



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 09:33 AM UTC

PDB ID : 9NLJ / pdb_00009nlj
EMDB ID : EMD-29399
Title : E.coli Initiation complex with Uup-EQ2
Authors : Singh, S.; Hunt, J.F.
Deposited on : 2025-03-03
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

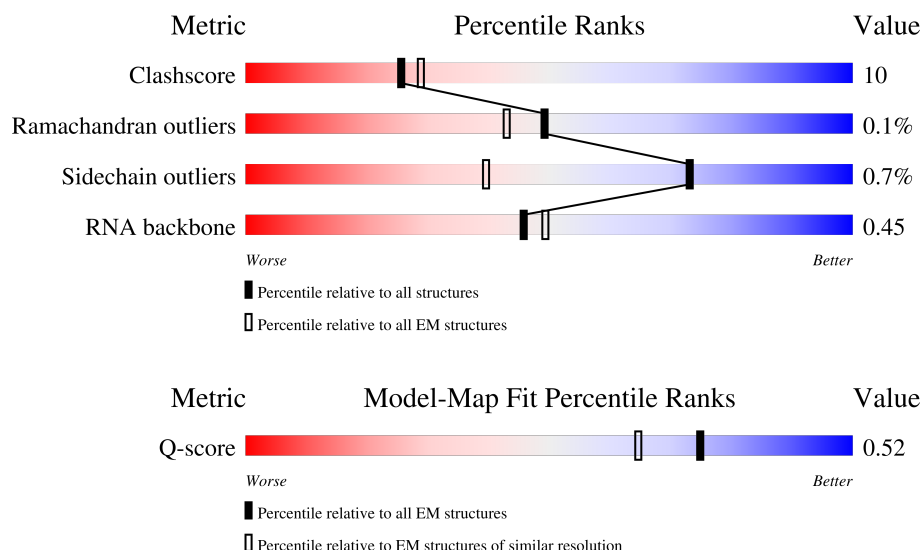
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14081 (2.50 - 3.50)

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	13	142	
2	14	122	
3	15	144	

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Mol	Chain	Length	Quality of chain
4	16	136	
5	17	120	
6	18	116	
7	19	114	
8	2	271	
9	20	117	
10	21	103	
11	22	110	
12	23	93	
13	24	102	
14	25	94	
15	27	85	
16	28	77	
17	29	63	
18	3	209	
19	30	58	
20	31	66	
21	32	56	
22	33	50	
23	34	46	
24	35	64	
25	36	38	
26	4	201	
27	5	177	
28	6	176	

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Mol	Chain	Length	Quality of chain
29	9	149	
30	R1	2903	
31	R2	119	
32	R3	1531	
33	sb	218	
34	sc	206	
35	sd	205	
36	se	157	
37	sf	100	
38	sg	151	
39	sh	129	
40	si	127	
41	sj	98	
42	sk	116	
43	sl	123	
44	sm	114	
45	sn	100	
46	so	88	
47	sp	82	
48	sq	80	
49	sr	65	
50	ss	79	
51	st	85	
52	su	65	
53	T	78	

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Mol	Chain	Length	Quality of chain
54	U	537	
55	1	220	
56	M	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	H2U	T	20	X	-	-	-
53	4OC	T	32	X	-	-	-
53	5MU	T	54	X	-	-	-
53	PSU	T	55	X	-	-	-
53	4SU	T	8	X	-	-	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150042 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 uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 2 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 3 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	15	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 5 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 6 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	18	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	20	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 10 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	24	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	25	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	27	85	Total	C	N	O	S	0	0
			642	396	130	114	2		

- Molecule 16 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	28	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	29	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 18 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	30	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	33	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 25 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R3	1531	Total	C	N	O	P	0	0
			32850	14652	6028	10640	1530		

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	st	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 52 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	T	78	Total	C	N	O	P S	0	0
			1649	740	295	536	76 2		

- Molecule 54 is a protein called Uup.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	U	537	Total	C	N	O	S	0	0
			4295	2690	778	810	17		

- Molecule 55 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

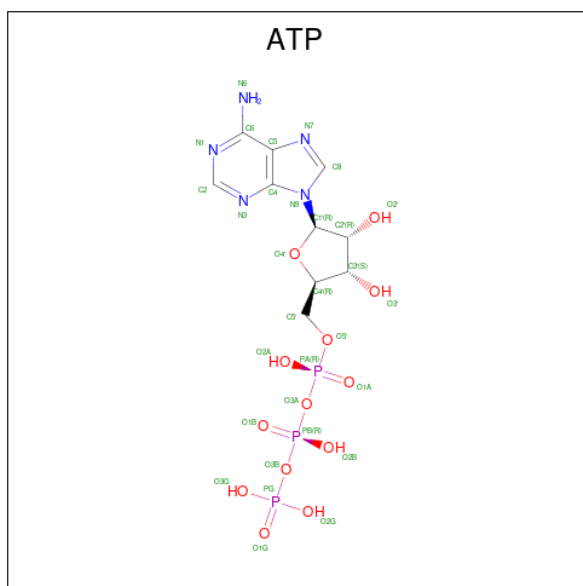
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total	Mg	0
			1	1	
57	2	1	Total	Mg	0
			1	1	
57	20	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	R1	192	Total	Mg	0
			192	192	
57	R3	81	Total	Mg	0
			81	81	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
58	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
58	U	1	Total	C	N	O	P	0
			31	10	5	13	3	

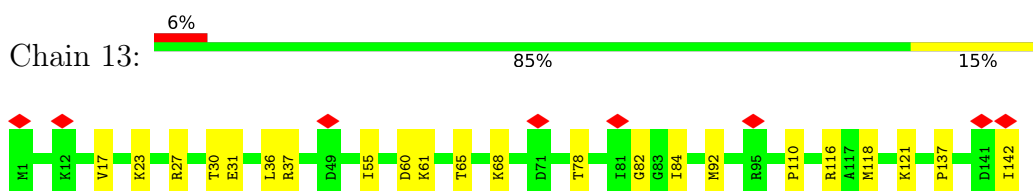
- Molecule 59 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
59	U	2	Total 2	Na 2	0

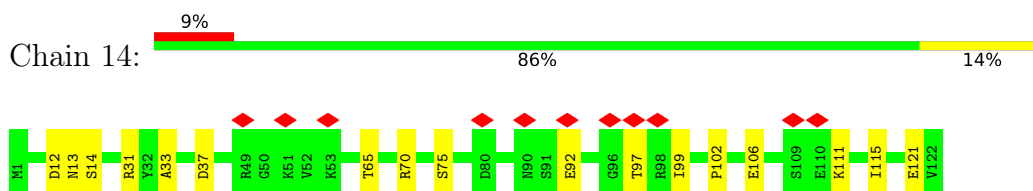
3 Residue-property plots [i](#)

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.

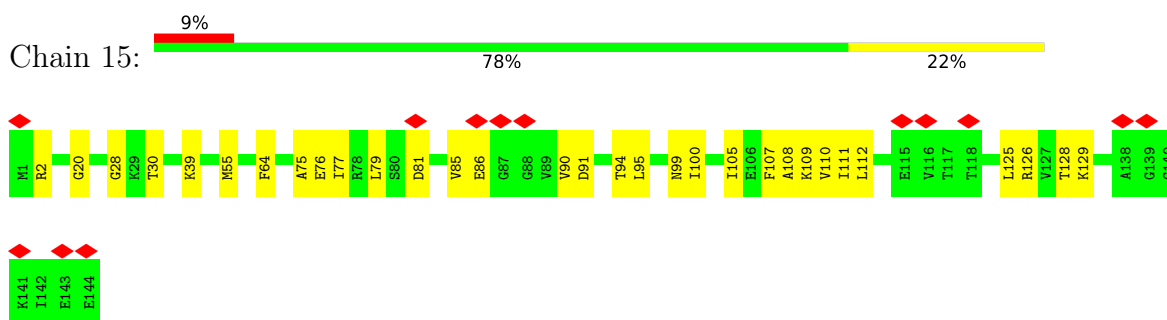
- Molecule 1: Large ribosomal subunit protein uL13



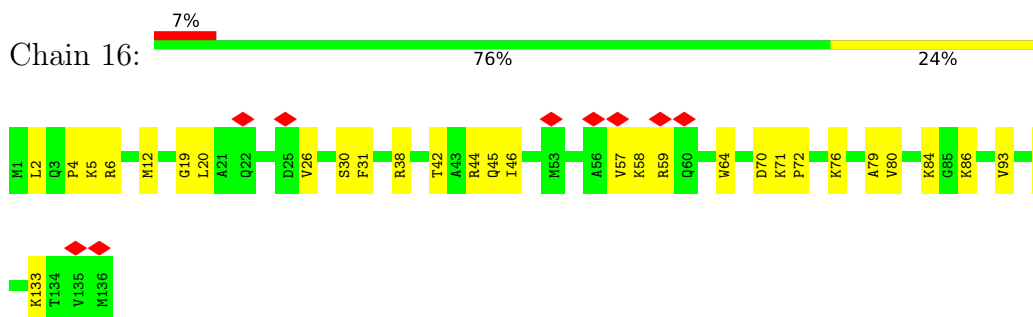
- Molecule 2: 50S ribosomal protein L14



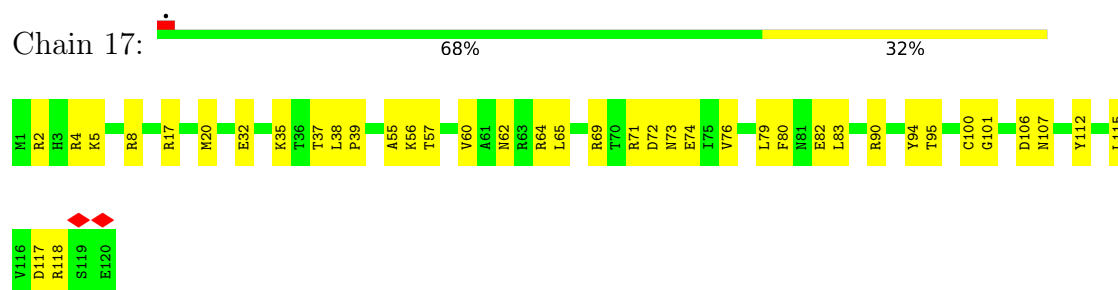
- Molecule 3: Large ribosomal subunit protein uL15



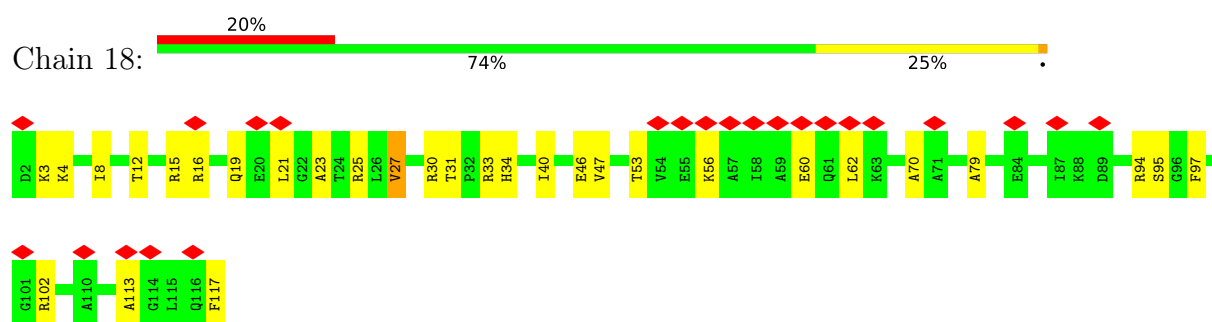
- Molecule 4: 50S ribosomal protein L16



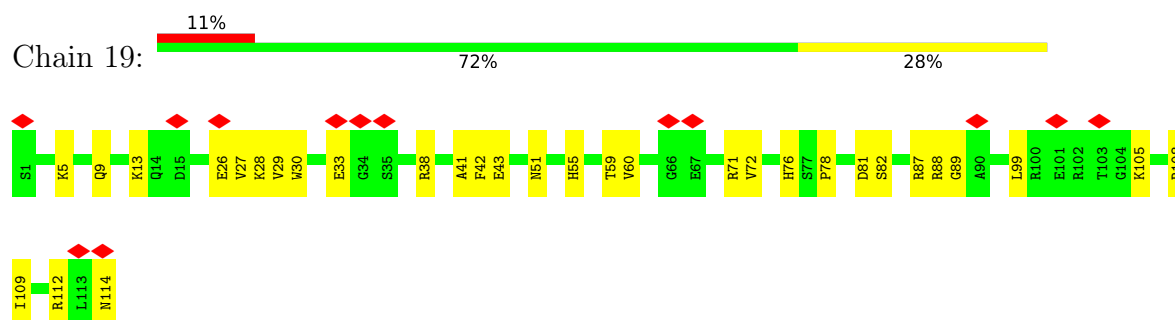
- Molecule 5: Large ribosomal subunit protein bL17



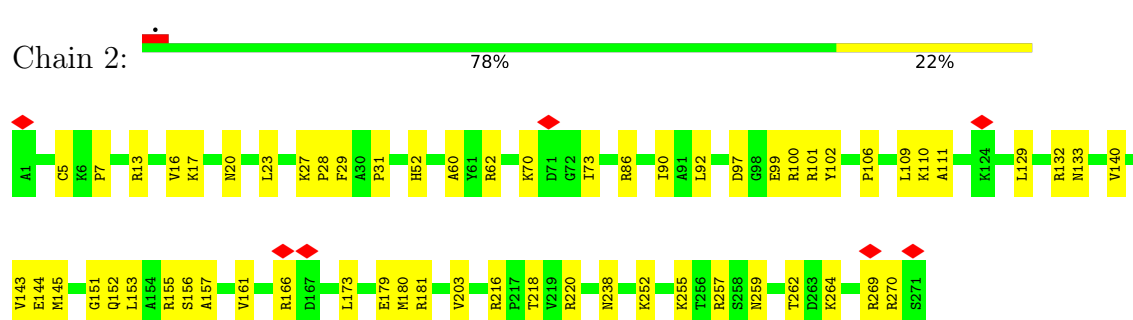
- Molecule 6: Large ribosomal subunit protein uL18



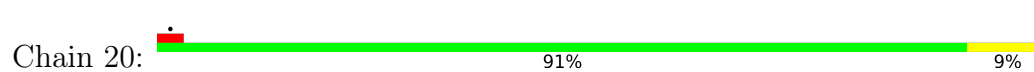
- Molecule 7: 50S ribosomal protein L19



- Molecule 8: 50S ribosomal protein L2

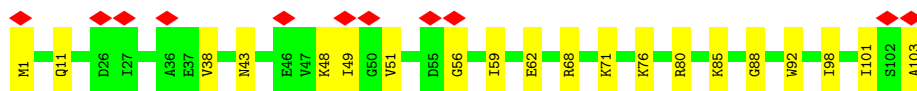
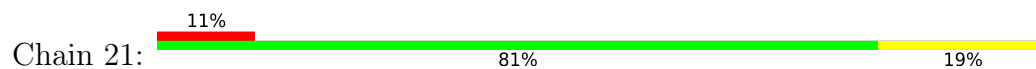


- Molecule 9: Large ribosomal subunit protein bL20

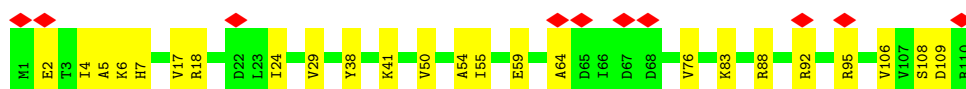
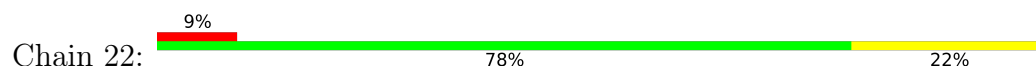




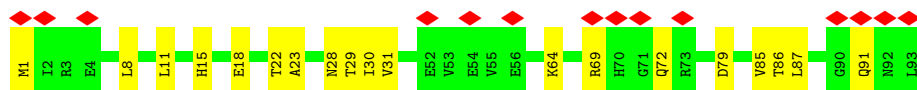
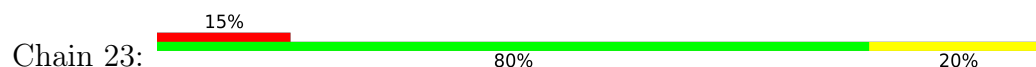
- Molecule 10: Large ribosomal subunit protein bL21



