wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 09:01 am GMT

PDB ID	:	5ADY
EMDB ID	:	EMD-3133
Title	:	Cryo-EM structures of the 50S ribosome subunit bound with HflX
Authors	:	Zhang, Y.; Mandava, C.S.; Cao, W.; Li, X.; Zhang, D.; Li, N.; Zhang, Y.; Zhang, X.; Qin, Y.; Mi, K.; Lei, J.; Sanyal, S.; Gao, N.
Deposited on	:	2015-08-25
Resolution	:	4.50 Å(reported)
Based on initial model	:	3FIK

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

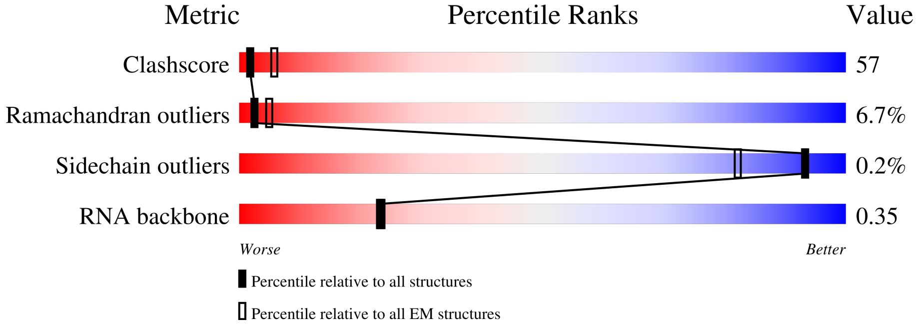
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

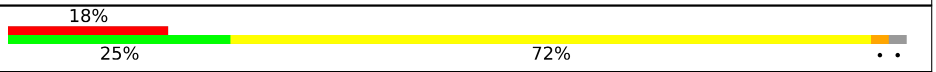
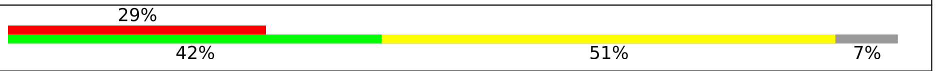
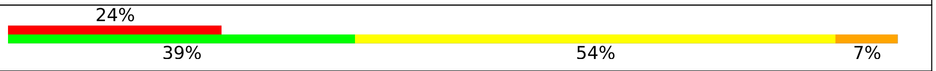
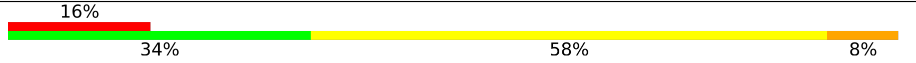
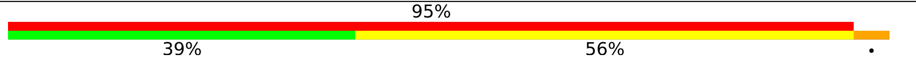
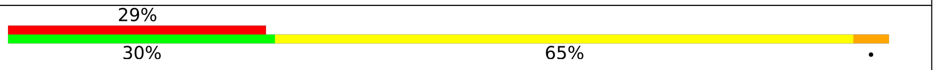
The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	234	
7	6	426	

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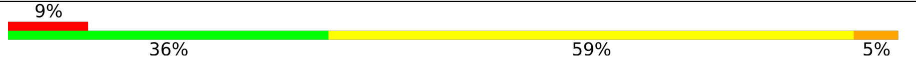
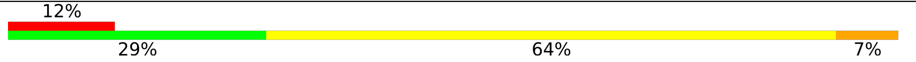
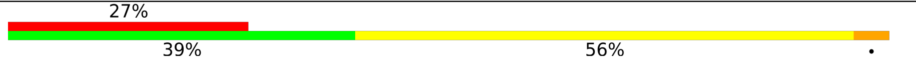
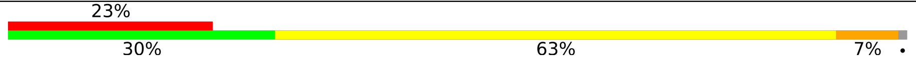
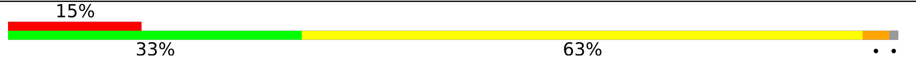
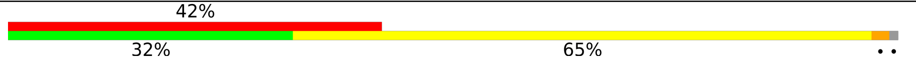
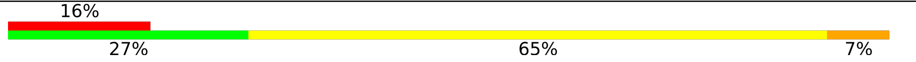
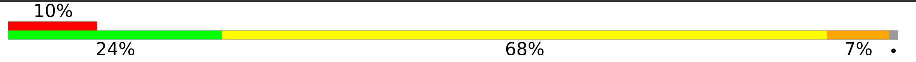
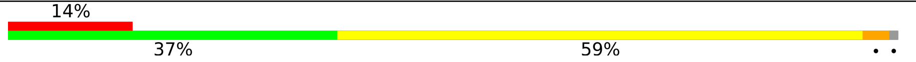
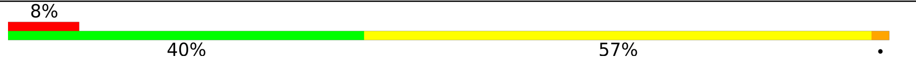
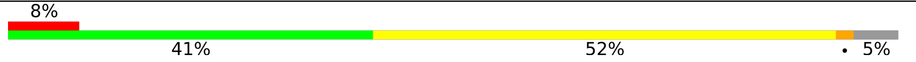
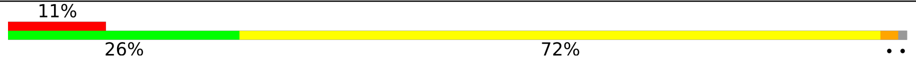
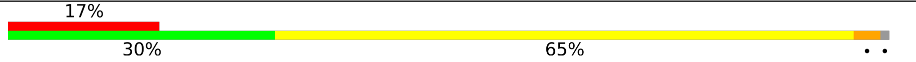
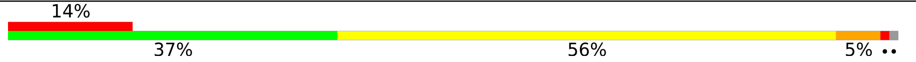
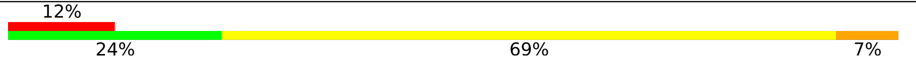
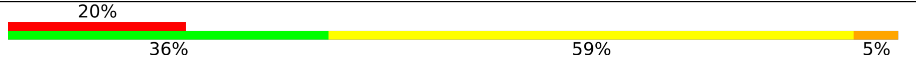
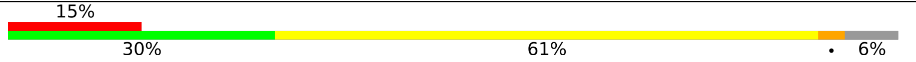
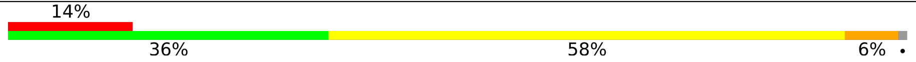
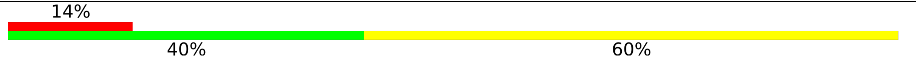
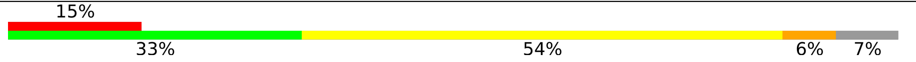
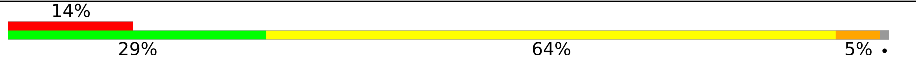
Mol	Chain	Length	Quality of chain
8	7	165	
9	A	120	
10	B	2903	
11	C	273	
12	D	209	
13	E	201	
14	F	179	
15	G	177	
16	H	149	
17	I	142	
18	J	142	
19	K	123	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	115	
25	Q	118	
26	R	103	
27	S	110	
28	T	100	
29	U	104	
30	V	94	
31	W	85	
32	X	78	

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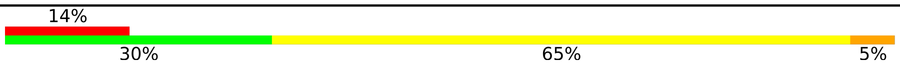
Mol	Chain	Length	Quality of chain
33	Y	63	
34	Z	59	

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
35	GNP	6	527	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 97364 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	51	410	263	76	71	0	1

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	234	1733	1081	315	330	7	0	0

- Molecule 7 is a protein called GTPASE HFLX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	426	Total 3403	C 2129	N 624	O 641	S 9	0	0

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	164	Total 1231	C 775	N 220	O 229	S 7	0	1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	117	Total 2504	C 1116	N 459	O 813	P 116	0	0

- Molecule 10 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	2903	Total 62317	C 27801	N 11467	O 20147	P 2902	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	C	G	conflict	GB 731469900
B	542	C	U	conflict	GB 731469900
B	846	U	C	conflict	GB 731469900
B	1211	C	U	conflict	GB 731469900
B	1220	G	A	conflict	GB 731469900
B	1229	C	U	conflict	GB 731469900
B	1723	G	A	conflict	GB 731469900
B	1725	U	C	conflict	GB 731469900
B	1726	C	G	conflict	GB 731469900
B	1727	C	A	conflict	GB 731469900
B	1730	C	U	conflict	GB 731469900
B	1733	G	U	conflict	GB 731469900
B	1734	G	C	conflict	GB 731469900
B	1735	A	G	conflict	GB 731469900
B	2794	C	U	conflict	GB 731469900
B	2796	U	C	conflict	GB 731469900
B	2799	A	G	conflict	GB 731469900

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2802	G	A	conflict	GB 731469900

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	272	2083	1288	424	364	7	0	1

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	141	1032	651	179	196	6	0	0

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	122	931	582	180	164	5	0	1

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	143	1045	649	206	189	1	0	0

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	121	961	593	197	166	5	0	1

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	94	739	466	140	131	2	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	U	103	780	492	147	141	0	1

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	79	596	367	120	108	1	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

