



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2026 – 08:14 pm BST

PDB ID : 9SXK / pdb_00009sxx
EMDB ID : EMD-55337
Title : Structural characterization of hibernating ribosomes in the Gram-negative pathogen *Klebsiella quasipneumoniae*
Authors : Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.D.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on : 2025-10-10
Resolution : 2.30 Å (reported)
Based on initial model : 8B0X

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

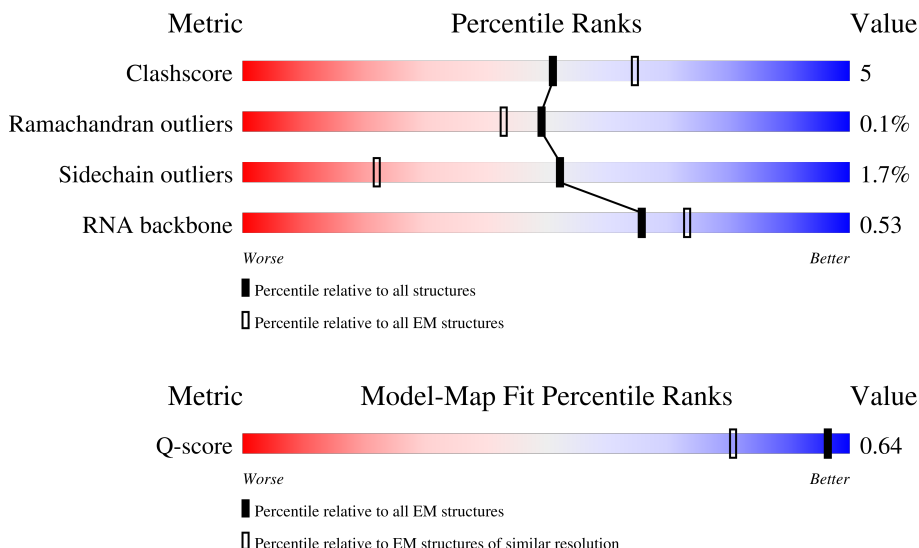
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	55	<div> <div>27%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
2	1	46	<div> <div></div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
3	2	65	<div> <div></div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1550	
7	B	241	
8	C	232	
9	D	206	
10	E	167	
11	F	131	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	W	15	
27	X	111	
28	a	2923	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	b	116	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	128	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 143298 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			418	268	76	73	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	70	Total	C	N	O	S	0	0
			540	333	103	98	6		

- Molecule 6 is a RNA chain called 16s rRNA (1538-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1538	Total	C	N	O	P	0	0
			33009	14730	6051	10690	1538		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1749	1106	315	320	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	206	Total	C	N	O	S	0	0
			1623	1028	305	287	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1644	1025	316	298	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1155	719	219	211	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			832	524	151	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	62	MET	LEU	variant	UNP A0A2N4W582

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1204	751	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			977	616	171	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	126	Total	C	N	O	S	0	0
			1010	628	202	177	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			788	493	151	143	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			877	541	173	160	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	HSE	ASN	conflict	UNP A0A1C1EGM1

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			958	592	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	116	Total	C	N	O	S	0	0
			907	564	181	158	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			805	500	164	138	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			710	438	144	127	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			636	397	127	111	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			639	402	121	112	4		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	62	Total	C	N	O	0	0
			507	321	94	92		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			667	426	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			669	413	138	115	3		

- Molecule 26 is a RNA chain called non-STOP mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	10	Total	C	N	O	P	0	0
			219	97	41	71	10		

- Molecule 27 is a protein called Ribosomal subunit interface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	98	Total	C	N	O	S	0	0
			778	484	149	142	3		

- Molecule 28 is a RNA chain called 23S rRNA (2901-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2901	Total	C	N	O	P	0	0
			62284	27795	11452	20136	2901		

- Molecule 29 is a RNA chain called 5S rRNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	116	Total	C	N	O	P	0	0
			2483	1106	453	808	116		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	271	Total	C	N	O	S	0	0
			2080	1286	423	364	7		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	209	Total	C	N	O	S	0	0
			1567	981	289	294	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	201	Total	C	N	O	S	0	0
			1554	975	284	290	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	176	Total	C	N	O	S	0	0
			1319	830	243	244	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	148	Total	C	N	O	S	0	0
			1099	693	197	208	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1134	716	211	202	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	123	Total	C	N	O	S	0	0
			947	594	181	166	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1063	658	211	191	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1074	685	204	179	6		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	119	Total	C	N	O	S	0	0
			950	588	195	162	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			816	517	153	144	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total	C	N	O	S	0	0
			855	530	166	156	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	93	Total	C	N	O	S	0	0
			739	467	139	131	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	u	94	Total	C	N	O	S	0
			749	477	136	134	2	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	v	78	Total	C	N	O	S	0
			592	367	118	106	1	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	x	62	Total	C	N	O	S	0
			499	308	98	92	1	0

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	y	58	Total	C	N	O	S	0
			447	279	87	79	2	0

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	z	56	Total	C	N	O	S	0
			443	269	94	79	1	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total 1	Zn 1	0
54	4	1	Total 1	Zn 1	0

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	95	Total 95	Mg 95	0
55	E	1	Total 1	Mg 1	0
55	a	254	Total 254	Mg 254	0
55	b	5	Total 5	Mg 5	0
55	c	1	Total 1	Mg 1	0
55	d	1	Total 1	Mg 1	0
55	p	1	Total 1	Mg 1	0
55	z	1	Total 1	Mg 1	0

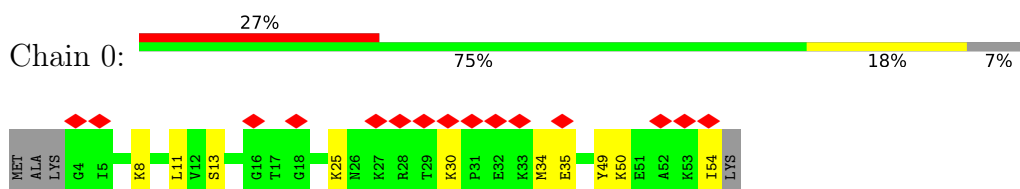
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	47	Total 47	K 47	0
56	a	114	Total 114	K 114	0
56	b	1	Total 1	K 1	0
56	c	4	Total 4	K 4	0
56	d	1	Total 1	K 1	0
56	e	1	Total 1	K 1	0
56	f	1	Total 1	K 1	0

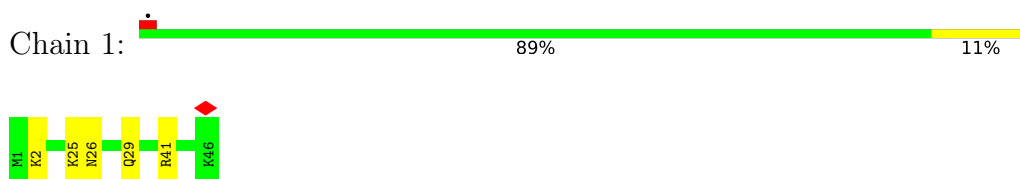
3 Residue-property plots [i](#)

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

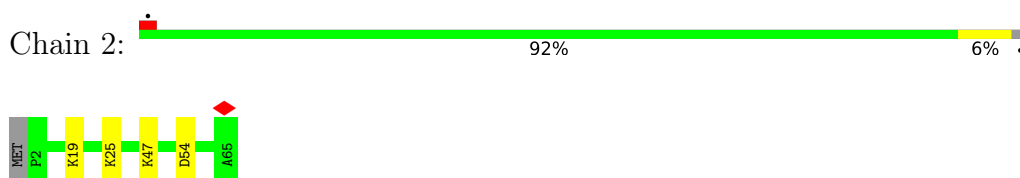
- Molecule 1: Large ribosomal subunit protein bL33



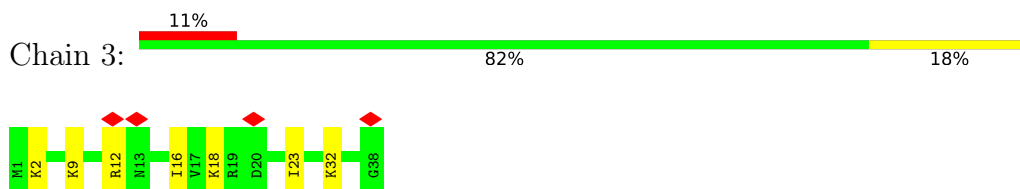
- Molecule 2: Large ribosomal subunit protein bL34



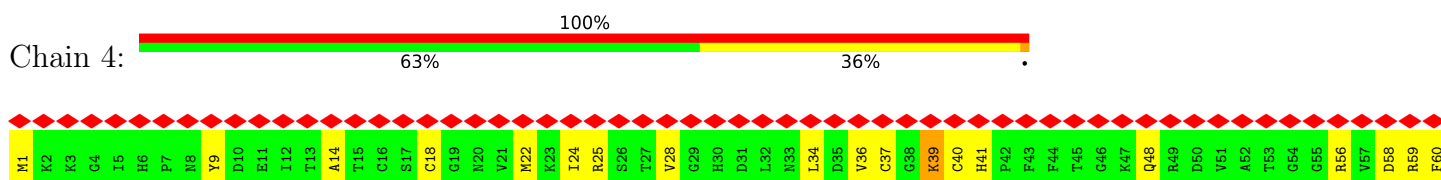
- Molecule 3: Large ribosomal subunit protein bL35

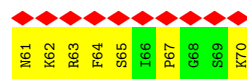


- Molecule 4: Large ribosomal subunit protein bL36

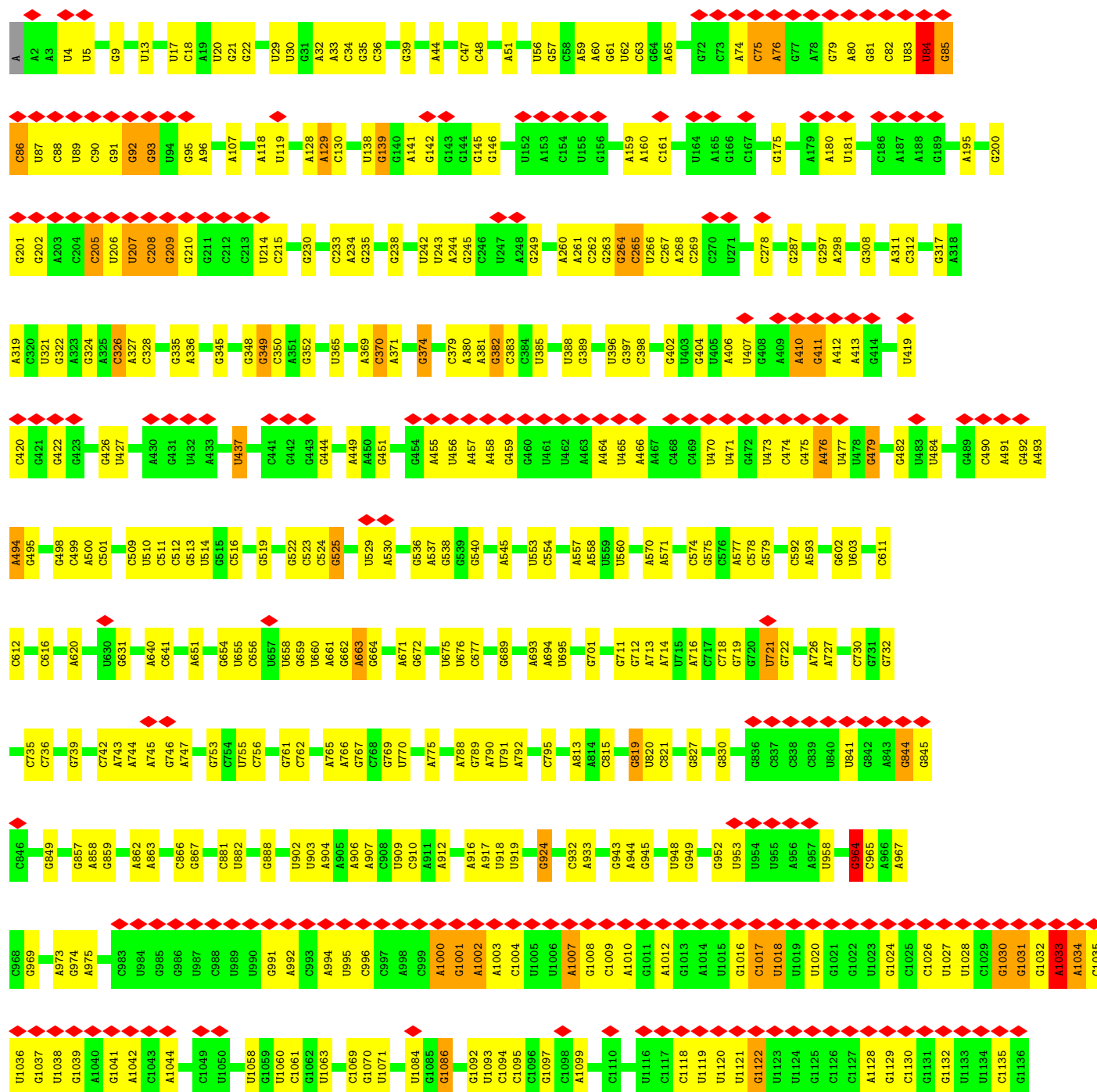


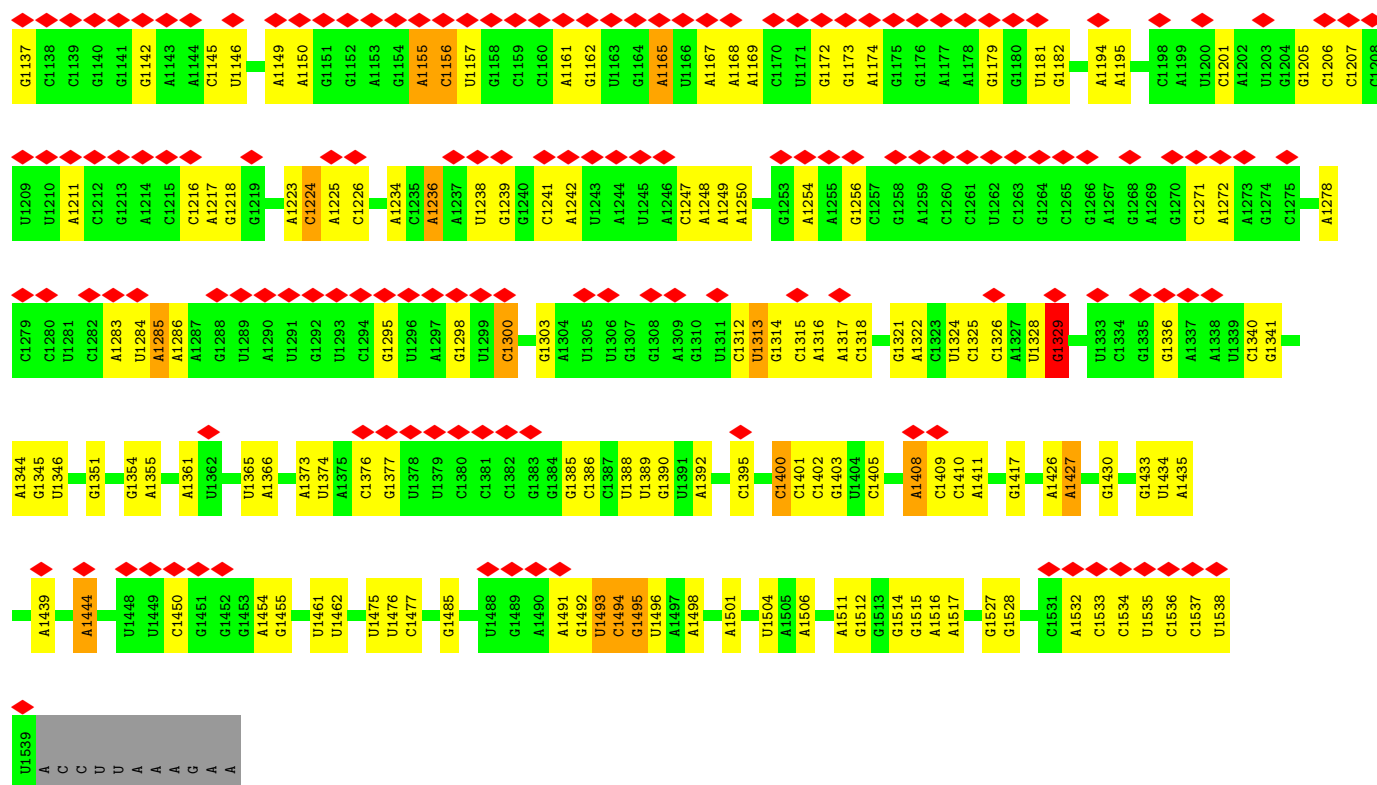
- Molecule 5: Large ribosomal subunit protein bL31