- Molecule 11: Large ribosomal subunit protein uL22



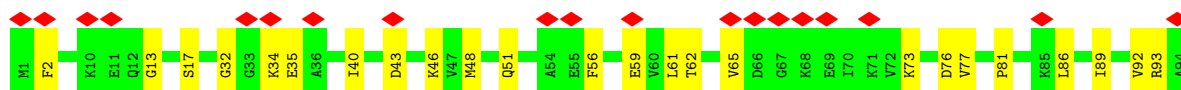
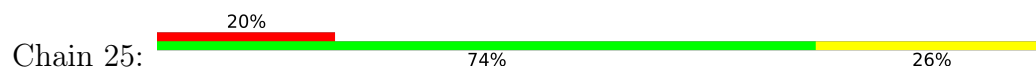
- Molecule 12: Large ribosomal subunit protein uL23



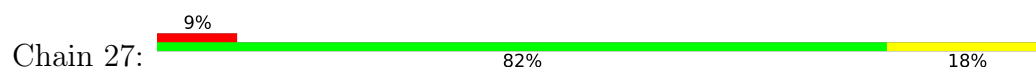
- Molecule 13: Large ribosomal subunit protein uL24



- Molecule 14: Large ribosomal subunit protein bL25

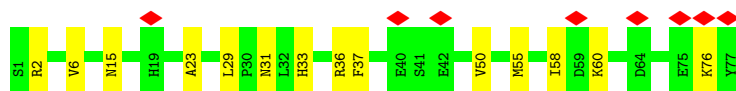
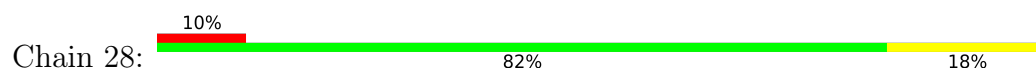


- Molecule 15: Large ribosomal subunit protein bL27

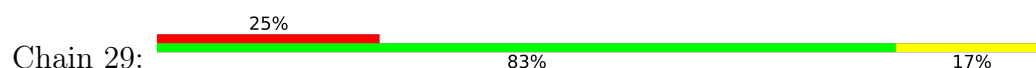




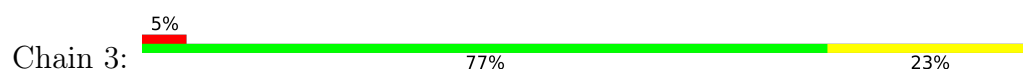
- Molecule 16: 50S ribosomal protein L28



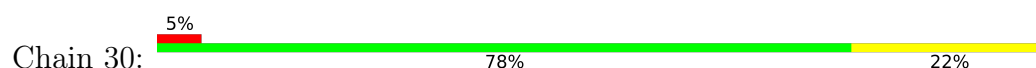
- Molecule 17: Large ribosomal subunit protein uL29



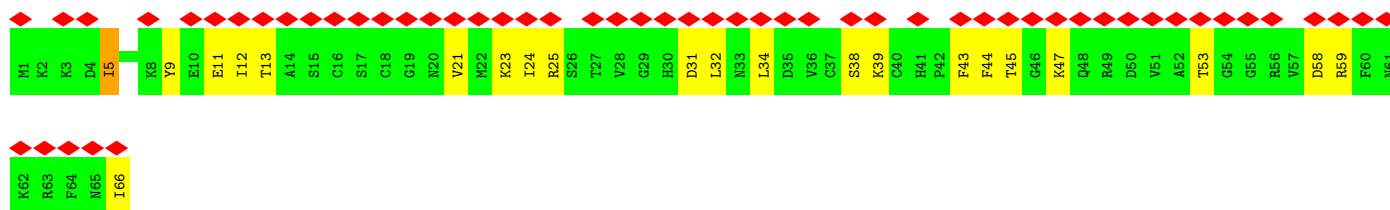
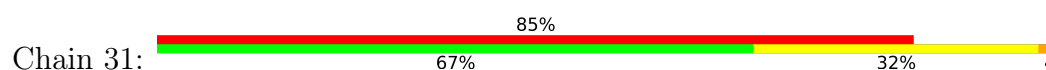
- Molecule 18: 50S ribosomal protein L3



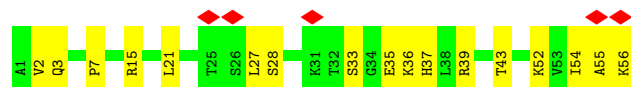
- Molecule 19: 50S ribosomal protein L30



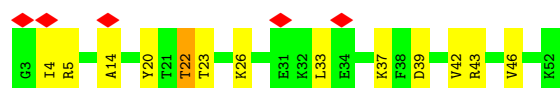
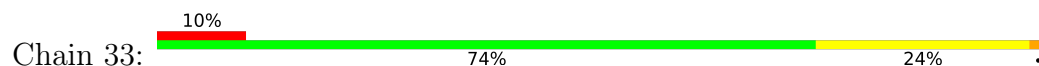
- Molecule 20: Large ribosomal subunit protein bL31



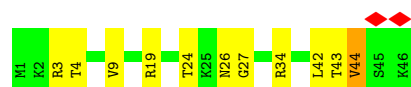
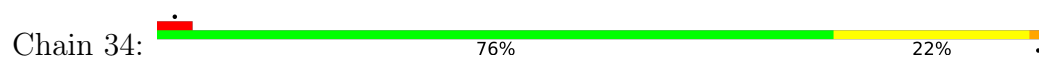
- Molecule 21: 50S ribosomal protein L32



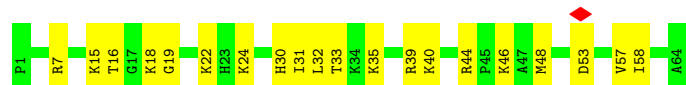
- Molecule 22: Large ribosomal subunit protein bL33



- Molecule 23: 50S ribosomal protein L34



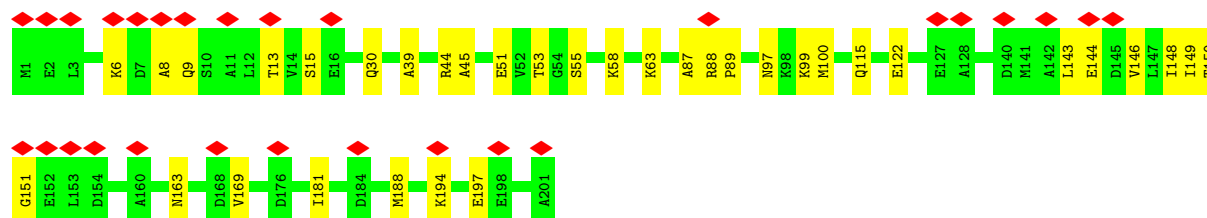
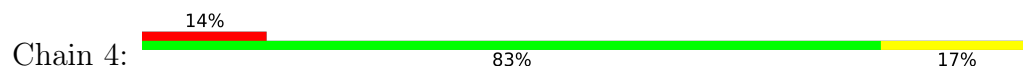
- Molecule 24: Large ribosomal subunit protein bL35



- Molecule 25: 50S ribosomal protein L36

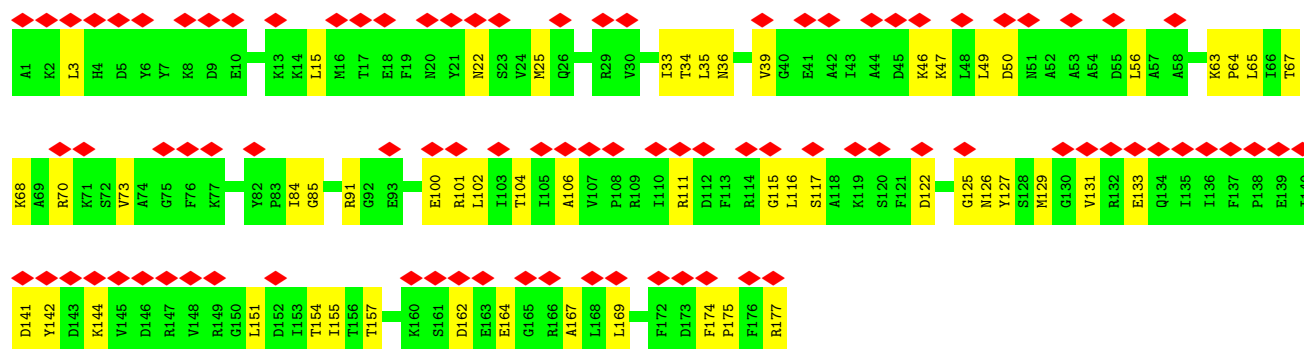


- Molecule 26: Large ribosomal subunit protein uL4

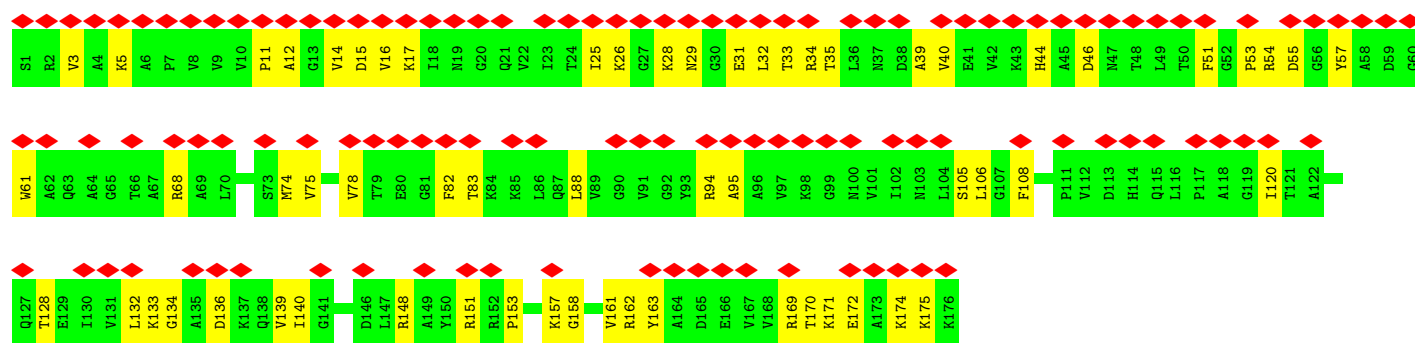


- Molecule 27: 50S ribosomal protein L5

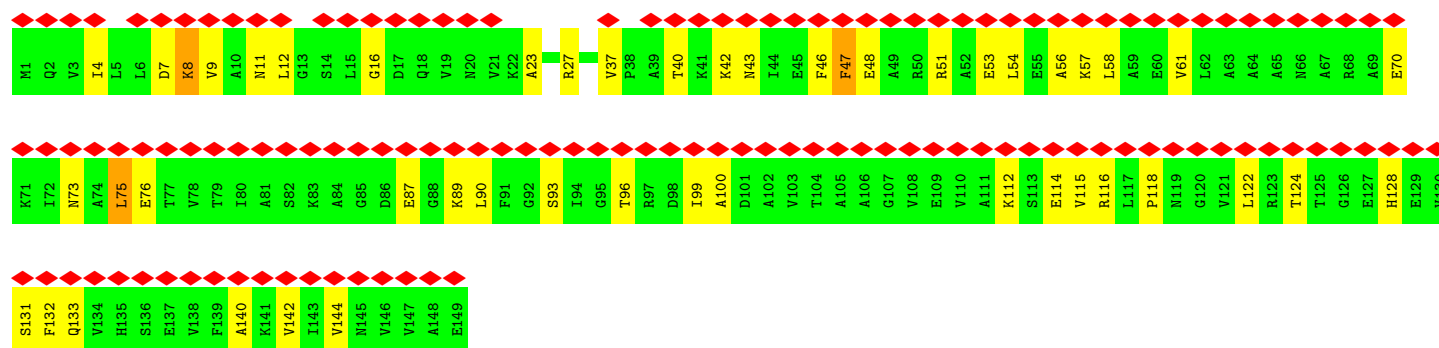
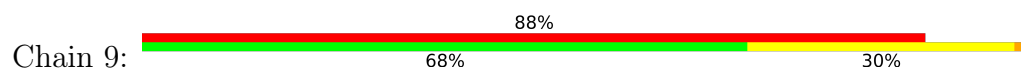




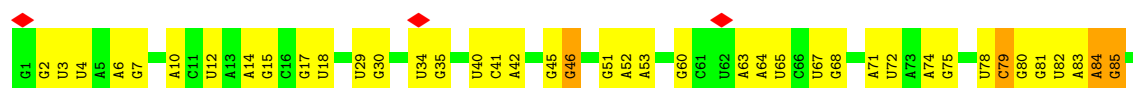
- Molecule 28: Large ribosomal subunit protein uL6



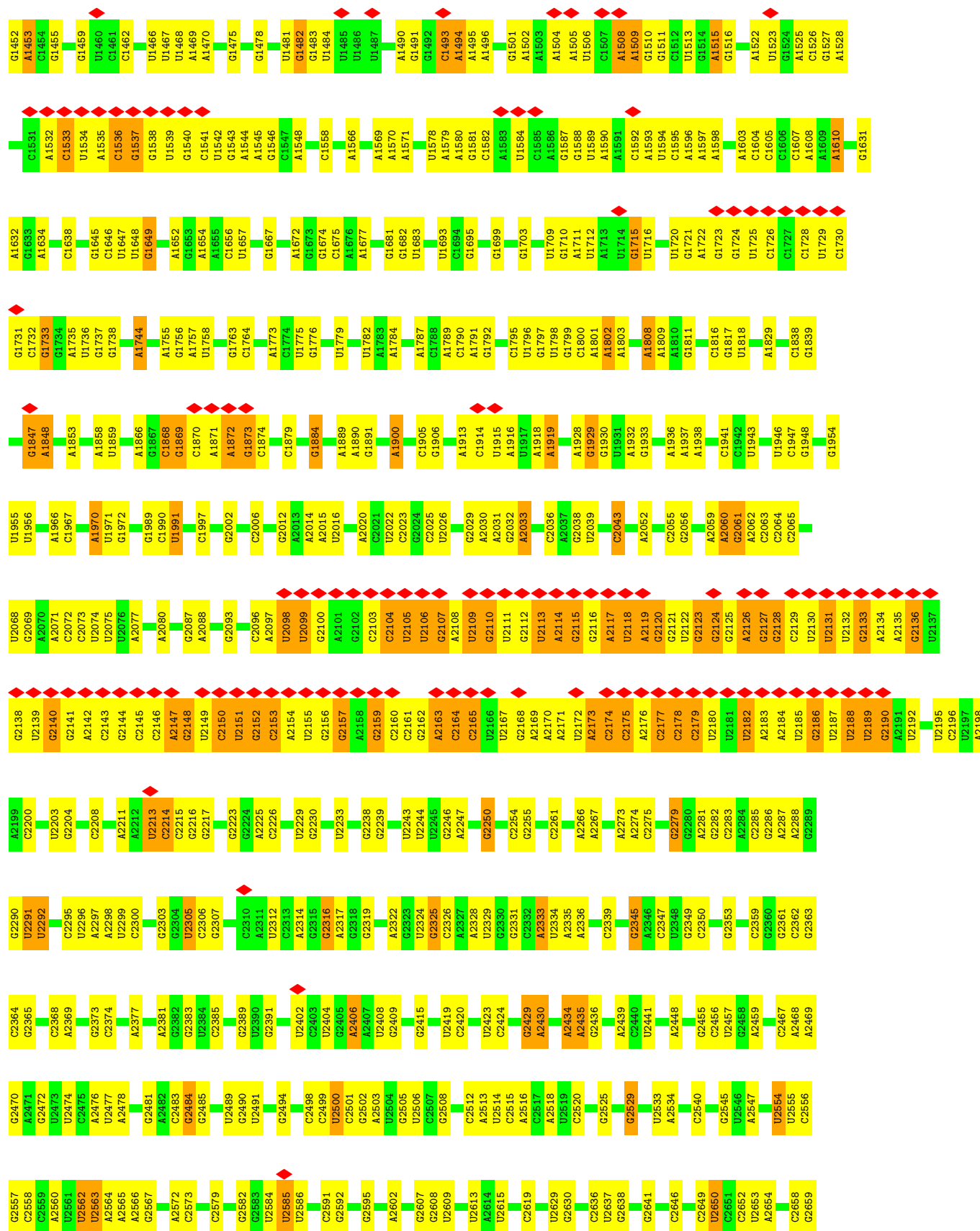
- Molecule 29: Large ribosomal subunit protein bL9