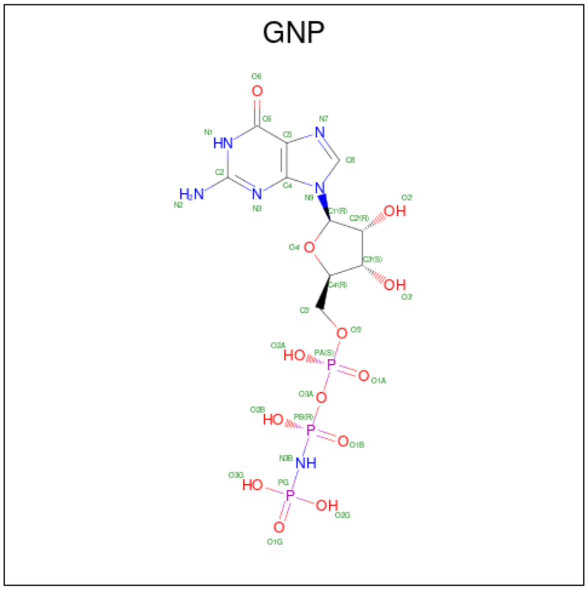
- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 35 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	6	1	32	10	6	13	3	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

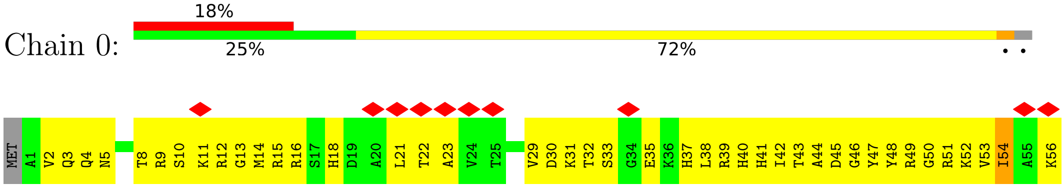
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	6	1	1	1	0

3 Residue-property plots ⓘ

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

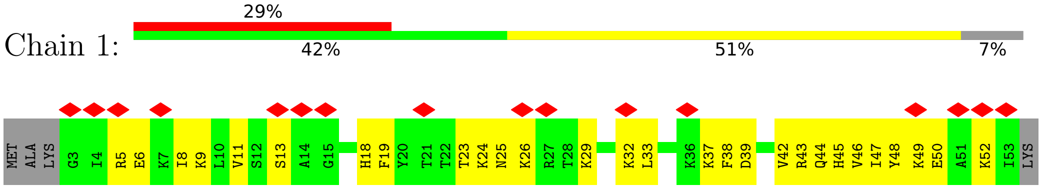
- Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:



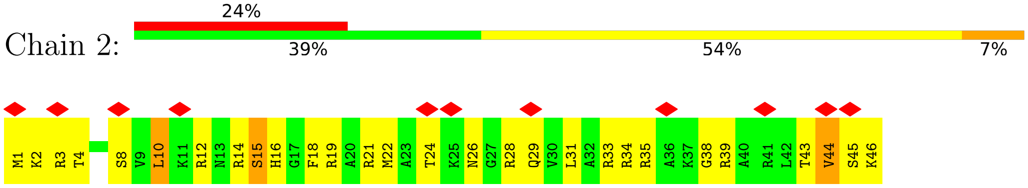
- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:



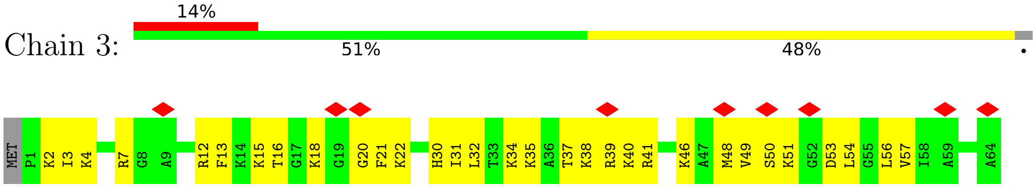
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:



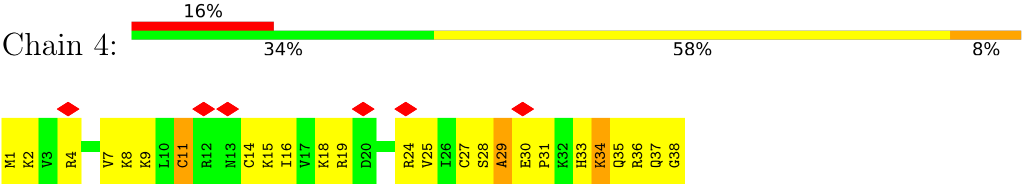
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:

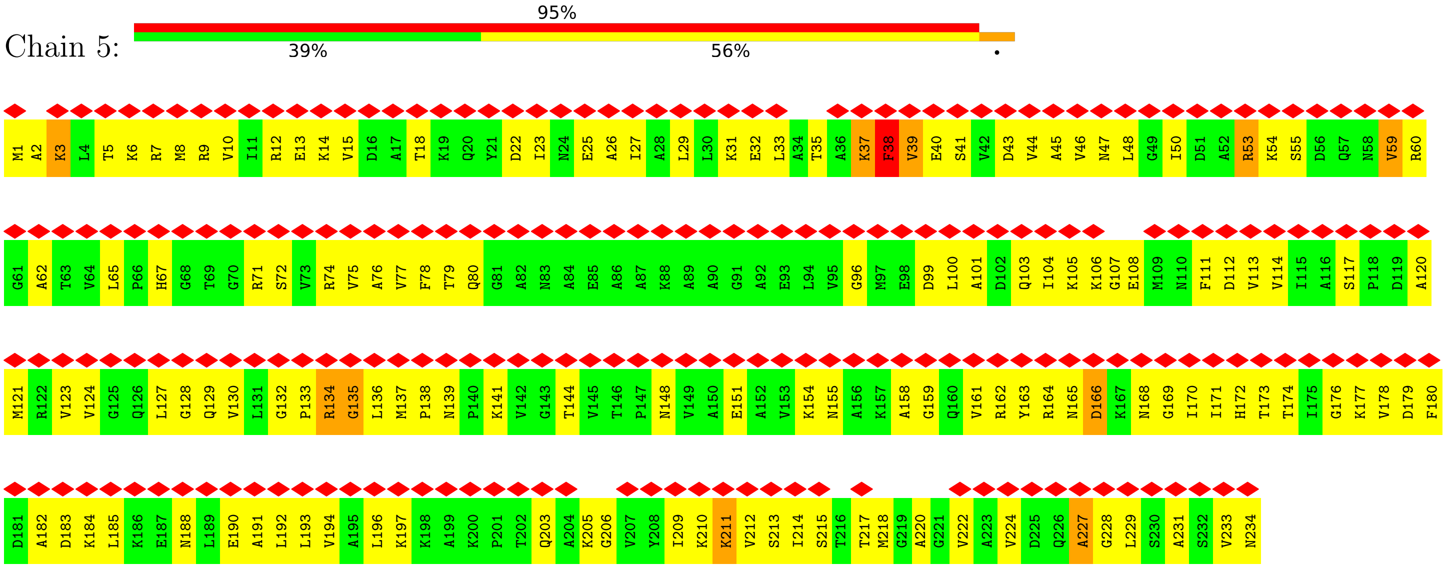


- Molecule 5: 50S RIBOSOMAL PROTEIN L36

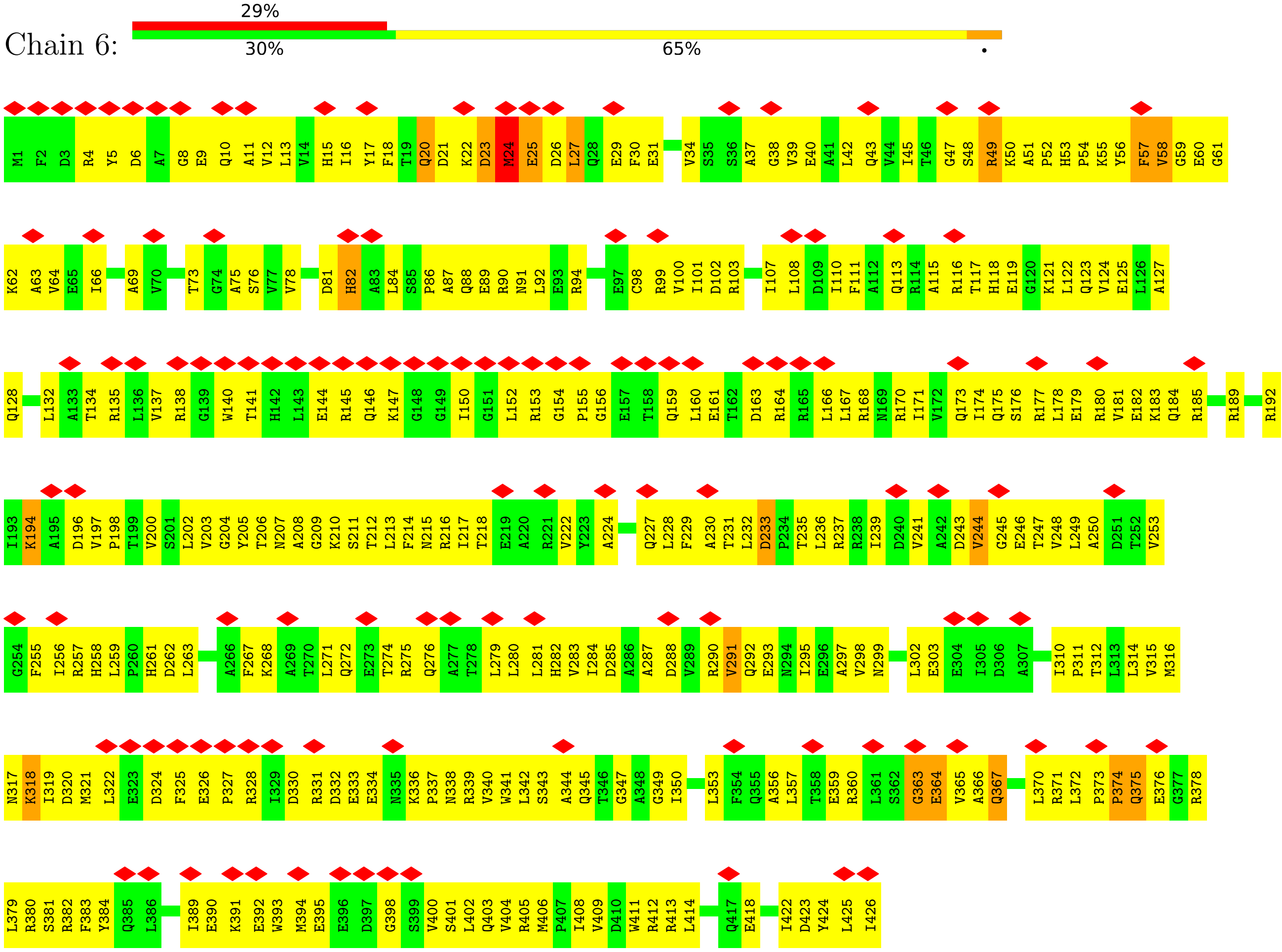
Chain 4:



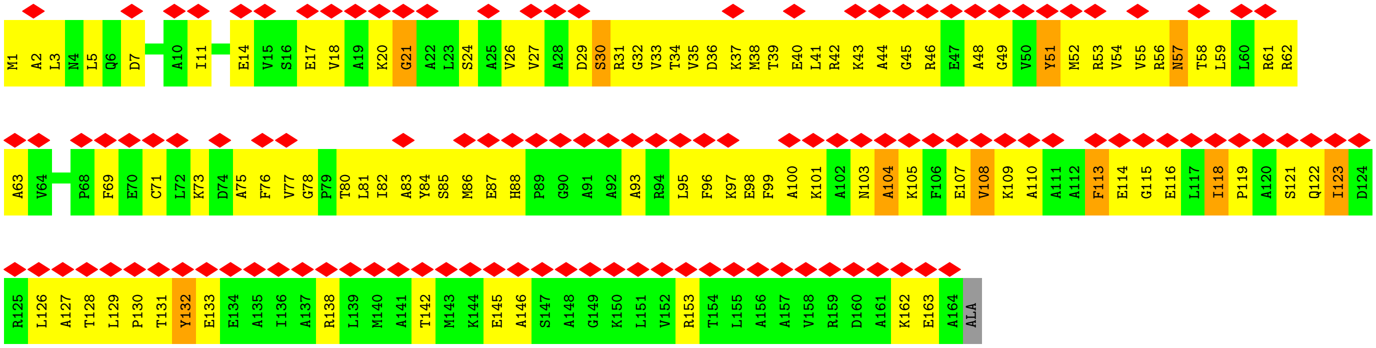
- Molecule 6: 50S RIBOSOMAL PROTEIN L1



- Molecule 7: GTPASE HFLX



- Molecule 8: 50S RIBOSOMAL PROTEIN L10



- Molecule 9: 5S RRNA

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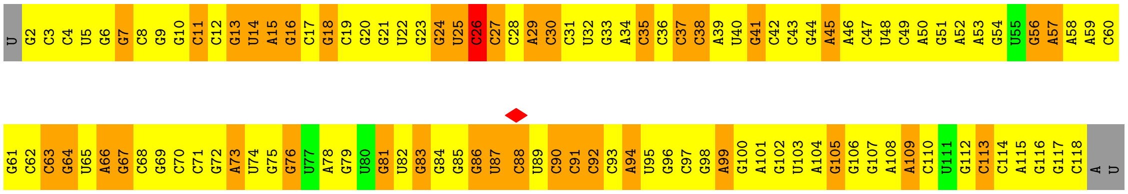
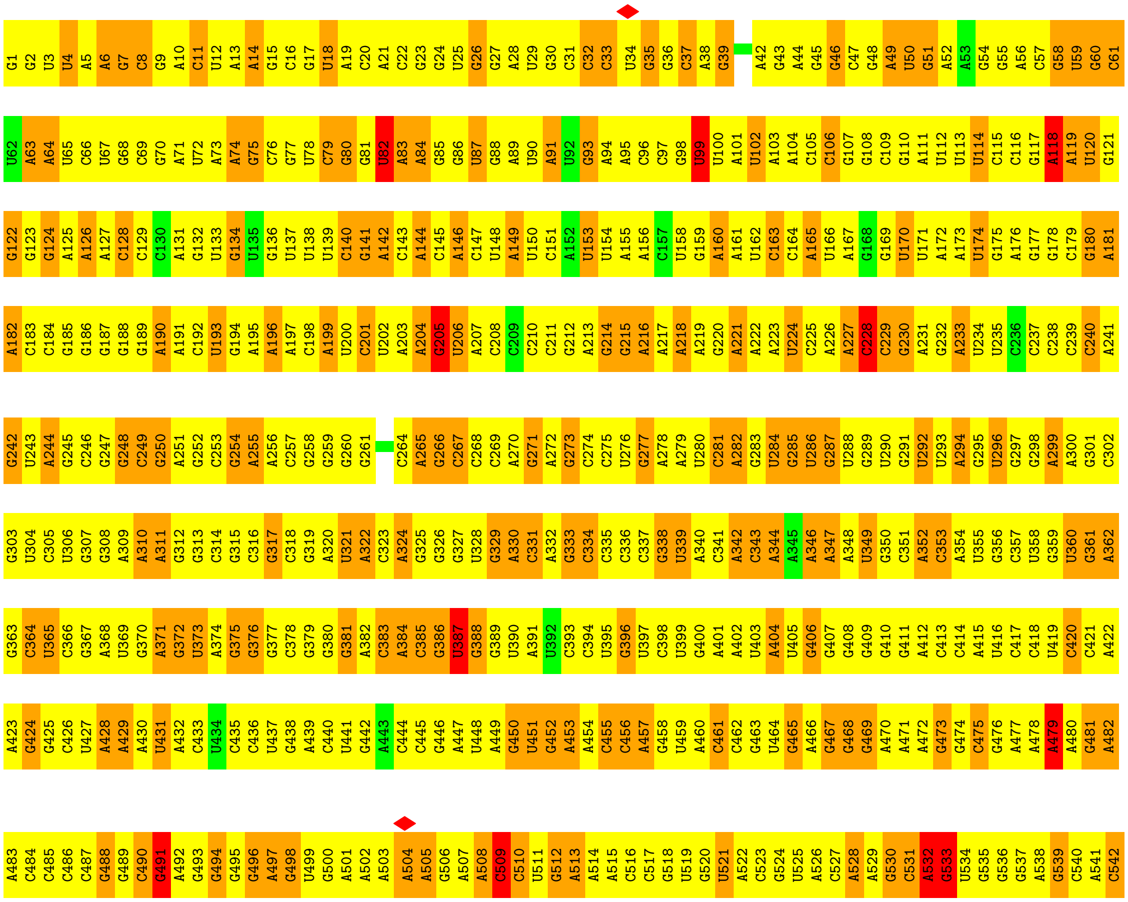
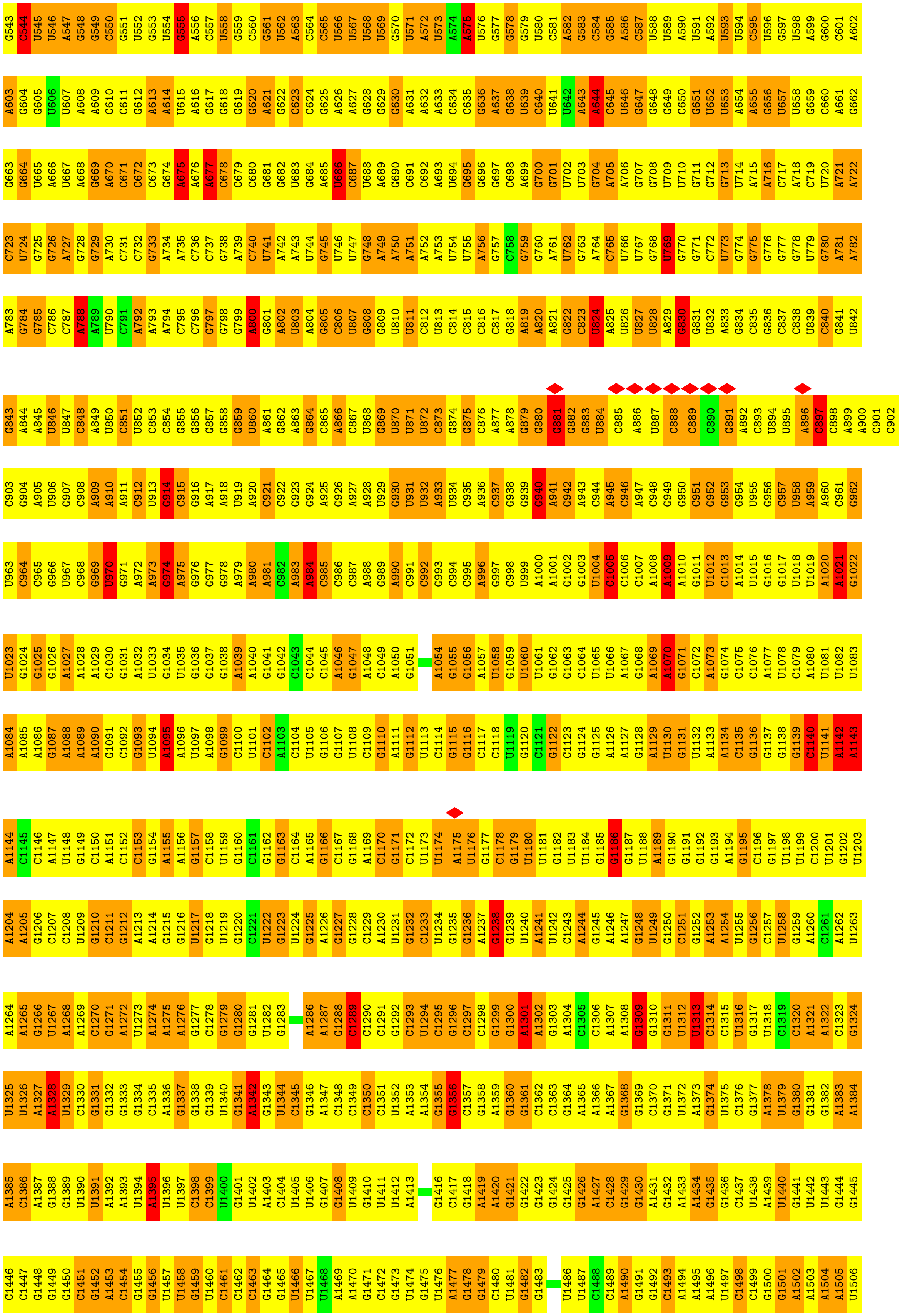


- Molecule 10: 23S RRNA

Chain B:

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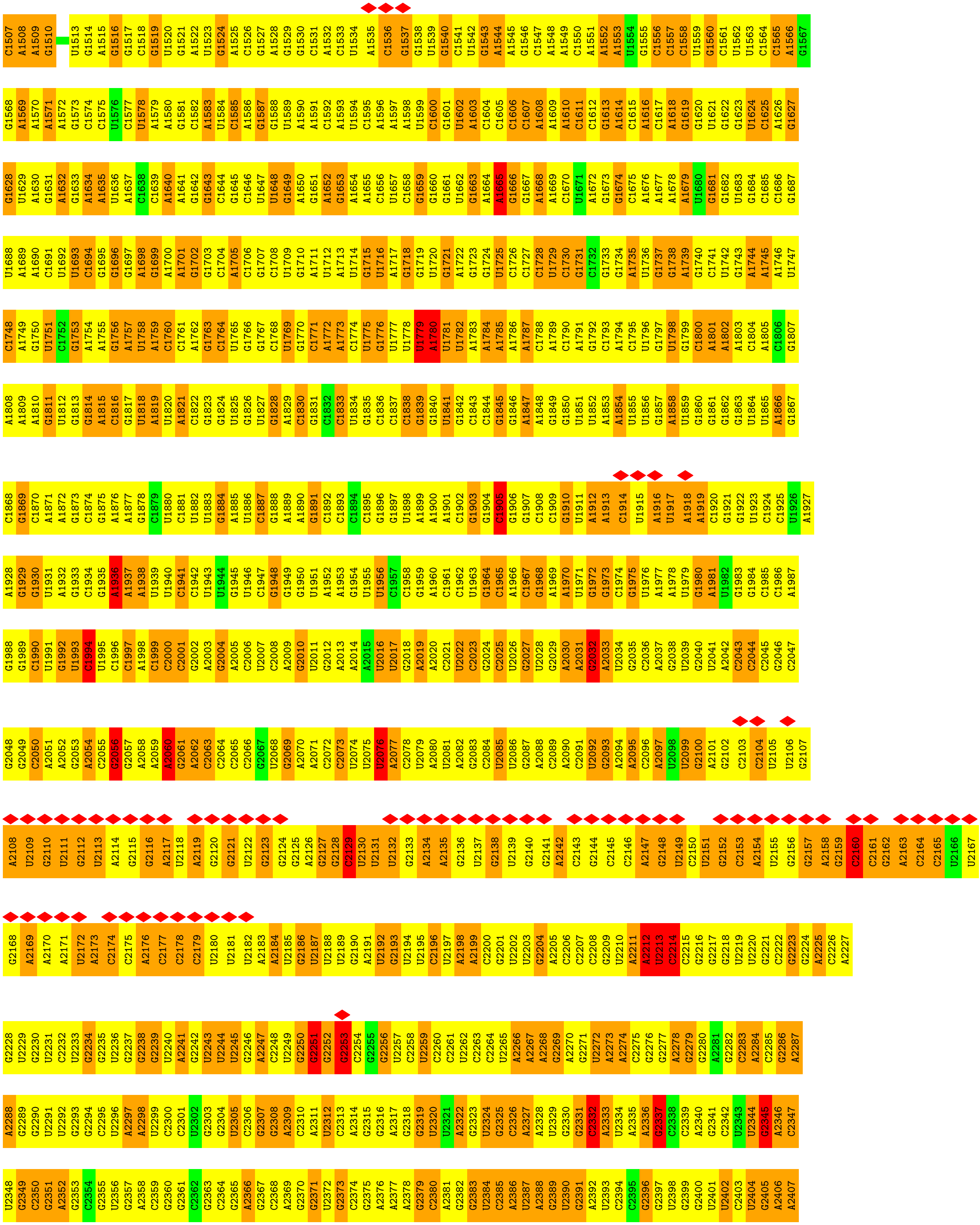
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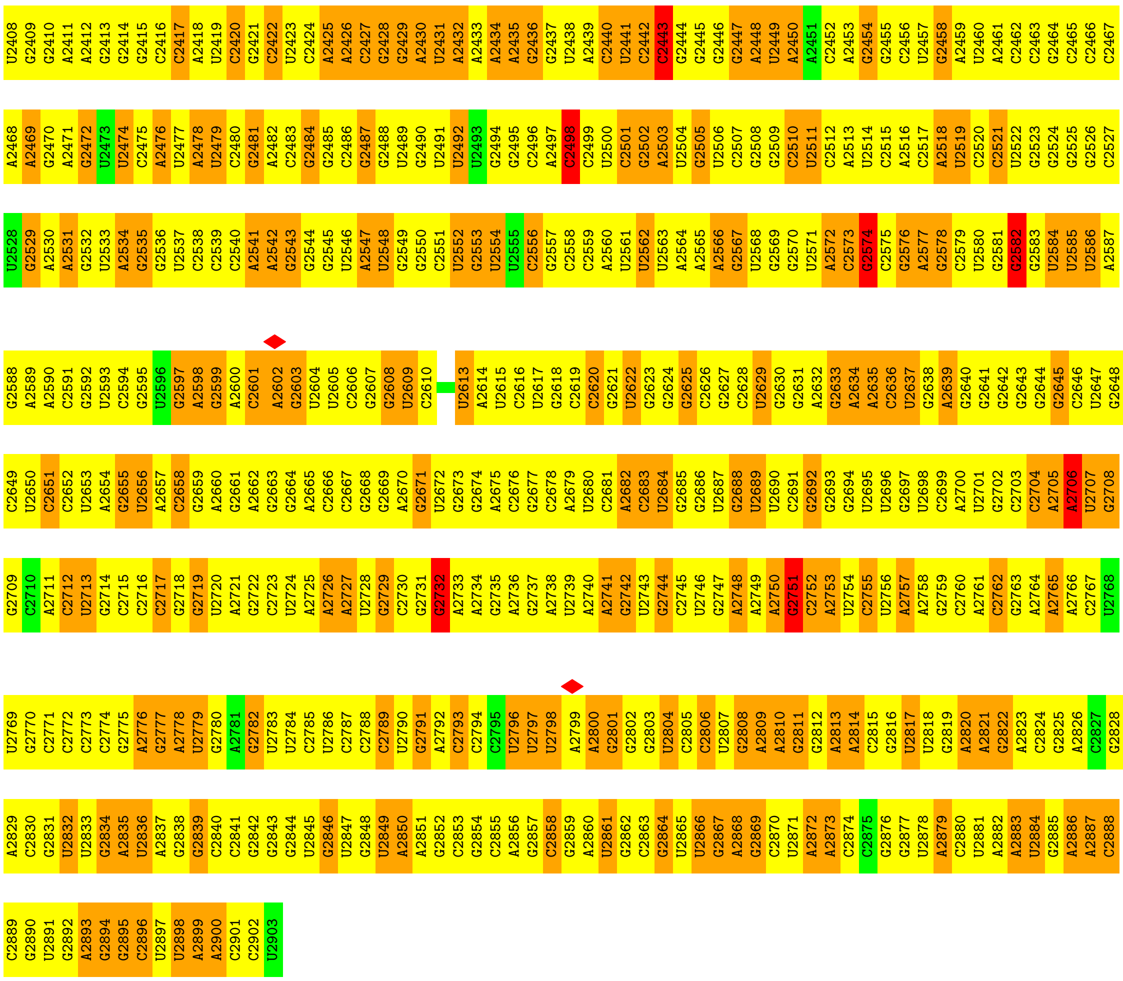
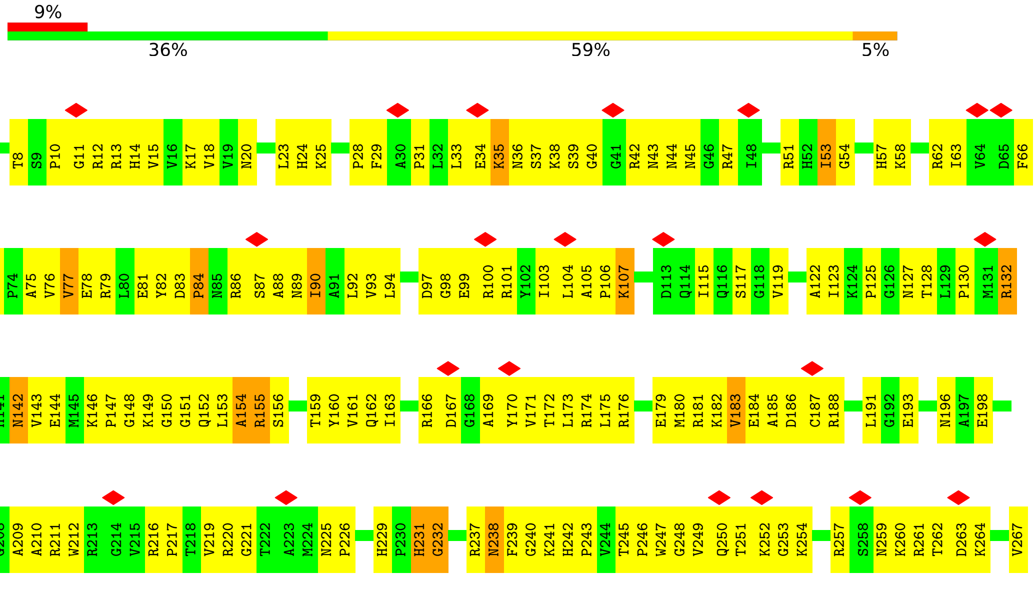
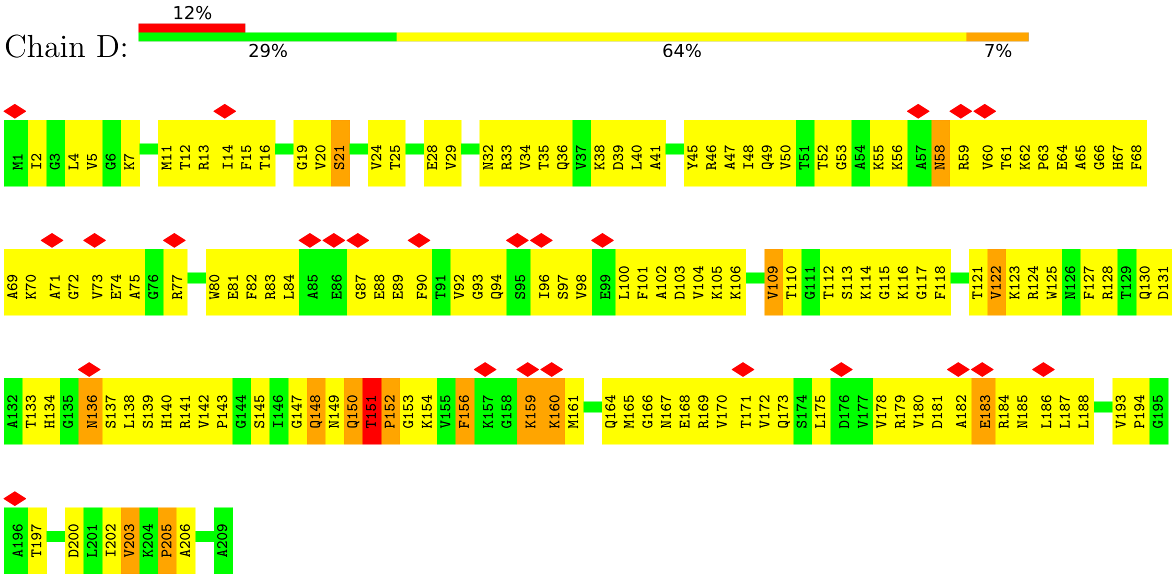