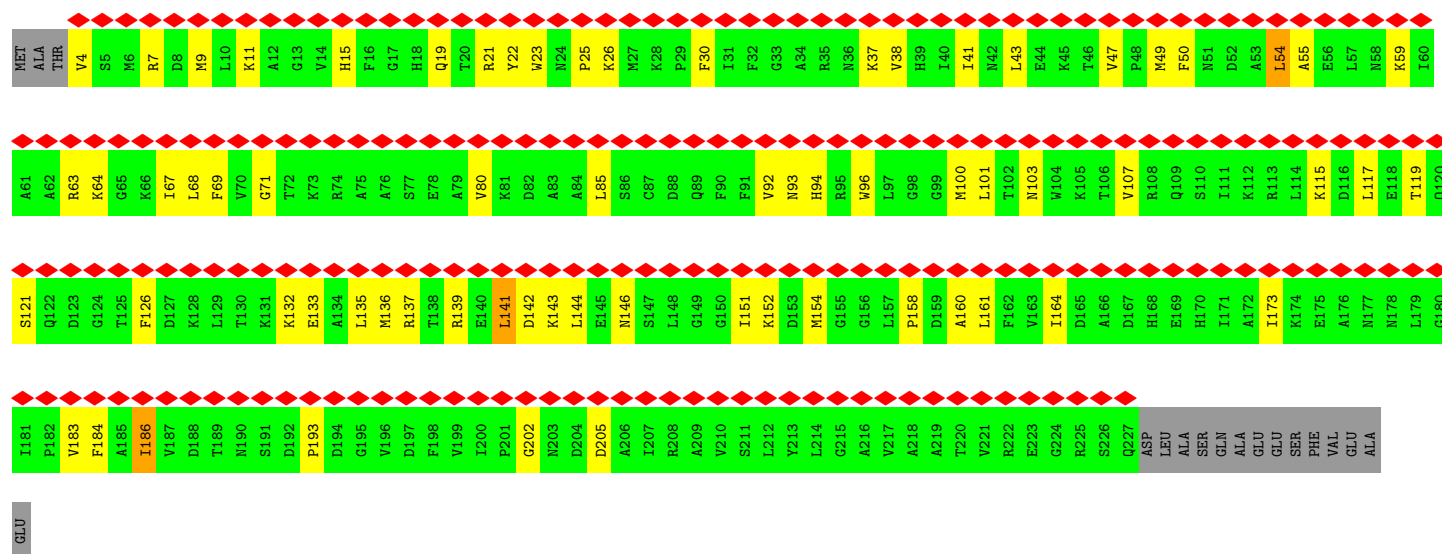


• Molecule 6: 16s rRNA (1538-MER)

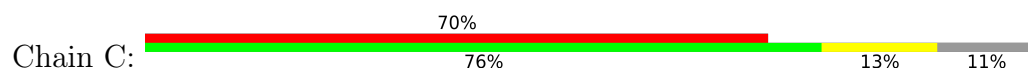
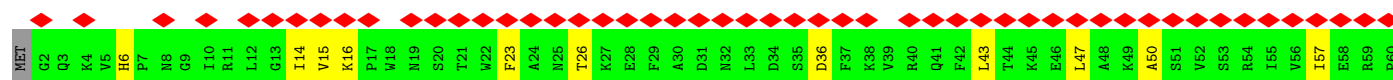


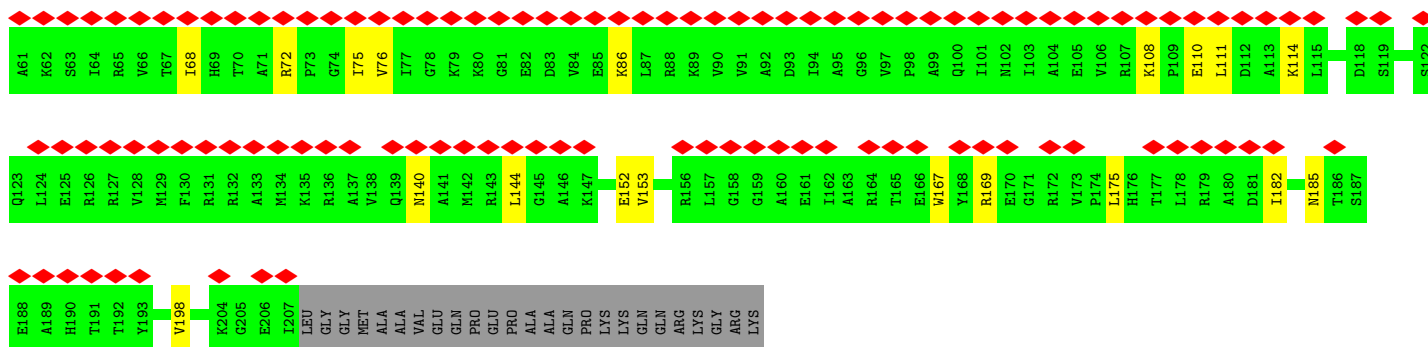


• Molecule 7: Small ribosomal subunit protein uS2

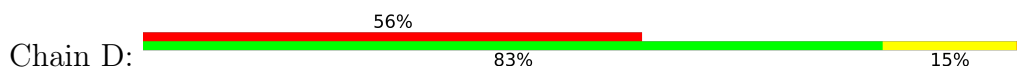
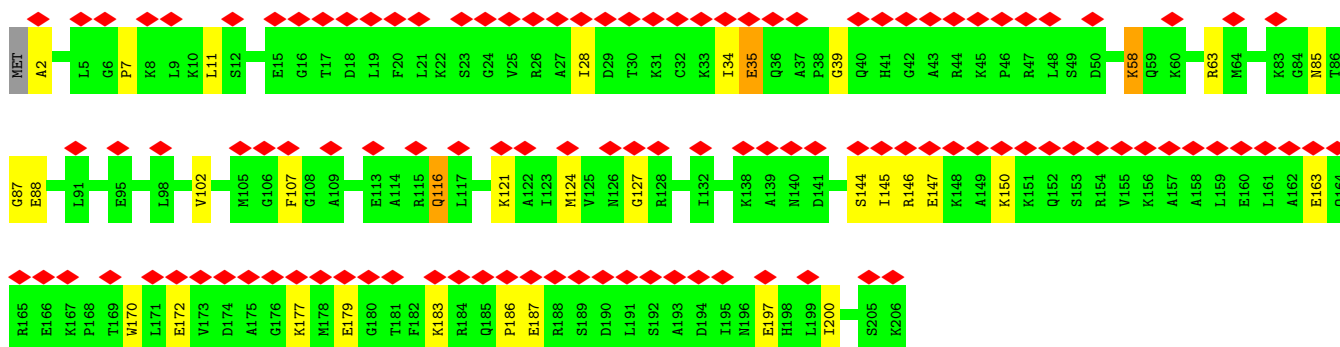


• Molecule 8: Small ribosomal subunit protein uS3

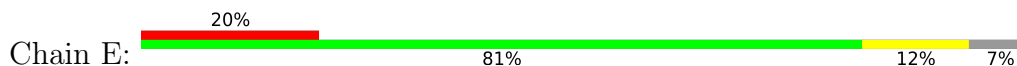
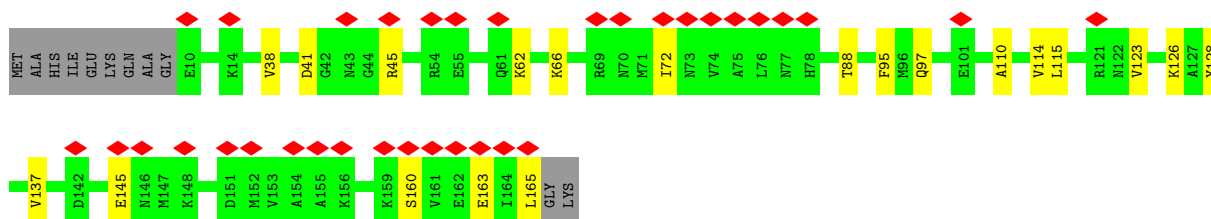




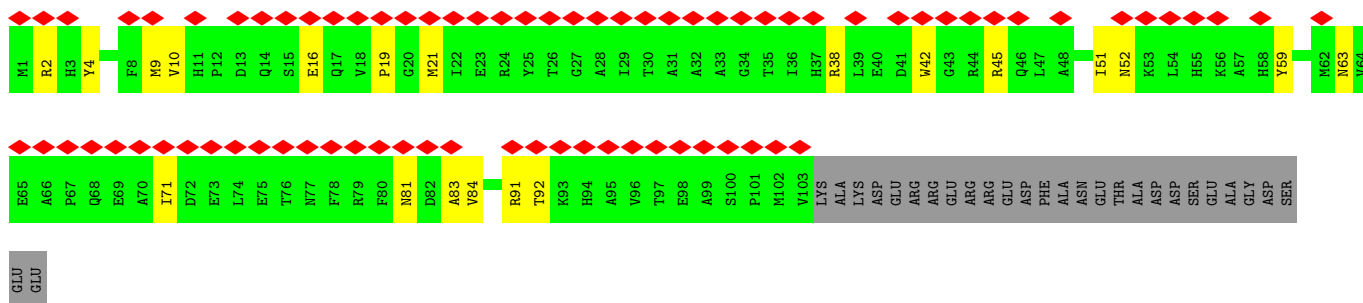
• Molecule 9: Small ribosomal subunit protein uS4



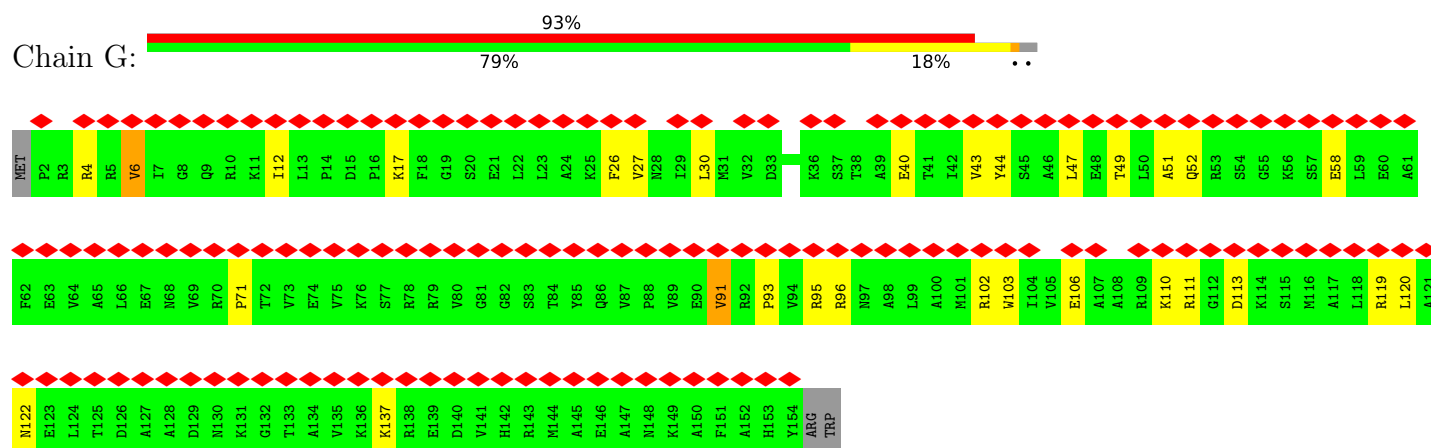
• Molecule 10: Small ribosomal subunit protein uS5



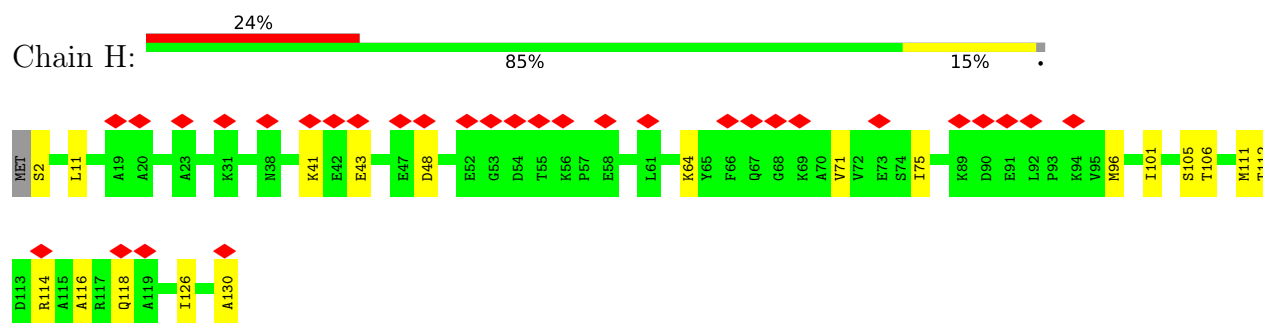
• Molecule 11: Small ribosomal subunit protein bS6



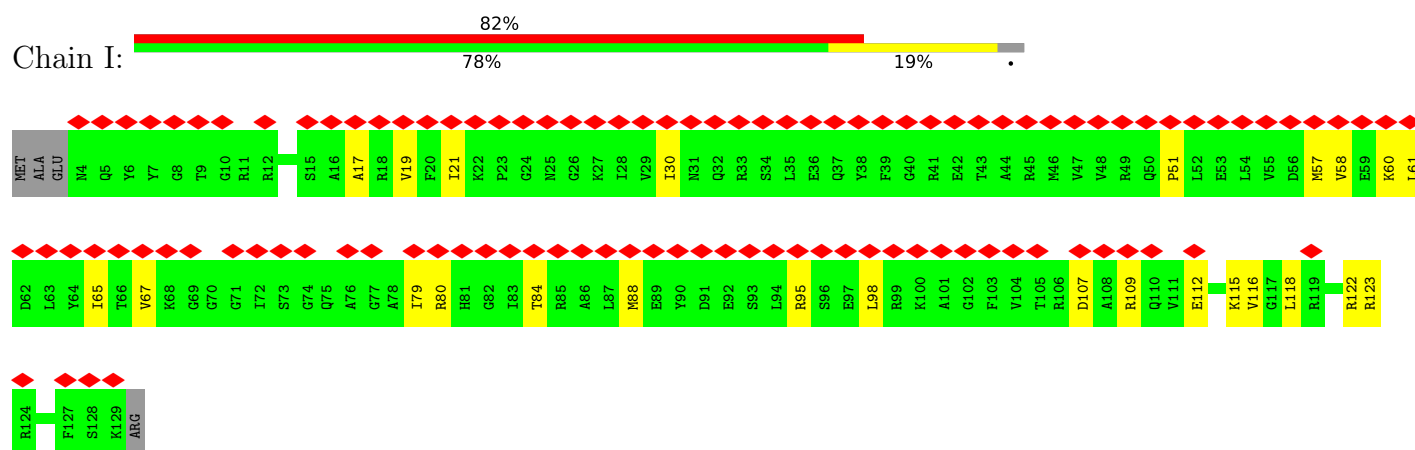
- Molecule 12: Small ribosomal subunit protein uS7



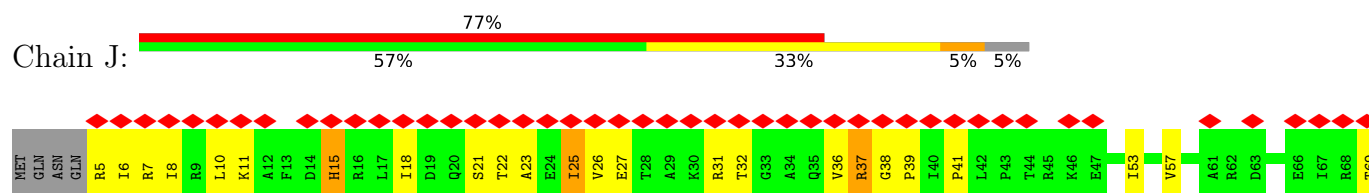
- Molecule 13: Small ribosomal subunit protein uS8



- Molecule 14: Small ribosomal subunit protein uS9

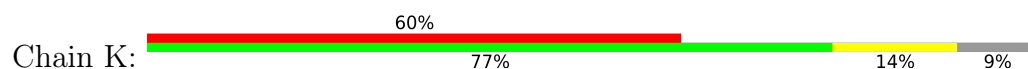
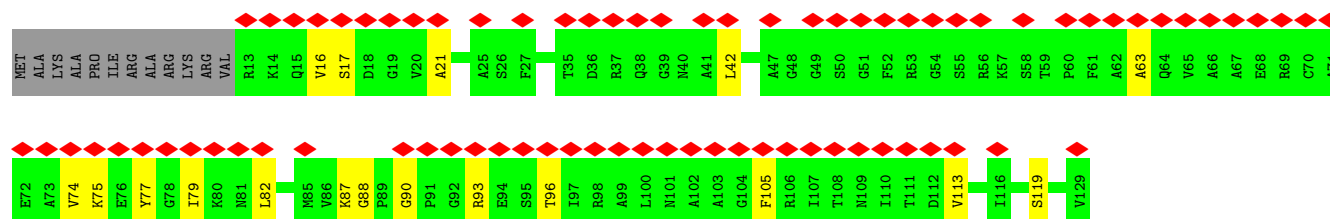