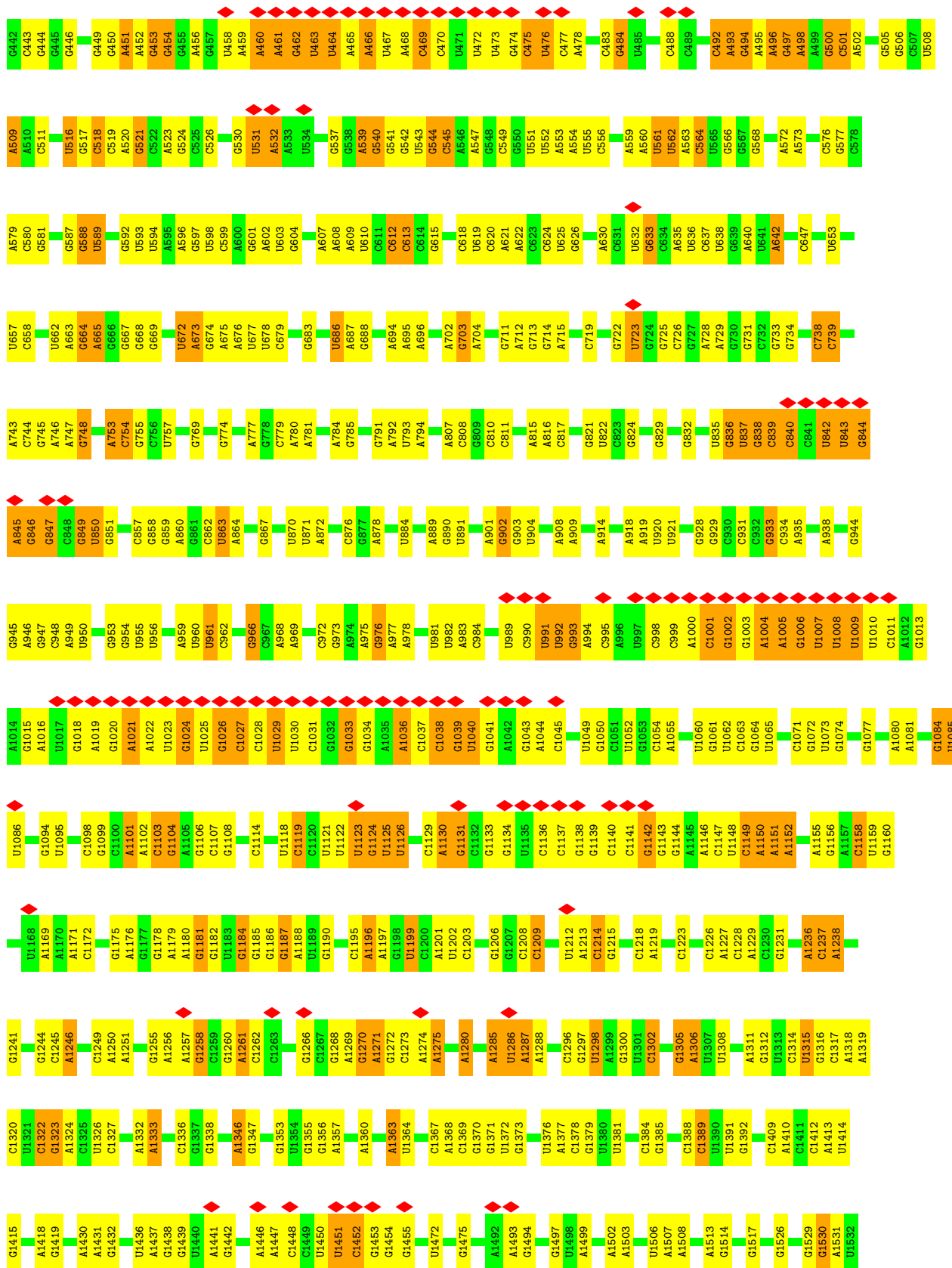


- Molecule 30: 23S ribosomal RNA

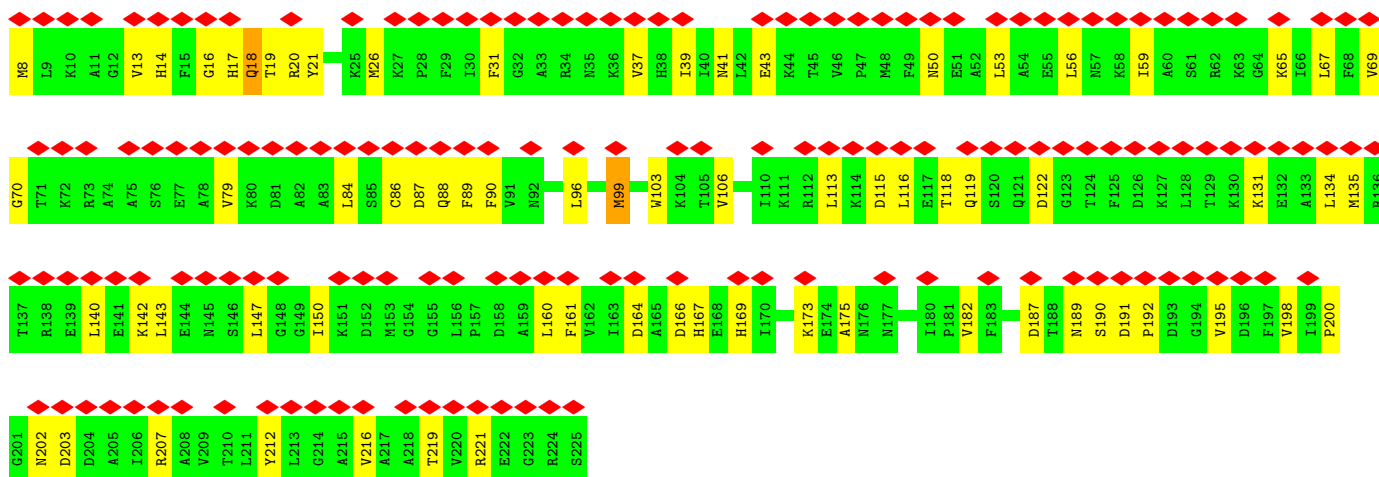
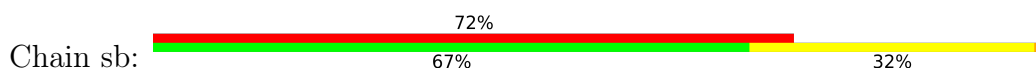








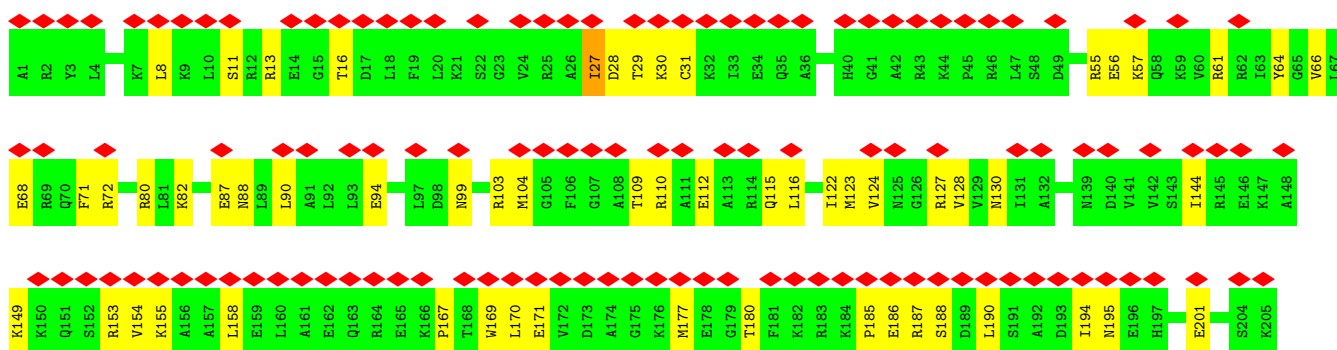
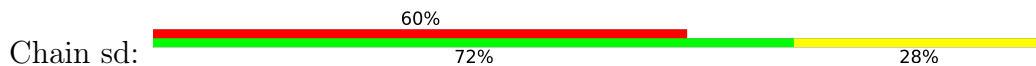
• Molecule 33: Small ribosomal subunit protein uS2



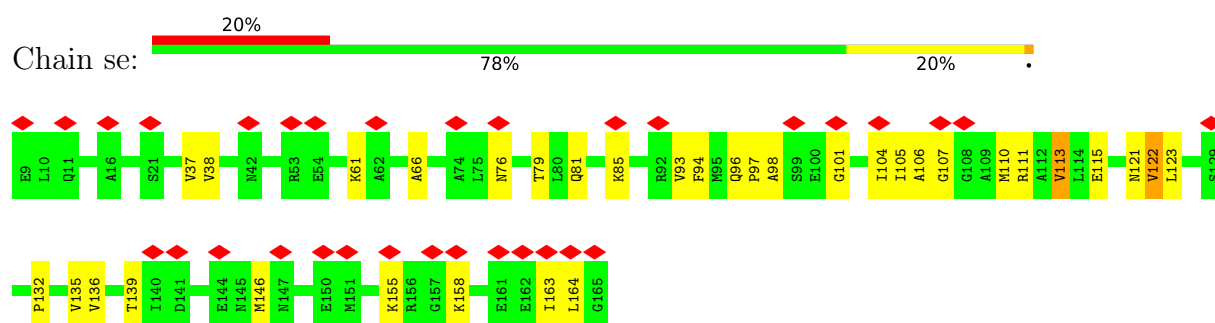
• Molecule 34: Small ribosomal subunit protein uS3



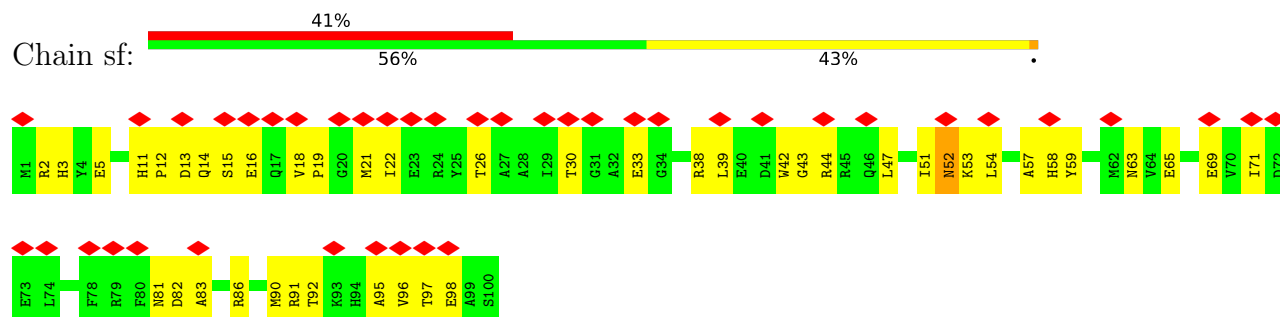
• Molecule 35: 30S ribosomal protein S4



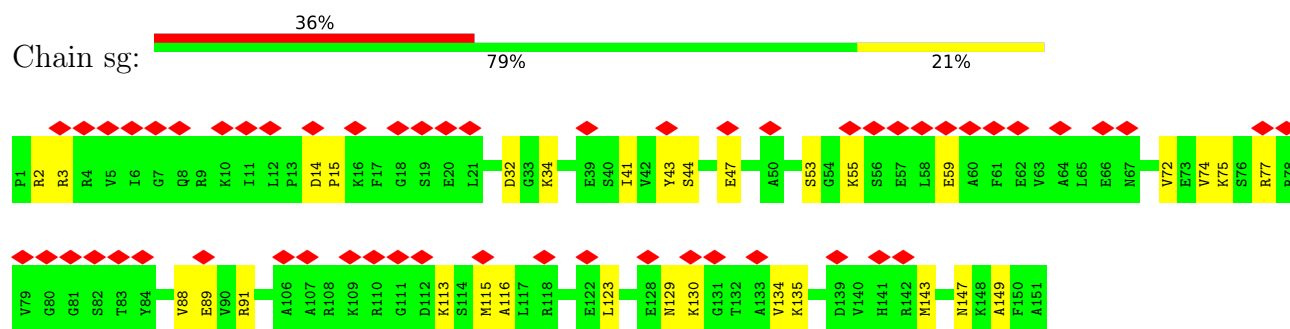
• Molecule 36: Small ribosomal subunit protein uS5



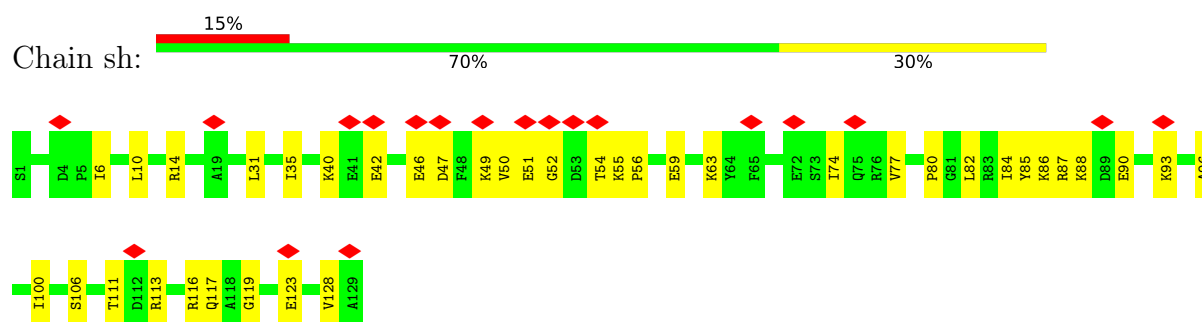
- Molecule 37: 30S ribosomal protein S6, non-modified isoform



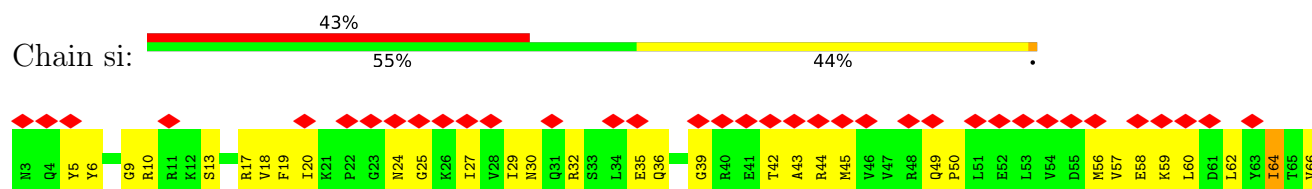
- Molecule 38: 30S ribosomal protein S7

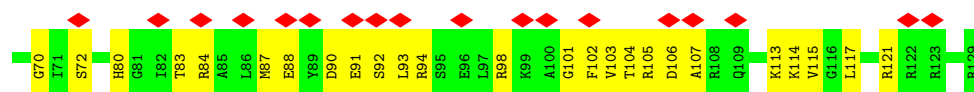


- Molecule 39: 30S ribosomal protein S8

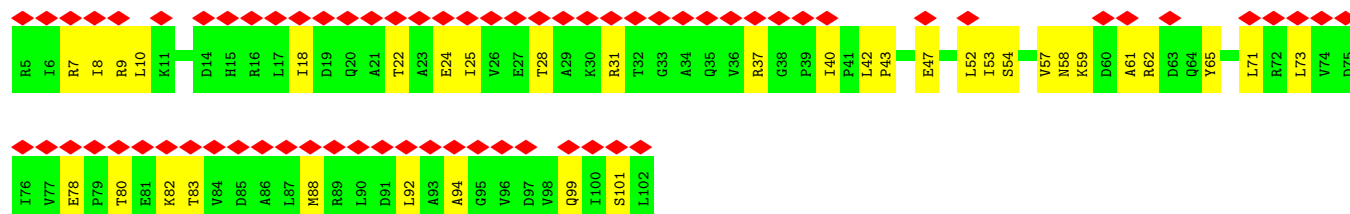


- Molecule 40: Small ribosomal subunit protein uS9

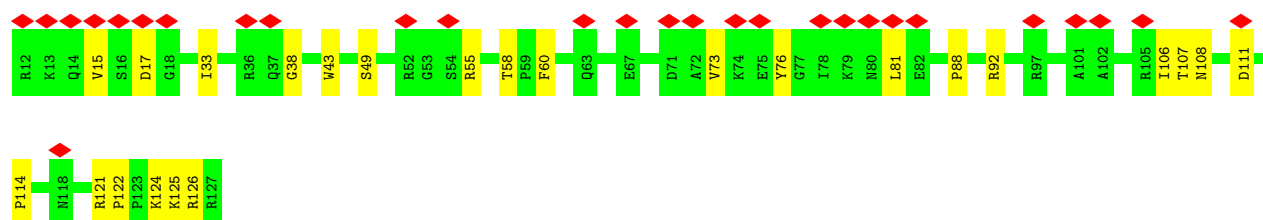
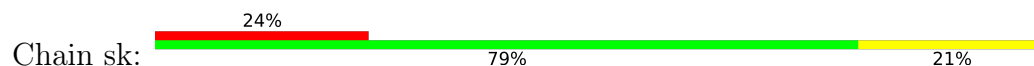




