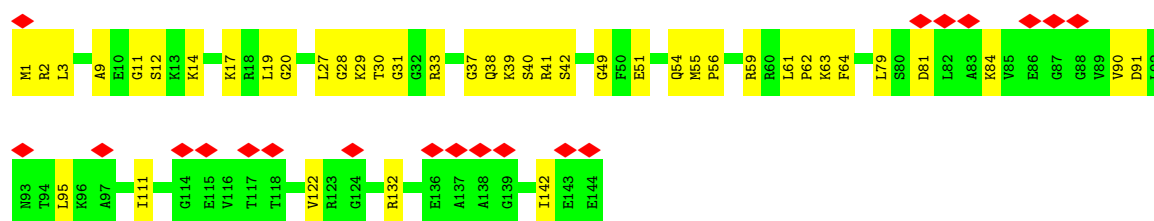




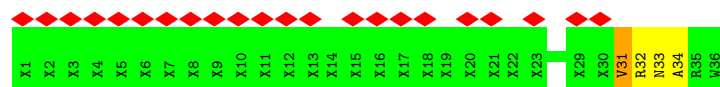
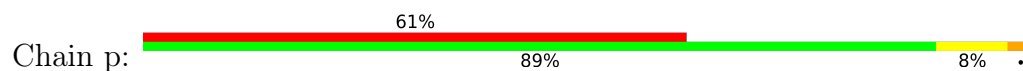
- Molecule 48: 50S ribosomal protein L14



- Molecule 49: 50S ribosomal protein L15



- Molecule 50: Nascent peptide

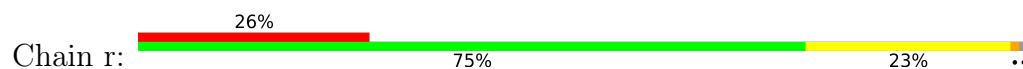


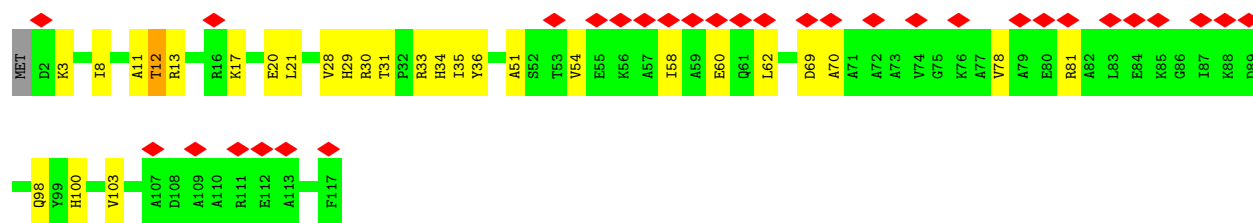
- Molecule 51: 50S ribosomal protein L17



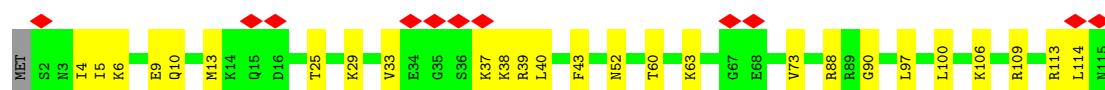
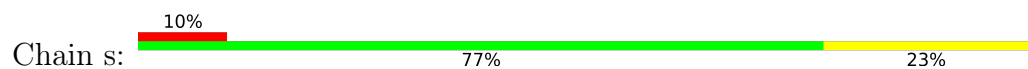
ALA
ALA
ALA
GLU

- Molecule 52: 50S ribosomal protein L18

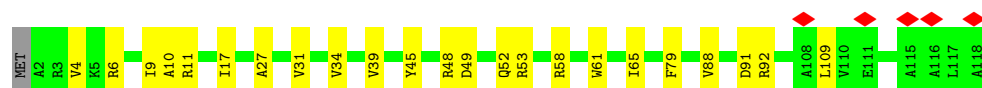
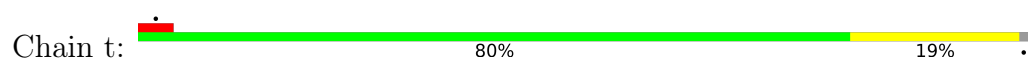




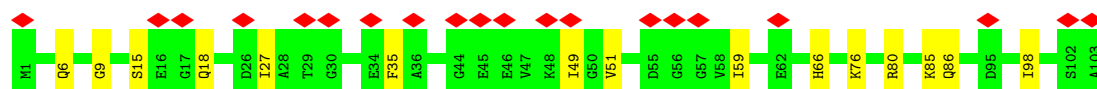
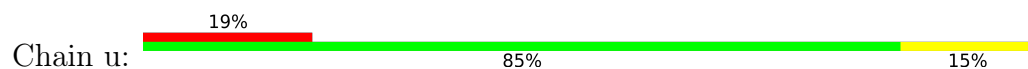
- Molecule 53: 50S ribosomal protein L19



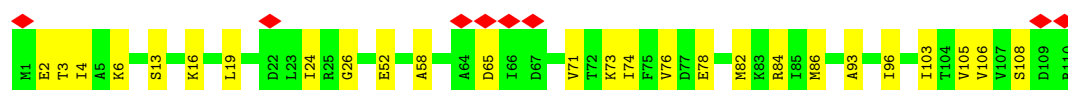
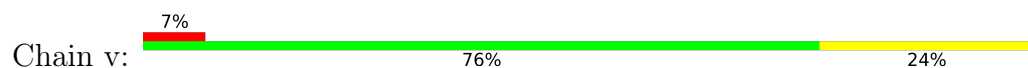
- Molecule 54: 50S ribosomal protein L20



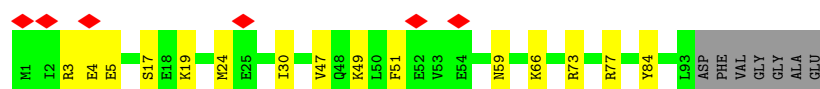
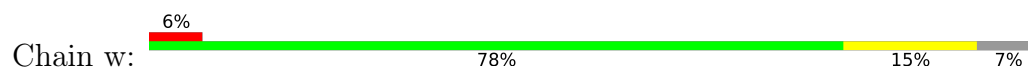
- Molecule 55: 50S ribosomal protein L21



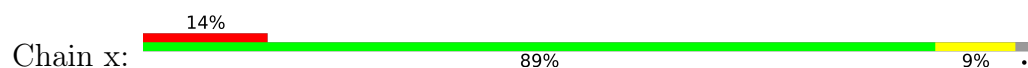
- Molecule 56: 50S ribosomal protein L22

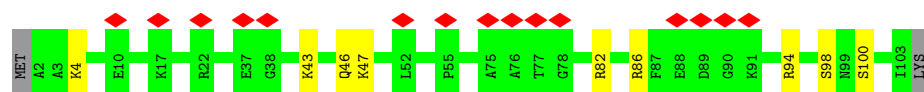


- Molecule 57: 50S ribosomal protein L23

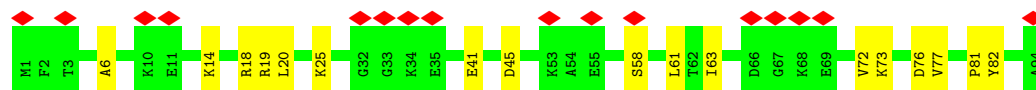
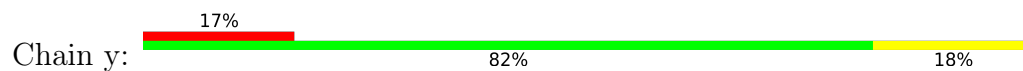


- Molecule 58: 50S ribosomal protein L24

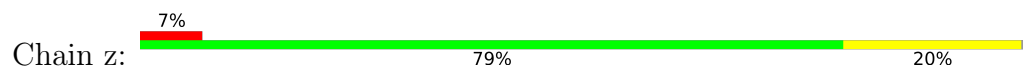




- Molecule 59: 50S ribosomal protein L25



- Molecule 60: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	26.876	Depositor
Minimum map value	-7.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	744.11993, 744.11993, 744.11993	wwPDB
Map dimensions	702, 702, 702	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, PSU, MA6, 3TD, OMC, PUT, 3AU, RSP, 4SU, 2MG, OMU, G7M, 6MZ, SPD, 4OC, MIA, OMG, ZN, MG, 1MG, 5MU, H2U, 2MA, UR3