- Molecule 15: Small ribosomal subunit protein uS10

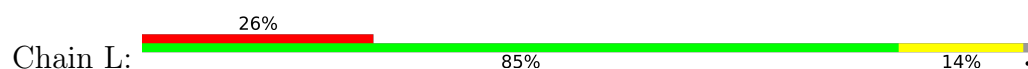
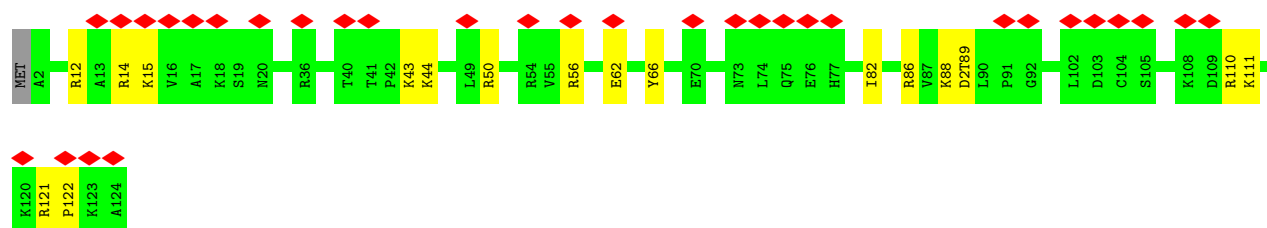




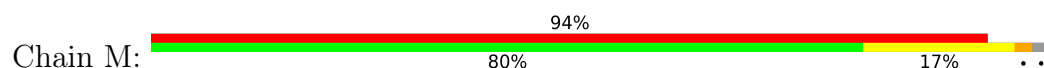
- Molecule 16: Small ribosomal subunit protein uS11



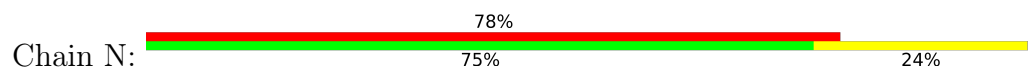
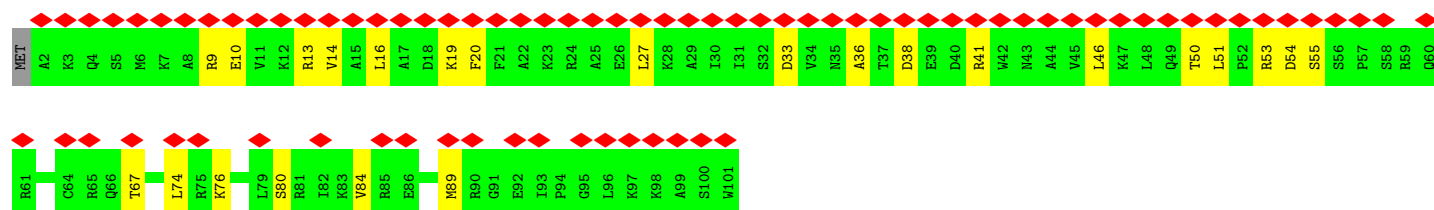
- Molecule 17: Small ribosomal subunit protein uS12



- Molecule 18: Small ribosomal subunit protein uS13

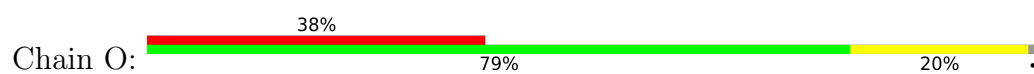
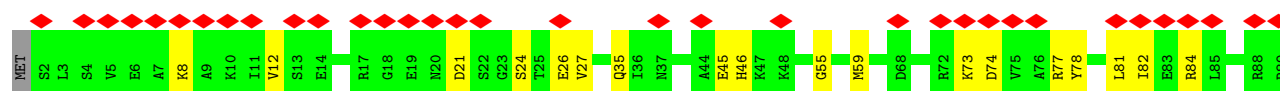


- Molecule 19: Small ribosomal subunit protein uS14

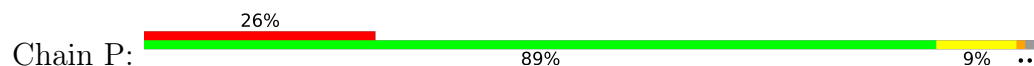
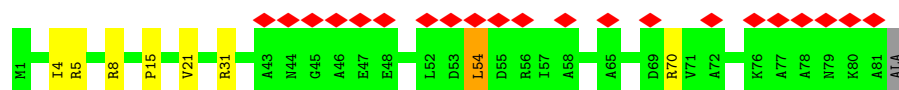


- Molecule 20: Small ribosomal subunit protein uS15

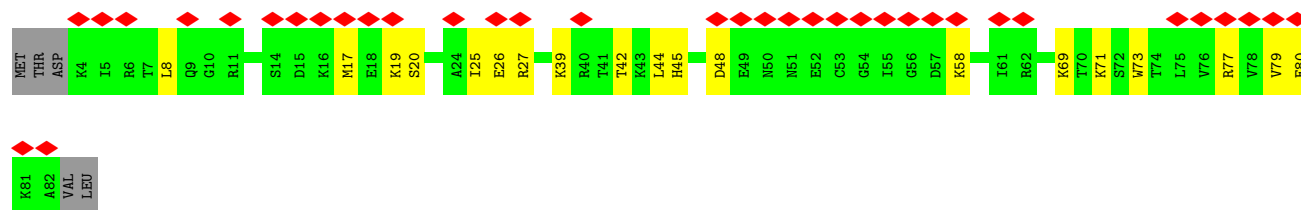




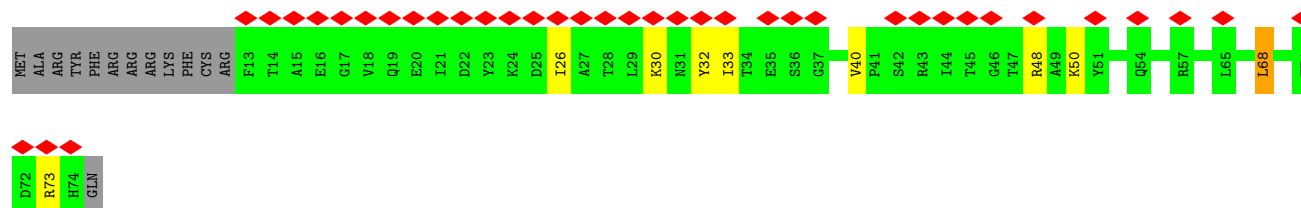
- Molecule 21: Small ribosomal subunit protein bS16



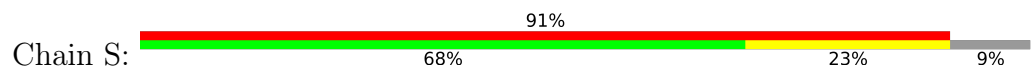
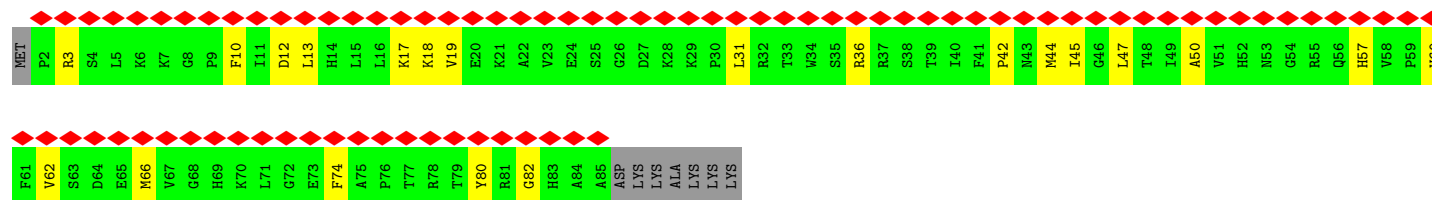
- Molecule 22: Small ribosomal subunit protein uS17



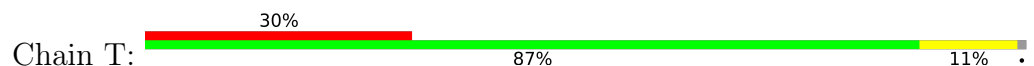
- Molecule 23: Small ribosomal subunit protein bS18

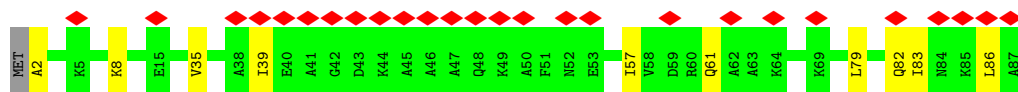


- Molecule 24: Small ribosomal subunit protein uS19

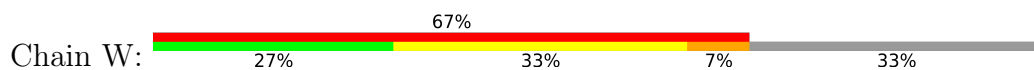


- Molecule 25: Small ribosomal subunit protein bS20

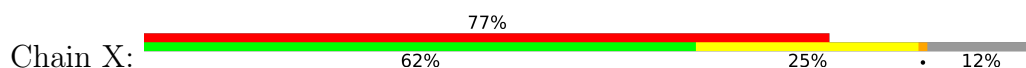
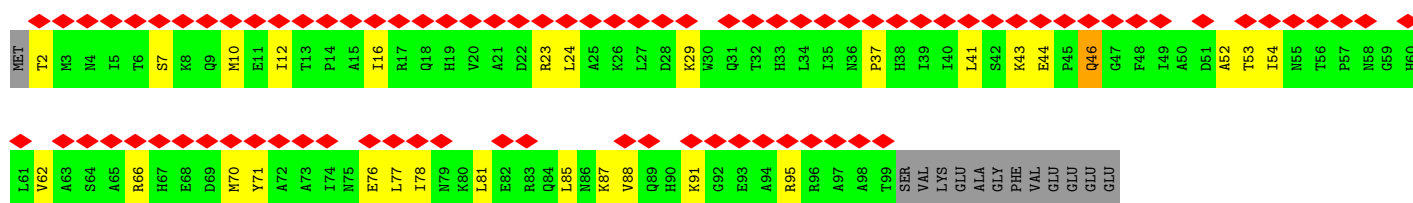