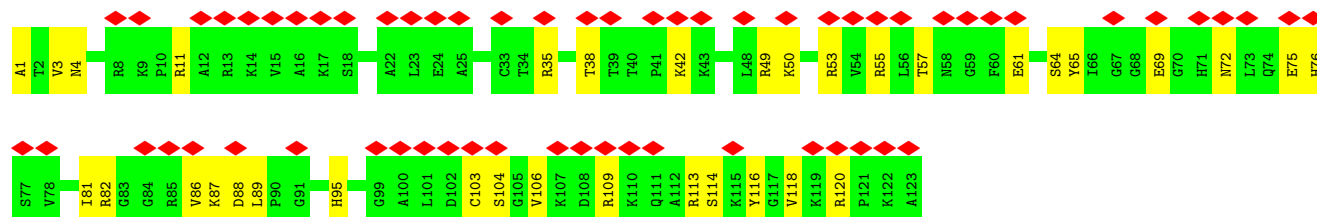
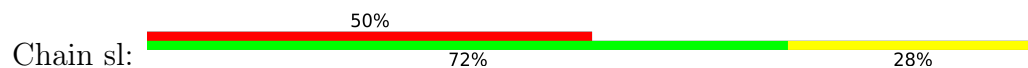
- Molecule 41: 30S ribosomal protein S10



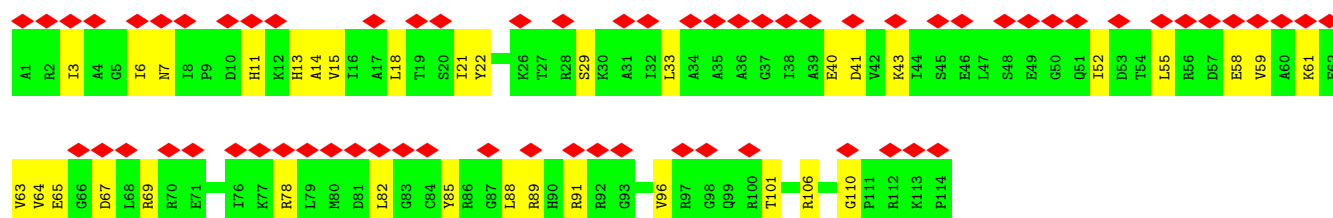
- Molecule 42: Small ribosomal subunit protein uS11



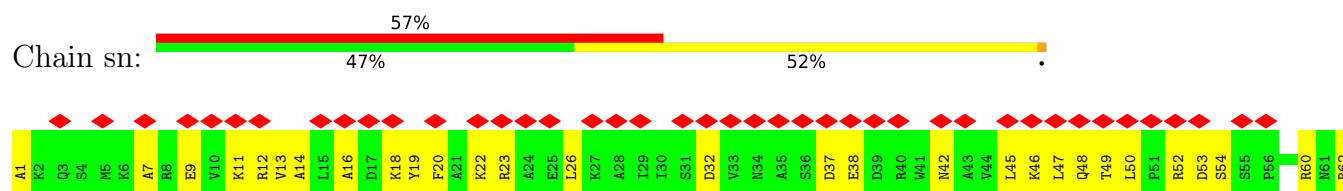
- Molecule 43: Small ribosomal subunit protein uS12



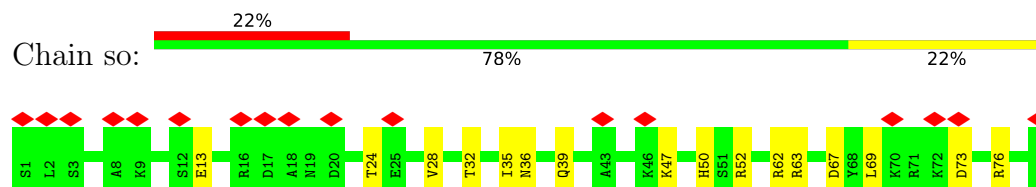
- Molecule 44: 30S ribosomal protein S13



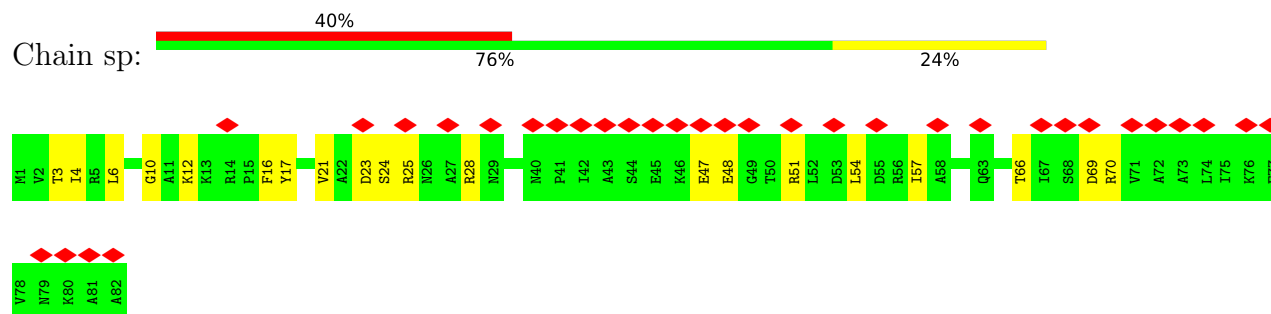
- Molecule 45: Small ribosomal subunit protein uS14



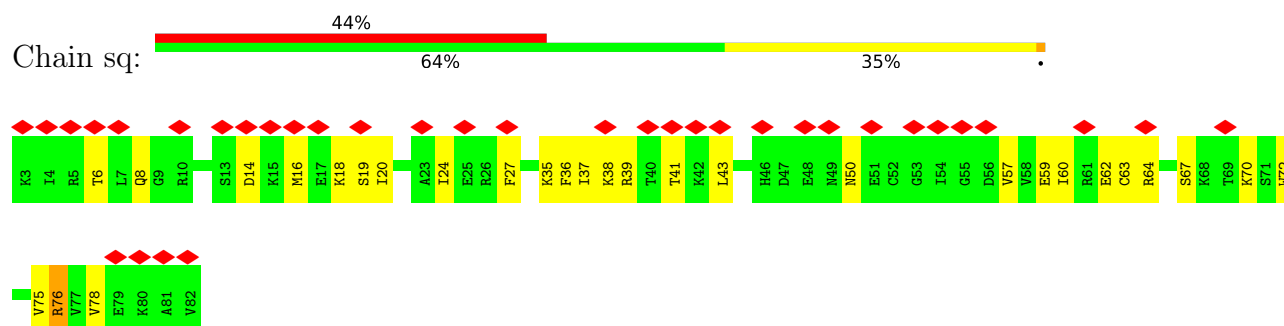
- Molecule 46: Small ribosomal subunit protein uS15



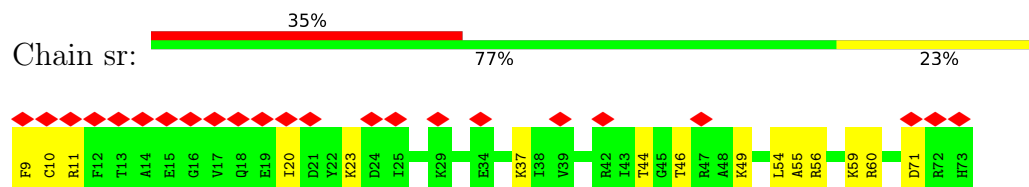
- Molecule 47: Small ribosomal subunit protein bS16



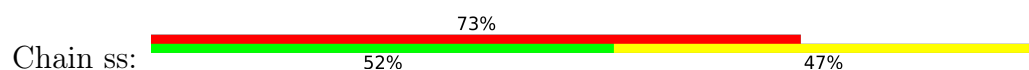
- Molecule 48: Small ribosomal subunit protein uS17



- Molecule 49: 30S ribosomal protein S18

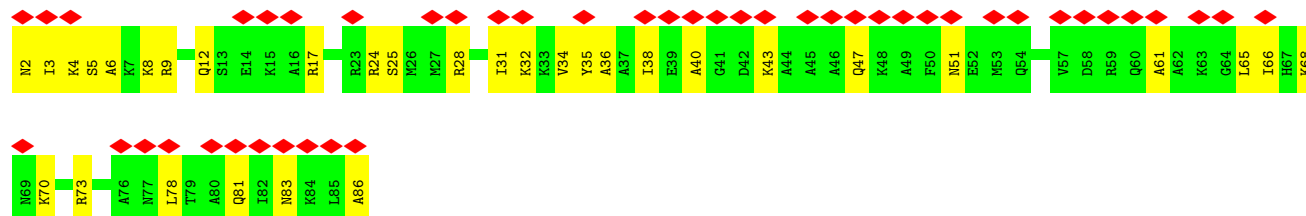


- Molecule 50: 30S ribosomal protein S19

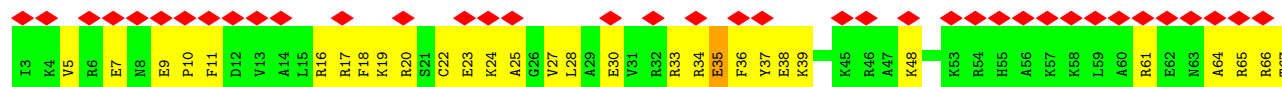




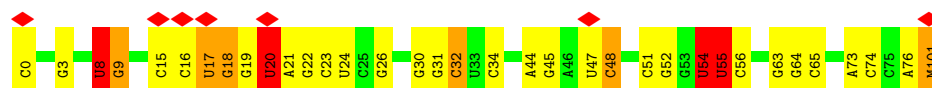
• Molecule 51: 30S ribosomal protein S20



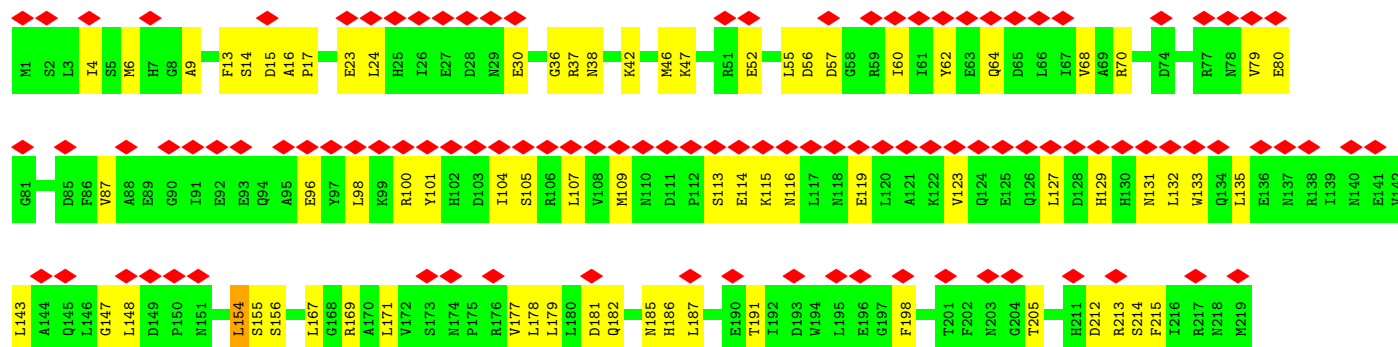
• Molecule 52: Small ribosomal subunit protein bS21

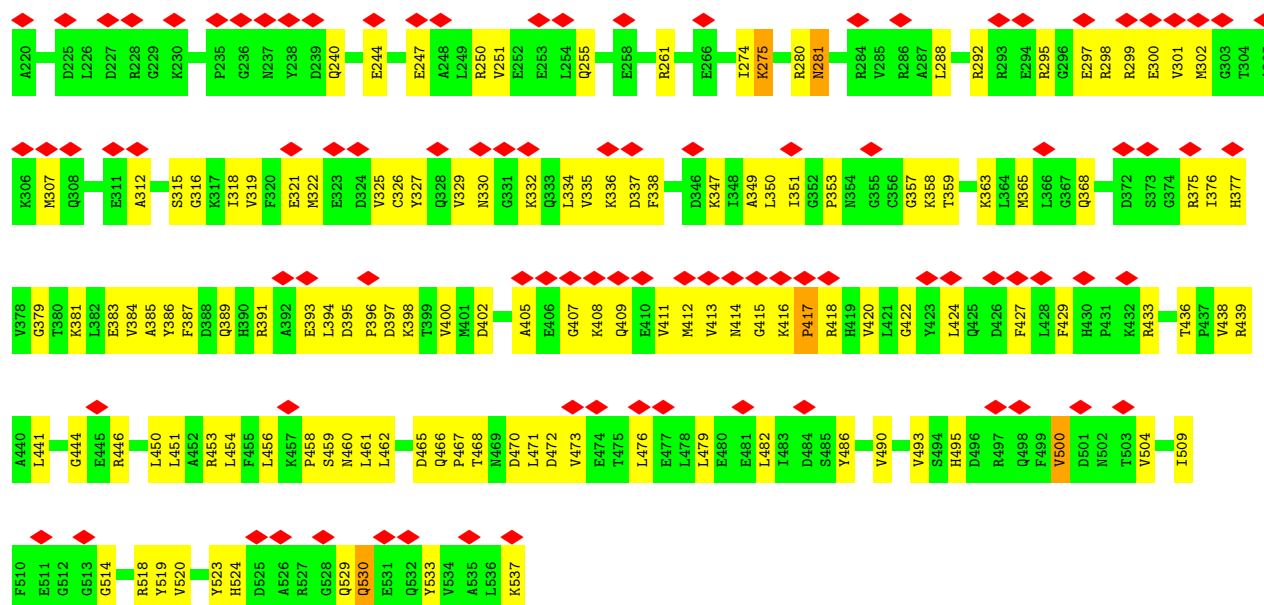


• Molecule 53: tRNA

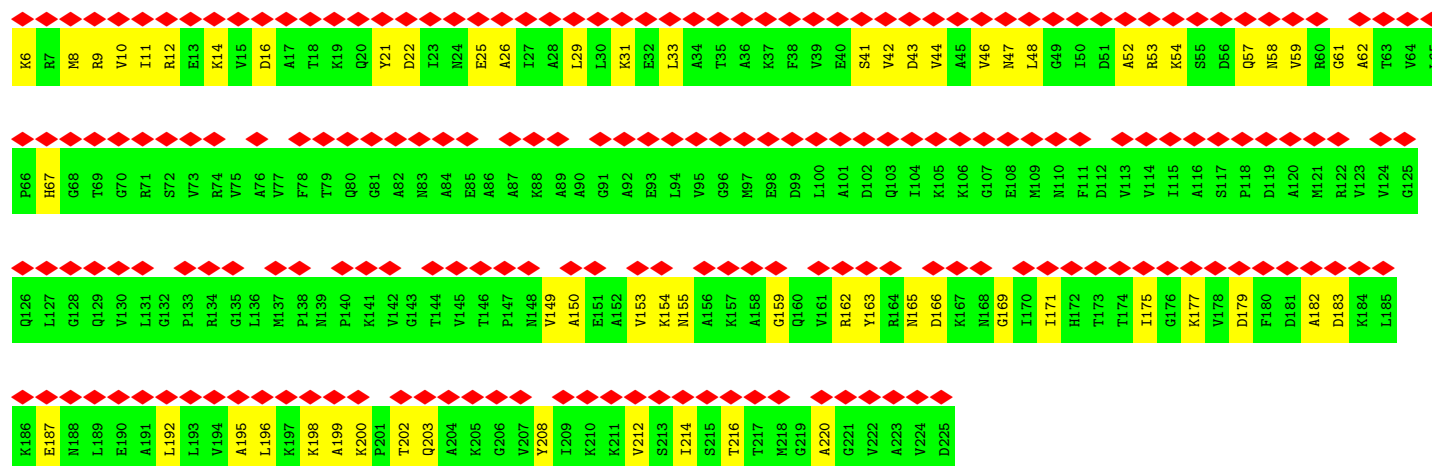
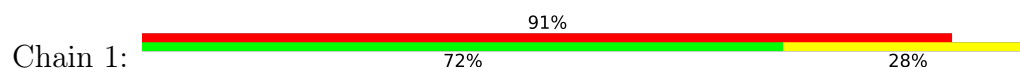


• Molecule 54: Uup

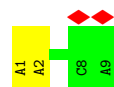
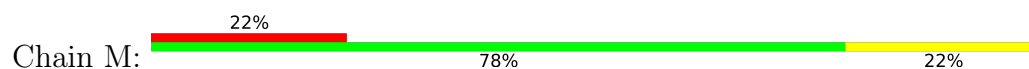




• Molecule 55: Large ribosomal subunit protein uL1



• Molecule 56: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.670	Depositor
Minimum map value	-2.176	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, 4SU, H2U, 4OC, ATP, PSU, FME, NA