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	0	0.16	0/303	0.39	0/397
2	1	0.12	0/635	0.32	0/848
3	2	0.10	0/510	0.31	0/677
4	3	0.25	0/453	0.45	0/605
5	4	0.24	0/543	0.53	0/726
6	5	0.12	0/450	0.30	0/599
7	6	0.10	0/513	0.33	0/676
8	7	0.15	0/69306	0.29	35/108116 (0.0%)
9	8	0.09	0/2876	0.21	0/4483
10	A	0.14	0/36637	0.29	0/57149
11	B	0.13	0/1807	0.43	0/2435
12	C	0.12	0/1685	0.36	0/2270
13	D	0.09	0/1665	0.30	0/2227
14	E	0.12	0/1179	0.33	0/1584
15	F	0.12	0/881	0.37	0/1189
16	G	0.11	0/1219	0.34	0/1635
17	H	0.11	0/989	0.33	0/1326
18	I	0.10	0/1034	0.31	0/1375
19	J	0.12	0/813	0.42	0/1100
20	K	0.12	0/900	0.34	0/1215
21	L	0.23	0/969	0.39	0/1300
22	M	0.12	0/919	0.34	0/1226
23	N	0.11	0/817	0.38	0/1088
24	O	0.10	0/722	0.37	0/964
25	P	0.11	0/659	0.32	0/884
26	Q	0.12	0/657	0.38	0/881
27	R	0.25	0/553	0.50	0/742
28	S	0.12	0/680	0.33	0/915
29	T	0.11	0/676	0.34	0/895
30	U	0.15	0/592	0.35	0/785
31	V	0.20	0/578	0.40	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	W	0.23	0/1604	0.37	2/2496 (0.1%)
33	X	0.40	2/1628 (0.1%)	0.38	0/2526
34	Y	0.23	0/1725	0.35	2/2687 (0.1%)
35	a	0.17	0/1033	0.30	0/1387
36	b	0.12	0/2121	0.35	0/2852
37	c	0.15	0/1586	0.36	0/2134
38	d	0.10	0/1571	0.26	0/2113
39	e	0.24	0/1444	0.44	0/1937
40	f	0.30	0/1343	0.47	0/1816
41	g	0.09	0/434	0.33	0/576
42	h	0.11	0/1104	0.31	0/1474
43	i	0.11	0/1122	0.38	0/1515
44	j	0.09	0/1037	0.29	0/1400
45	k	0.12	0/993	0.40	0/1341
46	l	0.11	0/380	0.29	0/498
47	m	0.23	0/1152	0.40	0/1551
48	n	0.15	0/955	0.38	0/1279
49	o	0.12	0/1062	0.35	0/1413
50	p	0.94	0/57	1.20	0/76
51	q	0.23	0/973	0.42	0/1301
52	r	0.11	0/901	0.36	0/1209
53	s	0.10	0/929	0.29	0/1242
54	t	0.11	0/960	0.27	0/1278
55	u	0.17	0/829	0.36	0/1107
56	v	0.12	0/864	0.34	0/1156
57	w	0.32	0/744	0.48	0/994
58	x	0.10	0/787	0.35	0/1051
59	y	0.09	0/766	0.29	0/1025
60	z	0.10	0/642	0.33	0/848
All	All	0.16	2/162966 (0.0%)	0.32	39/243493 (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
5	4	0	1
13	D	0	1
16	G	0	1
19	J	0	2
20	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	O	0	1
25	P	0	1
27	R	0	1
29	T	0	2
30	U	0	1
38	d	0	1
39	e	0	1
40	f	0	1
47	m	0	1
57	w	0	1
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	35	I	C5-C6	7.32	1.54	1.39
33	X	35	I	N3-C4	7.00	1.50	1.35

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	1860	G	P-O3'-C3'	-9.63	105.76	120.20
8	7	1856	U	P-O3'-C3'	-9.32	106.22	120.20
8	7	2237	G	P-O3'-C3'	-8.97	106.75	120.20
8	7	1859	U	P-O3'-C3'	-8.52	107.42	120.20
8	7	2885	G	P-O3'-C3'	-8.31	107.73	120.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4	25	ARG	Sidechain
13	D	104	ARG	Sidechain
16	G	78	ARG	Sidechain
19	J	37	ARG	Sidechain
19	J	48	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	0	302	0	340	12	0
2	1	625	0	652	11	0
3	2	509	0	543	4	0
4	3	449	0	488	18	0
5	4	533	0	530	16	0
6	5	444	0	458	15	0
7	6	504	0	572	12	0
8	7	62355	0	31381	498	0
9	8	2572	0	1302	22	0
10	A	32950	0	16602	537	0
11	B	1776	0	1802	57	0
12	C	1658	0	1732	63	0
13	D	1643	0	1707	42	0
14	E	1166	0	1212	29	0
15	F	862	0	864	24	0
16	G	1203	0	1254	25	0
17	H	979	0	1031	28	0
18	I	1022	0	1069	17	0
19	J	803	0	842	25	0
20	K	884	0	896	18	0
21	L	955	0	1016	27	0
22	M	910	0	978	22	0
23	N	805	0	844	34	0
24	O	714	0	734	13	0
25	P	649	0	666	21	0
26	Q	648	0	691	11	0
27	R	544	0	565	14	0
28	S	663	0	688	14	0
29	T	670	0	719	22	0
30	U	584	0	618	7	0
31	V	516	0	262	11	0
32	W	1630	0	839	20	0
33	X	1654	0	848	29	0
34	Y	1628	0	828	20	0
35	a	1026	0	1092	10	0
36	b	2082	0	2154	54	0
37	c	1565	0	1616	42	0
38	d	1552	0	1619	32	0
39	e	1420	0	1457	37	0
40	f	1323	0	1371	29	0
41	g	427	0	464	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	h	1085	0	1169	21	0
43	i	1111	0	1148	16	0
44	j	1023	0	1050	19	0
45	k	979	0	1028	23	0
46	l	377	0	418	16	0
47	m	1129	0	1162	31	0
48	n	946	0	1023	33	0
49	o	1053	0	1129	37	0
50	p	206	0	95	4	0
51	q	960	0	1000	22	0
52	r	891	0	923	22	0
53	s	917	0	962	20	0
54	t	947	0	1019	21	0
55	u	816	0	839	10	0
56	v	857	0	922	19	0
57	w	738	0	807	8	0
58	x	779	0	831	6	0
59	y	753	0	780	14	0
60	z	634	0	653	15	0
61	0	1	0	0	0	0
61	4	1	0	0	0	0
62	7	12	0	24	0	0
63	7	10	0	19	2	0
64	7	257	0	0	0	0
64	A	23	0	0	0	0
64	I	1	0	0	0	0
64	V	1	0	0	0	0
64	X	1	0	0	0	0
64	Y	1	0	0	0	0
64	b	1	0	0	0	0
64	q	1	0	0	0	0
64	r	1	0	0	0	0
65	Y	5	0	4	0	0
66	7	12	0	0	1	0
66	x	1	0	0	0	0
All	All	151734	0	102351	1911	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 8.

The worst 5 of 1911 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)
32:W:54:5MU:C4	32:W:54:5MU:C5	1.79	1.70
33:X:55:5MU:C4	33:X:55:5MU:C5	1.80	1.65
31:V:19:G:H1	33:X:36:C:H42	1.17	0.92
10:A:664:G:H22	10:A:741:G:H1	1.24	0.85
8:7:1278:C:H4'	51:q:34:ILE:HD11	1.58	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	2	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
4	3	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
5	4	66/70 (94%)	56 (85%)	9 (14%)	1 (2%)	8	32
6	5	54/57 (95%)	54 (100%)	0	0	100	100
7	6	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
11	B	225/241 (93%)	189 (84%)	29 (13%)	7 (3%)	3	18
12	C	210/233 (90%)	186 (89%)	23 (11%)	1 (0%)	24	57
13	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
14	E	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
15	F	104/135 (77%)	84 (81%)	19 (18%)	1 (1%)	12	41
16	G	151/179 (84%)	140 (93%)	10 (7%)	1 (1%)	18	49
17	H	127/130 (98%)	127 (100%)	0	0	100	100
18	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
19	J	98/103 (95%)	89 (91%)	8 (8%)	1 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	K	116/129 (90%)	102 (88%)	14 (12%)	0	100	100
21	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
22	M	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
23	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
24	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
25	P	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
26	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
27	R	64/75 (85%)	52 (81%)	12 (19%)	0	100	100
28	S	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	64 (94%)	3 (4%)	1 (2%)	8	32
35	a	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
37	c	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
38	d	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
39	e	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
40	f	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
41	g	50/55 (91%)	50 (100%)	0	0	100	100
42	h	135/136 (99%)	135 (100%)	0	0	100	100
43	i	147/149 (99%)	122 (83%)	25 (17%)	0	100	100
44	j	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
45	k	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
46	l	44/46 (96%)	44 (100%)	0	0	100	100
47	m	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	18	49
48	n	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
49	o	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
50	p	5/36 (14%)	2 (40%)	2 (40%)	1 (20%)	0	0
51	q	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
52	r	114/117 (97%)	110 (96%)	3 (3%)	1 (1%)	14	44
53	s	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
54	t	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	u	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
56	v	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	14	44
57	w	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
58	x	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
59	y	92/94 (98%)	92 (100%)	0	0	100	100
60	z	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
All	All	6037/6490 (93%)	5723 (95%)	297 (5%)	17 (0%)	37	67

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	U	64	ASN
11	B	117	LEU
11	B	118	GLU
15	F	38	ARG
19	J	94	ALA

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	0	34/34 (100%)	34 (100%)	0	100	100
2	1	67/68 (98%)	67 (100%)	0	100	100
3	2	55/55 (100%)	55 (100%)	0	100	100
4	3	48/49 (98%)	48 (100%)	0	100	100
5	4	60/62 (97%)	60 (100%)	0	100	100
6	5	47/48 (98%)	47 (100%)	0	100	100
7	6	51/52 (98%)	51 (100%)	0	100	100
11	B	189/199 (95%)	189 (100%)	0	100	100
12	C	172/190 (90%)	171 (99%)	1 (1%)	78	83
13	D	172/173 (99%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	E	120/126 (95%)	120 (100%)	0	100	100
15	F	92/116 (79%)	92 (100%)	0	100	100
16	G	126/147 (86%)	124 (98%)	2 (2%)	55	75
17	H	104/105 (99%)	104 (100%)	0	100	100
18	I	105/107 (98%)	105 (100%)	0	100	100
19	J	88/90 (98%)	88 (100%)	0	100	100
20	K	91/99 (92%)	91 (100%)	0	100	100
21	L	103/104 (99%)	103 (100%)	0	100	100
22	M	95/96 (99%)	95 (100%)	0	100	100
23	N	83/84 (99%)	83 (100%)	0	100	100
24	O	76/77 (99%)	76 (100%)	0	100	100
25	P	65/65 (100%)	65 (100%)	0	100	100
26	Q	74/78 (95%)	74 (100%)	0	100	100
27	R	57/65 (88%)	55 (96%)	2 (4%)	32	62
28	S	72/79 (91%)	72 (100%)	0	100	100
29	T	65/66 (98%)	65 (100%)	0	100	100
30	U	59/61 (97%)	59 (100%)	0	100	100
35	a	110/181 (61%)	110 (100%)	0	100	100
36	b	216/218 (99%)	216 (100%)	0	100	100
37	c	164/164 (100%)	164 (100%)	0	100	100
38	d	165/165 (100%)	165 (100%)	0	100	100
39	e	149/150 (99%)	148 (99%)	1 (1%)	76	82
40	f	137/138 (99%)	135 (98%)	2 (2%)	57	75
41	g	47/49 (96%)	47 (100%)	0	100	100
42	h	110/109 (101%)	110 (100%)	0	100	100
43	i	114/114 (100%)	114 (100%)	0	100	100
44	j	103/123 (84%)	103 (100%)	0	100	100
45	k	104/110 (94%)	104 (100%)	0	100	100
46	l	38/38 (100%)	38 (100%)	0	100	100
47	m	116/116 (100%)	115 (99%)	1 (1%)	70	80
48	n	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	o	103/103 (100%)	103 (100%)	0	100	100
50	p	5/5 (100%)	5 (100%)	0	100	100
51	q	100/103 (97%)	100 (100%)	0	100	100
52	r	86/87 (99%)	86 (100%)	0	100	100
53	s	99/100 (99%)	99 (100%)	0	100	100
54	t	89/90 (99%)	89 (100%)	0	100	100
55	u	84/84 (100%)	84 (100%)	0	100	100
56	v	93/93 (100%)	93 (100%)	0	100	100
57	w	80/84 (95%)	80 (100%)	0	100	100
58	x	83/85 (98%)	83 (100%)	0	100	100
59	y	78/78 (100%)	78 (100%)	0	100	100
60	z	62/63 (98%)	62 (100%)	0	100	100
All	All	5009/5249 (95%)	5000 (100%)	9 (0%)	85	89