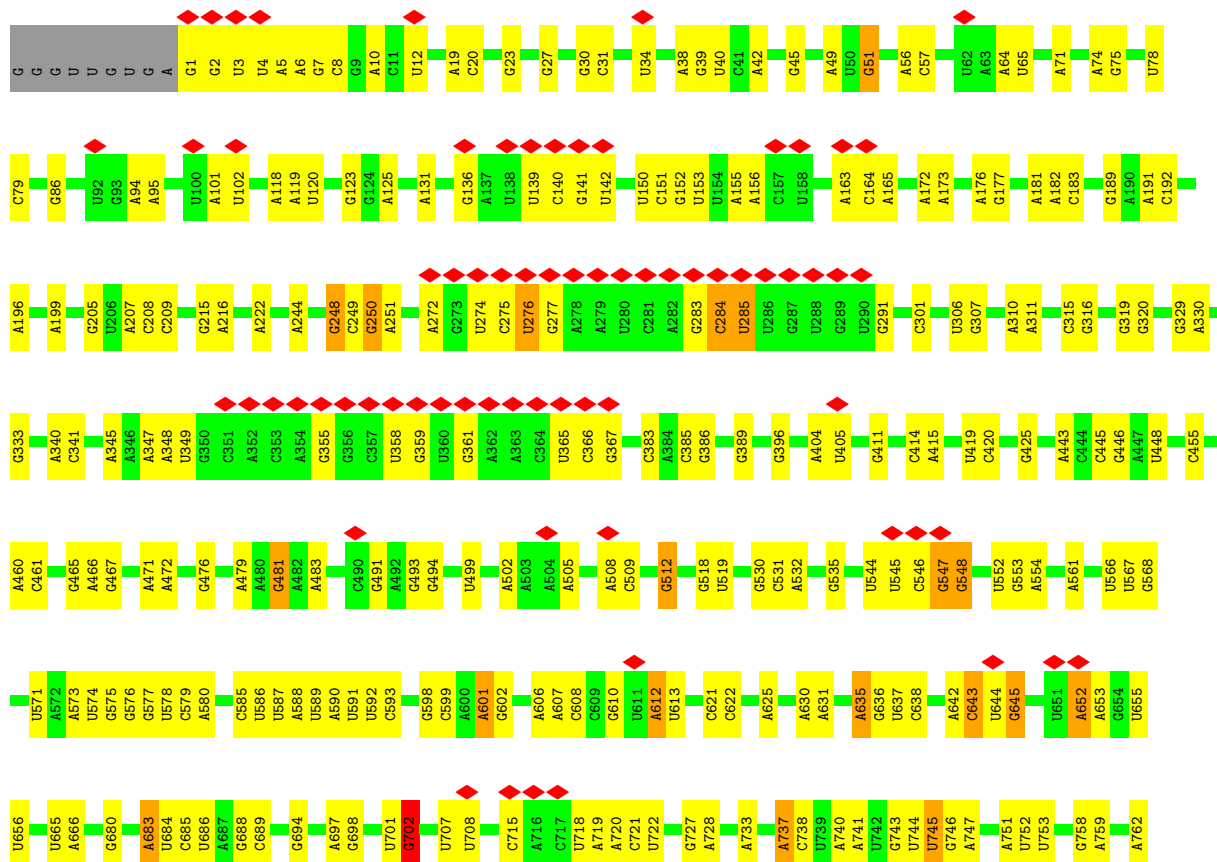
- Molecule 26: non-STOP mRNA

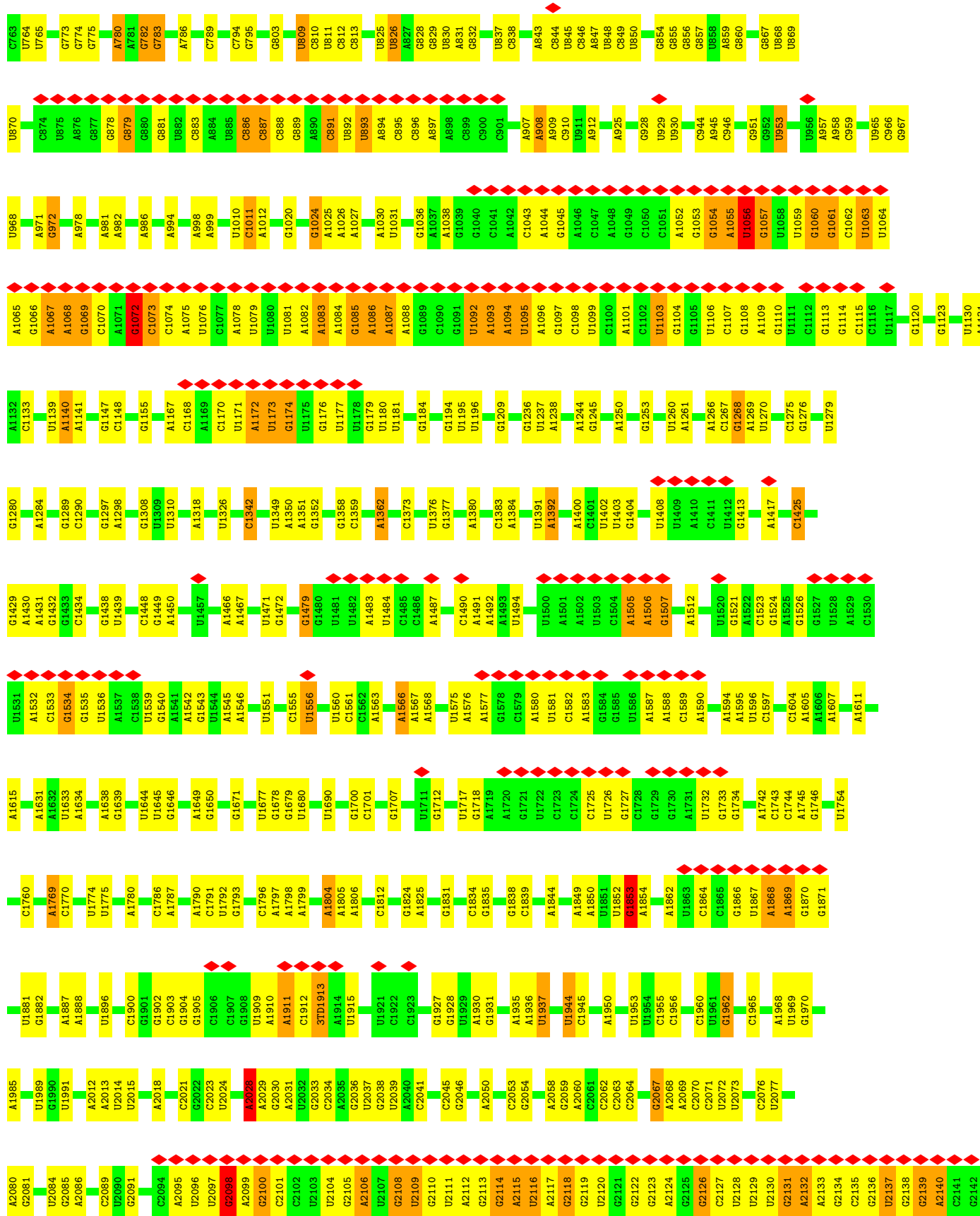


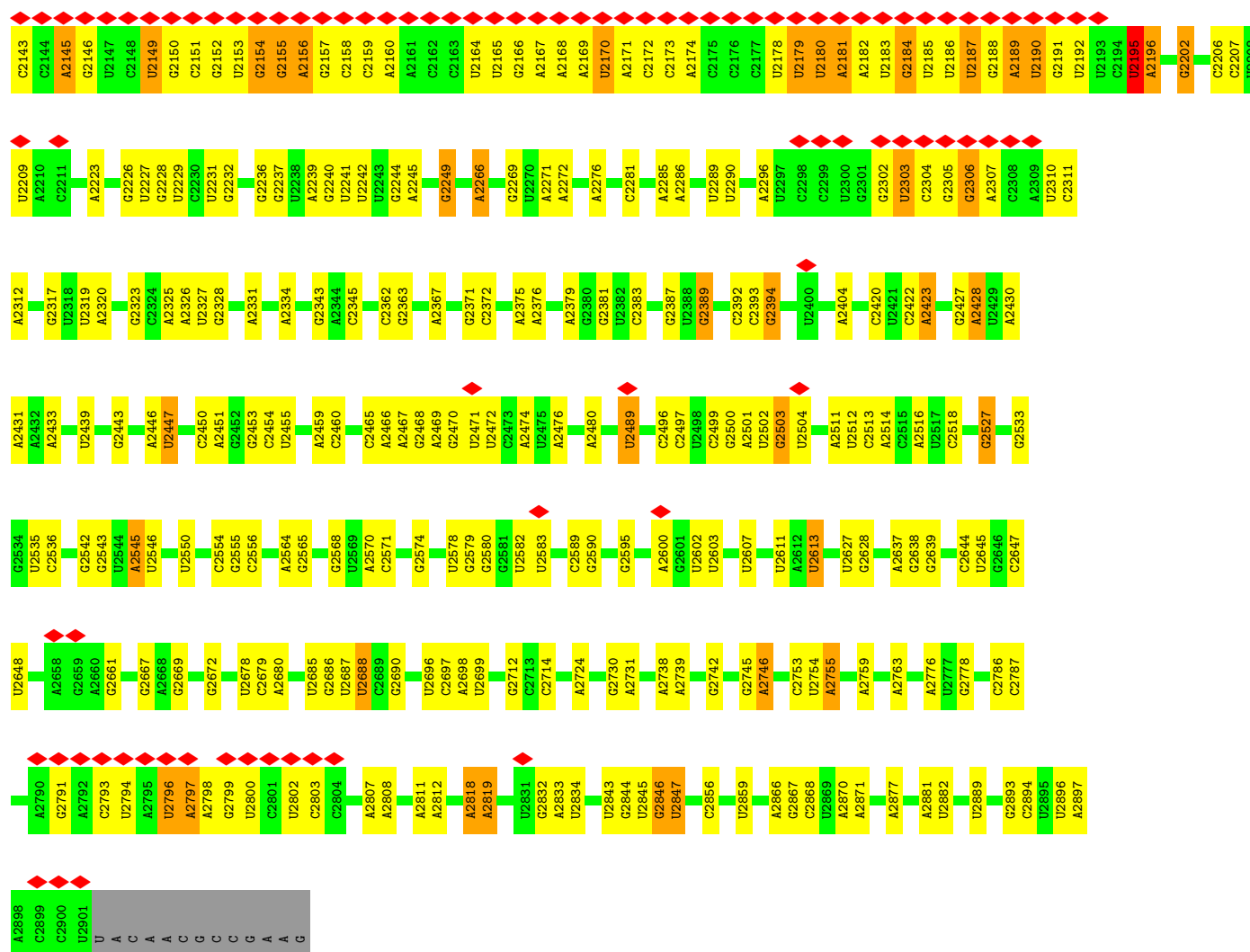
- Molecule 27: Ribosomal subunit interface protein



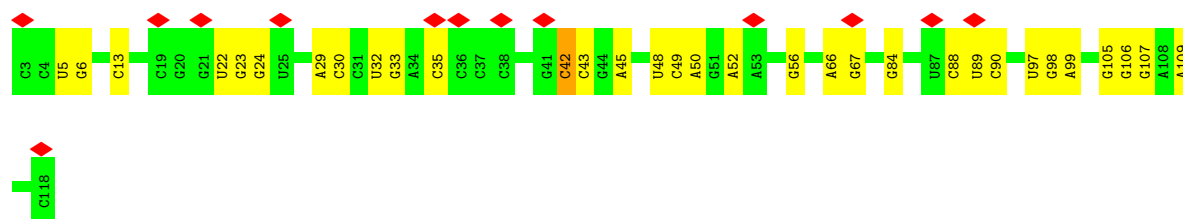
- Molecule 28: 23S rRNA (2901-MER)



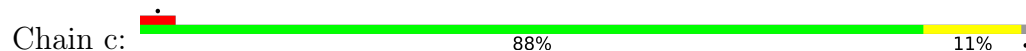
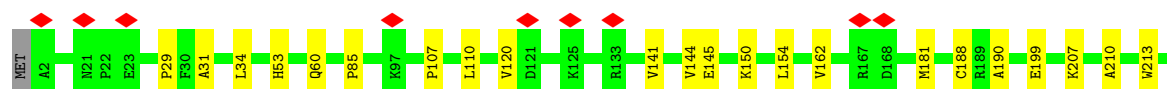


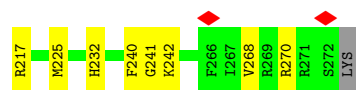


• Molecule 29: 5S rRNA (119-MER)

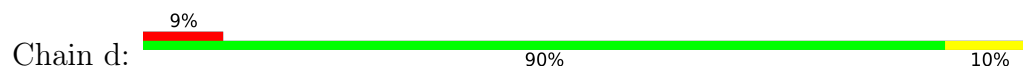


• Molecule 30: Large ribosomal subunit protein uL2

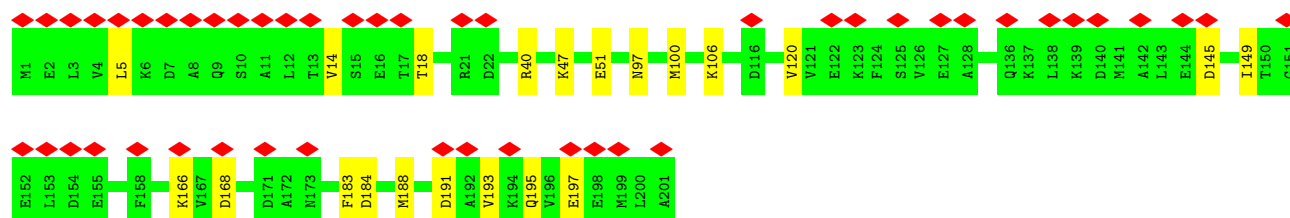




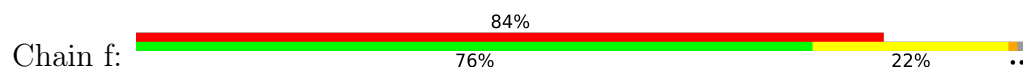
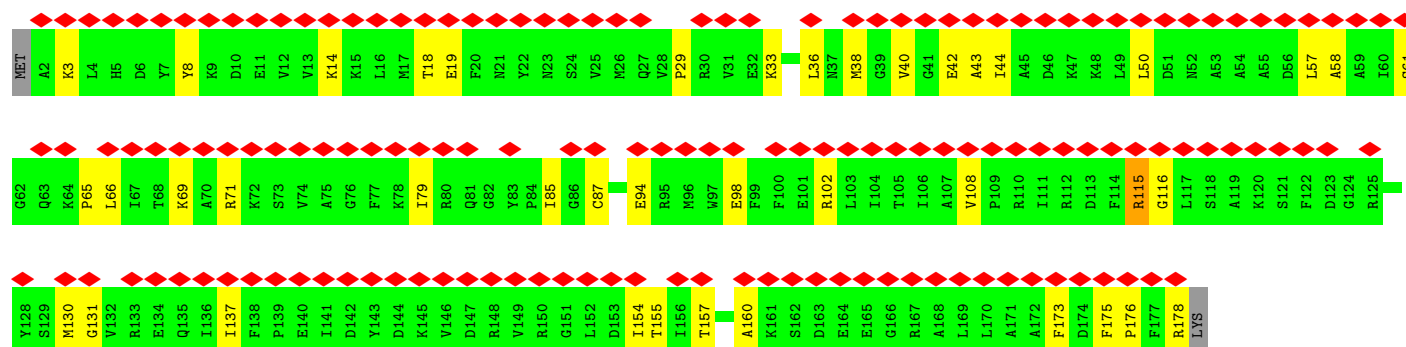
- Molecule 31: Large ribosomal subunit protein uL3



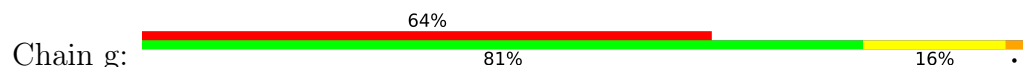
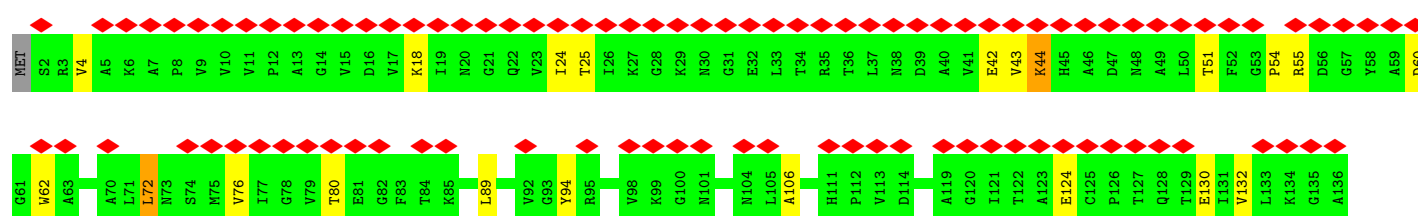
- Molecule 32: Large ribosomal subunit protein uL4



- Molecule 33: Large ribosomal subunit protein uL5

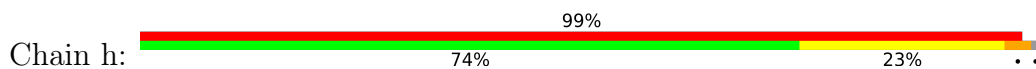
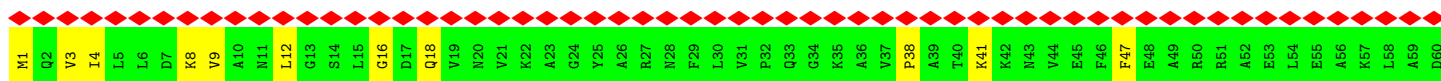


- Molecule 34: Large ribosomal subunit protein uL6

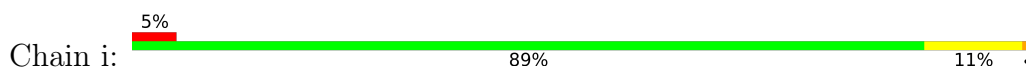




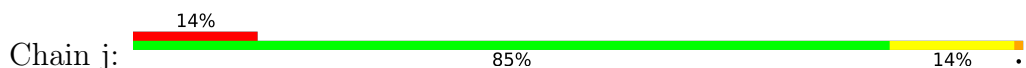
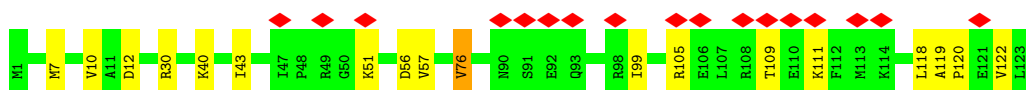
- Molecule 35: Large ribosomal subunit protein bL9



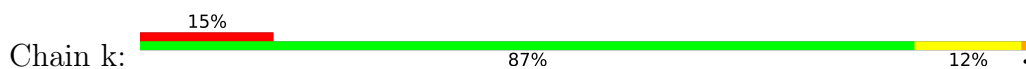
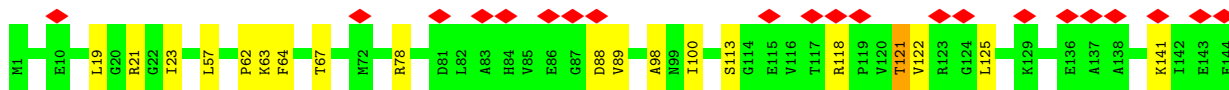
- Molecule 36: Large ribosomal subunit protein uL13



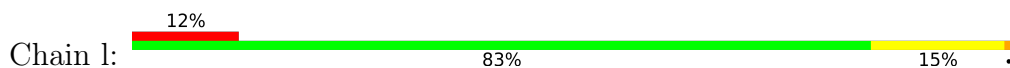
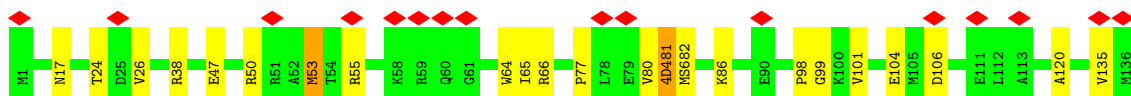
- Molecule 37: Large ribosomal subunit protein uL14



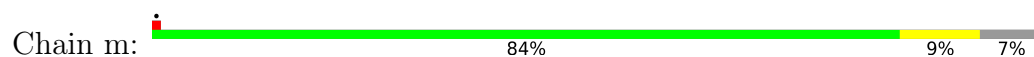
- Molecule 38: Large ribosomal subunit protein uL15



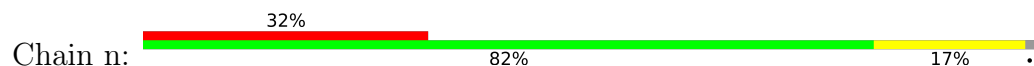
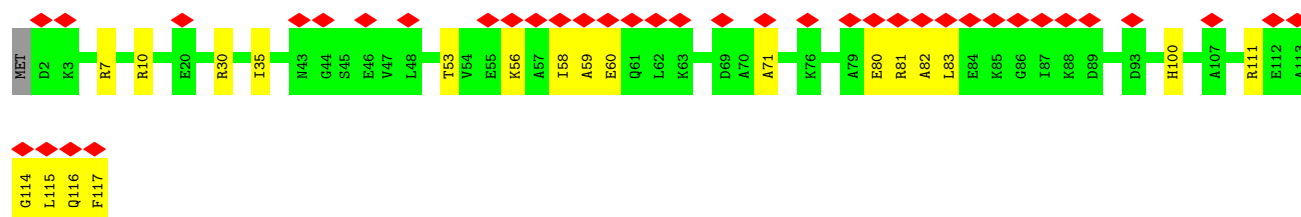
- Molecule 39: Large ribosomal subunit protein uL16



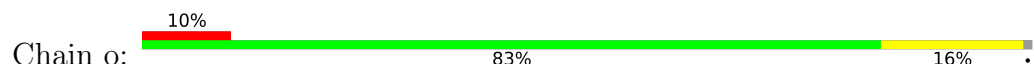
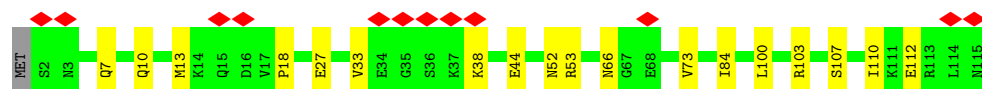
- Molecule 40: Large ribosomal subunit protein bL17



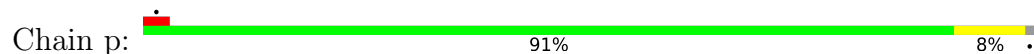
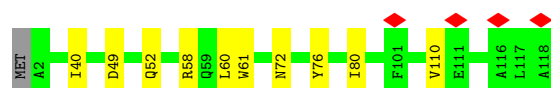
- Molecule 41: Large ribosomal subunit protein uL18



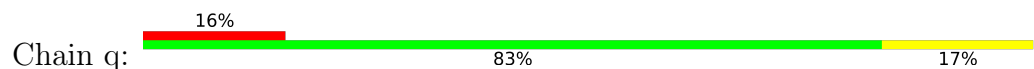
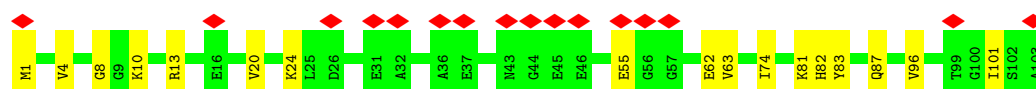
- Molecule 42: Large ribosomal subunit protein bL19