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	13	0.20	0/1152	0.30	0/1551
2	14	0.22	0/947	0.40	0/1268
3	15	0.23	0/1062	0.43	0/1413
4	16	0.21	0/1093	0.41	0/1460
5	17	0.24	0/973	0.39	0/1301
6	18	0.16	0/902	0.32	0/1209
7	19	0.21	0/929	0.32	0/1242
8	2	0.24	0/2121	0.38	0/2852
9	20	0.25	0/960	0.32	0/1278
10	21	0.22	0/829	0.42	0/1107
11	22	0.23	0/864	0.35	0/1156
12	23	0.20	0/744	0.31	0/994
13	24	0.17	0/787	0.37	0/1051
14	25	0.17	0/766	0.38	0/1025
15	27	0.22	0/650	0.35	0/858
16	28	0.23	0/635	0.32	0/848
17	29	0.14	0/510	0.28	0/677
18	3	0.24	0/1586	0.38	0/2134
19	30	0.22	0/453	0.35	0/605
20	31	0.14	0/531	0.50	1/709 (0.1%)
21	32	0.22	0/450	0.37	0/599
22	33	0.20	0/416	0.32	0/554
23	34	0.24	0/380	0.40	0/498
24	35	0.23	0/513	0.30	0/676
25	36	0.19	0/303	0.35	0/397
26	4	0.20	0/1571	0.33	0/2113
27	5	0.16	0/1434	0.36	0/1926
28	6	0.13	0/1343	0.35	0/1816
29	9	0.15	0/1122	0.45	0/1515
30	R1	0.26	0/69797	0.34	0/108890
31	R2	0.19	0/2847	0.29	0/4440
32	R3	0.19	0/36782	0.33	0/57377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	sb	0.14	0/1735	0.37	0/2338
34	sc	0.16	0/1651	0.36	1/2225 (0.0%)
35	sd	0.15	0/1665	0.37	0/2227
36	se	0.19	0/1169	0.45	0/1573
37	sf	0.16	0/835	0.43	0/1128
38	sg	0.16	0/1195	0.35	0/1602
39	sh	0.16	0/989	0.36	0/1326
40	si	0.18	0/1034	0.47	0/1375
41	sj	0.16	0/796	0.41	0/1077
42	sk	0.18	0/885	0.39	0/1195
43	sl	0.17	0/969	0.44	0/1300
44	sm	0.16	0/892	0.37	0/1193
45	sn	0.21	0/817	0.50	1/1088 (0.1%)
46	so	0.15	0/722	0.26	0/964
47	sp	0.14	0/659	0.34	0/884
48	sq	0.18	0/657	0.43	0/881
49	sr	0.15	0/544	0.31	0/731
50	ss	0.15	0/652	0.38	0/877
51	st	0.14	0/671	0.35	0/888
52	su	0.20	0/550	0.62	0/728
53	T	0.23	0/1716	0.30	0/2672
54	U	0.19	0/4363	0.41	2/5884 (0.0%)
55	1	0.12	0/1361	0.41	0/1796
56	M	0.17	0/219	0.25	0/339
All	All	0.22	0/162198	0.35	5/241830 (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
29	9	0	1
35	sd	0	1
45	sn	0	1
53	T	7	0
All	All	7	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	U	417	PRO	N-CD-CG	-7.02	92.67	103.20
34	sc	6	PRO	CA-N-CD	-6.81	102.47	112.00
45	sn	22	LYS	CB-CG-CD	6.23	125.63	111.30
54	U	417	PRO	CA-N-CD	-5.90	103.73	112.00
20	31	5	ILE	N-CA-C	-5.54	107.73	113.10

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C2',C3'
53	T	20	H2U	C2',C1'
53	T	32	4OC	C2'
53	T	54	5MU	C4'
53	T	55	PSU	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	9	8	LYS	Peptide
35	sd	27	ILE	Peptide
45	sn	86	ALA	Peptide

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	13	1129	0	1162	15	0
2	14	938	0	1012	12	0
3	15	1053	0	1129	28	0
4	16	1074	0	1157	26	0
5	17	960	0	1000	30	0
6	18	892	0	923	24	0
7	19	917	0	965	23	0
8	2	2082	0	2157	47	0
9	20	947	0	1022	14	0
10	21	816	0	839	18	0
11	22	857	0	922	21	0
12	23	738	0	807	15	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	24	779	0	834	22	0
14	25	753	0	780	15	0
15	27	642	0	665	15	0
16	28	625	0	655	13	0
17	29	509	0	543	9	0
18	3	1565	0	1616	35	0
19	30	449	0	491	11	0
20	31	522	0	524	18	0
21	32	444	0	461	16	0
22	33	409	0	440	10	0
23	34	377	0	418	10	0
24	35	504	0	574	15	0
25	36	302	0	343	10	0
26	4	1552	0	1619	34	0
27	5	1410	0	1447	39	0
28	6	1323	0	1374	44	0
29	9	1111	0	1148	37	0
30	R1	62318	0	31345	790	0
31	R2	2546	0	1292	43	0
32	R3	32850	0	16534	554	0
33	sb	1704	0	1732	53	0
34	sc	1624	0	1699	43	0
35	sd	1643	0	1710	52	0
36	se	1156	0	1199	30	0
37	sf	817	0	808	33	0
38	sg	1181	0	1240	25	0
39	sh	979	0	1034	26	0
40	si	1022	0	1070	52	0
41	sj	786	0	828	32	0
42	sk	869	0	878	22	0
43	sl	955	0	1019	31	0
44	sm	883	0	944	28	0
45	sn	805	0	847	49	0
46	so	714	0	737	15	0
47	sp	649	0	666	17	0
48	sq	648	0	691	20	0
49	sr	535	0	552	16	0
50	ss	637	0	665	31	0
51	st	665	0	714	32	0
52	su	544	0	579	33	0
53	T	1649	0	853	22	0
54	U	4295	0	4302	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1	1353	0	1159	44	0
56	M	195	0	99	1	0
57	15	1	0	0	0	0
57	2	1	0	0	0	0
57	20	1	0	0	0	0
57	32	1	0	0	0	0
57	R1	192	0	0	0	0
57	R3	81	0	0	0	0
58	U	62	0	24	4	0
59	U	2	0	0	0	0
All	All	150042	0	102247	2525	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 10.

The worst 5 of 2525 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)
30:R1:156:A:H2	30:R1:169:G:N1	1.28	1.26
30:R1:156:A:C2	30:R1:169:G:N1	2.03	1.24
32:R3:359:G:HO2'	32:R3:360:G:H8	1.03	0.97
30:R1:947:A:HO2'	30:R1:984:A:H2	1.09	0.92
30:R1:2073:C:H5	30:R1:2436:G:H1	1.20	0.89

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	13	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
2	14	120/122 (98%)	111 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	15	142/144 (99%)	126 (89%)	16 (11%)	0	100	100
4	16	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
5	17	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
6	18	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
7	19	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
8	2	269/271 (99%)	247 (92%)	22 (8%)	0	100	100
9	20	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
10	21	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
11	22	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
12	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
13	24	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	12	41
14	25	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
15	27	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
16	28	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
17	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	3	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
19	30	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
20	31	64/66 (97%)	52 (81%)	12 (19%)	0	100	100
21	32	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
22	33	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
23	34	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	23
24	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
26	4	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
27	5	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
28	6	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
29	9	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
33	sb	216/218 (99%)	193 (89%)	22 (10%)	1 (0%)	24	57
34	sc	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
35	sd	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
36	se	155/157 (99%)	129 (83%)	25 (16%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	sf	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
38	sg	149/151 (99%)	133 (89%)	16 (11%)	0	100	100
39	sh	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
40	si	125/127 (98%)	106 (85%)	19 (15%)	0	100	100
41	sj	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
42	sk	114/116 (98%)	102 (90%)	12 (10%)	0	100	100
43	sl	121/123 (98%)	92 (76%)	29 (24%)	0	100	100
44	sm	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
45	sn	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
46	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
47	sp	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
48	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
49	sr	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
50	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
51	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
52	su	63/65 (97%)	45 (71%)	17 (27%)	1 (2%)	7	30
54	U	535/537 (100%)	484 (90%)	50 (9%)	1 (0%)	43	73
55	1	218/220 (99%)	189 (87%)	29 (13%)	0	100	100
All	All	6342/6444 (98%)	5707 (90%)	629 (10%)	6 (0%)	49	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	24	88	ASP
52	su	35	GLU
54	U	275	LYS
36	se	122	VAL
33	sb	18	GLN

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	13	116/116 (100%)	115 (99%)	1 (1%)	70	80
2	14	103/103 (100%)	102 (99%)	1 (1%)	68	79
3	15	103/103 (100%)	103 (100%)	0	100	100
4	16	109/109 (100%)	109 (100%)	0	100	100
5	17	100/100 (100%)	100 (100%)	0	100	100
6	18	86/86 (100%)	85 (99%)	1 (1%)	63	78
7	19	99/99 (100%)	99 (100%)	0	100	100
8	2	216/216 (100%)	216 (100%)	0	100	100
9	20	89/89 (100%)	89 (100%)	0	100	100
10	21	84/84 (100%)	84 (100%)	0	100	100
11	22	93/93 (100%)	93 (100%)	0	100	100
12	23	80/80 (100%)	80 (100%)	0	100	100
13	24	83/83 (100%)	82 (99%)	1 (1%)	63	78
14	25	78/78 (100%)	78 (100%)	0	100	100
15	27	63/63 (100%)	63 (100%)	0	100	100
16	28	67/67 (100%)	67 (100%)	0	100	100
17	29	55/55 (100%)	55 (100%)	0	100	100
18	3	164/164 (100%)	162 (99%)	2 (1%)	63	78
19	30	48/48 (100%)	48 (100%)	0	100	100
20	31	59/59 (100%)	58 (98%)	1 (2%)	53	74
21	32	47/47 (100%)	47 (100%)	0	100	100
22	33	45/45 (100%)	44 (98%)	1 (2%)	45	71
23	34	38/38 (100%)	38 (100%)	0	100	100
24	35	51/51 (100%)	51 (100%)	0	100	100
25	36	34/34 (100%)	34 (100%)	0	100	100
26	4	165/165 (100%)	165 (100%)	0	100	100
27	5	148/148 (100%)	145 (98%)	3 (2%)	48	72
28	6	137/137 (100%)	135 (98%)	2 (2%)	57	75
29	9	114/114 (100%)	112 (98%)	2 (2%)	51	73
33	sb	180/180 (100%)	179 (99%)	1 (1%)	78	83
34	sc	170/170 (100%)	169 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	sd	172/172 (100%)	172 (100%)	0	100	100
36	se	119/119 (100%)	118 (99%)	1 (1%)	73	81
37	sf	87/87 (100%)	83 (95%)	4 (5%)	24	55
38	sg	124/124 (100%)	123 (99%)	1 (1%)	73	81
39	sh	104/104 (100%)	103 (99%)	1 (1%)	68	79
40	si	105/105 (100%)	104 (99%)	1 (1%)	68	79
41	sj	86/86 (100%)	86 (100%)	0	100	100
42	sk	89/89 (100%)	88 (99%)	1 (1%)	65	78
43	sl	103/103 (100%)	103 (100%)	0	100	100
44	sm	92/92 (100%)	92 (100%)	0	100	100
45	sn	83/83 (100%)	83 (100%)	0	100	100
46	so	76/76 (100%)	76 (100%)	0	100	100
47	sp	65/65 (100%)	65 (100%)	0	100	100
48	sq	74/74 (100%)	73 (99%)	1 (1%)	59	76
49	sr	56/56 (100%)	56 (100%)	0	100	100
50	ss	70/70 (100%)	69 (99%)	1 (1%)	59	76
51	st	65/65 (100%)	65 (100%)	0	100	100
52	su	55/55 (100%)	55 (100%)	0	100	100
54	U	462/462 (100%)	457 (99%)	5 (1%)	65	78
55	1	106/171 (62%)	105 (99%)	1 (1%)	70	80
All	All	5217/5282 (99%)	5183 (99%)	34 (1%)	73	82

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	U	154	LEU
54	U	281	ASN
54	U	530	GLN
28	6	170	THR
28	6	55	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
28	6	142	GLN
54	U	308	GLN
35	sd	119	HIS
54	U	110	ASN
54	U	495	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	R1	2902/2903 (99%)	621 (21%)	13 (0%)
31	R2	118/119 (99%)	22 (18%)	1 (0%)
32	R3	1529/1531 (99%)	433 (28%)	24 (1%)
53	T	76/78 (97%)	18 (23%)	3 (3%)
56	M	8/9 (88%)	0	0
All	All	4633/4640 (99%)	1094 (23%)	41 (0%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	R1	3	U
30	R1	4	U
30	R1	10	A
30	R1	12	U
30	R1	14	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	R3	753	A
32	R3	1270	G
32	R3	837	U
32	R3	1124	G
32	R3	1305	G

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

6 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
53	PSU	T	55	53	18,21,22	2.20	9 (50%)	21,30,33	1.87	4 (19%)
53	4SU	T	8	53	18,21,22	3.99	7 (38%)	25,30,33	2.34	6 (24%)
53	4OC	T	32	53	20,23,24	2.38	4 (20%)	25,32,35	2.02	5 (20%)
53	5MU	T	54	53	19,22,23	2.72	8 (42%)	27,32,35	2.26	8 (29%)
53	FME	T	101	53	8,9,10	0.95	0	8,9,11	1.20	1 (12%)
53	H2U	T	20	53	18,21,22	4.32	5 (27%)	19,30,33	4.14	6 (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
53	PSU	T	55	53	1/1/5/5	1/7/25/26	0/2/2/2
53	4SU	T	8	53	2/2/5/5	3/7/25/26	0/2/2/2
53	4OC	T	32	53	1/1/5/6	4/9/29/30	0/2/2/2
53	5MU	T	54	53	1/1/5/5	3/7/25/26	0/2/2/2
53	FME	T	101	53	-	2/7/9/11	-
53	H2U	T	20	53	2/2/8/9	5/7/38/39	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	8	4SU	O2-C2	11.92	1.44	1.23
53	T	20	H2U	O4-C4	10.47	1.44	1.23
53	T	8	4SU	C4-S4	9.54	1.85	1.68
53	T	54	5MU	O4-C4	-9.24	1.06	1.23
53	T	20	H2U	C2-N1	9.14	1.48	1.35

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	T	20	H2U	O2-C2-N1	-11.63	109.12	123.10
53	T	20	H2U	O4-C4-N3	-7.68	108.46	120.30
53	T	8	4SU	C4-N3-C2	-6.65	120.94	127.31
53	T	20	H2U	O4-C4-C5	-6.62	108.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	T	20	H2U	O2-C2-N3	-6.23	110.00	121.49

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C2'
53	T	8	4SU	C3'
53	T	20	H2U	C2'
53	T	20	H2U	C1'
53	T	32	4OC	C2'

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	T	20	H2U	O4'-C4'-C5'-O5'
53	T	20	H2U	O4'-C1'-N1-C6
53	T	20	H2U	C2'-C1'-N1-C2
53	T	54	5MU	C4'-C5'-O5'-P
53	T	101	FME	CB-CA-N-CN

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	T	55	PSU	2	0
53	T	8	4SU	1	0
53	T	32	4OC	2	0
53	T	54	5MU	3	0
53	T	101	FME	1	0
53	T	20	H2U	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 281 ligands modelled in this entry, 279 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	ATP	U	602	59	32,33,33	0.39	0	48,52,52	0.32	0
58	ATP	U	601	59	32,33,33	0.40	0	48,52,52	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ATP	U	602	59	-	6/22/38/38	0/3/3/3
58	ATP	U	601	59	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	U	602	ATP	C5'-O5'-PA-O2A
58	U	602	ATP	O4'-C4'-C5'-O5'
58	U	602	ATP	C3'-C4'-C5'-O5'
58	U	602	ATP	C5'-O5'-PA-O1A
58	U	602	ATP	C5'-O5'-PA-O3A