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	f	72	LEU
47	m	99	ARG
27	R	11	CYS
27	R	74	HIS
39	e	175	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
40	f	101	ASN
45	k	105	GLN
40	f	115	HIS
43	i	43	ASN
47	m	80	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1534/1535 (99%)	396 (25%)	30 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	V	23/24 (95%)	13 (56%)	3 (13%)
32	W	75/76 (98%)	24 (32%)	4 (5%)
33	X	76/77 (98%)	28 (36%)	6 (7%)
34	Y	75/76 (98%)	22 (29%)	2 (2%)
8	7	2903/2921 (99%)	465 (16%)	31 (1%)
9	8	119/120 (99%)	14 (11%)	3 (2%)
All	All	4805/4829 (99%)	962 (20%)	79 (1%)

5 of 962 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	10	A
8	7	15	G
8	7	34	U
8	7	44	A
8	7	46	G

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1168	U
33	X	1	G
10	A	1201	A
31	V	17	G
33	X	47	G7M

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

54 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	$\# Z > 2$
34	5MU	Y	54	34	19,22,23	0.27	0	28,32,35	0.29	0
10	5MC	A	1407	10	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	5MU	X	55	33	19,22,23	7.20	7 (36%)	28,32,35	3.32	10 (35%)
34	PSU	Y	55	34	18,21,22	4.66	8 (44%)	22,30,33	1.87	5 (22%)
10	UR3	A	1498	10	19,22,23	2.76	8 (42%)	26,32,35	1.32	2 (7%)
33	PSU	X	56	33	18,21,22	4.69	8 (44%)	22,30,33	1.81	5 (22%)
10	5MC	A	967	10	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
33	RSP	X	33	33	17,21,22	4.13	7 (41%)	22,30,33	0.82	0
8	5MU	7	747	8	19,22,23	0.23	0	28,32,35	0.34	0
32	G7M	W	46	32	23,26,27	2.85	9 (39%)	35,39,42	1.94	8 (22%)
8	PSU	7	2504	8	18,21,22	4.67	8 (44%)	22,30,33	1.84	5 (22%)
8	OMG	7	2251	32,8	23,26,27	2.57	7 (30%)	33,38,41	2.43	10 (30%)
8	PSU	7	2605	8	18,21,22	4.65	8 (44%)	22,30,33	1.80	5 (22%)
8	2MA	7	2503	8,64	22,25,26	4.06	8 (36%)	33,37,40	3.39	12 (36%)
10	G7M	A	527	10	23,26,27	2.84	9 (39%)	35,39,42	1.75	8 (22%)
8	2MG	7	1835	8	23,26,27	0.35	0	32,38,41	0.46	0
32	5MU	W	54	32	19,22,23	7.19	7 (36%)	28,32,35	3.31	9 (32%)
33	H2U	X	17	33	18,21,22	3.10	5 (27%)	21,30,33	1.95	4 (19%)
34	H2U	Y	17	34	18,21,22	3.09	5 (27%)	21,30,33	2.03	5 (23%)
32	PSU	W	32	32	18,21,22	4.66	8 (44%)	22,30,33	1.87	5 (22%)
8	PSU	7	746	8,64	18,21,22	4.67	9 (50%)	22,30,33	1.78	5 (22%)
32	MIA	W	37	32	28,31,32	2.42	5 (17%)	40,44,47	2.74	17 (42%)
33	H2U	X	21	33	18,21,22	3.09	5 (27%)	21,30,33	1.99	5 (23%)
10	MA6	A	1518	10	23,26,27	1.35	3 (13%)	34,38,41	3.31	14 (41%)
8	OMC	7	2498	8,64	19,22,23	3.24	8 (42%)	26,31,34	0.77	0
33	4SU	X	8	33	18,21,22	3.79	7 (38%)	26,30,33	2.26	4 (15%)
33	2MA	X	38	33	22,25,26	4.15	8 (36%)	33,37,40	3.60	10 (30%)
32	H2U	W	20	32	18,21,22	3.06	5 (27%)	21,30,33	2.01	5 (23%)
10	MA6	A	1519	10	23,26,27	1.35	4 (17%)	34,38,41	3.34	14 (41%)
8	G7M	7	2069	8	23,26,27	2.82	9 (39%)	35,39,42	1.73	7 (20%)
8	5MC	7	1962	8	18,22,23	4.03	7 (38%)	26,32,35	1.03	2 (7%)
10	2MG	A	1207	10	23,26,27	3.10	8 (34%)	32,38,41	2.50	11 (34%)
10	4OC	A	1402	10	20,23,24	3.24	8 (40%)	26,32,35	0.90	1 (3%)
8	6MZ	7	2030	8	22,25,26	2.85	5 (22%)	30,36,39	2.42	11 (36%)
8	6MZ	7	1618	8	22,25,26	2.75	4 (18%)	30,36,39	2.48	10 (33%)
8	3TD	7	1915	8	19,22,23	4.04	7 (36%)	21,32,35	1.72	2 (9%)
33	3AU	X	48	33	24,28,29	2.84	7 (29%)	33,40,43	1.30	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	7	955	8	18,21,22	4.63	8 (44%)	22,30,33	1.87	5 (22%)
8	1MG	7	745	8	22,26,27	2.72	5 (22%)	33,39,42	2.31	8 (24%)
8	5MU	7	1939	8	19,22,23	0.27	0	28,32,35	0.27	0
10	2MG	A	1516	10	23,26,27	3.11	8 (34%)	32,38,41	2.49	11 (34%)
8	PSU	7	2580	8	18,21,22	4.62	9 (50%)	22,30,33	1.89	6 (27%)
8	H2U	7	2449	8	18,21,22	3.02	5 (27%)	21,30,33	2.04	5 (23%)
8	PSU	7	2457	8	18,21,22	4.62	8 (44%)	22,30,33	1.94	5 (22%)
32	H2U	W	17	32	18,21,22	3.08	5 (27%)	21,30,33	2.00	5 (23%)
32	PSU	W	55	32	18,21,22	4.68	8 (44%)	22,30,33	1.84	5 (22%)
32	H2U	W	16	32	18,21,22	3.07	5 (27%)	21,30,33	1.94	5 (23%)
8	PSU	7	2604	8	18,21,22	4.63	8 (44%)	22,30,33	1.85	5 (22%)
10	2MG	A	966	10	23,26,27	3.13	8 (34%)	32,38,41	2.50	11 (34%)
32	4SU	W	8	32	18,21,22	3.79	7 (38%)	26,30,33	2.25	5 (19%)
8	2MG	7	2445	8	23,26,27	3.09	8 (34%)	32,38,41	2.50	11 (34%)
34	G7M	Y	46	34	23,26,27	2.84	9 (39%)	35,39,42	1.74	7 (20%)
8	OMU	7	2552	8	19,22,23	3.20	8 (42%)	26,31,34	1.71	5 (19%)
33	G7M	X	47	33	23,26,27	2.85	8 (34%)	35,39,42	1.95	8 (22%)

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
34	5MU	Y	54	34	-	2/7/25/26	0/2/2/2
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
33	5MU	X	55	33	-	2/7/25/26	0/2/2/2
34	PSU	Y	55	34	-	0/7/25/26	0/2/2/2
10	UR3	A	1498	10	-	2/7/25/26	0/2/2/2
33	PSU	X	56	33	-	1/7/25/26	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
33	RSP	X	33	33	-	1/7/25/26	0/2/2/2
8	5MU	7	747	8	-	1/7/25/26	0/2/2/2
32	G7M	W	46	32	-	5/7/25/26	0/3/3/3
8	PSU	7	2504	8	-	0/7/25/26	0/2/2/2
8	OMG	7	2251	32,8	-	3/9/27/28	0/3/3/3
8	PSU	7	2605	8	-	0/7/25/26	0/2/2/2
8	2MA	7	2503	8,64	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	G7M	A	527	10	-	2/7/25/26	0/3/3/3
8	2MG	7	1835	8	-	0/9/27/28	0/3/3/3
32	5MU	W	54	32	-	2/7/25/26	0/2/2/2
33	H2U	X	17	33	-	5/7/38/39	0/2/2/2
34	H2U	Y	17	34	-	7/7/38/39	0/2/2/2
32	PSU	W	32	32	-	0/7/25/26	0/2/2/2
8	PSU	7	746	8,64	-	1/7/25/26	0/2/2/2
32	MIA	W	37	32	-	3/15/33/34	0/3/3/3
33	H2U	X	21	33	-	2/7/38/39	0/2/2/2
10	MA6	A	1518	10	-	0/11/29/30	0/3/3/3
8	OMC	7	2498	8,64	-	2/9/27/28	0/2/2/2
33	4SU	X	8	33	-	2/7/25/26	0/2/2/2
33	2MA	X	38	33	-	5/7/25/26	0/3/3/3
32	H2U	W	20	32	-	1/7/38/39	0/2/2/2
10	MA6	A	1519	10	-	3/11/29/30	0/3/3/3
8	G7M	7	2069	8	-	3/7/25/26	0/3/3/3
8	5MC	7	1962	8	-	0/7/25/26	0/2/2/2
10	2MG	A	1207	10	-	0/9/27/28	0/3/3/3
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
8	6MZ	7	2030	8	-	3/9/27/28	0/3/3/3
8	6MZ	7	1618	8	-	4/9/27/28	0/3/3/3
8	3TD	7	1915	8	-	2/7/25/26	0/2/2/2
33	3AU	X	48	33	-	4/16/34/35	0/2/2/2
8	PSU	7	955	8	-	0/7/25/26	0/2/2/2
8	1MG	7	745	8	-	0/7/25/26	0/3/3/3
8	5MU	7	1939	8	-	0/7/25/26	0/2/2/2
10	2MG	A	1516	10	-	0/9/27/28	0/3/3/3
8	PSU	7	2580	8	-	0/7/25/26	0/2/2/2
8	H2U	7	2449	8	-	0/7/38/39	0/2/2/2
8	PSU	7	2457	8	-	1/7/25/26	0/2/2/2
32	H2U	W	17	32	-	2/7/38/39	0/2/2/2
32	PSU	W	55	32	-	0/7/25/26	0/2/2/2
32	H2U	W	16	32	-	1/7/38/39	0/2/2/2
8	PSU	7	2604	8	-	0/7/25/26	0/2/2/2
10	2MG	A	966	10	-	0/9/27/28	0/3/3/3
32	4SU	W	8	32	-	2/7/25/26	0/2/2/2
8	2MG	7	2445	8	-	0/9/27/28	0/3/3/3
34	G7M	Y	46	34	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMU	7	2552	8	-	0/9/27/28	0/2/2/2
33	G7M	X	47	33	-	3/7/25/26	0/3/3/3