- Molecule 11: 50S RIBOSOMAL PROTEIN L2

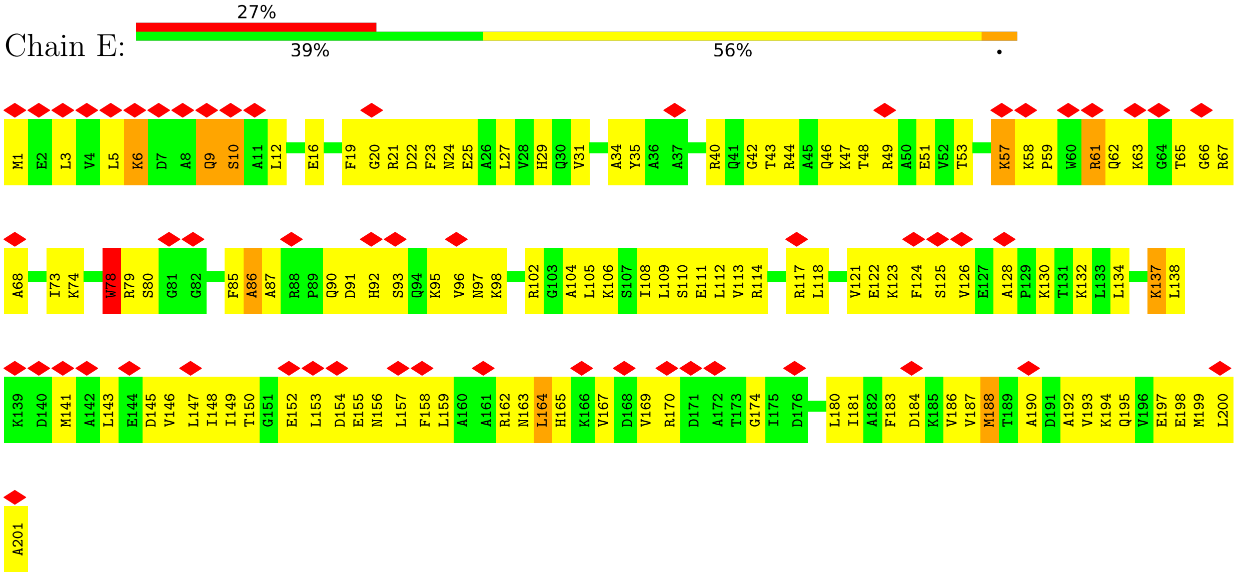
Chain C:



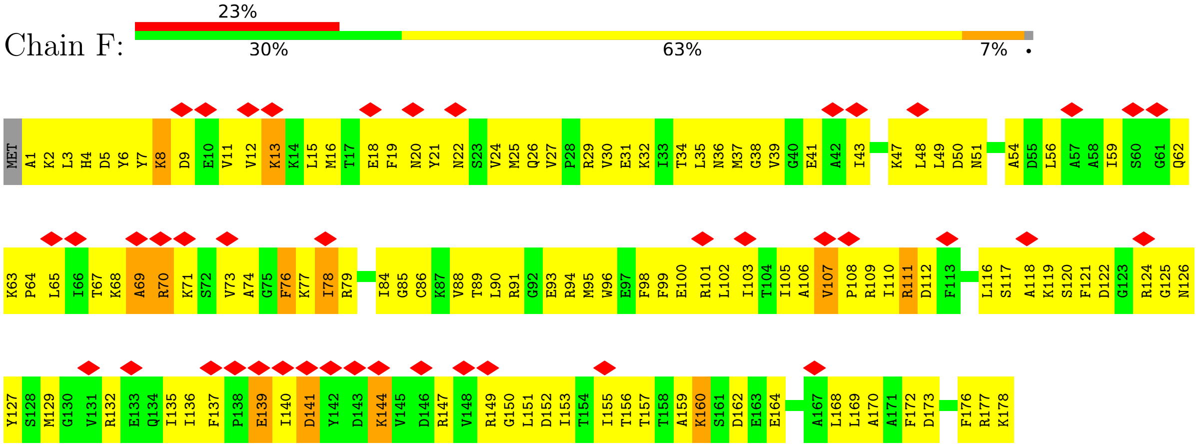
- Molecule 12: 50S RIBOSOMAL PROTEIN L3



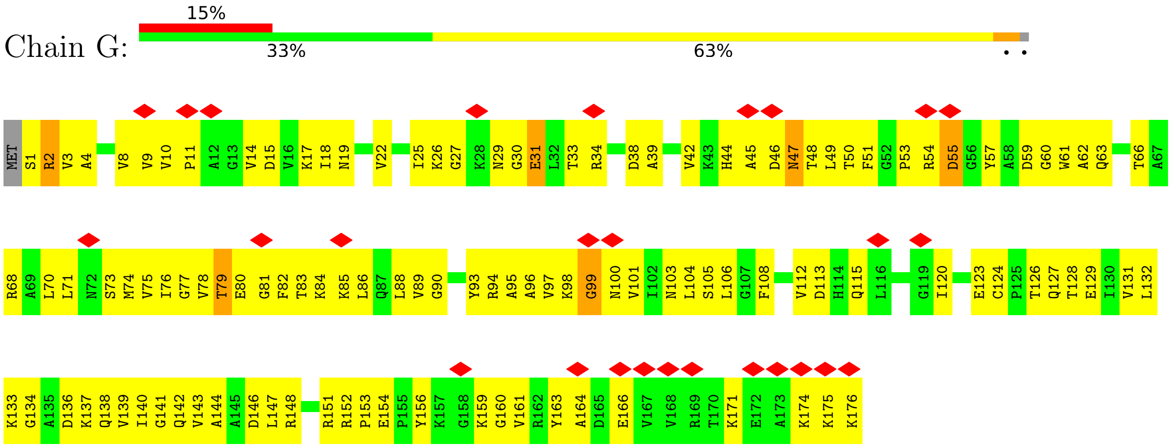
- Molecule 13: 50S RIBOSOMAL PROTEIN L4



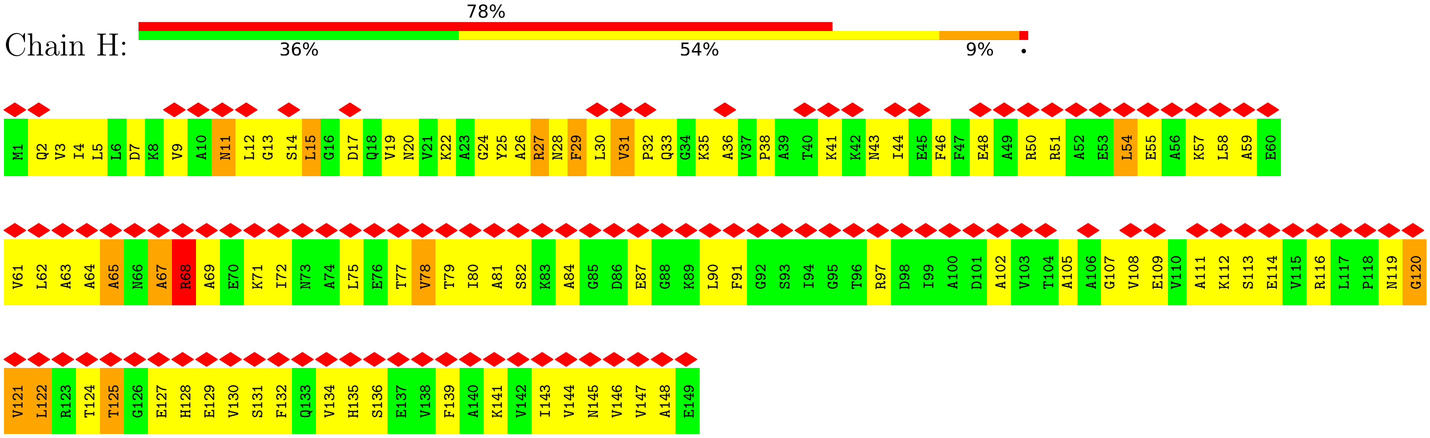
- Molecule 14: 50S RIBOSOMAL PROTEIN L5



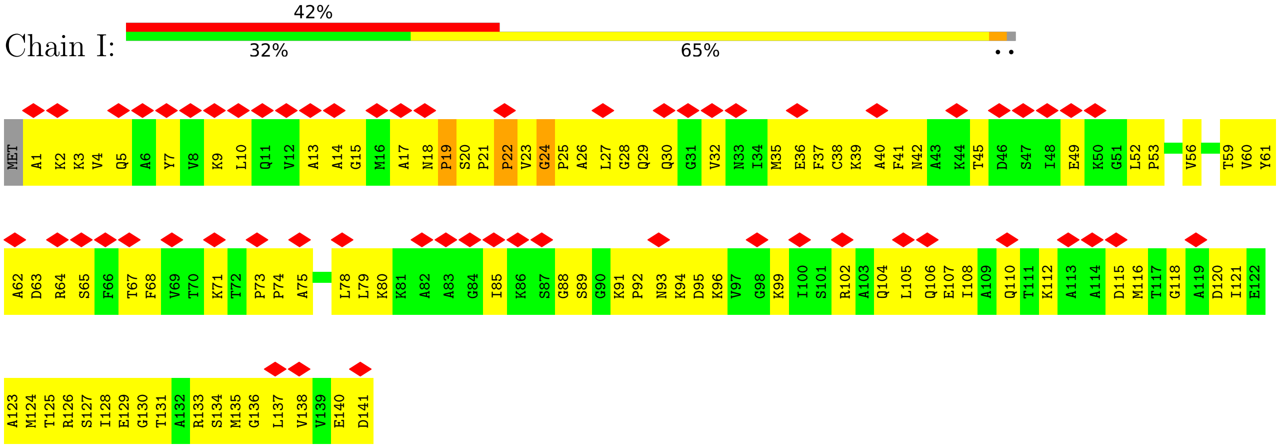
- Molecule 15: 50S RIBOSOMAL PROTEIN L6



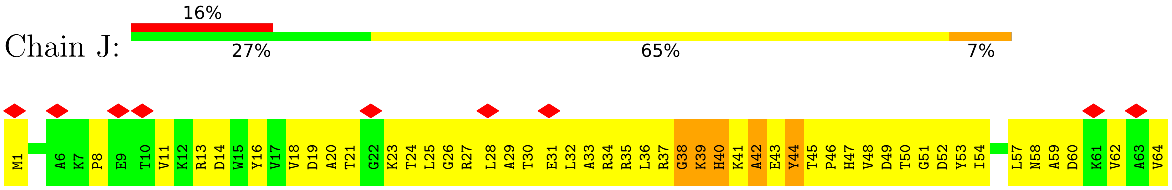
- Molecule 16: 50S RIBOSOMAL PROTEIN L9

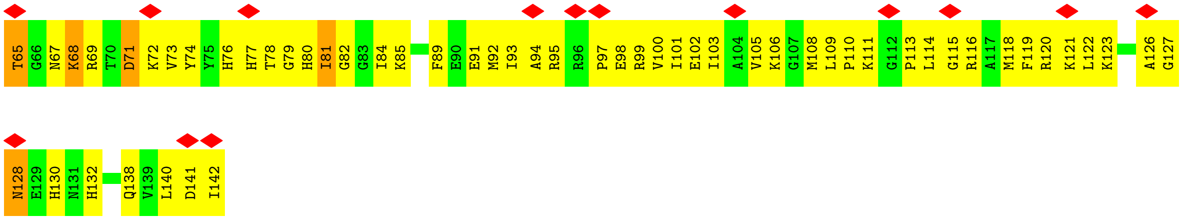


- Molecule 17: 50S RIBOSOMAL PROTEIN L11



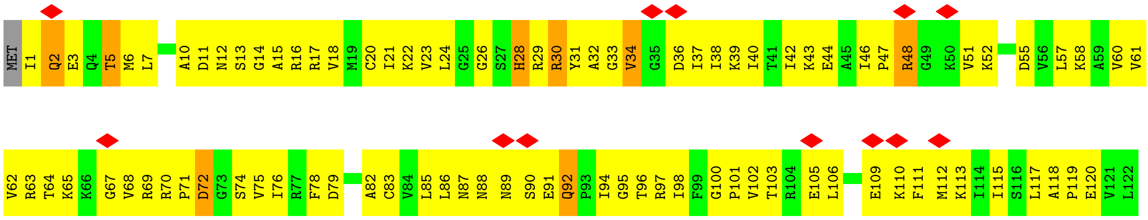
- Molecule 18: 50S RIBOSOMAL PROTEIN L13