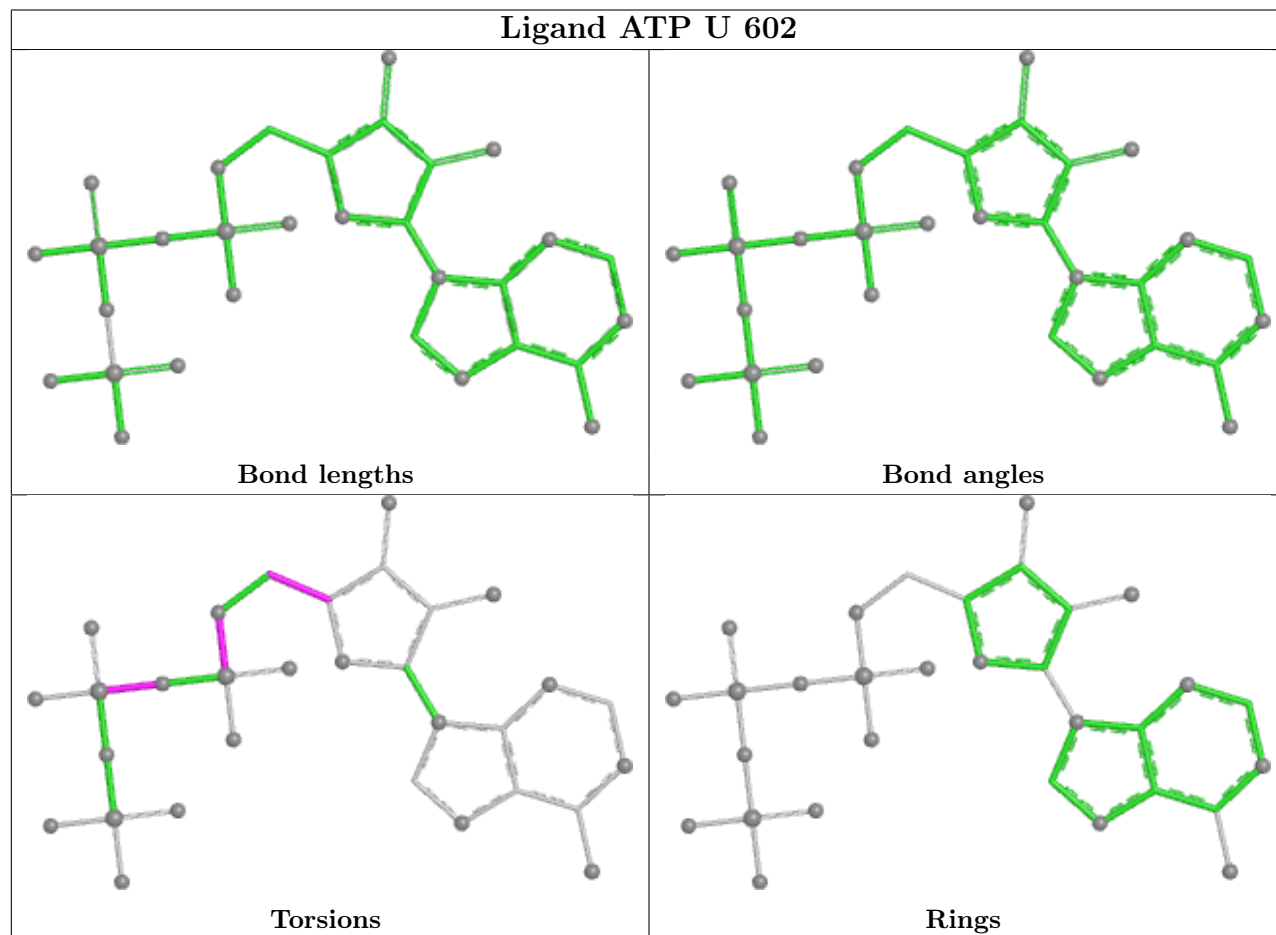
There are no ring outliers.

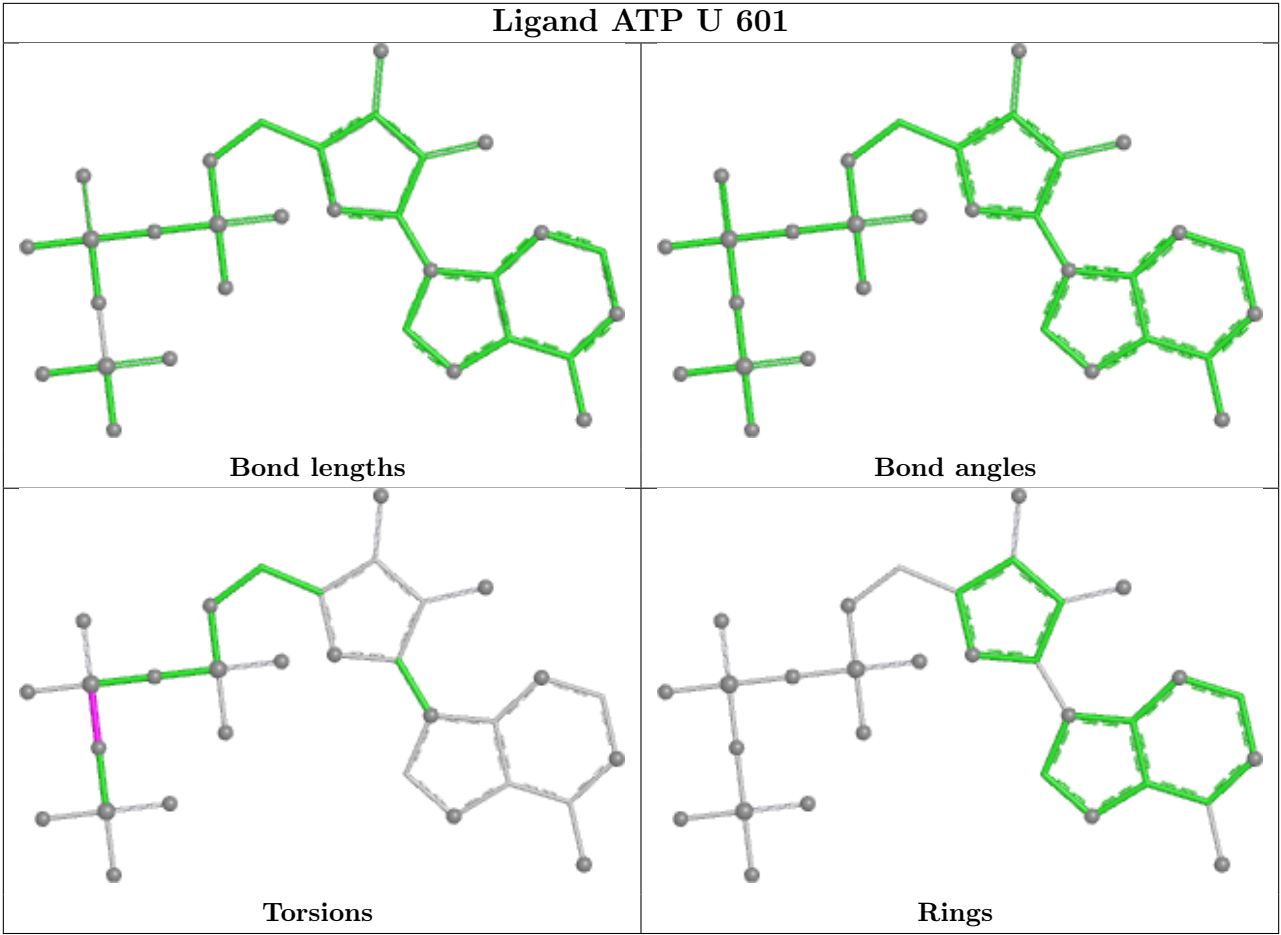
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	602	ATP	2	0
58	U	601	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	210:C	O3'	211:G	P	7.40
1	R3	460:A	O3'	461:A	P	4.00

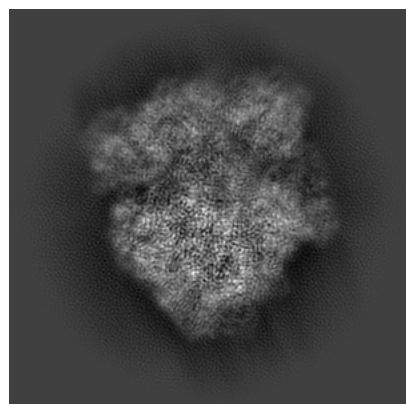
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29399. These allow visual inspection of the internal detail of the map and identification of artifacts.

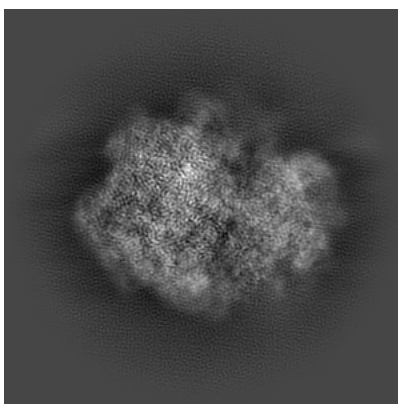
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

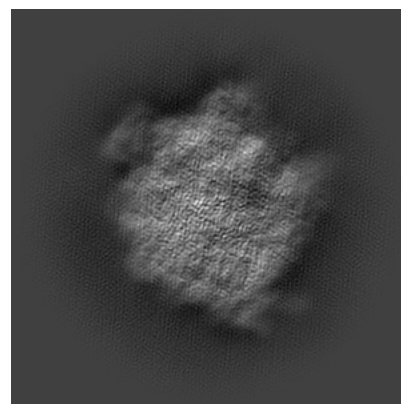
6.1.1 Primary map



X

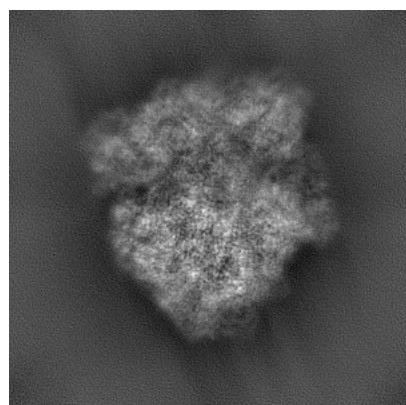


Y

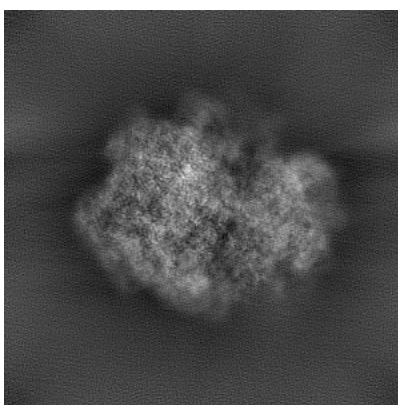


Z

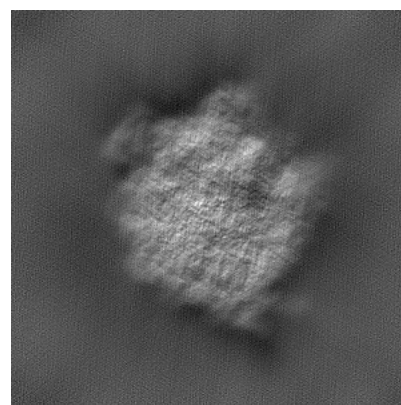
6.1.2 Raw map



X



Y

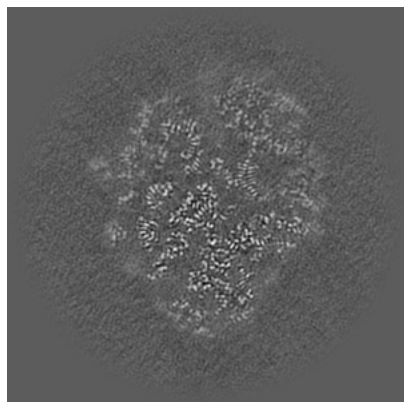


Z

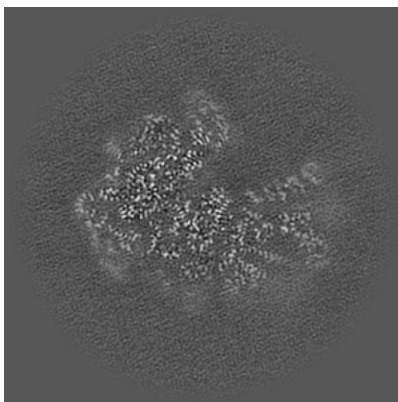
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

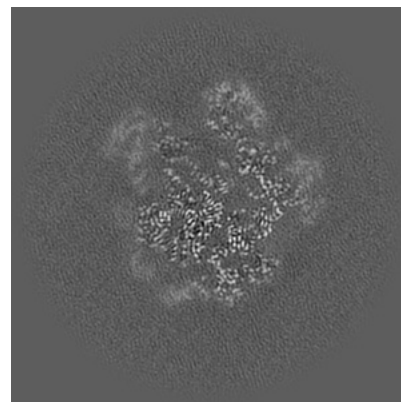
6.2.1 Primary map



X Index: 200

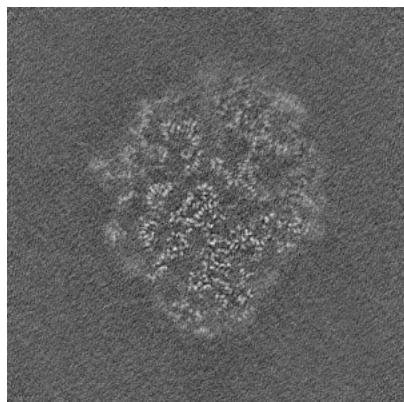


Y Index: 200

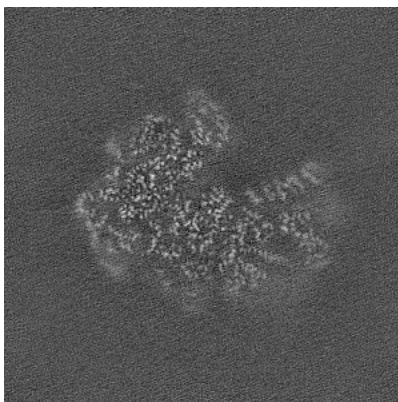


Z Index: 200

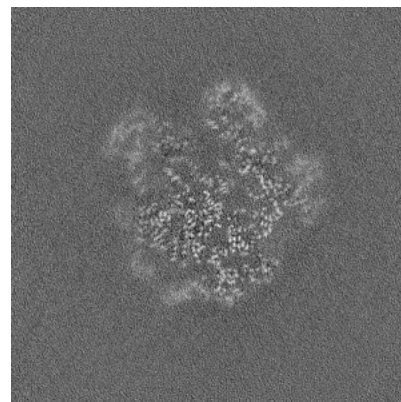
6.2.2 Raw map



X Index: 200



Y Index: 200

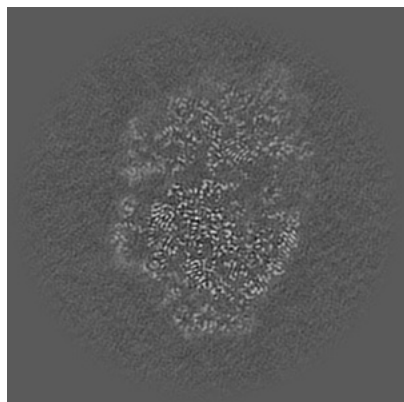


Z Index: 200

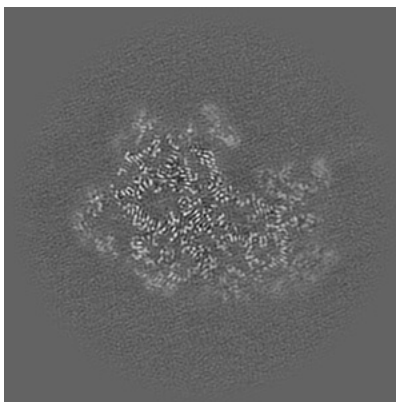
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

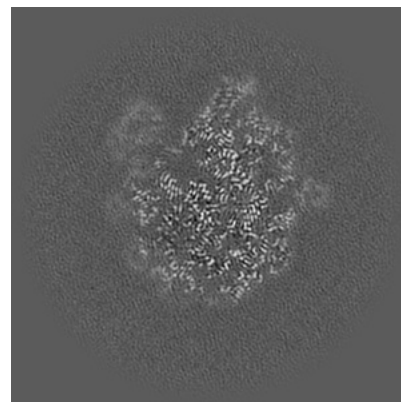
6.3.1 Primary map



X Index: 188

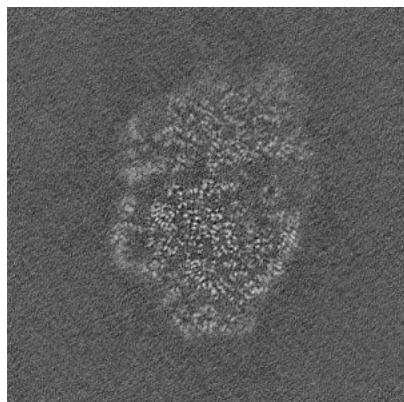


Y Index: 184

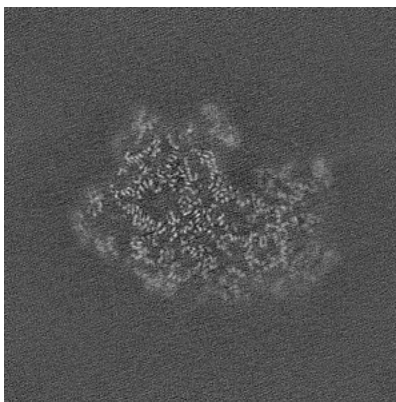


Z Index: 184

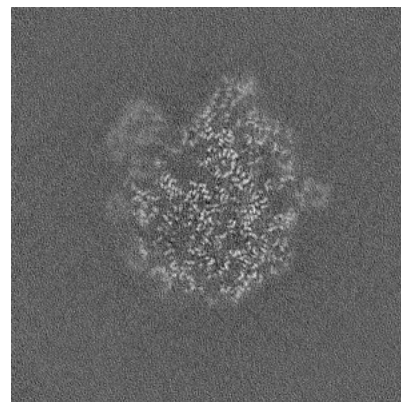
6.3.2 Raw map



X Index: 188



Y Index: 184

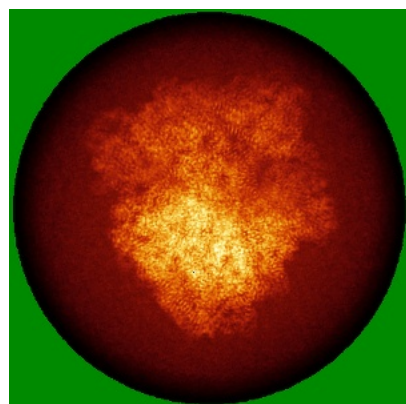


Z Index: 184

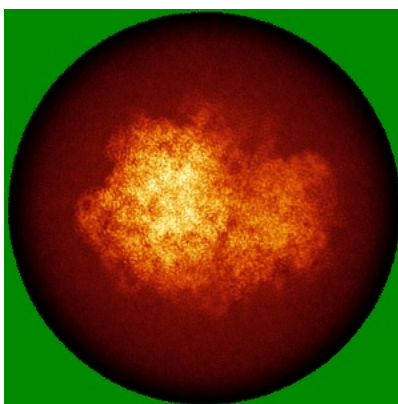
The images above show the largest variance slices of the map in three orthogonal directions.