The worst 5 of 352 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	55	5MU	C4-C5	21.25	1.80	1.44
32	W	54	5MU	C4-C5	21.10	1.79	1.44
32	W	54	5MU	C6-N1	15.74	1.64	1.38
33	X	55	5MU	C6-N1	15.72	1.64	1.38
33	X	38	2MA	C4-N3	12.66	1.50	1.34

The worst 5 of 325 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	X	38	2MA	C1'-N9-C8	-12.89	98.03	127.14
10	A	1519	MA6	N1-C6-N6	-12.29	103.65	117.08
8	7	2503	2MA	C1'-N9-C8	-12.05	99.93	127.14
10	A	1518	MA6	N1-C6-N6	-11.81	104.17	117.08
33	X	38	2MA	C4-N9-C1'	11.55	154.12	126.59

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	527	G7M	O4'-C4'-C5'-O5'
10	A	527	G7M	C3'-C4'-C5'-O5'
34	Y	17	H2U	O4'-C4'-C5'-O5'
34	Y	17	H2U	C3'-C4'-C5'-O5'
34	Y	17	H2U	O4'-C1'-N1-C6

There are no ring outliers.

23 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Y	54	5MU	4	0
33	X	55	5MU	1	0
34	Y	55	PSU	1	0
33	X	56	PSU	1	0
8	7	747	5MU	1	0
32	W	46	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	7	2251	OMG	1	0
8	7	2503	2MA	3	0
32	W	54	5MU	2	0
32	W	37	MIA	2	0
10	A	1518	MA6	1	0
33	X	38	2MA	3	0
10	A	1402	4OC	2	0
8	7	2030	6MZ	3	0
8	7	1915	3TD	1	0
33	X	48	3AU	2	0
8	7	1939	5MU	1	0
8	7	2449	H2U	1	0
32	W	17	H2U	1	0
32	W	16	H2U	3	0
8	7	2604	PSU	1	0
34	Y	46	G7M	1	0
33	X	47	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 293 ligands modelled in this entry, 289 are monoatomic - leaving 4 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	$\# Z > 2$
62	PUT	7	3001	-	5,5,5	0.25	0	4,4,4	0.52	0
62	PUT	7	3002	-	5,5,5	0.25	0	4,4,4	0.54	0
63	SPD	7	3003	-	9,9,9	0.32	0	8,8,8	0.85	0
65	ALA	Y	102	34	3,4,5	1.17	1 (33%)	2,4,6	3.11	1 (50%)

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
62	PUT	7	3001	-	-	1/3/3/3	-
62	PUT	7	3002	-	-	0/3/3/3	-
63	SPD	7	3003	-	-	0/7/7/7	-
65	ALA	Y	102	34	-	0/0/2/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	Y	102	ALA	O-C	2.01	1.27	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Y	102	ALA	O-C-CA	-4.39	110.38	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	7	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	7	3003	SPD	2	0

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.

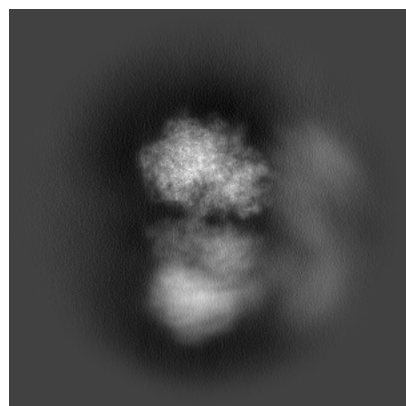
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17743. These allow visual inspection of the internal detail of the map and identification of artifacts.

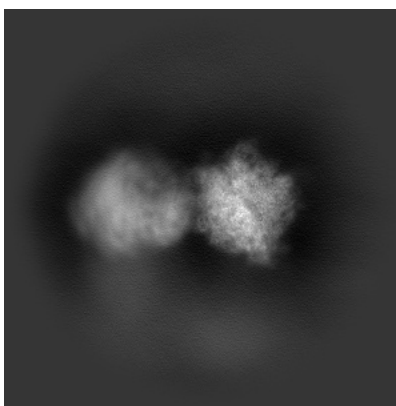
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

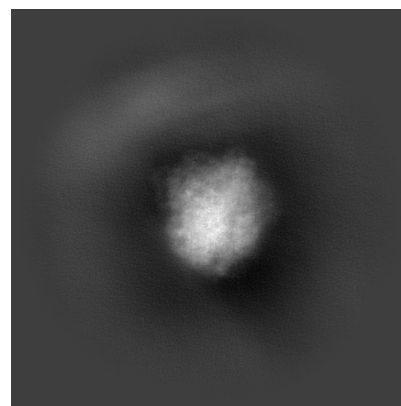
6.1.1 Primary map



X

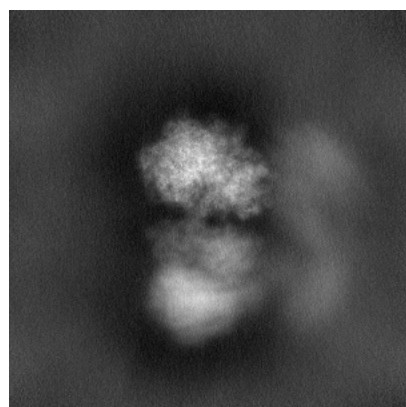


Y

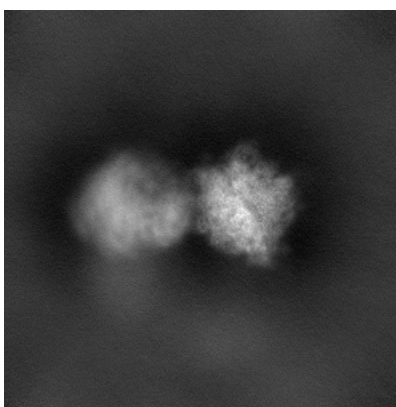


Z

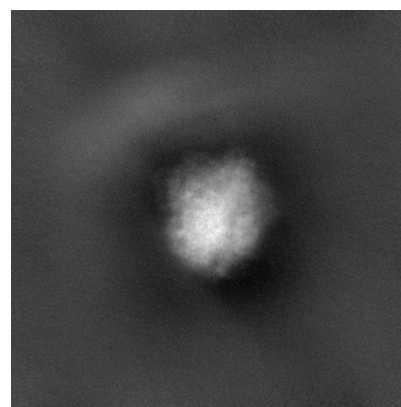
6.1.2 Raw map



X



Y

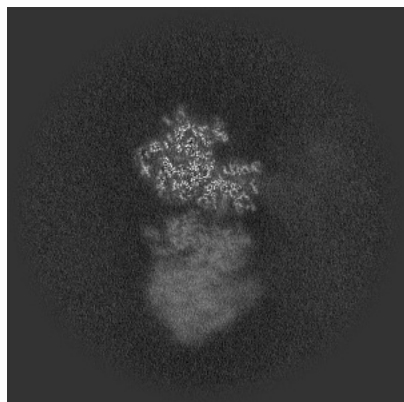


Z

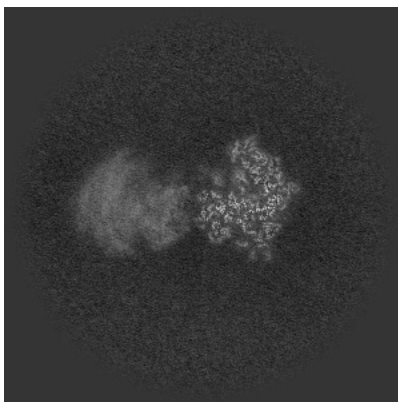
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