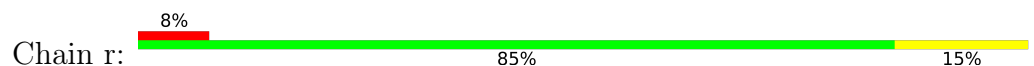
- Molecule 43: Large ribosomal subunit protein bL20



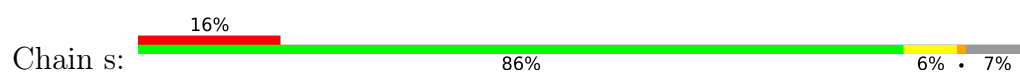
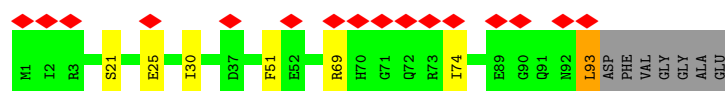
- Molecule 44: Large ribosomal subunit protein bL21



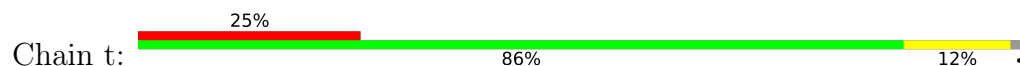
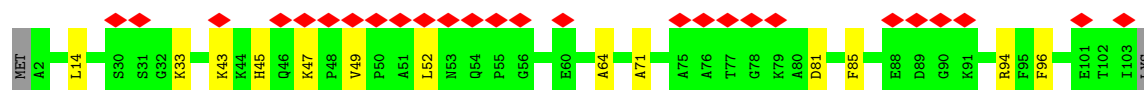
- Molecule 45: Large ribosomal subunit protein uL22



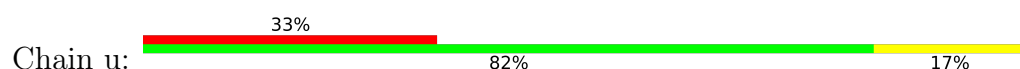
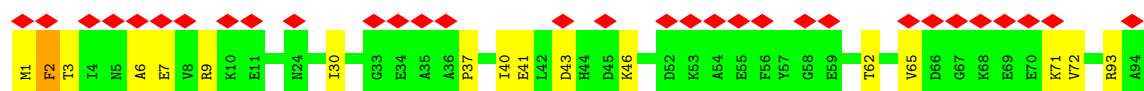
- Molecule 46: Large ribosomal subunit protein uL23



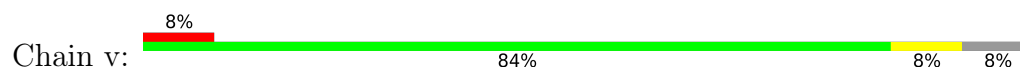
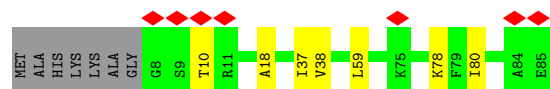
- Molecule 47: Large ribosomal subunit protein uL24



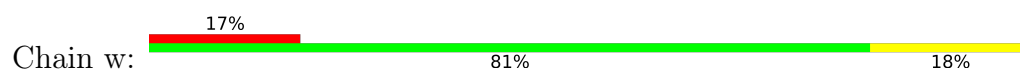
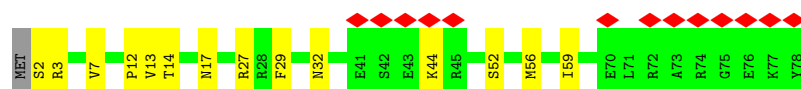
- Molecule 48: Large ribosomal subunit protein bL25



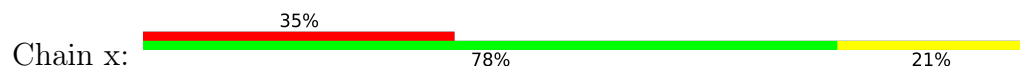
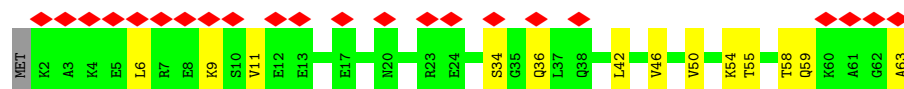
- Molecule 49: Large ribosomal subunit protein bL27



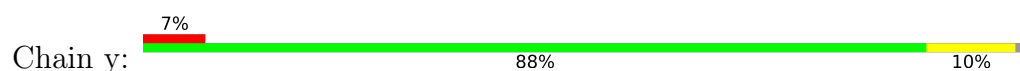
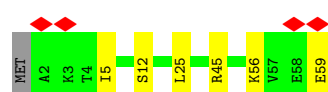
- Molecule 50: Large ribosomal subunit protein bL28



- Molecule 51: Large ribosomal subunit protein uL29

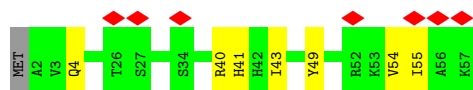


- Molecule 52: Large ribosomal subunit protein uL30



- Molecule 53: Large ribosomal subunit protein bL32

Chain z:  12% 86% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	374079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.494	Depositor
Minimum map value	-1.683	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	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: HSE, G7M, K, OMU, 4OC, 1MG, PSU, 5MU, UR3, 5MC, 4D4, MS6, MEQ, OMG, D2T, 2MA, 6MZ, H2U, MA6, MG, 2MG, ZN, 3TD, OMC

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	0.33	0/425	0.42	0/566
2	1	0.38	0/380	0.44	0/498
3	2	0.38	0/513	0.41	0/676
4	3	0.36	0/303	0.42	0/397
5	4	0.21	0/550	0.46	0/734
6	A	0.79	0/36680	0.84	10/57215 (0.0%)
7	B	0.18	0/1780	0.40	0/2398
8	C	0.24	0/1650	0.33	0/2223
9	D	0.25	0/1665	0.32	0/2225
10	E	0.32	0/1168	0.37	0/1570
11	F	0.26	0/851	0.38	0/1152
12	G	0.21	0/1220	0.36	0/1638
13	H	0.29	0/987	0.35	0/1323
14	I	0.23	0/1022	0.33	0/1361
15	J	0.25	0/798	0.48	0/1078
16	K	0.25	0/885	0.33	0/1192
17	L	0.31	0/961	0.38	0/1287
18	M	0.21	0/916	0.35	0/1225
19	N	0.24	0/817	0.35	0/1088
20	O	0.29	0/718	0.35	0/955
21	P	0.34	0/646	0.38	0/870
22	Q	0.27	0/647	0.41	0/865
23	R	0.29	0/515	0.40	0/693
24	S	0.21	0/684	0.33	0/920
25	T	0.30	0/675	0.37	0/894
26	W	0.37	0/245	0.85	0/381
27	X	0.25	0/791	0.38	0/1069
28	a	1.06	1/69183 (0.0%)	0.95	48/107924 (0.0%)
29	b	0.80	0/2776	0.82	0/4328
30	c	0.38	0/2118	0.41	0/2846
31	d	0.38	0/1577	0.42	0/2122

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.36	0/1573	0.38	0/2115
33	f	0.25	0/1434	0.41	0/1926
34	g	0.25	0/1339	0.35	0/1811
35	h	0.17	0/1110	0.38	0/1500
36	i	0.37	0/1157	0.37	0/1556
37	j	0.39	0/956	0.42	0/1281
38	k	0.35	0/1073	0.39	0/1427
39	l	0.34	0/1072	0.39	0/1434
40	m	0.39	0/963	0.42	0/1288
41	n	0.28	0/902	0.42	0/1209
42	o	0.38	0/929	0.39	0/1242
43	p	0.40	0/960	0.40	0/1278
44	q	0.37	0/829	0.39	0/1106
45	r	0.36	0/862	0.40	0/1154
46	s	0.34	0/745	0.45	0/996
47	t	0.31	0/787	0.38	0/1051
48	u	0.31	0/763	0.43	0/1024
49	v	0.39	0/599	0.39	0/795
50	w	0.37	0/635	0.41	0/848
51	x	0.30	0/500	0.37	0/665
52	y	0.32	0/451	0.36	0/603
53	z	0.36	0/449	0.43	0/597
All	All	0.83	1/154234 (0.0%)	0.81	58/230619 (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
15	J	0	2
39	l	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1377	G	C8-N7	-5.17	1.27	1.30

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2098	G	OP1-P-O3'	-11.72	72.83	108.00
28	a	2098	G	OP2-P-O3'	-8.50	82.50	108.00
28	a	512	G	O4'-C1'-N9	8.34	114.87	108.20
28	a	2846	G	O4'-C1'-N9	7.71	114.36	108.20
28	a	1056	U	C2-N1-C1'	7.44	126.62	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	J	37	ARG	Peptide
15	J	38	GLY	Peptide
39	l	81	4D4	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	418	0	449	6	0
2	1	377	0	418	5	0
3	2	504	0	572	4	0
4	3	302	0	340	3	0
5	4	540	0	537	19	0
6	A	33009	0	16624	280	0
7	B	1749	0	1774	44	0
8	C	1623	0	1696	20	0
9	D	1644	0	1706	22	0
10	E	1155	0	1206	10	0
11	F	832	0	821	15	0
12	G	1204	0	1256	19	0
13	H	977	0	1031	11	0
14	I	1010	0	1057	21	0
15	J	788	0	830	26	0
16	K	877	0	884	11	0
17	L	958	0	1019	9	0
18	M	907	0	977	16	0
19	N	805	0	846	16	0
20	O	710	0	735	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	P	636	0	649	7	0
22	Q	639	0	684	10	0
23	R	507	0	525	7	0
24	S	667	0	691	11	0
25	T	669	0	717	5	0
26	W	219	0	108	7	0
27	X	778	0	793	21	0
28	a	62284	0	31324	487	0
29	b	2483	0	1258	13	0
30	c	2080	0	2152	21	0
31	d	1567	0	1619	11	0
32	e	1554	0	1620	12	0
33	f	1410	0	1444	29	0
34	g	1319	0	1367	21	0
35	h	1099	0	1139	23	0
36	i	1134	0	1161	11	0
37	j	947	0	1025	11	0
38	k	1063	0	1130	14	0
39	l	1074	0	1138	13	0
40	m	950	0	994	6	0
41	n	892	0	923	11	0
42	o	917	0	962	10	0
43	p	947	0	1019	6	0
44	q	816	0	841	9	0
45	r	855	0	915	10	0
46	s	739	0	809	6	0
47	t	779	0	830	7	0
48	u	749	0	763	9	0
49	v	592	0	612	4	0
50	w	625	0	652	11	0
51	x	499	0	534	6	0
52	y	447	0	484	5	0
53	z	443	0	458	4	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	95	0	0	0	0
55	E	1	0	0	0	0
55	a	254	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	d	1	0	0	0	0
55	p	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	z	1	0	0	0	0
56	A	47	0	0	0	0
56	a	114	0	0	0	0
56	b	1	0	0	0	0
56	c	4	0	0	0	0
56	d	1	0	0	0	0
56	e	1	0	0	0	0
56	f	1	0	0	0	0
All	All	143298	0	96118	1302	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 5.

The worst 5 of 1302 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)
6:A:76:A:N6	6:A:91:G:H1	1.35	1.23
12:G:111:ARG:HH21	12:G:122:ASN:HB3	1.31	0.91
6:A:1122:G:H3'	15:J:37:ARG:HH21	1.38	0.89
28:a:1055:A:H5''	28:a:1087:A:H61	1.38	0.88
28:a:544:U:O2	28:a:547:G:O6	1.92	0.86

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	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	68/70 (97%)	57 (84%)	11 (16%)	0	100	100
7	B	222/241 (92%)	205 (92%)	17 (8%)	0	100	100
8	C	204/232 (88%)	196 (96%)	8 (4%)	0	100	100
9	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
10	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
11	F	101/131 (77%)	98 (97%)	3 (3%)	0	100	100
12	G	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
13	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	I	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
15	J	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	12	15
16	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
17	L	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
18	M	114/118 (97%)	106 (93%)	8 (7%)	0	100	100
19	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
22	Q	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
23	R	60/75 (80%)	57 (95%)	3 (5%)	0	100	100
24	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
25	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
27	X	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
30	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
31	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
32	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
33	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
34	g	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
35	h	146/149 (98%)	133 (91%)	12 (8%)	1 (1%)	18	23
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
40	m	117/128 (91%)	113 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
45	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
46	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
47	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
48	u	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	11	13
49	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5625/5926 (95%)	5422 (96%)	200 (4%)	3 (0%)	49	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	h	115	VAL
15	J	57	VAL
48	u	2	PHE

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	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	32 (94%)	2 (6%)	18	26
5	4	60/60 (100%)	57 (95%)	3 (5%)	22	33
7	B	185/198 (93%)	180 (97%)	5 (3%)	39	58
8	C	170/189 (90%)	170 (100%)	0	100	100
9	D	171/172 (99%)	166 (97%)	5 (3%)	37	55
10	E	119/126 (94%)	118 (99%)	1 (1%)	73	86
11	F	88/111 (79%)	87 (99%)	1 (1%)	65	81
12	G	126/129 (98%)	123 (98%)	3 (2%)	43	62
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	104/107 (97%)	103 (99%)	1 (1%)	68	82
15	J	87/91 (96%)	82 (94%)	5 (6%)	18	27
16	K	89/98 (91%)	89 (100%)	0	100	100
17	L	102/103 (99%)	99 (97%)	3 (3%)	37	55
18	M	96/98 (98%)	93 (97%)	3 (3%)	35	52
19	N	83/84 (99%)	82 (99%)	1 (1%)	63	79
20	O	75/76 (99%)	74 (99%)	1 (1%)	61	77
21	P	63/63 (100%)	62 (98%)	1 (2%)	55	73
22	Q	73/78 (94%)	71 (97%)	2 (3%)	39	58
23	R	53/65 (82%)	52 (98%)	1 (2%)	50	69
24	S	72/79 (91%)	69 (96%)	3 (4%)	26	40
25	T	65/66 (98%)	64 (98%)	1 (2%)	57	75
27	X	83/94 (88%)	80 (96%)	3 (4%)	31	47
30	c	215/217 (99%)	214 (100%)	1 (0%)	81	90
31	d	163/163 (100%)	162 (99%)	1 (1%)	78	89
32	e	165/165 (100%)	165 (100%)	0	100	100
33	f	148/150 (99%)	145 (98%)	3 (2%)	48	67
34	g	135/136 (99%)	128 (95%)	7 (5%)	21	31
35	h	112/113 (99%)	108 (96%)	4 (4%)	31	47
36	i	116/116 (100%)	114 (98%)	2 (2%)	53	72
37	j	104/104 (100%)	102 (98%)	2 (2%)	50	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	k	105/105 (100%)	104 (99%)	1 (1%)	68	82
39	l	107/107 (100%)	105 (98%)	2 (2%)	50	69
40	m	98/103 (95%)	97 (99%)	1 (1%)	68	82
41	n	86/87 (99%)	84 (98%)	2 (2%)	44	63
42	o	99/100 (99%)	97 (98%)	2 (2%)	48	67
43	p	89/90 (99%)	89 (100%)	0	100	100
44	q	83/83 (100%)	80 (96%)	3 (4%)	31	47
45	r	92/92 (100%)	92 (100%)	0	100	100
46	s	80/84 (95%)	79 (99%)	1 (1%)	61	77
47	t	83/85 (98%)	82 (99%)	1 (1%)	63	79
48	u	76/76 (100%)	76 (100%)	0	100	100
49	v	60/64 (94%)	59 (98%)	1 (2%)	53	72
50	w	67/68 (98%)	67 (100%)	0	100	100
51	x	53/54 (98%)	52 (98%)	1 (2%)	50	69
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4668/4824 (97%)	4588 (98%)	80 (2%)	52	72

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	h	8	LYS
42	o	7	GLN
35	h	114	GLU
38	k	121	THR
44	q	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
37	j	9	ASN
51	x	25	GLN
40	m	9	GLN
41	n	104	GLN
51	x	39	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	W	9/15 (60%)	2 (22%)	0
28	a	2899/2923 (99%)	426 (14%)	0
29	b	115/116 (99%)	17 (14%)	0
6	A	1537/1550 (99%)	213 (13%)	4 (0%)
All	All	4560/4604 (99%)	658 (14%)	4 (0%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	9	G
6	A	13	U
6	A	32	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1001	G
6	A	1033	A
6	A	1392	A
6	A	1492	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