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

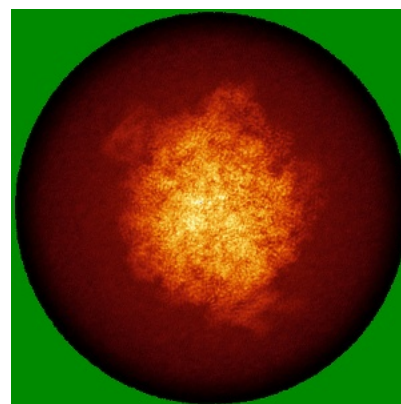
6.4.1 Primary map



X

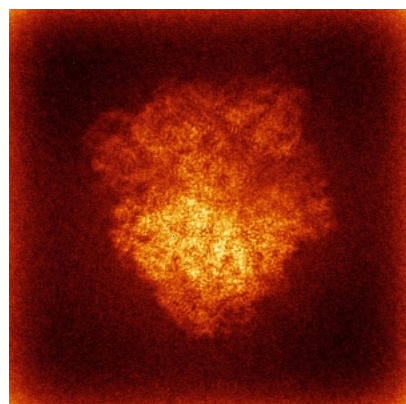


Y

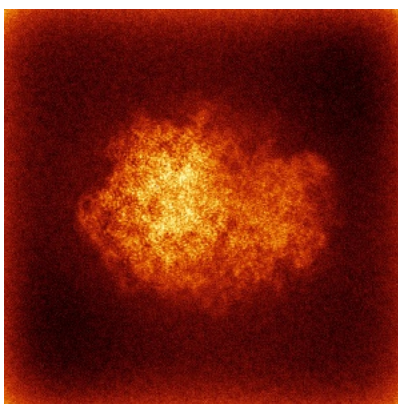


Z

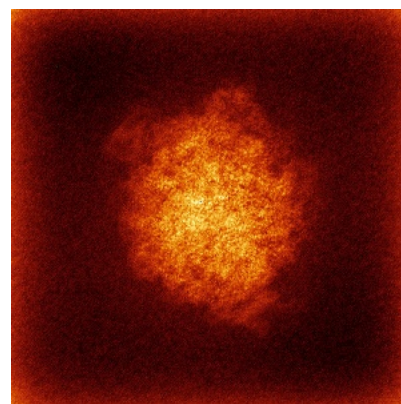
6.4.2 Raw map



X



Y

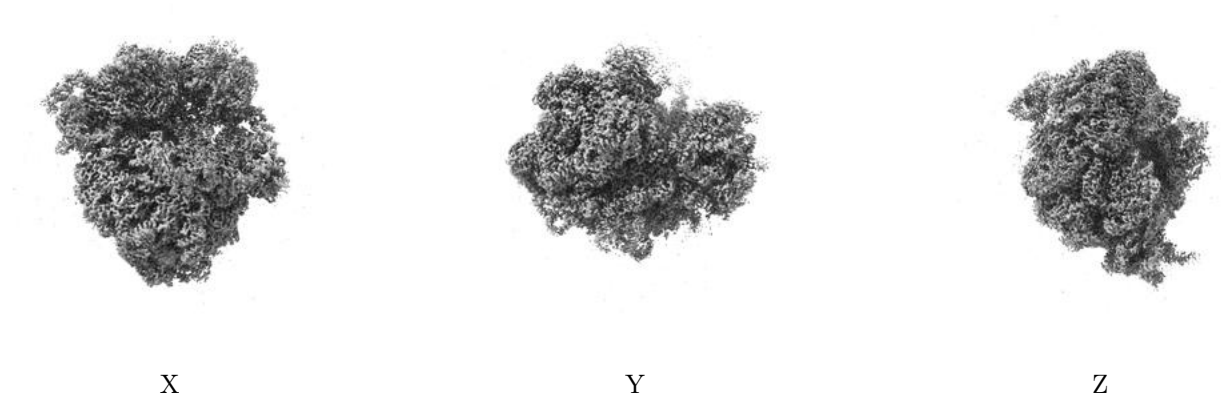


Z

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.

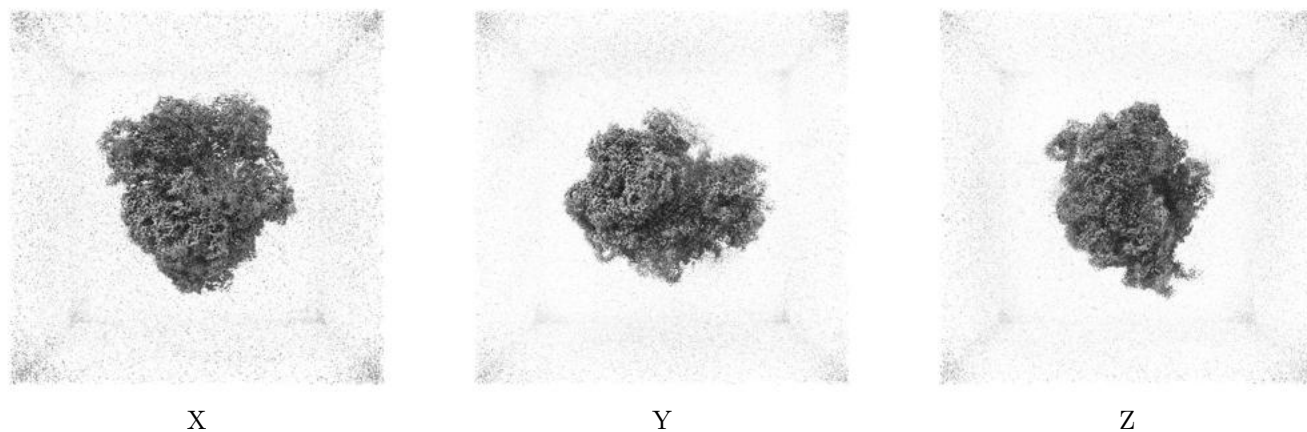
6.5 Orthogonal surface views [i](#)

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.

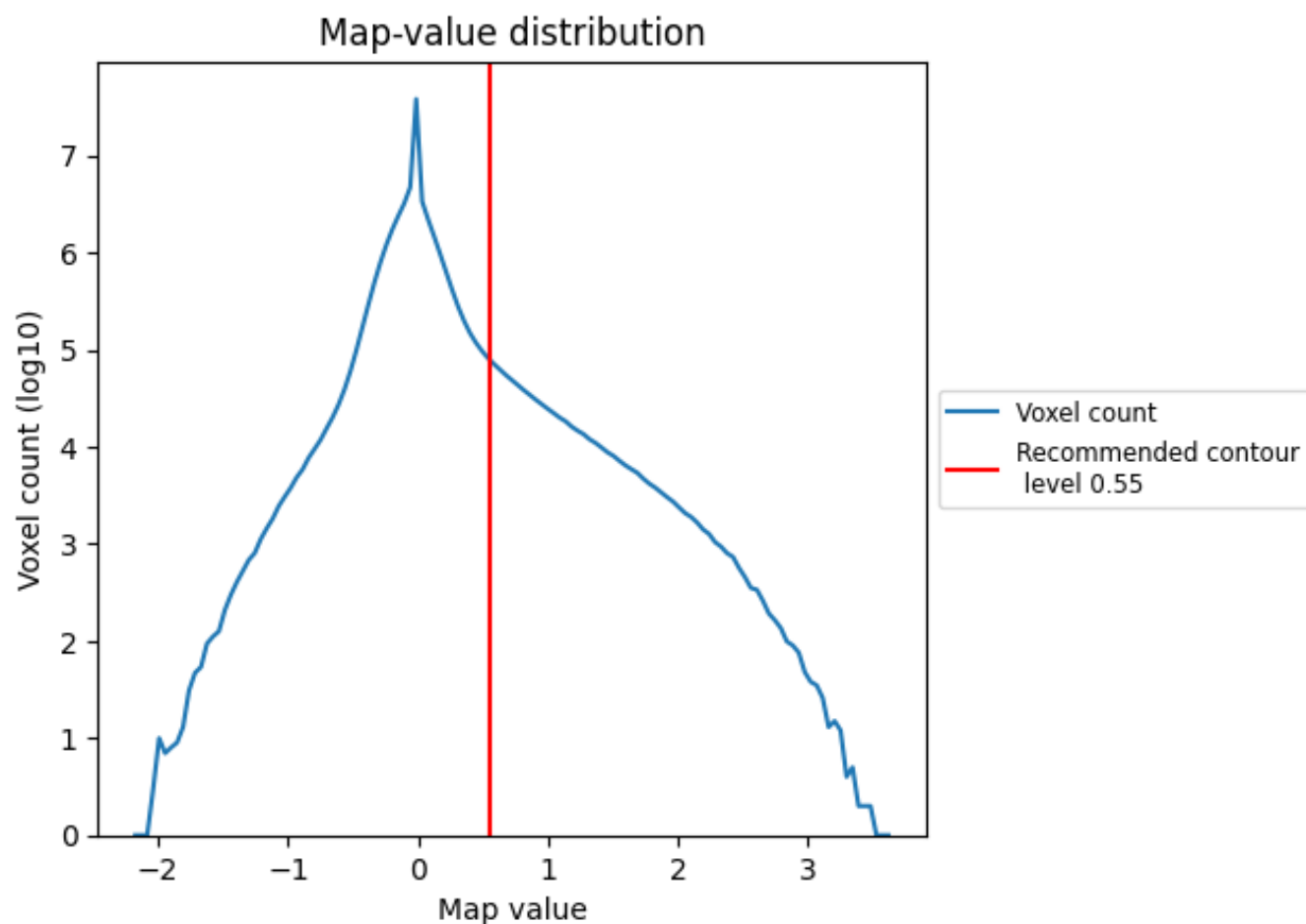
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

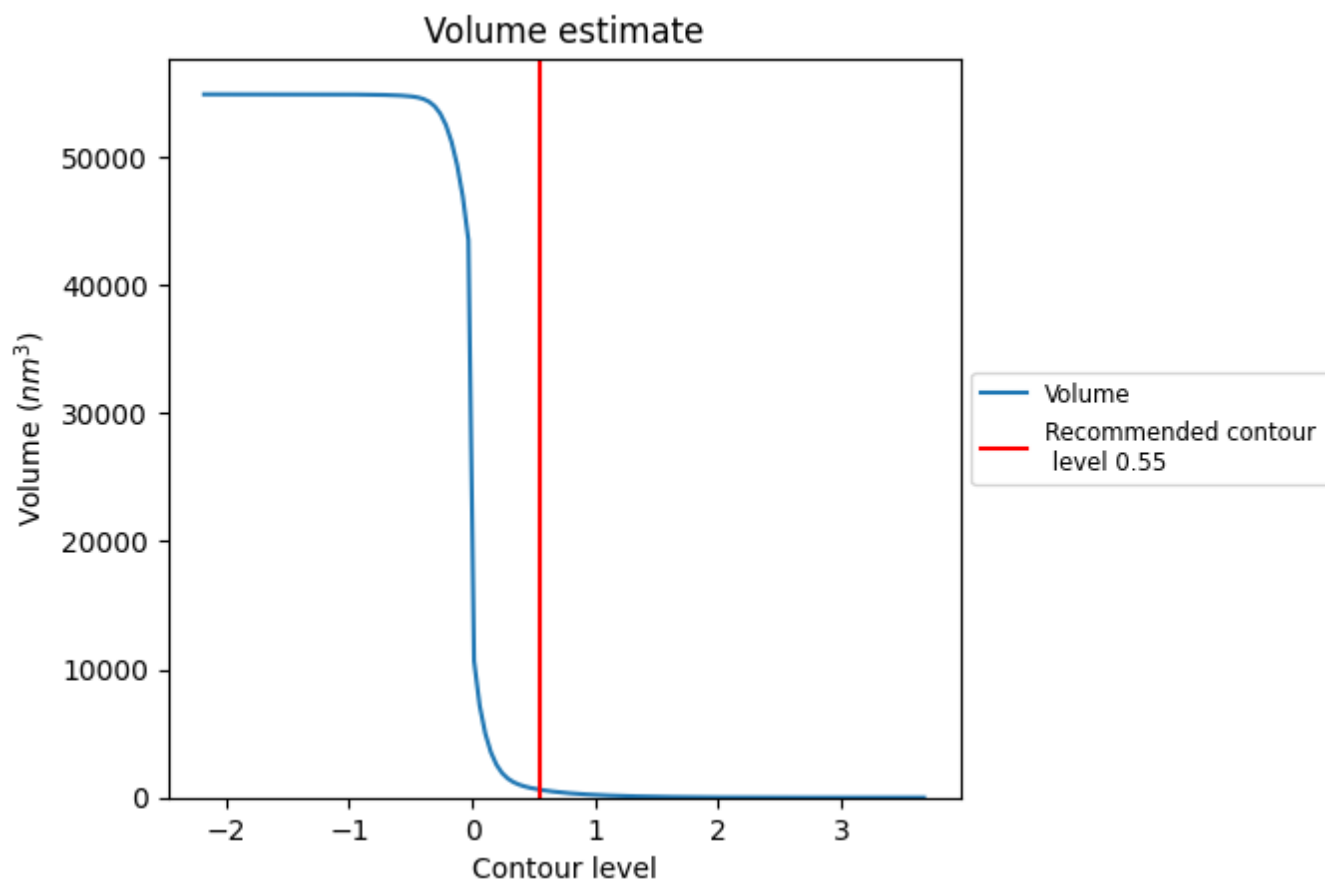
This section contains the results of statistical analysis of the map.

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.