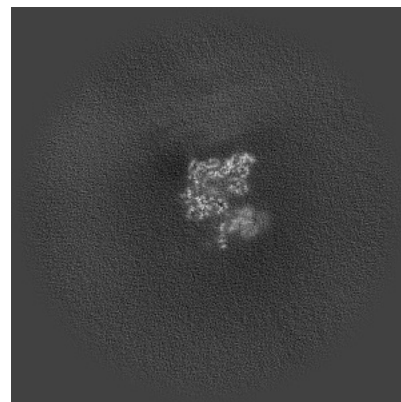
6.2.1 Primary map



X Index: 351

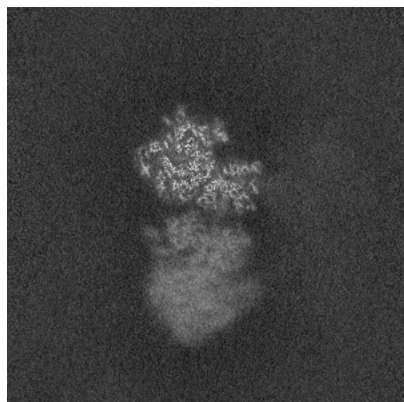


Y Index: 351

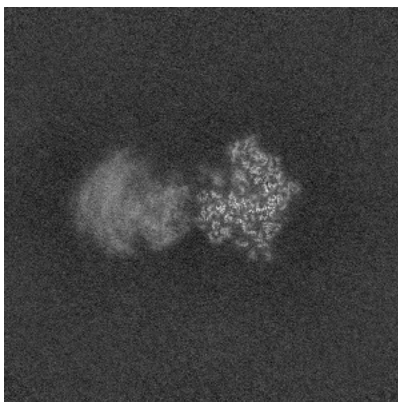


Z Index: 351

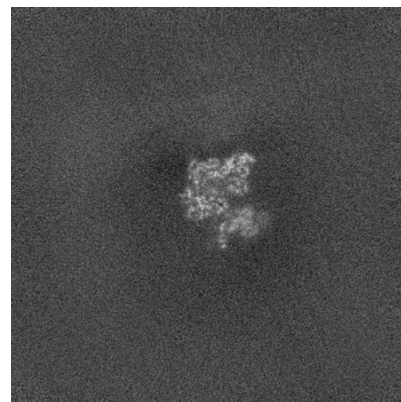
6.2.2 Raw map



X Index: 351



Y Index: 351

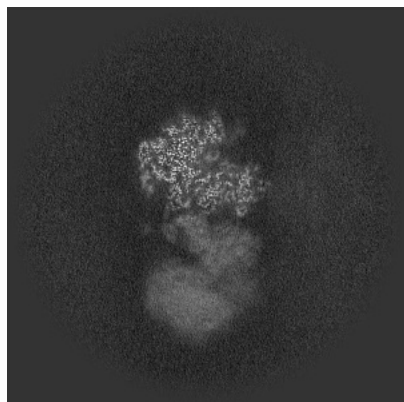


Z Index: 351

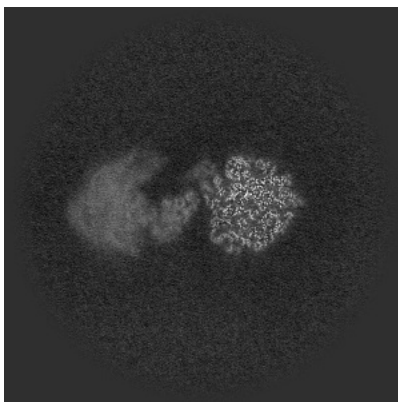
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

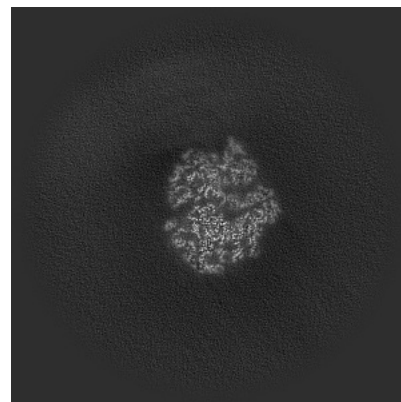
6.3.1 Primary map



X Index: 369

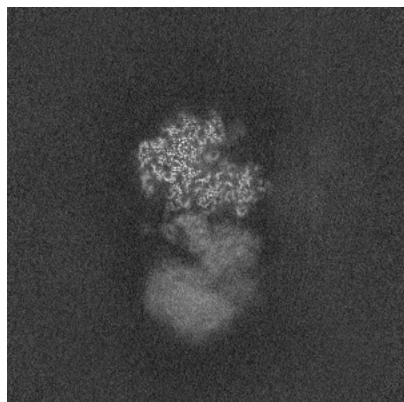


Y Index: 312

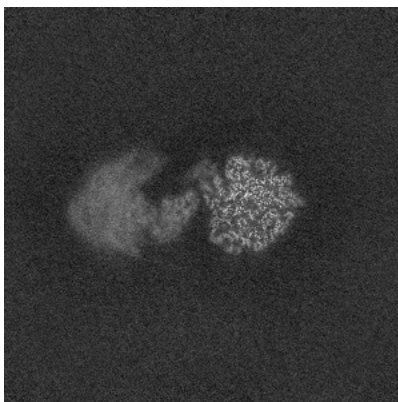


Z Index: 411

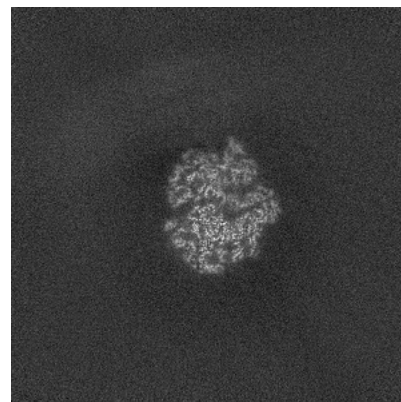
6.3.2 Raw map



X Index: 369



Y Index: 312

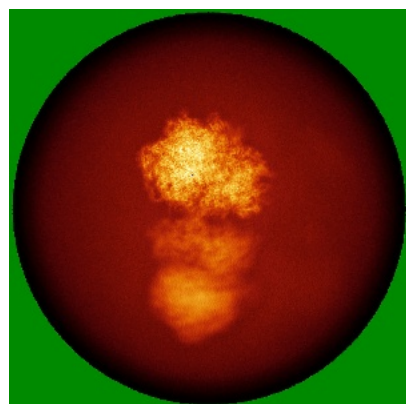


Z Index: 411

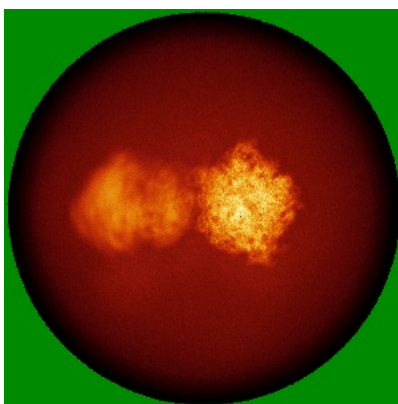
The images above show the largest variance slices of the map in three orthogonal directions.

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

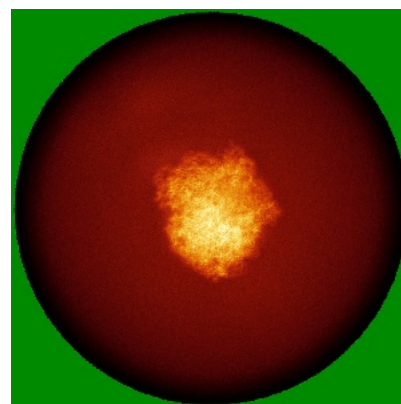
6.4.1 Primary map



X

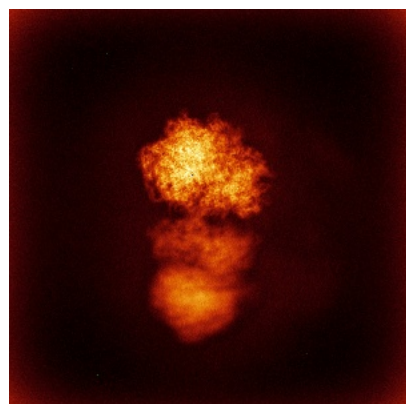


Y

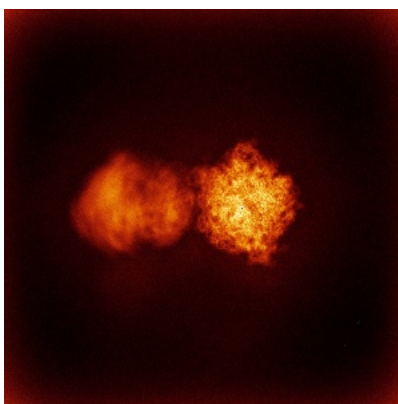


Z

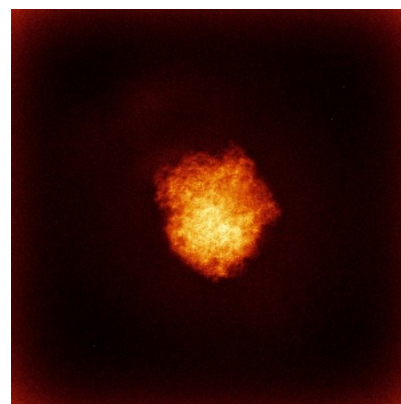
6.4.2 Raw map



X



Y

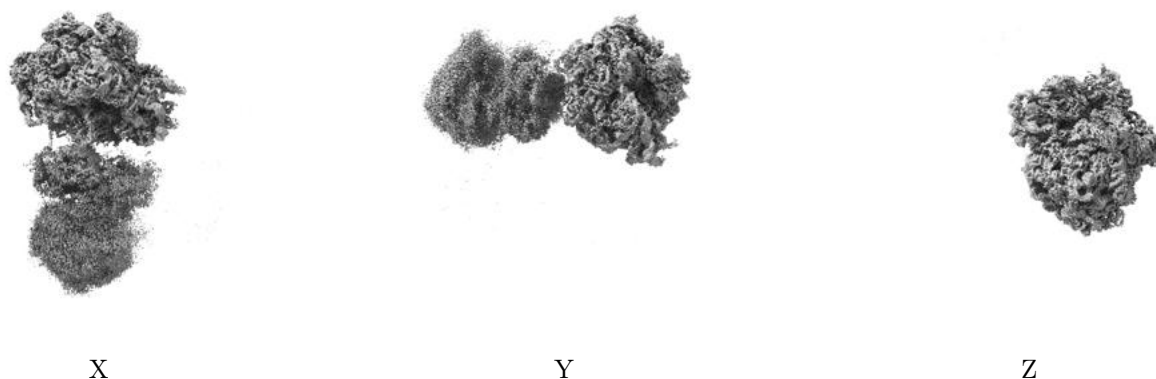


Z

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.