40 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	$\# Z > 2$
28	2MG	a	2443	28	23,26,27	2.60	7 (30%)	32,38,41	2.16	9 (28%)
28	PSU	a	2578	28,56	18,21,22	2.43	9 (50%)	22,30,33	1.92	4 (18%)
39	MS6	l	82	39	5,7,8	0.67	0	2,7,9	1.60	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	UR3	A	1496	6	19,22,23	2.53	6 (31%)	26,32,35	1.30	1 (3%)
28	6MZ	a	1615	28	22,25,26	2.41	4 (18%)	30,36,39	2.24	9 (30%)
28	PSU	a	2603	28	18,21,22	2.33	7 (38%)	22,30,33	2.07	4 (18%)
6	5MC	A	1405	6	18,22,23	1.93	6 (33%)	26,32,35	1.24	2 (7%)
28	PSU	a	2602	28	18,21,22	2.34	8 (44%)	22,30,33	1.98	6 (27%)
31	MEQ	d	150	31	8,9,10	0.90	0	5,10,12	1.27	1 (20%)
28	PSU	a	2502	28,56	18,21,22	2.34	7 (38%)	22,30,33	2.02	3 (13%)
6	G7M	A	525	56,6	23,26,27	2.17	5 (21%)	35,39,42	1.87	7 (20%)
28	1MG	a	743	28	22,26,27	2.48	5 (22%)	33,39,42	1.90	7 (21%)
28	PSU	a	953	28	18,21,22	2.21	7 (38%)	22,30,33	1.85	3 (13%)
28	H2U	a	2447	28	18,21,22	3.93	5 (27%)	21,30,33	5.60	7 (33%)
28	PSU	a	1909	28	18,21,22	2.08	7 (38%)	22,30,33	1.91	3 (13%)
28	5MU	a	1937	28,56	19,22,23	2.76	7 (36%)	28,32,35	3.65	9 (32%)
6	MA6	A	1516	6	23,26,27	1.30	3 (13%)	34,38,41	2.24	9 (26%)
28	5MC	a	1960	28,56	18,22,23	1.95	6 (33%)	26,32,35	1.22	1 (3%)
28	OMU	a	2550	28,55,56	19,22,23	2.70	7 (36%)	26,31,34	1.71	5 (19%)
6	PSU	A	514	55,6	18,21,22	2.15	8 (44%)	22,30,33	1.89	4 (18%)
28	2MA	a	2501	28,55,56	22,25,26	1.34	3 (13%)	33,37,40	2.18	8 (24%)
39	4D4	l	81	39	9,11,12	0.79	0	8,13,15	2.14	3 (37%)
28	PSU	a	744	28,55	18,21,22	2.29	8 (44%)	22,30,33	1.91	3 (13%)
6	2MG	A	964	6	23,26,27	2.56	6 (26%)	32,38,41	2.13	10 (31%)
6	MA6	A	1517	6	23,26,27	1.29	3 (13%)	34,38,41	2.29	9 (26%)
16	HSE	K	119	16	5,6,7	0.90	0	2,6,8	0.60	0
28	OMC	a	2496	28,55	19,22,23	1.81	5 (26%)	26,31,34	1.14	2 (7%)
28	6MZ	a	2028	28	22,25,26	2.52	5 (22%)	30,36,39	2.20	9 (30%)
28	5MU	a	745	28	19,22,23	2.56	7 (36%)	28,32,35	3.79	10 (35%)
6	4OC	A	1400	6	20,23,24	2.20	4 (20%)	26,32,35	1.06	3 (11%)
28	G7M	a	2067	28,56	23,26,27	2.14	5 (21%)	35,39,42	1.95	7 (20%)
6	5MC	A	965	6	18,22,23	1.92	6 (33%)	26,32,35	1.31	3 (11%)
28	PSU	a	1915	28	18,21,22	2.06	7 (38%)	22,30,33	1.80	3 (13%)
6	2MG	A	1205	56,6	23,26,27	2.56	5 (21%)	32,38,41	2.08	12 (37%)
17	D2T	L	89	17	7,9,10	1.18	1 (14%)	6,11,13	1.62	2 (33%)
28	3TD	a	1913	28	18,22,23	2.73	7 (38%)	22,32,35	1.65	2 (9%)
28	2MG	a	1831	28	23,26,27	2.53	7 (30%)	32,38,41	2.17	10 (31%)
28	PSU	a	2455	28	18,21,22	2.41	8 (44%)	22,30,33	2.09	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OMG	a	2249	28,56	23,26,27	2.32	6 (26%)	33,38,41	1.92	10 (30%)
6	2MG	A	1514	6	23,26,27	2.57	7 (30%)	32,38,41	2.14	10 (31%)

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
28	2MG	a	2443	28	-	1/9/27/28	0/3/3/3
28	PSU	a	2578	28,56	-	0/7/25/26	0/2/2/2
39	MS6	l	82	39	-	1/4/6/8	-
6	UR3	A	1496	6	-	0/7/25/26	0/2/2/2
28	6MZ	a	1615	28	-	0/9/27/28	0/3/3/3
28	PSU	a	2603	28	-	0/7/25/26	0/2/2/2
6	5MC	A	1405	6	-	0/7/25/26	0/2/2/2
28	PSU	a	2602	28	-	0/7/25/26	0/2/2/2
31	MEQ	d	150	31	-	4/8/9/11	-
28	PSU	a	2502	28,56	-	2/7/25/26	0/2/2/2
6	G7M	A	525	56,6	-	3/7/25/26	0/3/3/3
28	1MG	a	743	28	-	0/7/25/26	0/3/3/3
28	PSU	a	953	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2447	28	-	2/7/38/39	0/2/2/2
28	PSU	a	1909	28	-	0/7/25/26	0/2/2/2
28	5MU	a	1937	28,56	-	0/7/25/26	0/2/2/2
6	MA6	A	1516	6	-	0/11/29/30	0/3/3/3
28	5MC	a	1960	28,56	-	1/7/25/26	0/2/2/2
28	OMU	a	2550	28,55,56	-	0/9/27/28	0/2/2/2
6	PSU	A	514	55,6	-	0/7/25/26	0/2/2/2
28	2MA	a	2501	28,55,56	-	3/7/25/26	0/3/3/3
39	4D4	l	81	39	-	1/11/12/14	-
28	PSU	a	744	28,55	-	1/7/25/26	0/2/2/2
6	2MG	A	964	6	-	0/9/27/28	0/3/3/3
6	MA6	A	1517	6	-	4/11/29/30	0/3/3/3
16	HSE	K	119	16	-	1/4/5/7	-
28	OMC	a	2496	28,55	-	0/9/27/28	0/2/2/2
28	6MZ	a	2028	28	-	2/9/27/28	0/3/3/3
28	5MU	a	745	28	-	0/7/25/26	0/2/2/2
6	4OC	A	1400	6	-	0/9/29/30	0/2/2/2
28	G7M	a	2067	28,56	-	2/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MC	A	965	6	-	0/7/25/26	0/2/2/2
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
6	2MG	A	1205	56,6	-	2/9/27/28	0/3/3/3
17	D2T	L	89	17	-	5/7/12/14	-
28	3TD	a	1913	28	-	0/7/25/26	0/2/2/2
28	2MG	a	1831	28	-	0/9/27/28	0/3/3/3
28	PSU	a	2455	28	-	0/7/25/26	0/2/2/2
28	OMG	a	2249	28,56	-	1/9/27/28	0/3/3/3
6	2MG	A	1514	6	-	0/9/27/28	0/3/3/3

The worst 5 of 214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2028	6MZ	C6-N6	9.80	1.44	1.34
28	a	2447	H2U	O4-C4	9.77	1.43	1.23
28	a	1615	6MZ	C6-N6	9.47	1.44	1.34
6	A	964	2MG	O6-C6	9.00	1.40	1.23
6	A	1205	2MG	O6-C6	8.83	1.40	1.23

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2447	H2U	C4-N3-C2	-19.23	109.84	125.79
28	a	2447	H2U	O2-C2-N1	-9.89	110.70	123.11
28	a	745	5MU	C5M-C5-C4	8.76	128.41	118.77
28	a	1937	5MU	C4-N3-C2	-8.45	116.42	127.35
28	a	1937	5MU	N3-C2-N1	8.37	126.01	114.89

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1205	2MG	N1-C2-N2-CM2
6	A	1205	2MG	N3-C2-N2-CM2
6	A	1517	MA6	C5-C6-N6-C10
17	L	89	D2T	CG-CB-SB-CB1
17	L	89	D2T	CA-CB-CG-OD1

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	953	PSU	1	0
28	a	1937	5MU	1	0
6	A	964	2MG	1	0
16	K	119	HSE	1	0
28	a	2028	6MZ	2	0
6	A	1400	4OC	1	0
28	a	1913	3TD	1	0
28	a	2249	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 530 ligands modelled in this entry, 530 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1913:3TD	O3'	1914:A	P	4.68

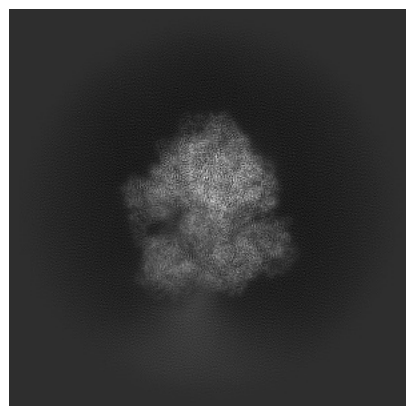
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55337. These allow visual inspection of the internal detail of the map and identification of artifacts.

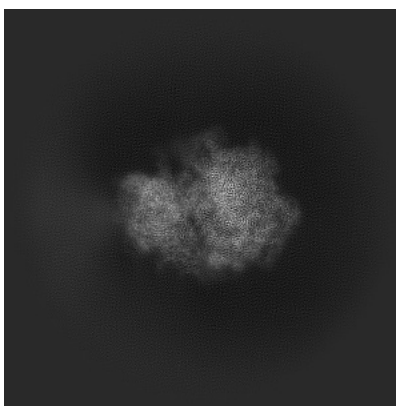
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

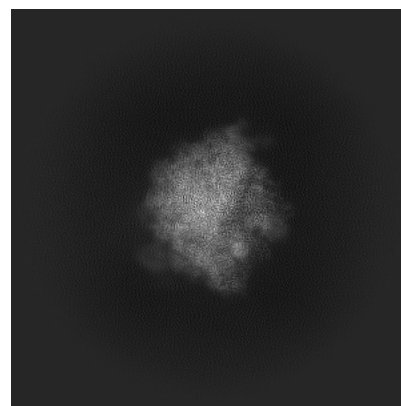
6.1.1 Primary map



X

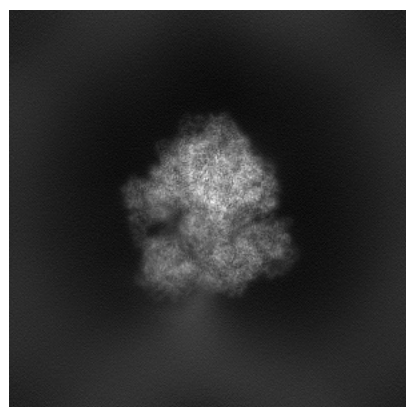


Y

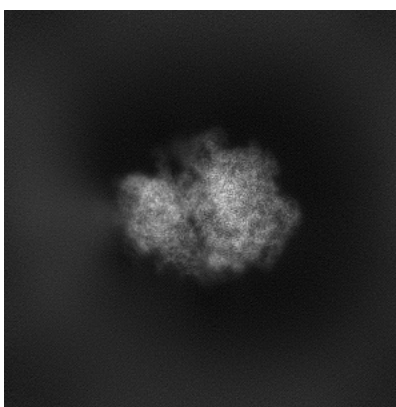


Z

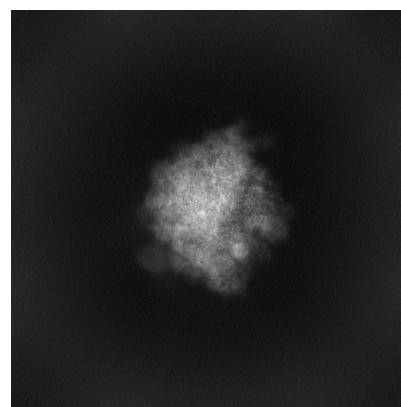
6.1.2 Raw map



X



Y

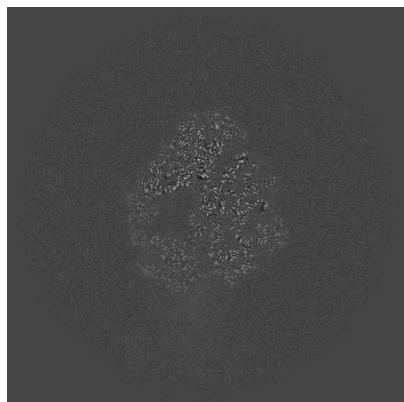


Z

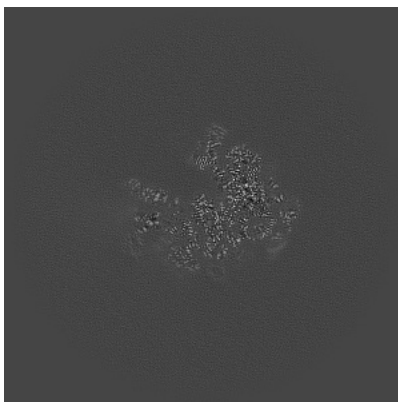
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

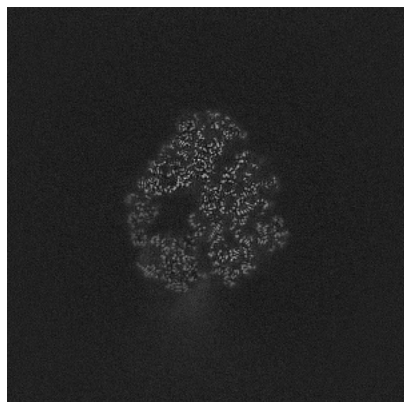


Y Index: 256

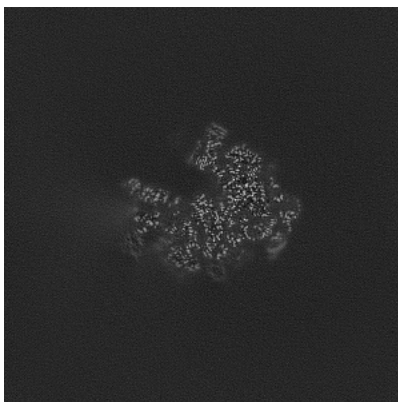


Z Index: 256

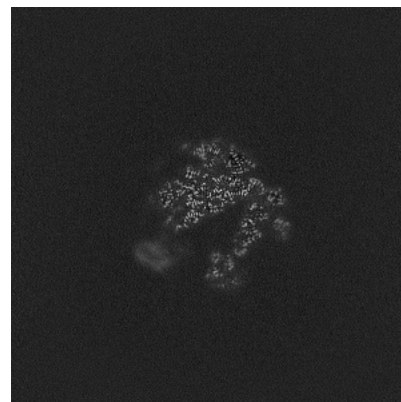
6.2.2 Raw map



X Index: 256



Y Index: 256

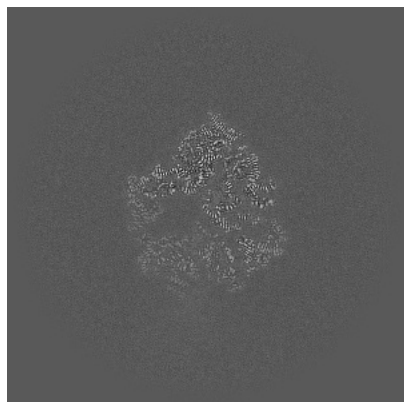


Z Index: 256

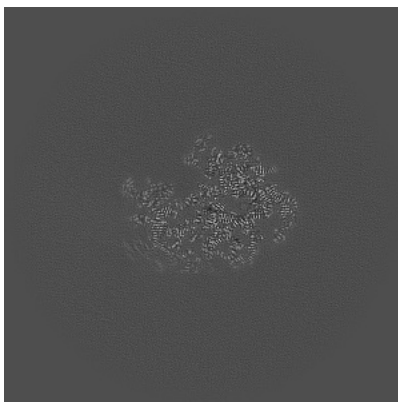
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

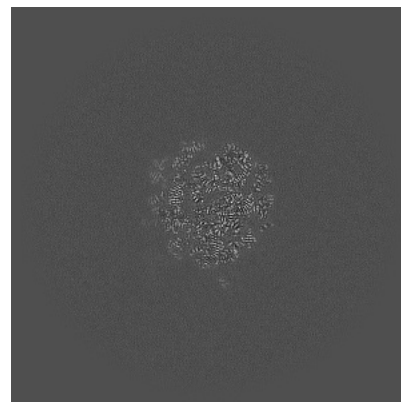
6.3.1 Primary map



X Index: 264

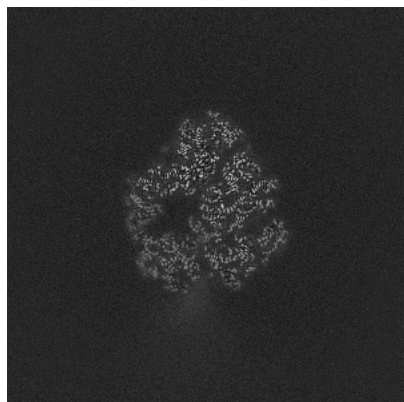


Y Index: 267

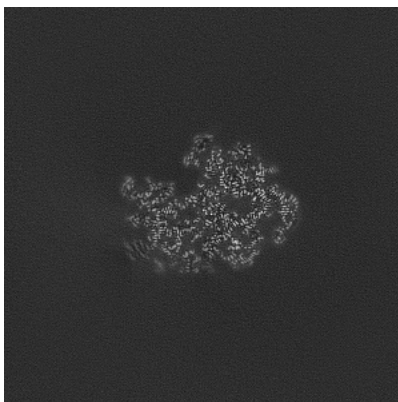


Z Index: 298

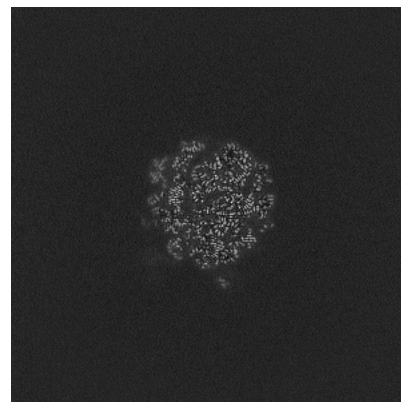
6.3.2 Raw map



X Index: 260



Y Index: 268

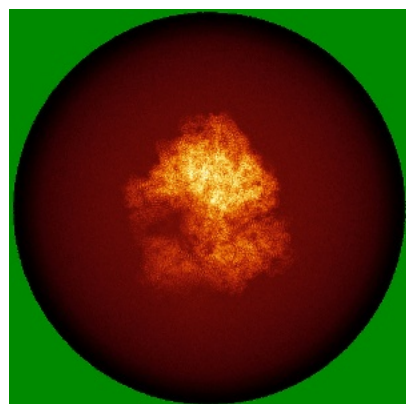


Z Index: 298

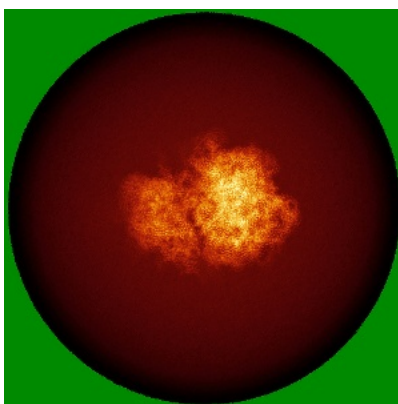
The images above show the largest variance slices of the map in three orthogonal directions.