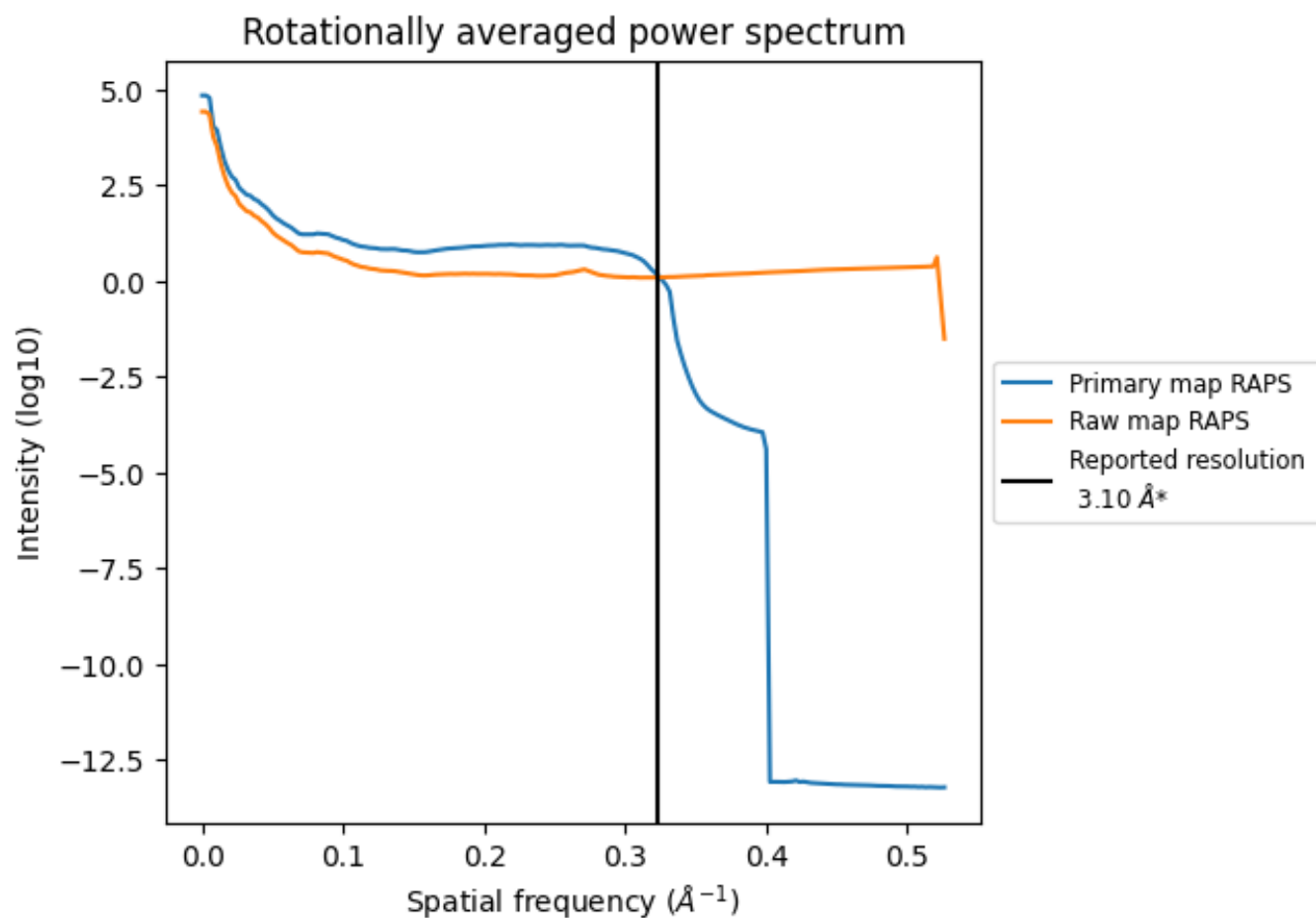
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 616 nm³; this corresponds to an approximate mass of 556 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 ⓘ

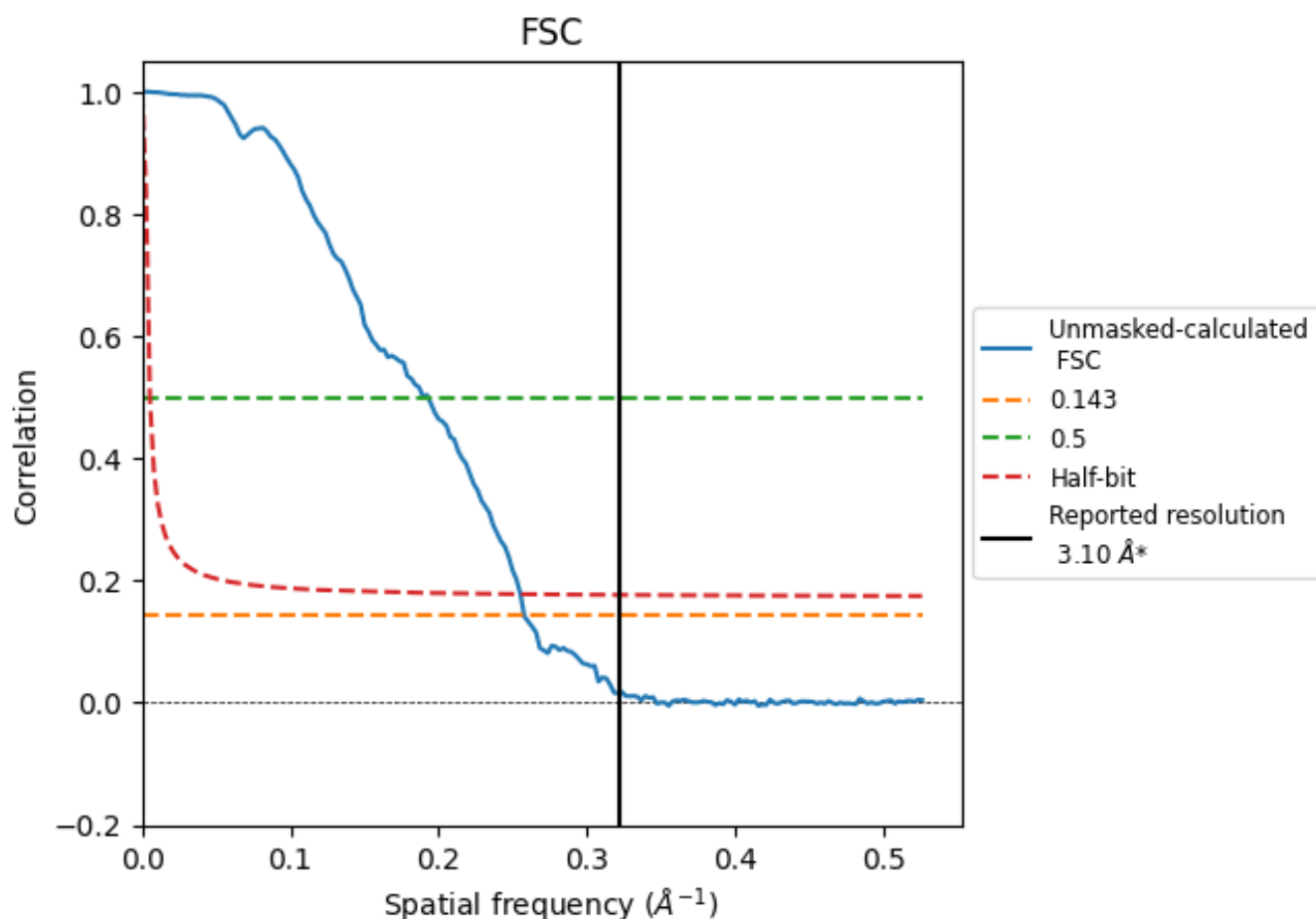


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

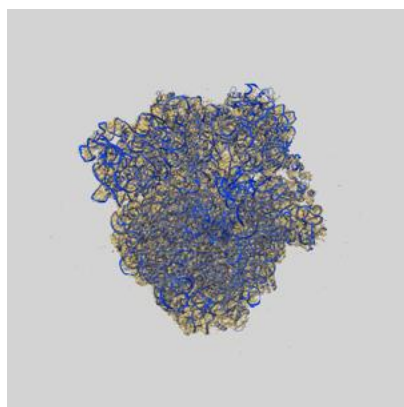
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	5.19	3.92

*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 3.88 differs from the reported value 3.1 by more than 10 %

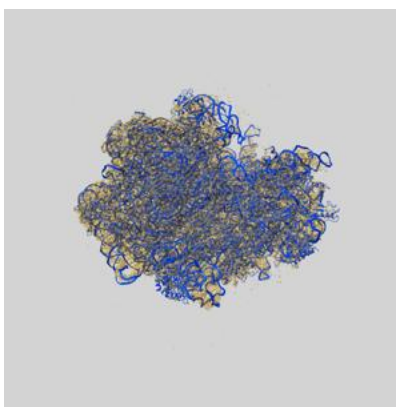
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29399 and PDB model 9NLJ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

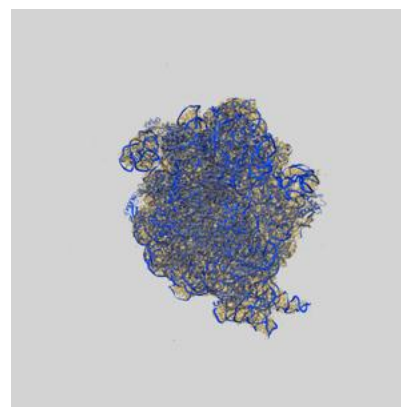
9.1 Map-model overlay [i](#)



X



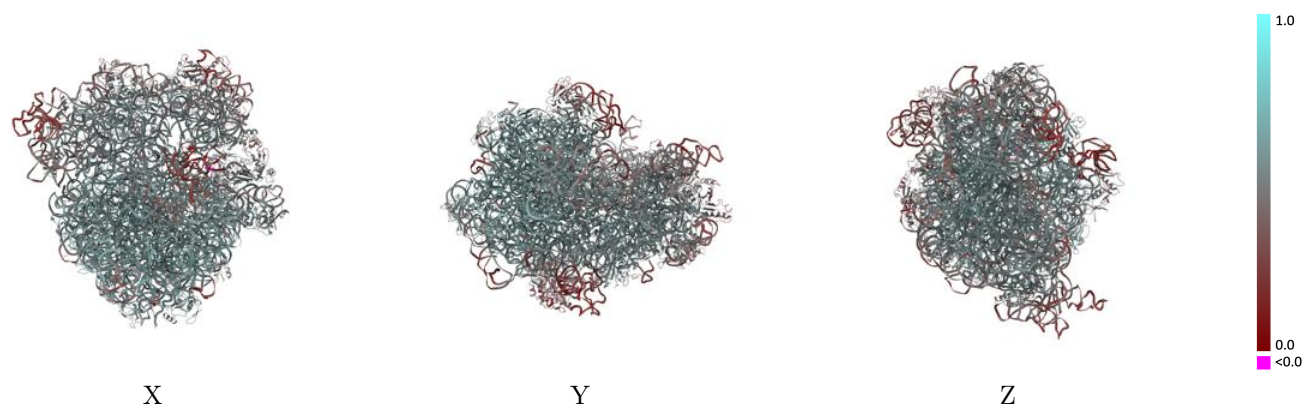
Y



Z

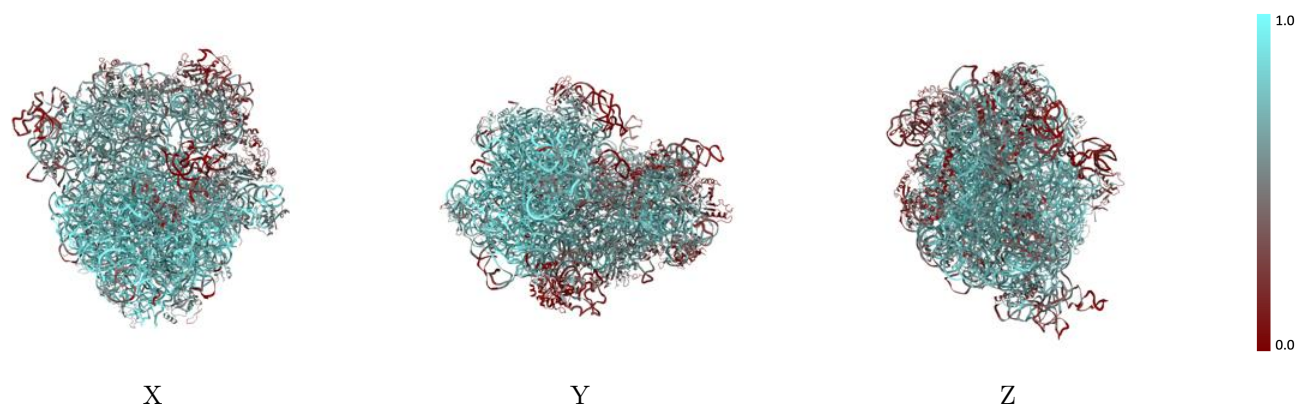
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



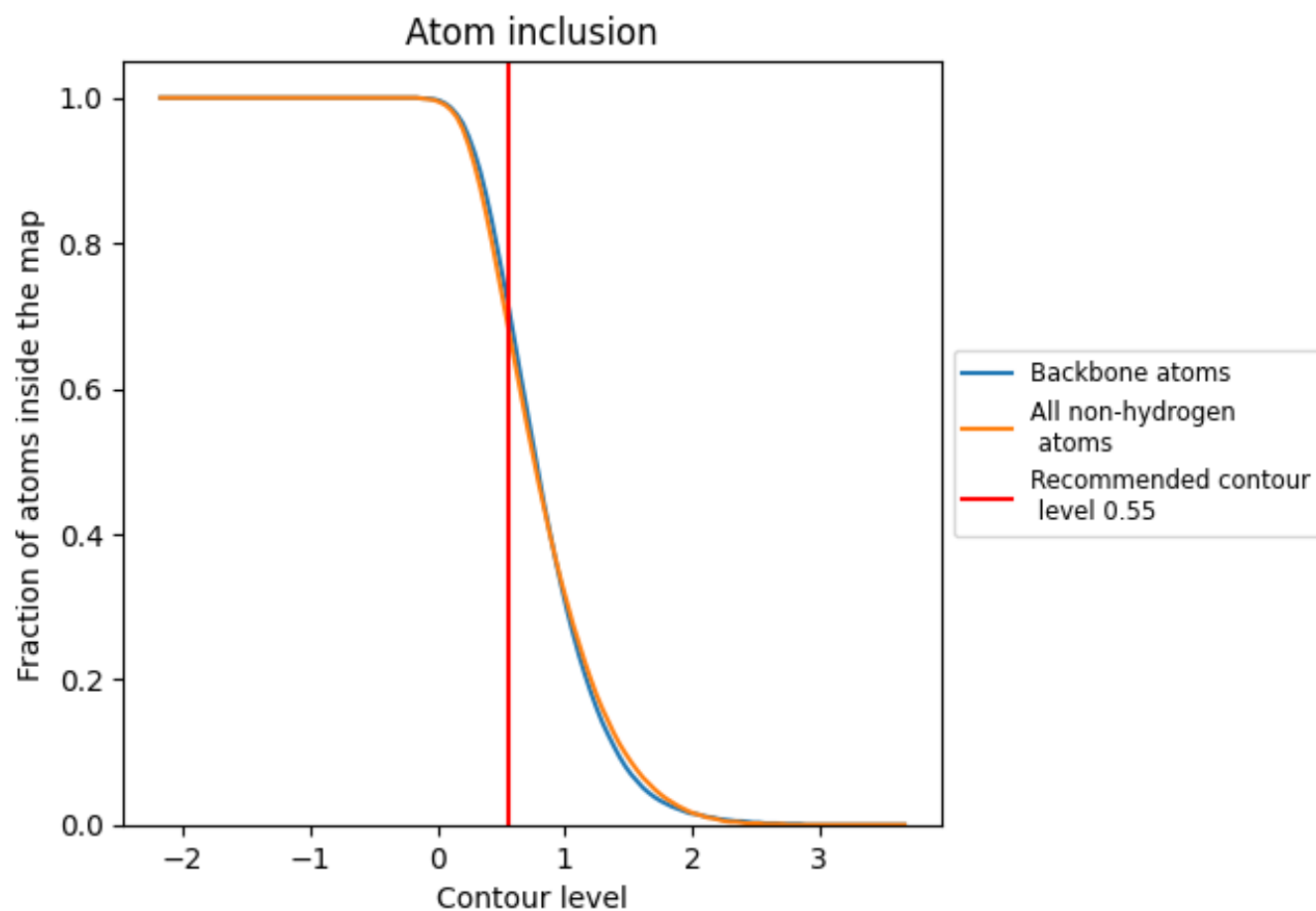
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 69% 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	 0.6900	 0.5200
1	 0.1170	 0.3350
13	 0.7500	 0.5890
14	 0.7150	 0.5820
15	 0.7360	 0.5620
16	 0.7170	 0.5740
17	 0.8160	 0.5810
18	 0.5540	 0.5190
19	 0.6900	 0.5700
2	 0.7360	 0.5870
20	 0.7940	 0.5910
21	 0.6670	 0.5520
22	 0.7200	 0.5710
23	 0.6190	 0.5480
24	 0.5410	 0.5200
25	 0.5980	 0.5270
27	 0.7430	 0.5800
28	 0.6960	 0.5740
29	 0.5760	 0.5130
3	 0.7740	 0.5800
30	 0.7390	 0.5700
31	 0.1740	 0.3730
32	 0.7370	 0.5750
33	 0.7080	 0.5760
34	 0.8030	 0.5970
35	 0.8310	 0.6080
36	 0.6540	 0.5610
4	 0.6520	 0.5520
5	 0.4030	 0.4830
6	 0.2940	 0.4200
9	 0.1110	 0.3510
M	 0.6560	 0.5380
R1	 0.8100	 0.5400
R2	 0.7600	 0.4990
R3	 0.6950	 0.4920



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Chain	Atom inclusion	Q-score
T	 0.7420	 0.5500
U	 0.4790	 0.5230
sb	 0.2780	 0.4310
sc	 0.4320	 0.5000
sd	 0.3490	 0.4730
se	 0.5690	 0.5190
sf	 0.4850	 0.4790
sg	 0.4850	 0.5090
sh	 0.5820	 0.5330
si	 0.4310	 0.4760
sj	 0.2820	 0.4450
sk	 0.5850	 0.5470
sl	 0.4160	 0.5130
sm	 0.3840	 0.4790
sn	 0.3760	 0.4700
so	 0.5640	 0.5170
sp	 0.4510	 0.4960
sq	 0.4640	 0.4960
sr	 0.5040	 0.5020
ss	 0.2880	 0.4460
st	 0.4080	 0.4750
su	 0.3480	 0.4410