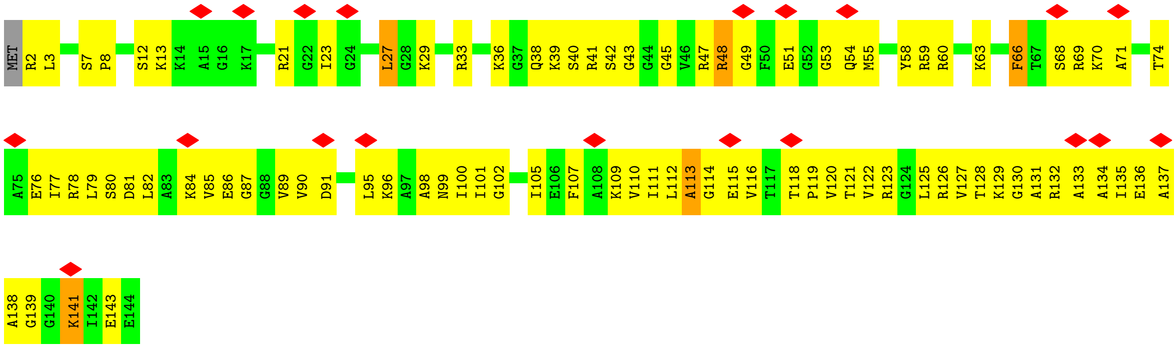
- Molecule 19: 50S RIBOSOMAL PROTEIN L14

Chain K:



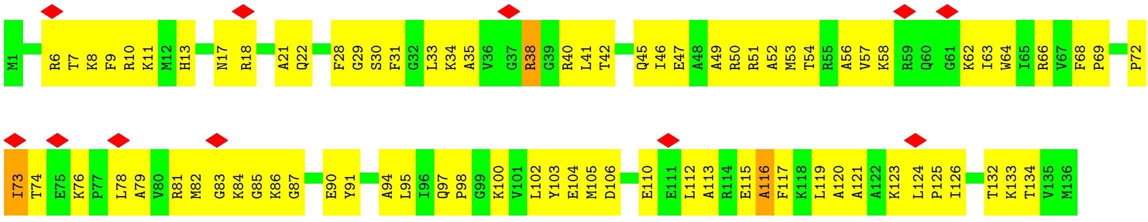
- Molecule 20: 50S RIBOSOMAL PROTEIN L15

Chain L:



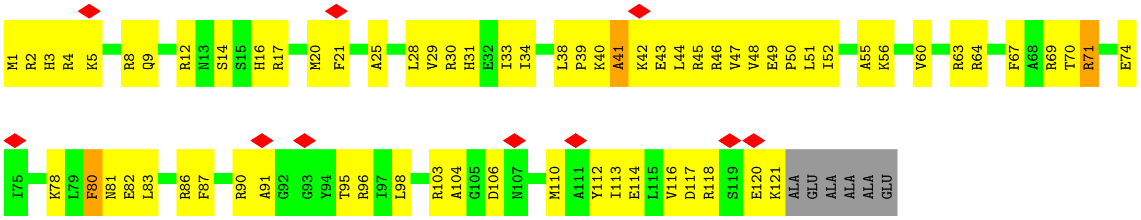
- Molecule 21: 50S RIBOSOMAL PROTEIN L16

Chain M:



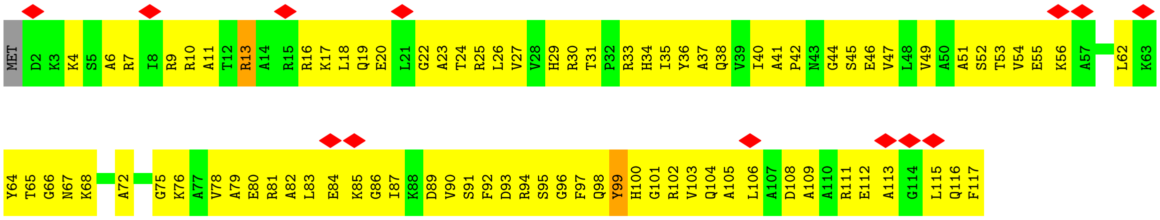
- Molecule 22: 50S RIBOSOMAL PROTEIN L17

Chain N:



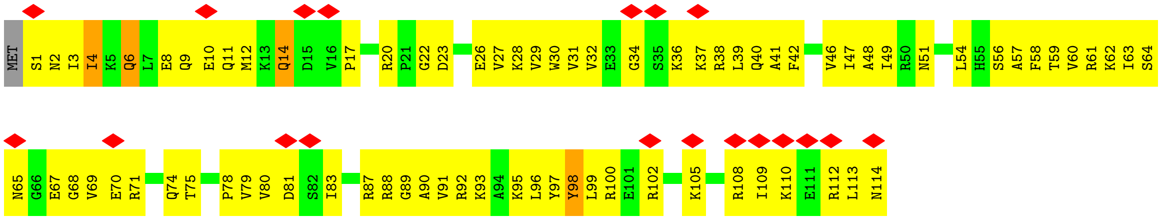
- Molecule 23: 50S RIBOSOMAL PROTEIN L18

Chain O:



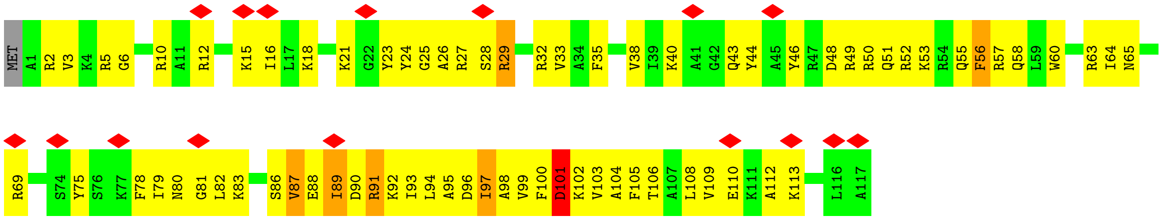
- Molecule 24: 50S RIBOSOMAL PROTEIN L19

Chain P:



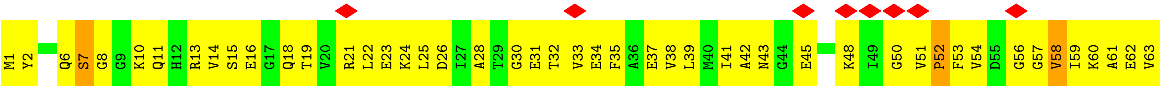
- Molecule 25: 50S RIBOSOMAL PROTEIN L20

Chain Q:



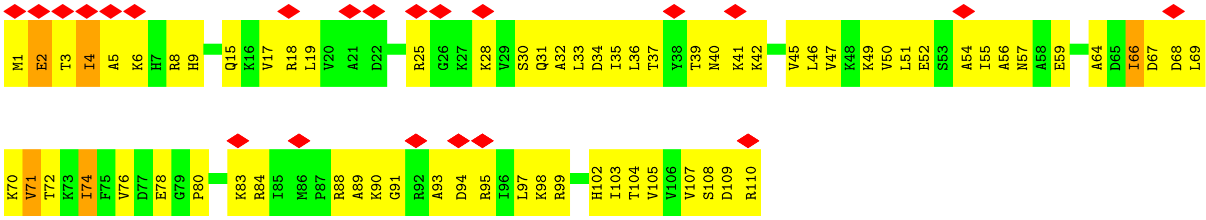
- Molecule 26: 50S RIBOSOMAL PROTEIN L21

Chain R:



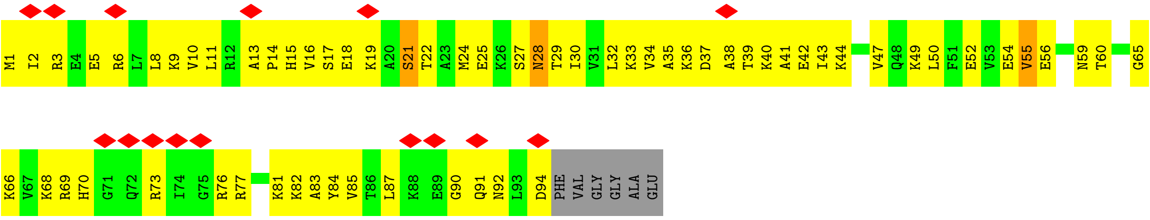
- Molecule 27: 50S RIBOSOMAL PROTEIN L22

Chain S:



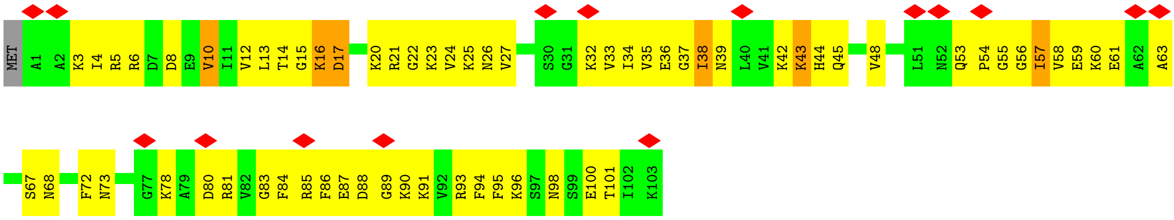
- Molecule 28: 50S RIBOSOMAL PROTEIN L23

Chain T:



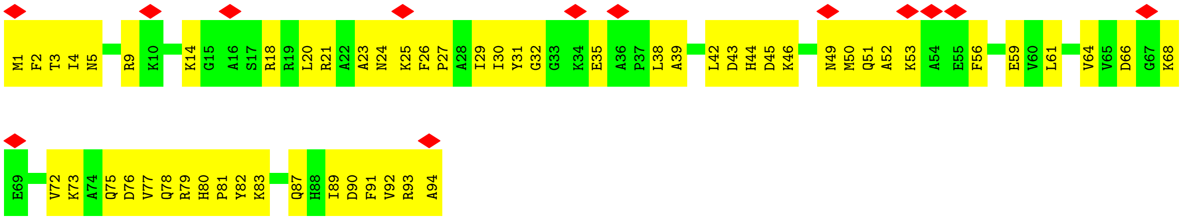
- Molecule 29: 50S RIBOSOMAL PROTEIN L24