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

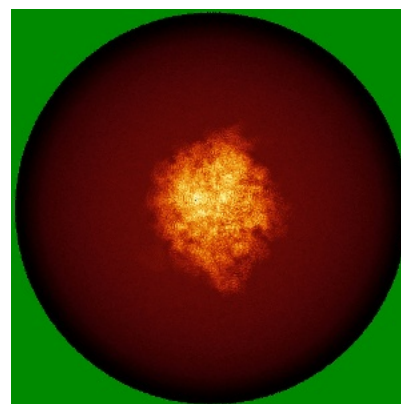
6.4.1 Primary map



X

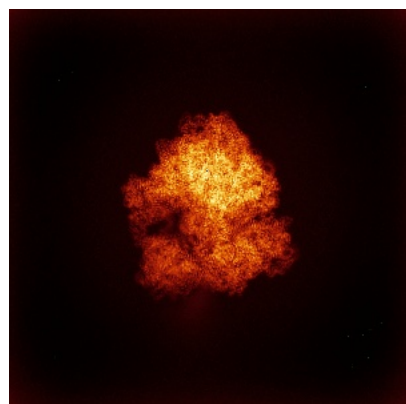


Y

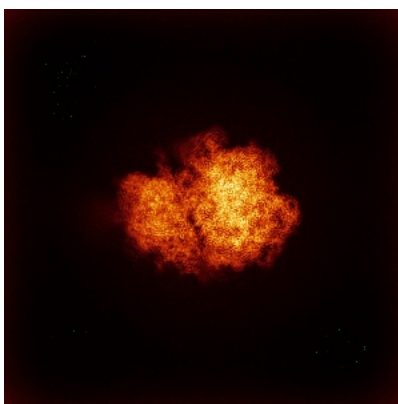


Z

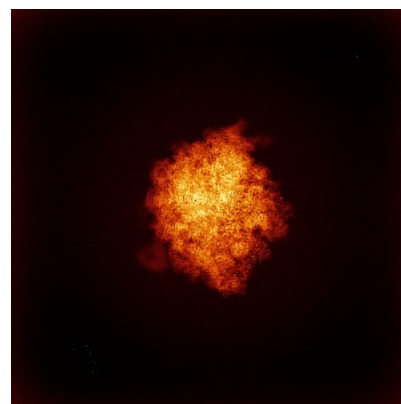
6.4.2 Raw map



X



Y

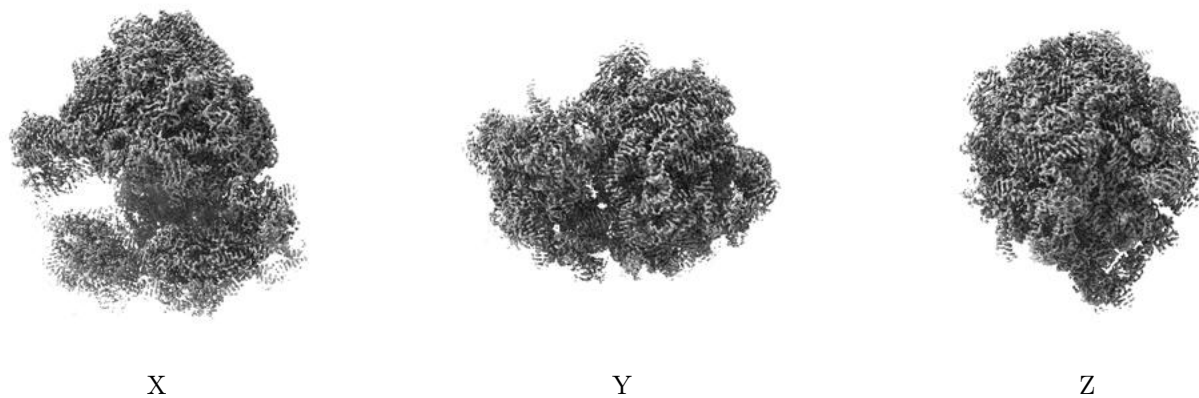


Z

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.

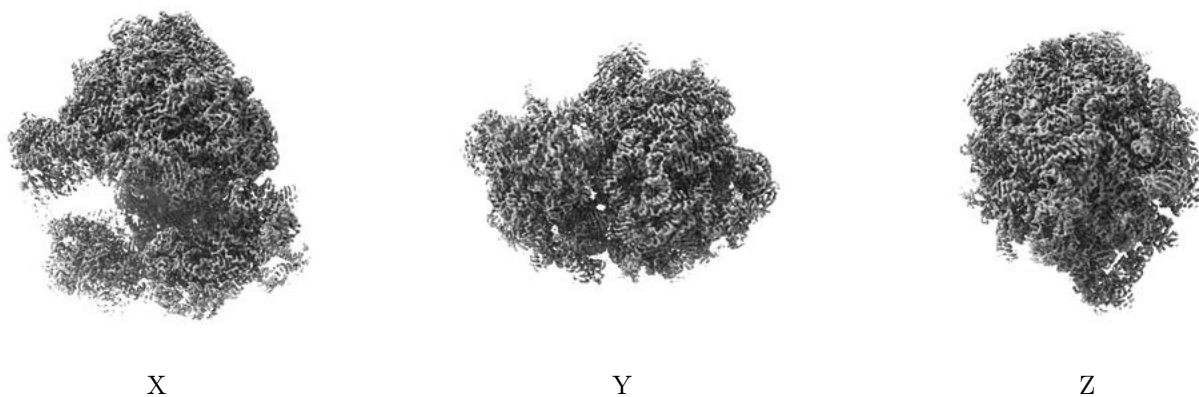
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

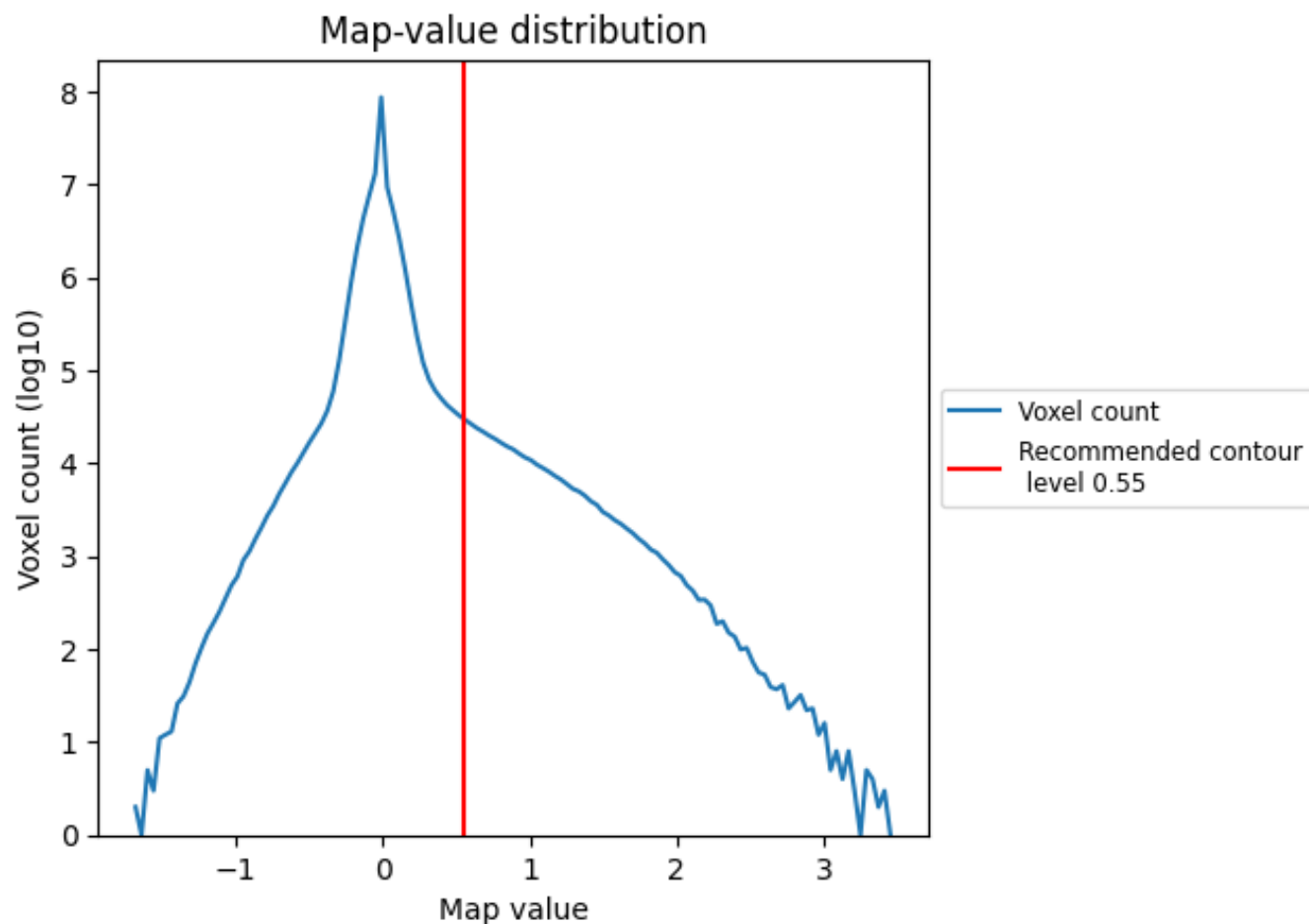
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

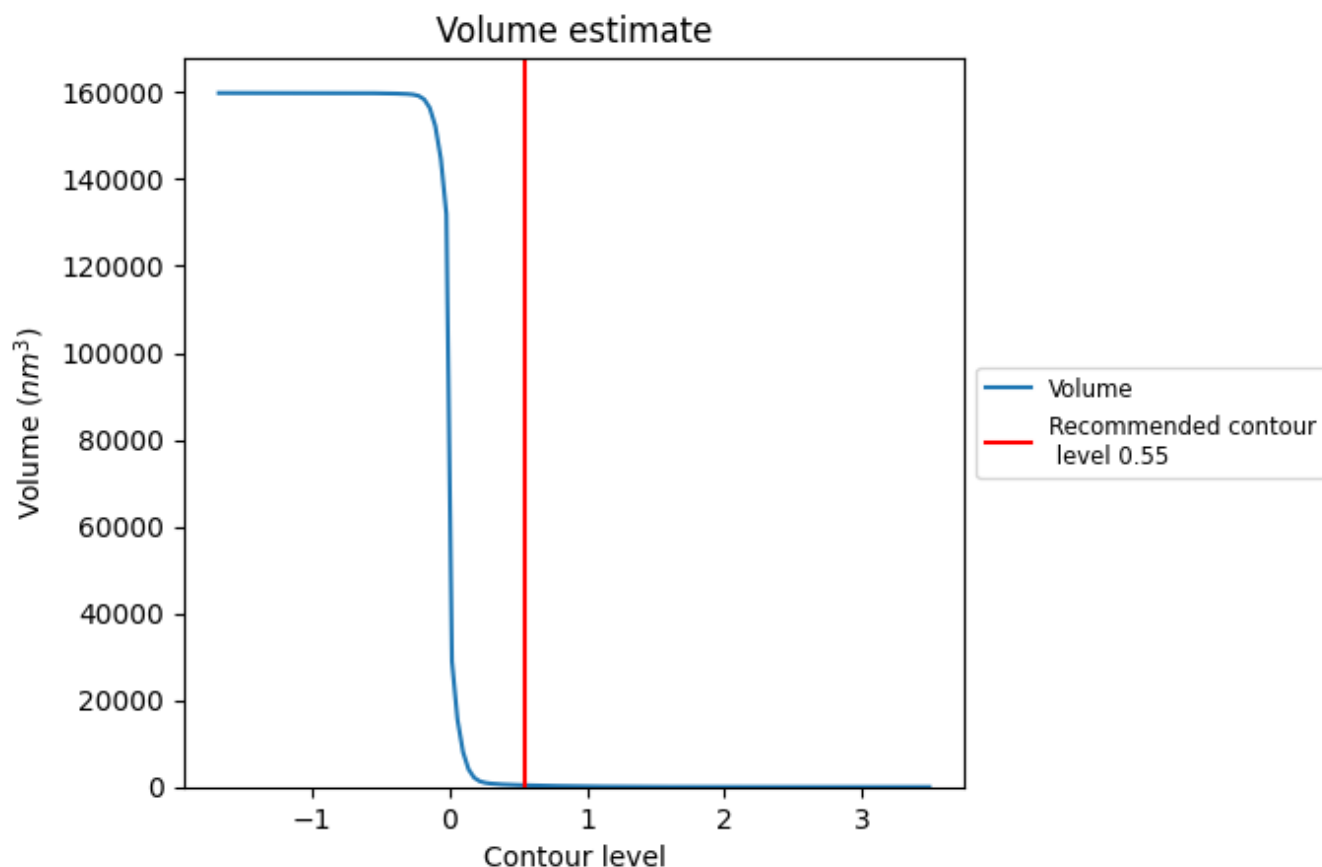
This section contains the results of statistical analysis of the map.

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.