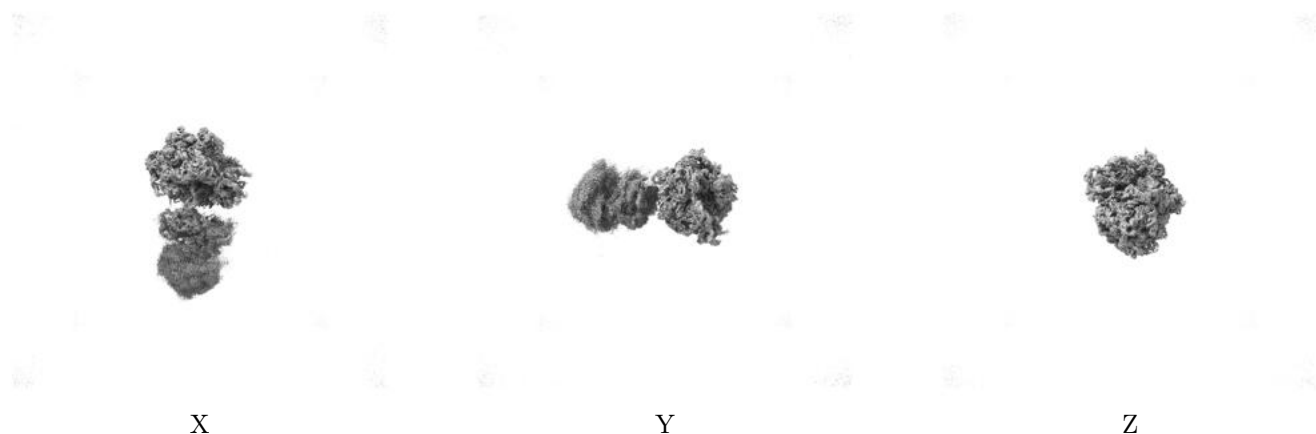
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. 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.

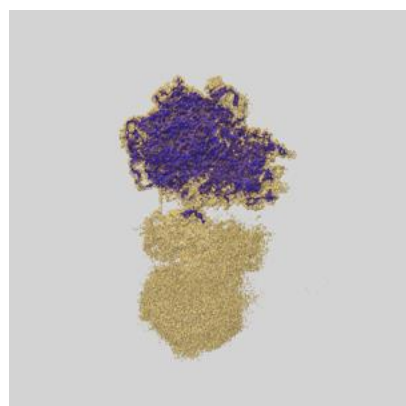
6.6 Mask visualisation [i](#)

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

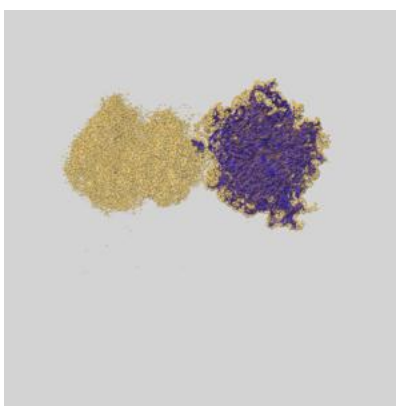
A mask typically either:

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

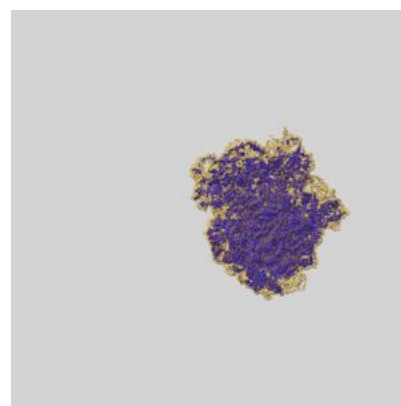
6.6.1 emd_17743_msk_1.map [i](#)



X



Y

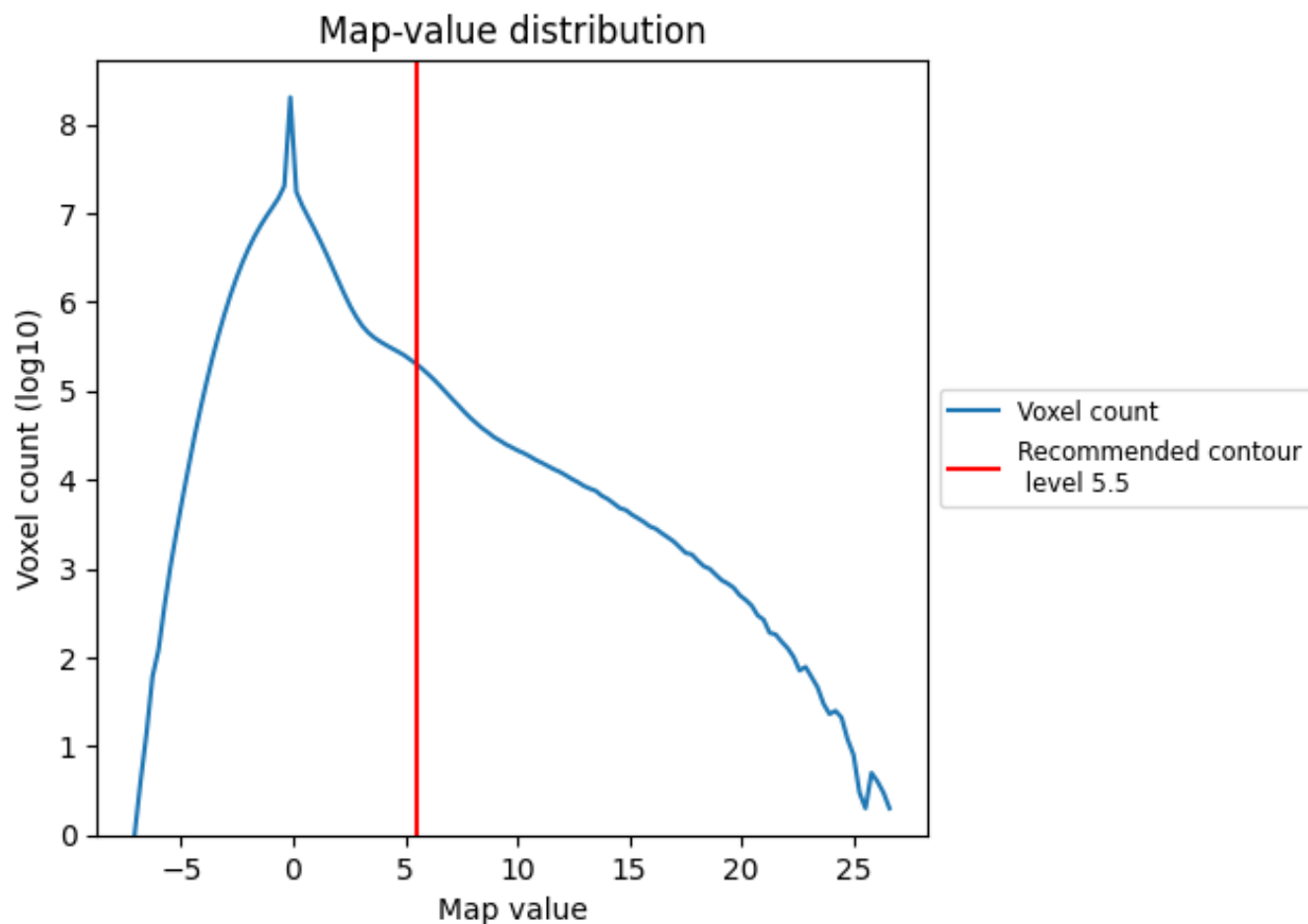


Z

7 Map analysis [i](#)

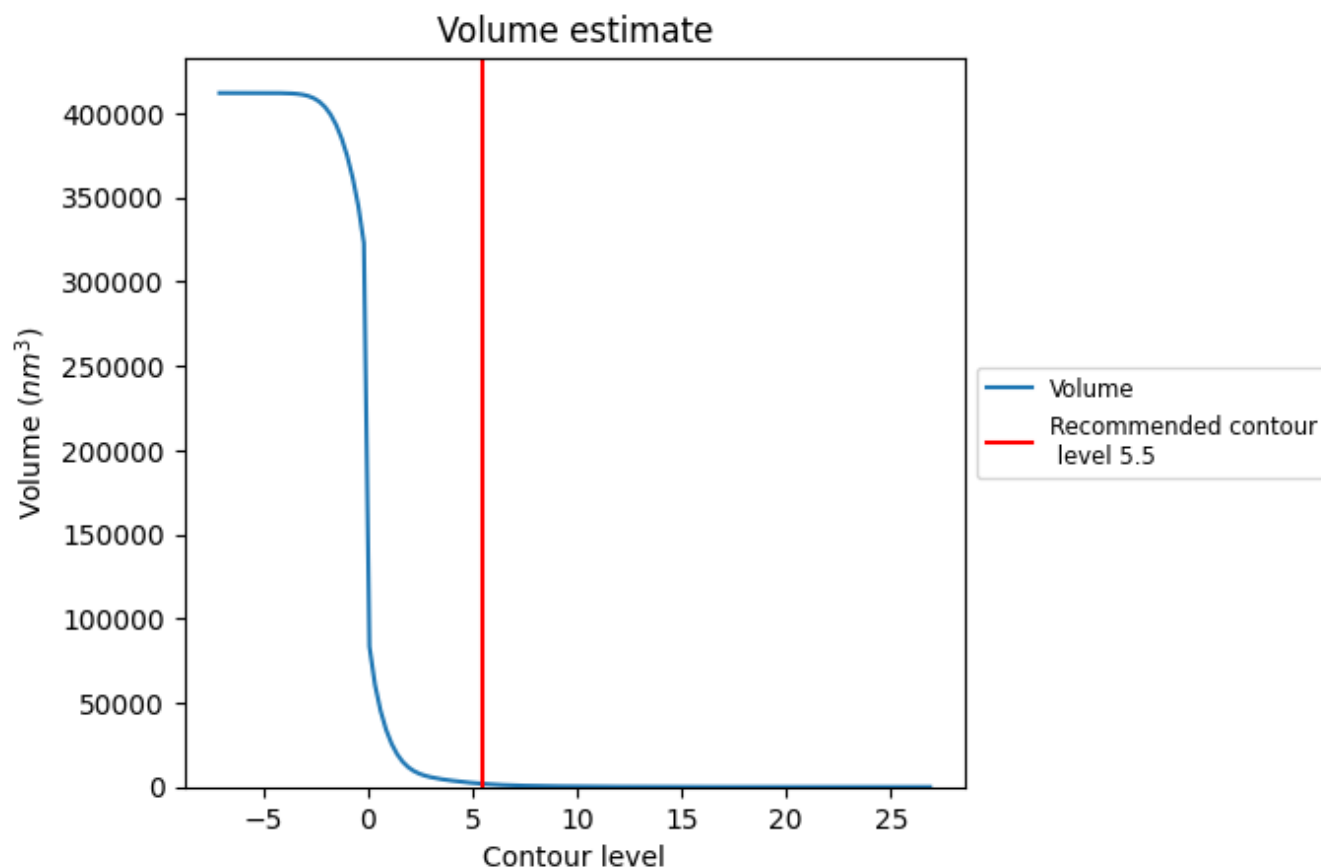
This section contains the results of statistical analysis of the map.