Chain U:

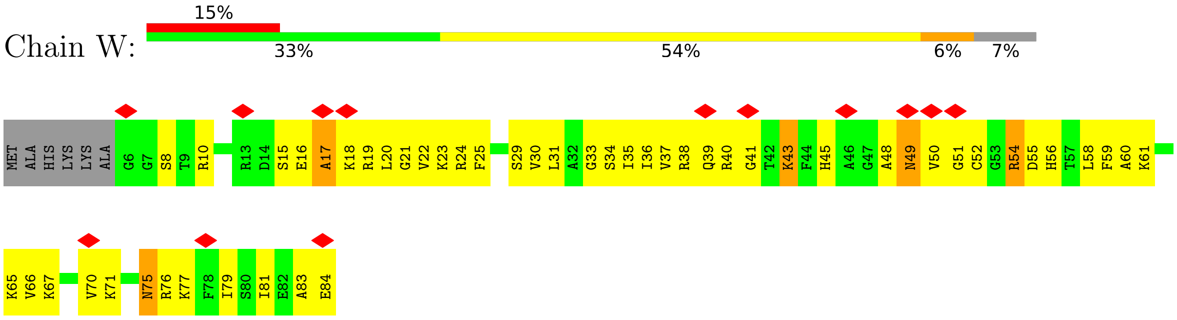


- Molecule 30: 50S RIBOSOMAL PROTEIN L25

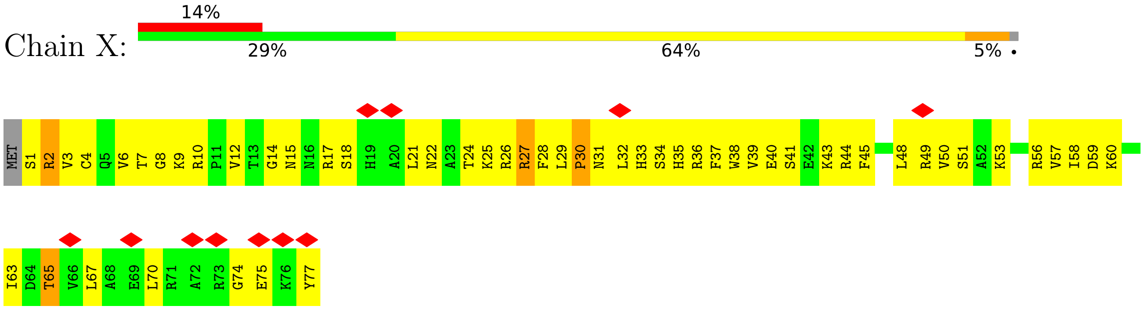
Chain V:



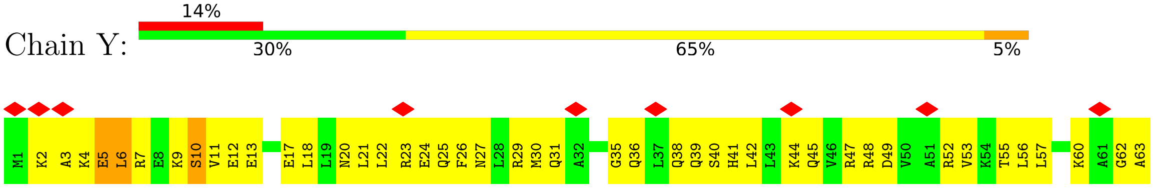
- Molecule 31: 50S RIBOSOMAL PROTEIN L27



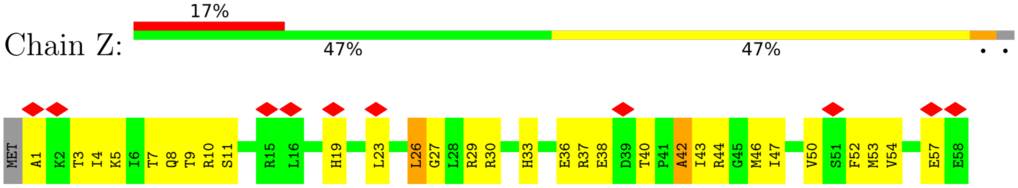
- Molecule 32: 50S RIBOSOMAL PROTEIN L28



- Molecule 33: 50S RIBOSOMAL PROTEIN L29



- Molecule 34: 50S RIBOSOMAL PROTEIN L30



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	384206	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	75000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	5.850	Depositor
Minimum map value	-2.336	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.416	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	349.77, 349.77, 349.77	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1659, 1.1659, 1.1659	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG

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	0.65	0/450	0.77	0/599
2	1	0.57	0/417	0.68	0/556
3	2	0.69	0/380	0.78	0/498
4	3	0.64	0/513	0.76	0/676
5	4	0.65	0/303	0.77	0/397
6	5	0.35	0/1748	0.64	1/2355 (0.0%)
7	6	0.55	0/3456	0.76	1/4675 (0.0%)
8	7	0.39	0/1245	0.63	0/1677
9	A	1.01	0/2800	1.16	6/4367 (0.1%)
10	B	1.18	47/69796 (0.1%)	1.22	227/108888 (0.2%)
11	C	0.63	0/2122	0.72	0/2854
12	D	0.66	0/1586	0.75	0/2134
13	E	0.58	0/1571	0.73	0/2113
14	F	0.46	0/1444	0.69	0/1937
15	G	0.57	0/1343	0.71	0/1816
16	H	0.46	0/1122	0.64	0/1515
17	I	0.41	0/1046	0.64	0/1410
18	J	0.64	0/1152	0.75	0/1551
19	K	0.60	0/940	0.75	0/1260
20	L	0.58	0/1054	0.79	1/1403 (0.1%)
21	M	0.68	0/1093	0.71	0/1460
22	N	0.66	0/974	0.74	0/1303
23	O	0.54	0/902	0.70	0/1209
24	P	0.61	0/929	0.71	0/1242
25	Q	0.78	0/960	0.77	0/1278
26	R	0.64	0/829	0.71	0/1107
27	S	0.66	0/864	0.84	0/1156
28	T	0.61	0/745	0.77	0/996
29	U	0.53	0/788	0.72	0/1053
30	V	0.60	0/766	0.72	0/1025
31	W	0.64	0/603	0.80	0/797
32	X	0.62	0/635	0.71	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.53	0/510	0.68	0/677
34	Z	0.60	0/453	0.77	1/605 (0.2%)
All	All	1.03	47/105539 (0.0%)	1.10	237/157437 (0.2%)

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
6	5	0	1
13	E	0	1
14	F	0	1
24	P	0	1
25	Q	0	1
All	All	0	5

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	788	A	N9-C4	-8.84	1.32	1.37
10	B	118	A	N9-C4	-7.60	1.33	1.37
10	B	677	A	N9-C4	-6.86	1.33	1.37
10	B	1142	A	N9-C4	-6.60	1.33	1.37
10	B	1254	A	N9-C4	-6.54	1.33	1.37

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	828	U	C2-N1-C1'	8.23	127.58	117.70
10	B	205	G	C2-N3-C4	-8.04	107.88	111.90
10	B	1816	C	C2-N1-C1'	8.01	127.61	118.80
10	B	544	C	C2-N1-C1'	7.58	127.14	118.80
10	B	1238	G	N3-C4-C5	7.58	132.39	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	59	VAL	Peptide
13	E	59	PRO	Peptide

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Mol	Chain	Res	Type	Group
14	F	76	PHE	Peptide
24	P	14	GLN	Peptide
25	Q	101	ASP	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	0	444	0	461	53	0
2	1	410	0	440	42	0
3	2	377	0	418	42	0
4	3	504	0	574	60	0
5	4	302	0	343	35	0
6	5	1733	0	1823	197	0
7	6	3403	0	3433	388	0
8	7	1231	0	1282	124	0
9	A	2504	0	1271	246	0
10	B	62317	0	31345	6165	0
11	C	2083	0	2157	244	0
12	D	1565	0	1616	238	0
13	E	1552	0	1619	130	0
14	F	1420	0	1460	169	0
15	G	1323	0	1374	136	0
16	H	1111	0	1148	191	0
17	I	1032	0	1088	142	0
18	J	1129	0	1162	144	0
19	K	931	0	1003	116	0
20	L	1045	0	1117	121	0
21	M	1074	0	1157	105	0
22	N	961	0	1000	107	0
23	O	892	0	923	130	0
24	P	917	0	965	101	0
25	Q	947	0	1022	143	0
26	R	816	0	839	106	0
27	S	857	0	922	100	0
28	T	739	0	807	74	0
29	U	780	0	834	89	0
30	V	753	0	780	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	W	596	0	610	94	0
32	X	625	0	655	93	0
33	Y	509	0	543	52	0
34	Z	449	0	491	26	0
35	6	32	0	13	23	0
36	6	1	0	0	0	0
All	All	97364	0	66695	9065	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 57.

The worst 5 of 9065 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)
16:H:68:ARG:CD	16:H:132:PHE:CE1	1.84	1.55
16:H:68:ARG:HG3	16:H:132:PHE:CD2	1.40	1.55
16:H:68:ARG:HG3	16:H:132:PHE:CE2	1.37	1.53
16:H:68:ARG:HD2	16:H:132:PHE:CE1	1.43	1.52
7:6:365:VAL:CG2	7:6:405:ARG:NH2	1.69	1.43