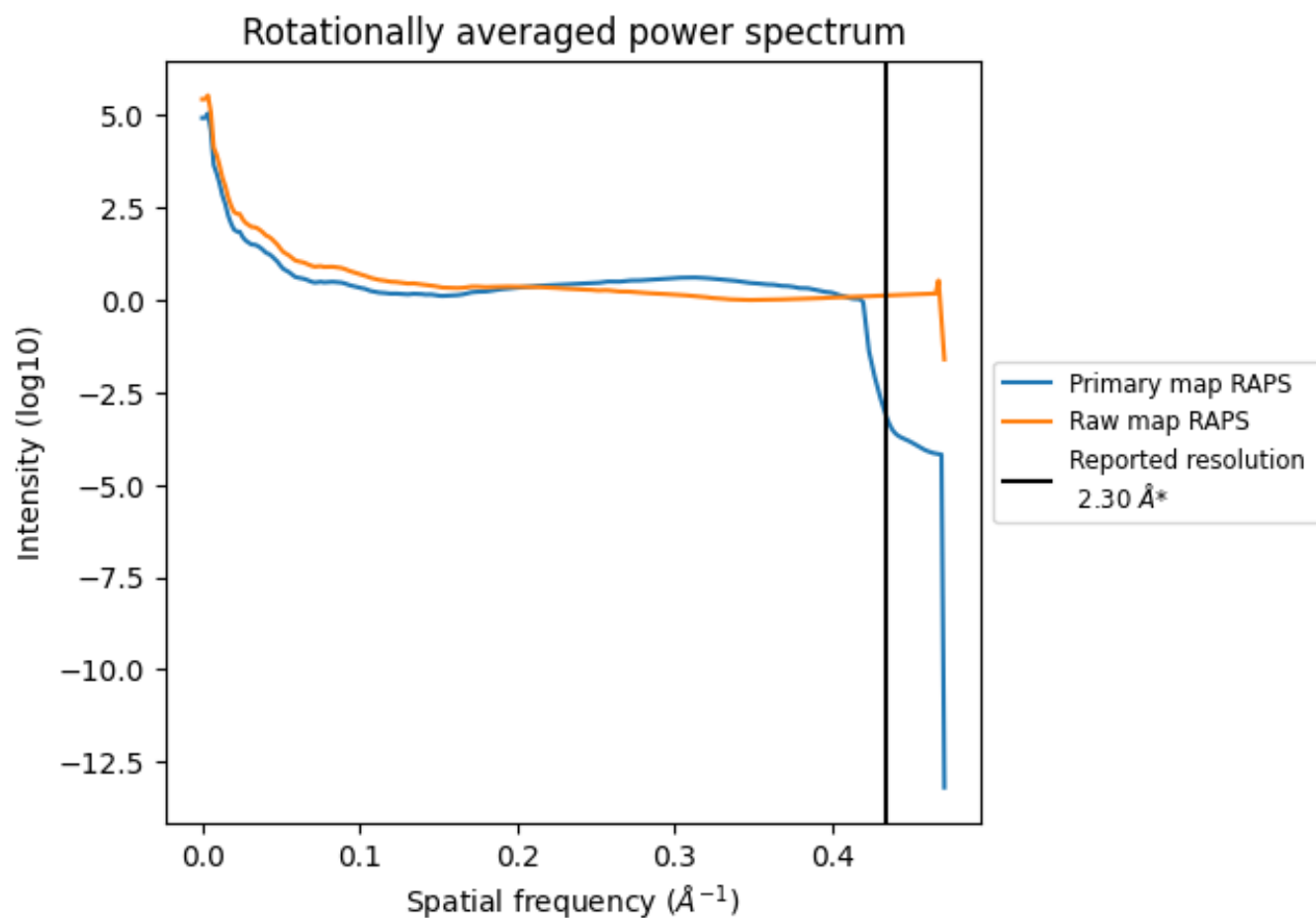
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm^3 ; this corresponds to an approximate mass of 346 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 ⓘ

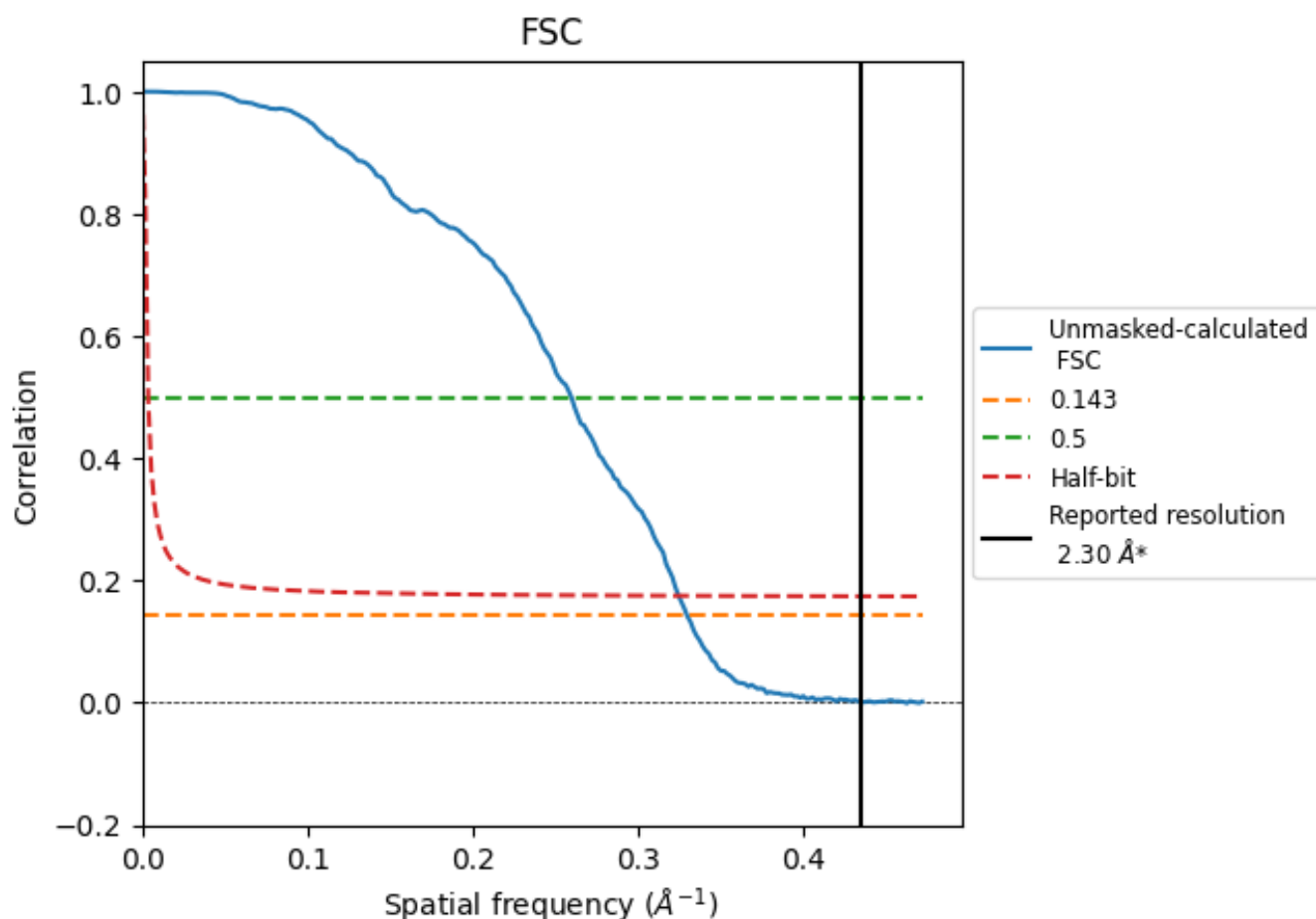


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

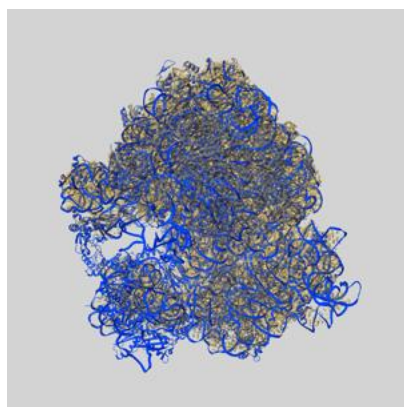
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.03	3.85	3.08

*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 3.03 differs from the reported value 2.3 by more than 10 %

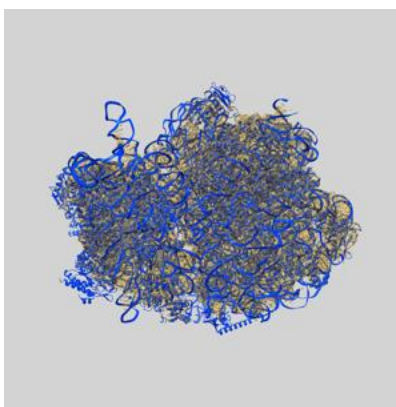
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55337 and PDB model 9SXX. Per-residue inclusion information can be found in section 3 on page 14.

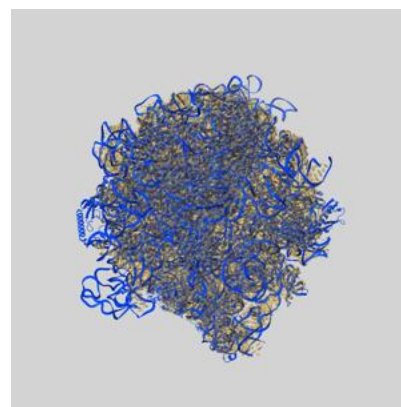
9.1 Map-model overlay [i](#)



X



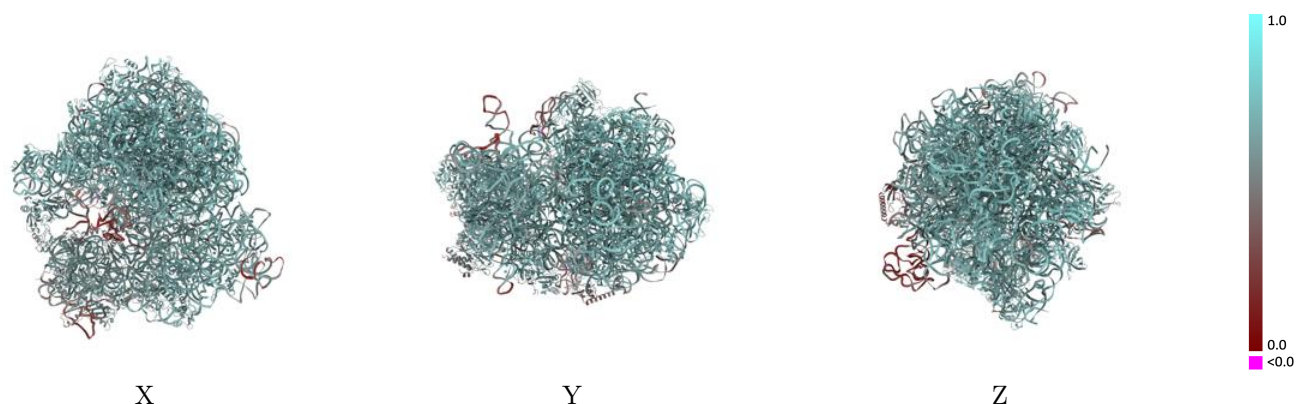
Y



Z

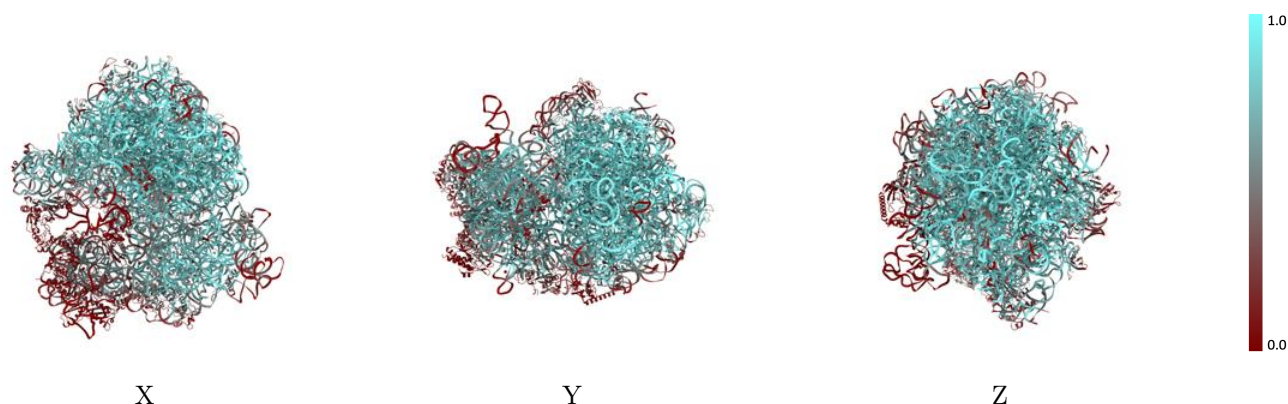
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



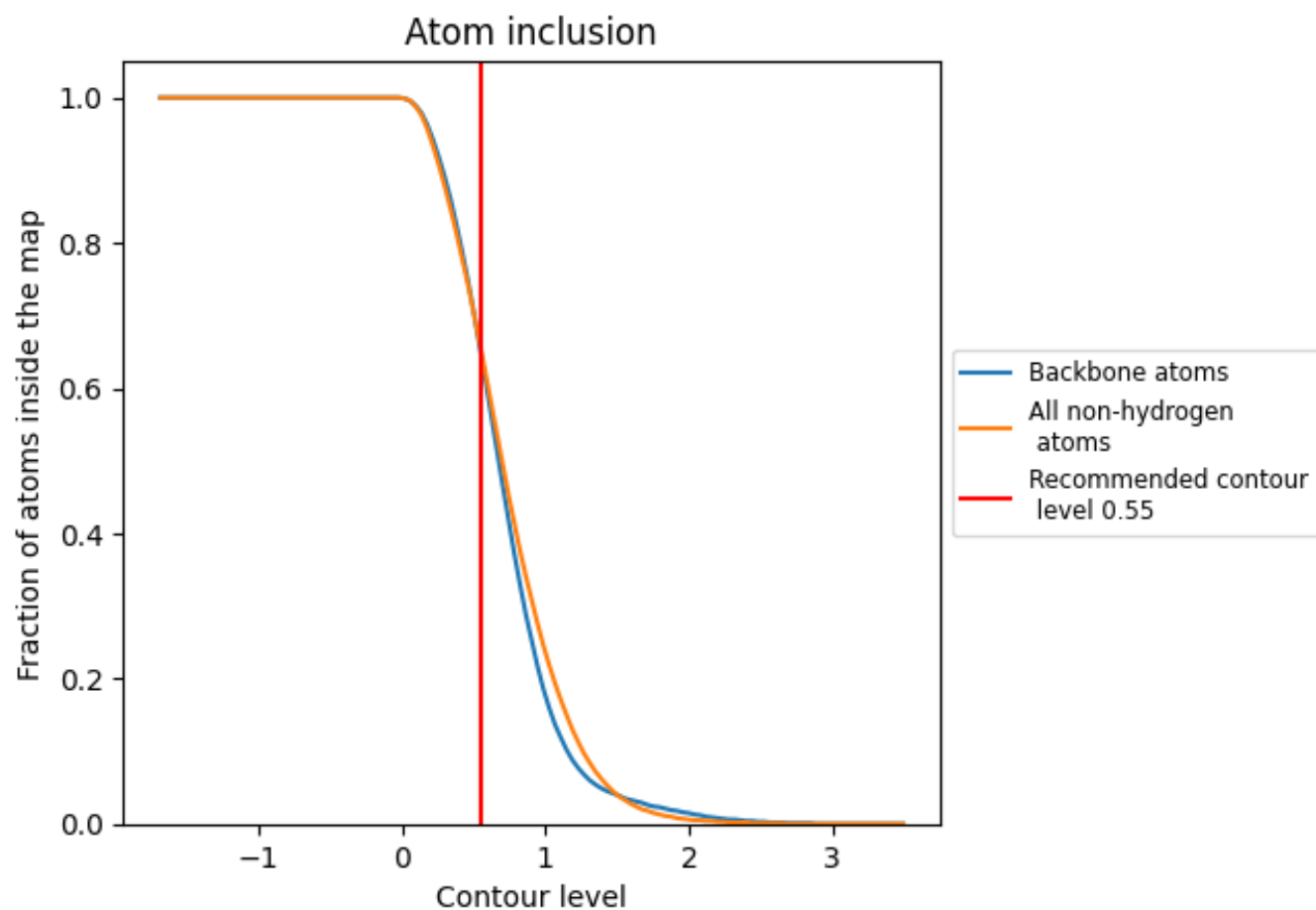
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 66% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.6400
0	 0.5600	 0.6780
1	 0.9150	 0.7080
2	 0.9100	 0.7100
3	 0.7580	 0.6900
4	 0.0300	 0.5090
A	 0.6140	 0.6260
B	 0.0060	 0.4970
C	 0.2460	 0.6080
D	 0.3670	 0.6400
E	 0.5850	 0.6640
F	 0.2580	 0.6060
G	 0.1010	 0.5900
H	 0.5690	 0.6620
I	 0.1640	 0.5810
J	 0.1570	 0.5370
K	 0.3080	 0.6180
L	 0.5770	 0.6670
M	 0.1030	 0.5800
N	 0.2260	 0.6050
O	 0.5160	 0.6540
P	 0.6080	 0.6590
Q	 0.4580	 0.6410
R	 0.3570	 0.5940
S	 0.0420	 0.5650
T	 0.5370	 0.6570
W	 0.0000	 0.4250
X	 0.1950	 0.6020
a	 0.7910	 0.6480
b	 0.6730	 0.6460
c	 0.8230	 0.7010
d	 0.8080	 0.6970
e	 0.6670	 0.6780
f	 0.1770	 0.5940
g	 0.3120	 0.6170



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.0150	 0.4490
i	 0.8150	 0.6940
j	 0.7310	 0.6910
k	 0.7400	 0.6890
l	 0.7340	 0.6860
m	 0.8890	 0.7060
n	 0.5110	 0.6530
o	 0.7330	 0.6910
p	 0.8660	 0.7070
q	 0.6860	 0.6800
r	 0.8070	 0.6960
s	 0.6510	 0.6710
t	 0.5910	 0.6570
u	 0.5680	 0.6640
v	 0.7920	 0.6930
w	 0.7340	 0.6890
x	 0.5110	 0.6530
y	 0.7880	 0.6900
z	 0.7760	 0.6950