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.

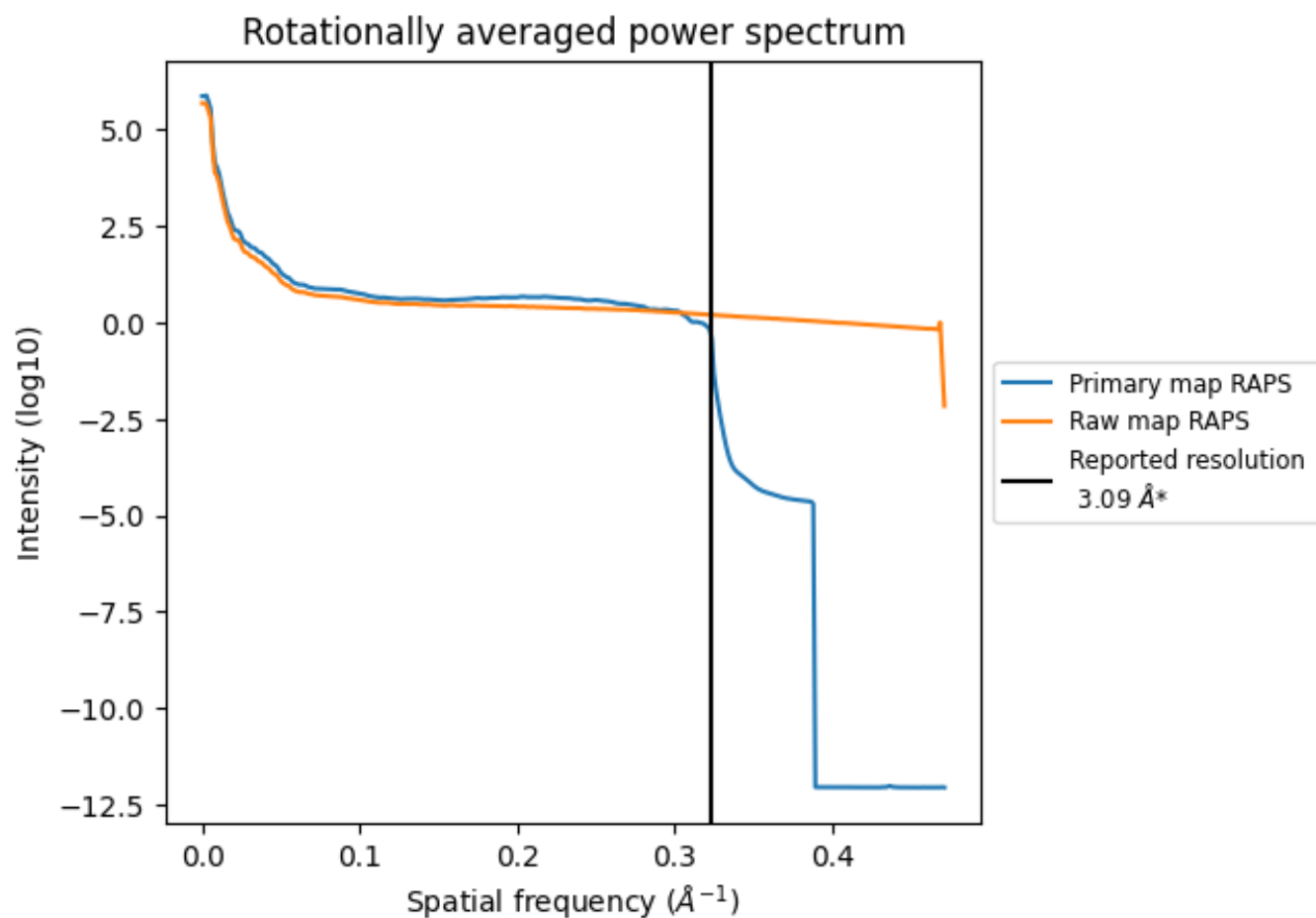
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1904 nm^3 ; this corresponds to an approximate mass of 1720 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 ⓘ

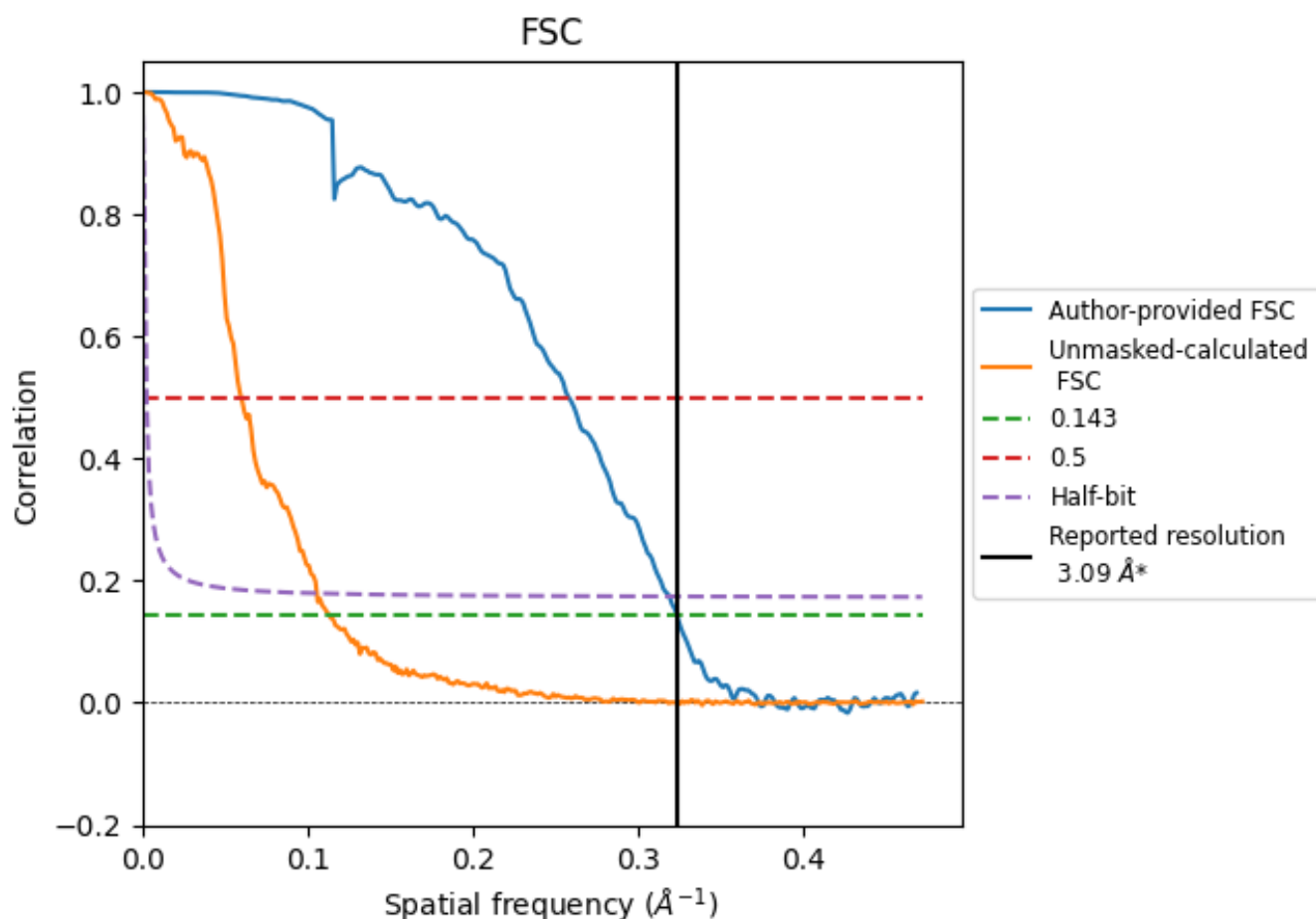


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

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 0.324 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

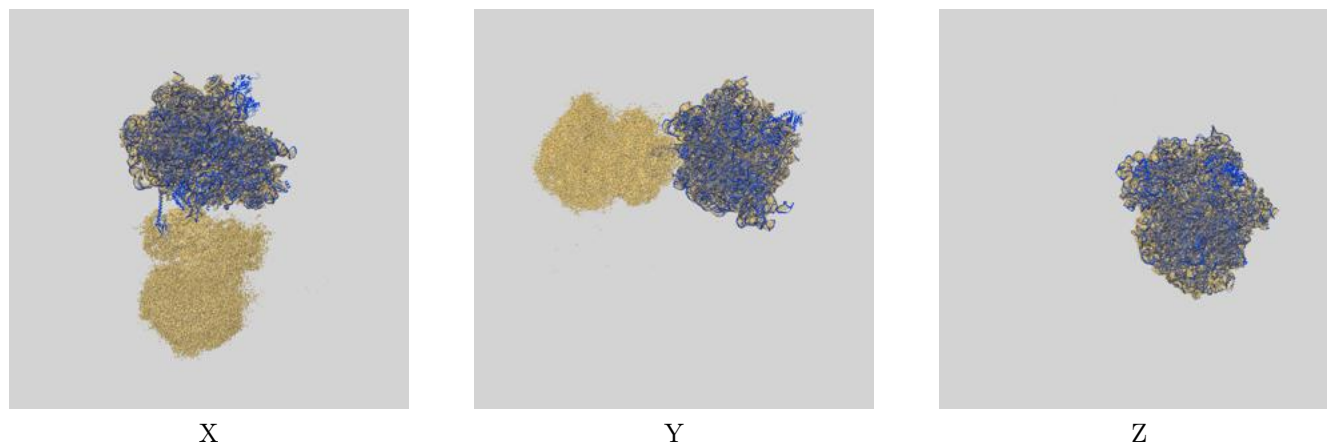
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.88	3.14
Unmasked-calculated*	8.83	16.72	9.47

*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 8.83 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

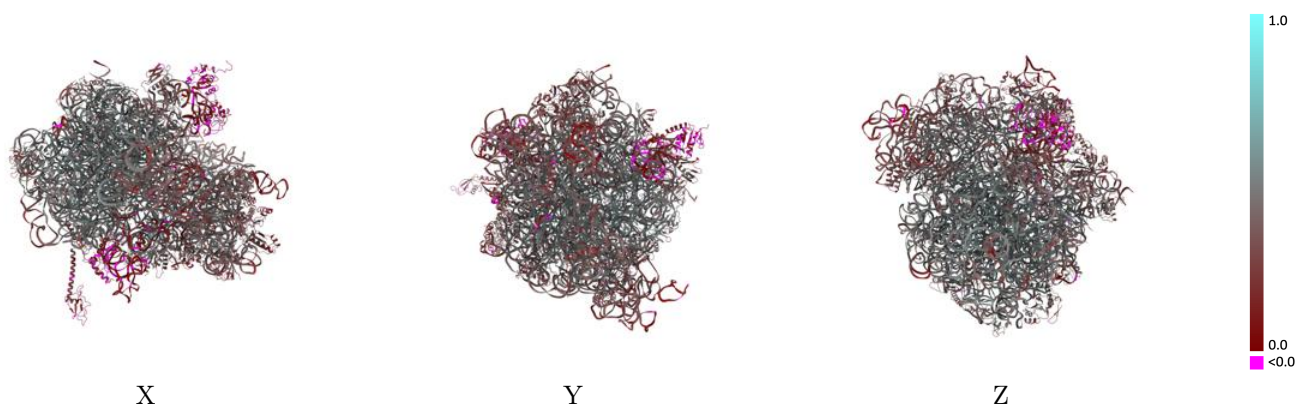
This section contains information regarding the fit between EMDB map EMD-17743 and PDB model 8PKL. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



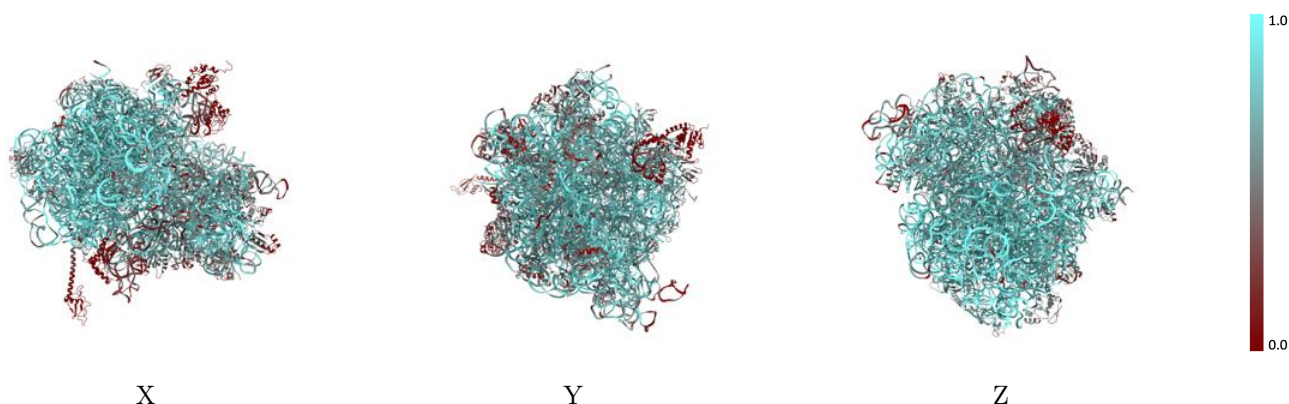
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



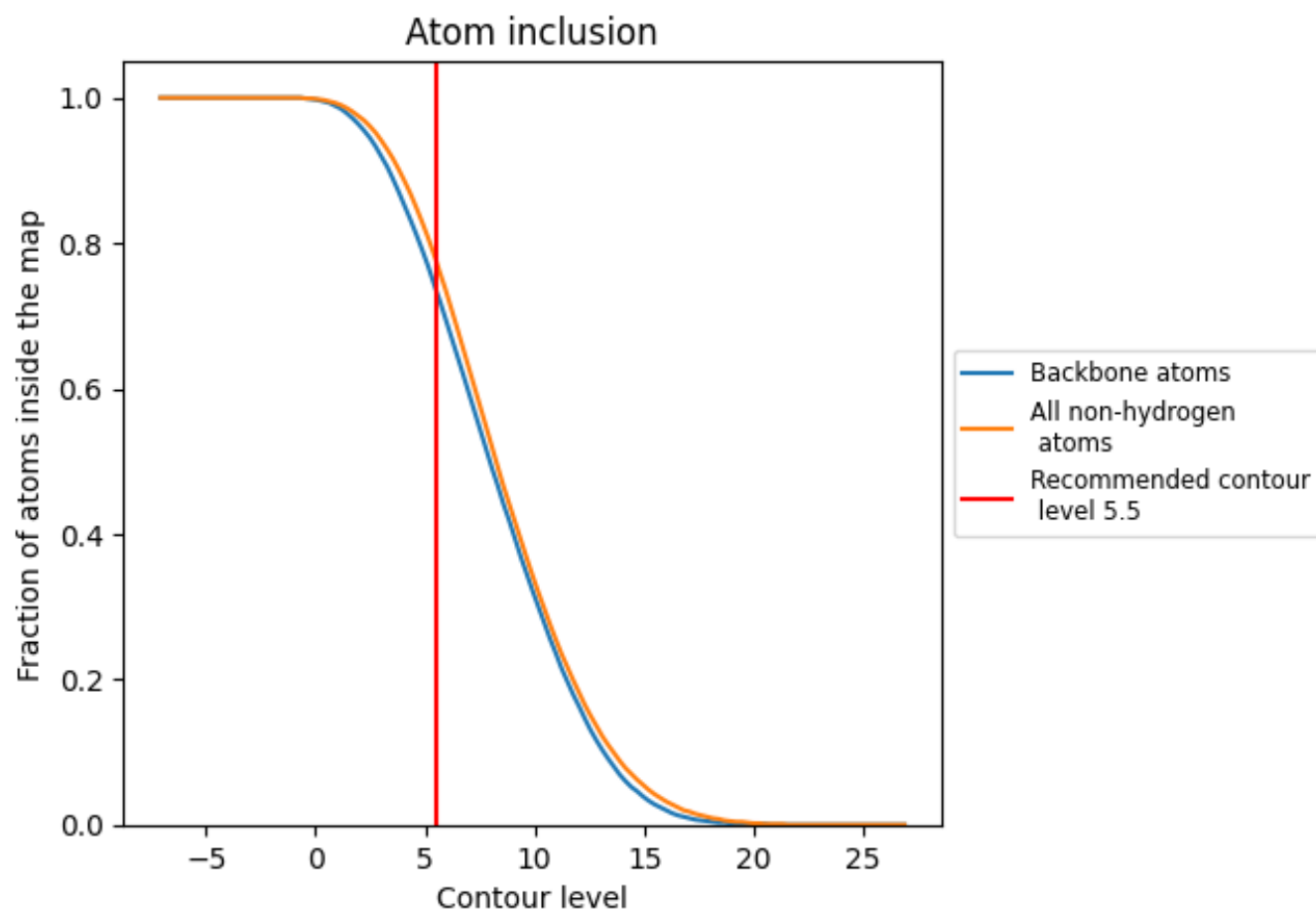
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 78% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.4140
0	 0.7850	 0.4090
1	 0.7440	 0.4470
2	 0.5860	 0.3790
3	 0.7050	 0.3980
4	 0.3520	 0.2890
5	 0.7500	 0.4200
6	 0.8390	 0.4680
7	 0.9070	 0.4640
8	 0.8620	 0.4070
A	 0.8520	 0.4170
B	 0.3770	 0.3190
C	 0.5310	 0.3430
D	 0.3880	 0.3240
E	 0.5930	 0.4000
F	 0.4590	 0.3680
G	 0.5640	 0.3560
H	 0.5330	 0.3850
I	 0.5530	 0.3570
J	 0.4010	 0.2920
K	 0.6380	 0.4070
L	 0.7040	 0.4000
M	 0.5470	 0.3370
N	 0.5980	 0.3490
O	 0.5970	 0.3590
P	 0.5090	 0.3680
Q	 0.5540	 0.3710
R	 0.5930	 0.4290
S	 0.5660	 0.3590
T	 0.5620	 0.2880
U	 0.4910	 0.3340
V	 0.5400	 0.2600
W	 0.8680	 0.3690
X	 0.3800	 0.1560
Y	 0.6400	 0.3290



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Chain	Atom inclusion	Q-score
a	 0.0280	 0.0810
b	 0.7870	 0.4670
c	 0.7280	 0.4470
d	 0.6570	 0.4130
e	 0.5260	 0.3060
f	 0.5230	 0.3470
g	 0.6970	 0.4000
h	 0.7560	 0.4370
i	 0.1760	 0.2140
j	 0.0040	 0.0530
k	 0.0030	 0.0530
l	 0.8680	 0.4860
m	 0.7950	 0.4450
n	 0.7080	 0.4280
o	 0.6900	 0.4300
p	 0.3680	 0.2100
q	 0.7830	 0.4440
r	 0.5830	 0.3550
s	 0.6790	 0.4210
t	 0.8070	 0.4630
u	 0.6410	 0.4170
v	 0.7520	 0.4520
w	 0.7180	 0.4240
x	 0.6150	 0.3940
y	 0.6340	 0.3780
z	 0.7770	 0.4470