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	54/57 (95%)	45 (83%)	5 (9%)	4 (7%)	1	16
2	1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
3	2	44/46 (96%)	35 (80%)	6 (14%)	3 (7%)	1	17
4	3	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
5	4	36/38 (95%)	26 (72%)	5 (14%)	5 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	232/234 (99%)	190 (82%)	27 (12%)	15 (6%)	1	18
7	6	424/426 (100%)	364 (86%)	39 (9%)	21 (5%)	2	23
8	7	162/165 (98%)	128 (79%)	23 (14%)	11 (7%)	1	17
11	C	270/273 (99%)	219 (81%)	34 (13%)	17 (6%)	1	19
12	D	207/209 (99%)	166 (80%)	20 (10%)	21 (10%)	0	10
13	E	199/201 (99%)	160 (80%)	21 (11%)	18 (9%)	1	12
14	F	176/179 (98%)	131 (74%)	30 (17%)	15 (8%)	1	13
15	G	174/177 (98%)	142 (82%)	21 (12%)	11 (6%)	1	19
16	H	147/149 (99%)	97 (66%)	29 (20%)	21 (14%)	0	4
17	I	139/142 (98%)	122 (88%)	13 (9%)	4 (3%)	4	32
18	J	140/142 (99%)	109 (78%)	19 (14%)	12 (9%)	1	13
19	K	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	1	13
20	L	141/144 (98%)	113 (80%)	20 (14%)	8 (6%)	1	20
21	M	134/136 (98%)	113 (84%)	13 (10%)	8 (6%)	1	19
22	N	119/127 (94%)	96 (81%)	18 (15%)	5 (4%)	3	25
23	O	114/117 (97%)	105 (92%)	6 (5%)	3 (3%)	5	35
24	P	112/115 (97%)	89 (80%)	18 (16%)	5 (4%)	2	24
25	Q	115/118 (98%)	102 (89%)	7 (6%)	6 (5%)	2	22
26	R	101/103 (98%)	78 (77%)	13 (13%)	10 (10%)	0	10
27	S	108/110 (98%)	93 (86%)	8 (7%)	7 (6%)	1	18
28	T	92/100 (92%)	73 (79%)	13 (14%)	6 (6%)	1	18
29	U	101/104 (97%)	79 (78%)	14 (14%)	8 (8%)	1	14
30	V	92/94 (98%)	81 (88%)	10 (11%)	1 (1%)	14	52
31	W	77/85 (91%)	58 (75%)	12 (16%)	7 (9%)	1	12
32	X	75/78 (96%)	61 (81%)	9 (12%)	5 (7%)	1	18
33	Y	61/63 (97%)	49 (80%)	6 (10%)	6 (10%)	0	10
34	Z	56/59 (95%)	51 (91%)	3 (5%)	2 (4%)	3	28
All	All	4133/4234 (98%)	3374 (82%)	484 (12%)	275 (7%)	2	18

5 of 275 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	11	CYS

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Mol	Chain	Res	Type
5	4	34	LYS
6	5	38	PHE
6	5	39	VAL
6	5	135	GLY

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	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
6	5	181/181 (100%)	179 (99%)	2 (1%)	73	85
7	6	364/364 (100%)	363 (100%)	1 (0%)	92	95
8	7	123/123 (100%)	123 (100%)	0	100	100
11	C	216/218 (99%)	216 (100%)	0	100	100
12	D	164/164 (100%)	163 (99%)	1 (1%)	86	92
13	E	165/165 (100%)	164 (99%)	1 (1%)	86	92
14	F	149/150 (99%)	149 (100%)	0	100	100
15	G	137/138 (99%)	137 (100%)	0	100	100
16	H	114/114 (100%)	113 (99%)	1 (1%)	78	87
17	I	109/110 (99%)	109 (100%)	0	100	100
18	J	116/116 (100%)	116 (100%)	0	100	100
19	K	102/104 (98%)	102 (100%)	0	100	100
20	L	102/103 (99%)	102 (100%)	0	100	100
21	M	109/109 (100%)	109 (100%)	0	100	100
22	N	100/103 (97%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	O	86/87 (99%)	86 (100%)	0	100	100
24	P	99/100 (99%)	99 (100%)	0	100	100
25	Q	89/90 (99%)	88 (99%)	1 (1%)	73	85
26	R	84/84 (100%)	84 (100%)	0	100	100
27	S	93/93 (100%)	93 (100%)	0	100	100
28	T	80/84 (95%)	80 (100%)	0	100	100
29	U	83/85 (98%)	83 (100%)	0	100	100
30	V	78/78 (100%)	78 (100%)	0	100	100
31	W	59/63 (94%)	59 (100%)	0	100	100
32	X	67/68 (98%)	67 (100%)	0	100	100
33	Y	55/55 (100%)	55 (100%)	0	100	100
34	Z	48/49 (98%)	48 (100%)	0	100	100
All	All	3387/3419 (99%)	3380 (100%)	7 (0%)	93	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	D	151	THR
13	E	78	TRP
25	Q	56	PHE
16	H	68	ARG
7	6	24	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
26	R	11	GLN
30	V	80	HIS
26	R	91	GLN
28	T	92	ASN
32	X	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	2902/2903 (99%)	1015 (34%)	56 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	116/120 (96%)	35 (30%)	2 (1%)
All	All	3018/3023 (99%)	1050 (34%)	58 (1%)

5 of 1050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	7	G
9	A	11	C
9	A	13	G
9	A	14	U
9	A	15	A

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	B	1385	A
10	B	2810	A
10	B	1779	U
10	B	2808	G
10	B	2389	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
35	GNP	6	527	36	29,34,34	2.07	9 (31%)	33,54,54	2.52	10 (30%)

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
35	GNP	6	527	36	-	4/14/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	6	527	GNP	PB-O3A	-7.03	1.50	1.59
35	6	527	GNP	PB-O2B	-3.47	1.47	1.56
35	6	527	GNP	C6-N1	3.29	1.38	1.33
35	6	527	GNP	PG-O1G	2.92	1.50	1.46
35	6	527	GNP	C8-N7	-2.67	1.29	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	6	527	GNP	C5-C6-N1	-8.46	111.86	123.43
35	6	527	GNP	C2-N1-C6	5.19	124.17	115.93
35	6	527	GNP	PB-O3A-PA	-5.07	114.77	132.62
35	6	527	GNP	O2B-PB-O1B	3.71	117.71	109.92
35	6	527	GNP	C2-N3-C4	-3.67	111.17	115.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	6	527	GNP	PB-N3B-PG-O1G
35	6	527	GNP	PG-N3B-PB-O1B
35	6	527	GNP	PA-O3A-PB-O1B
35	6	527	GNP	O4'-C4'-C5'-O5'

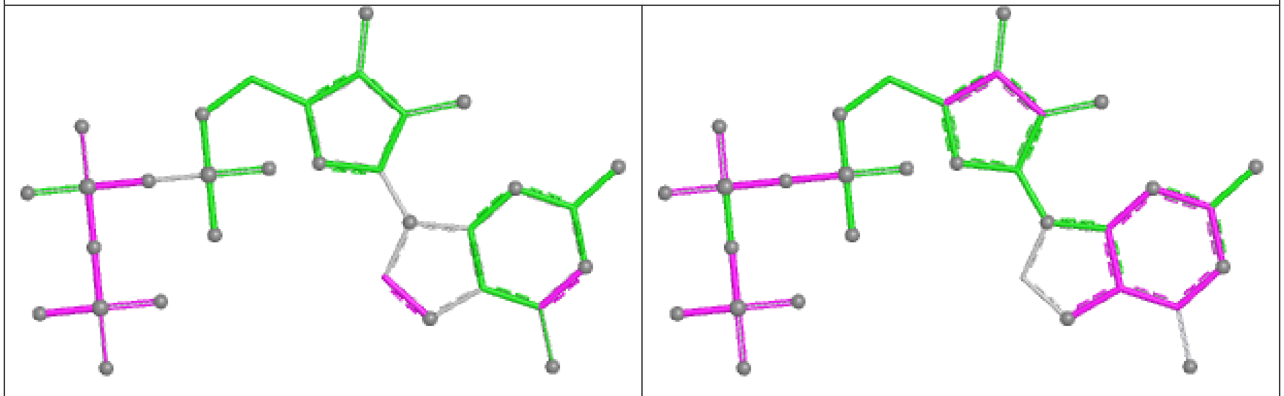
There are no ring outliers.

1 monomer is involved in 23 short contacts:

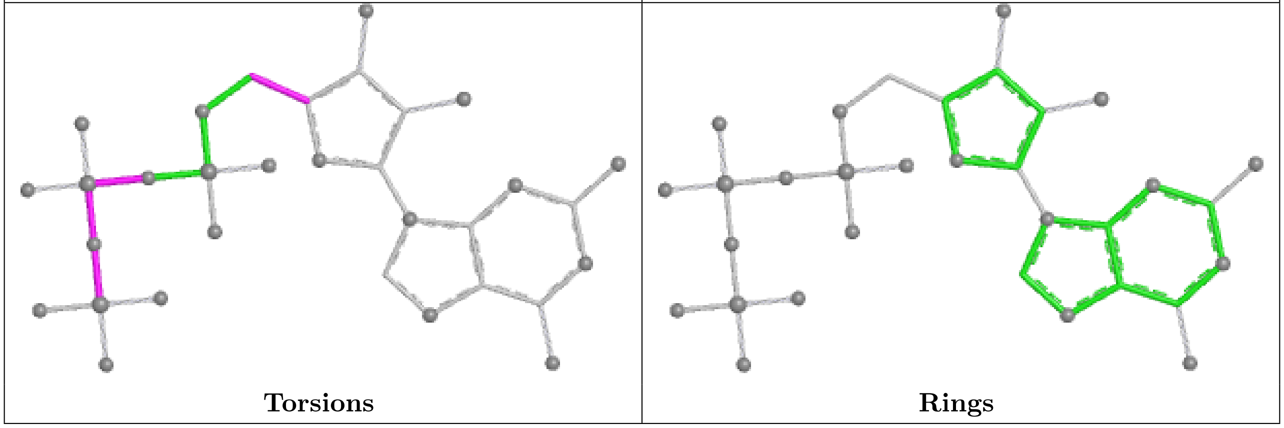
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	6	527	GNP	23	0

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 then 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.

Ligand GNP 6 527



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

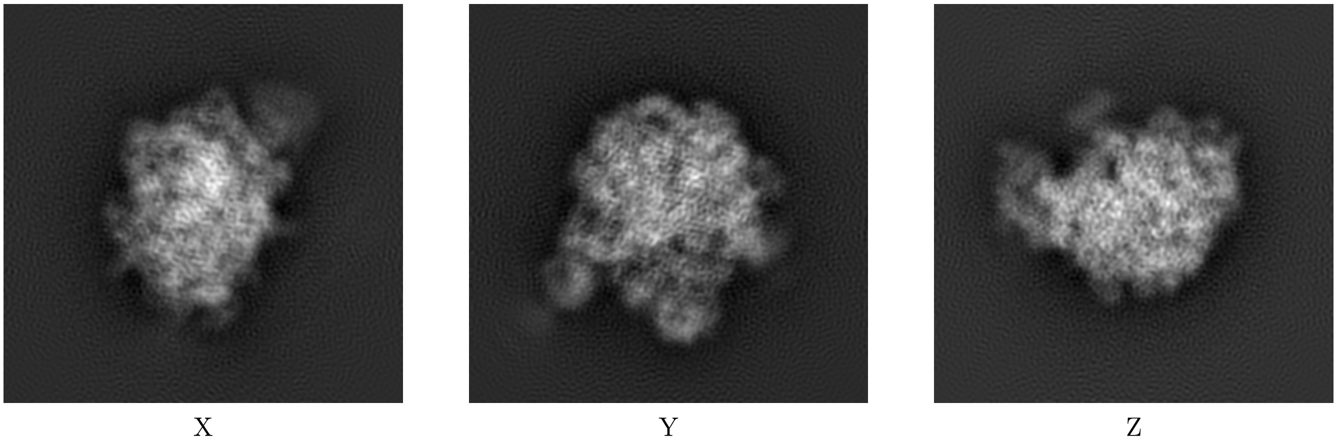
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3133. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

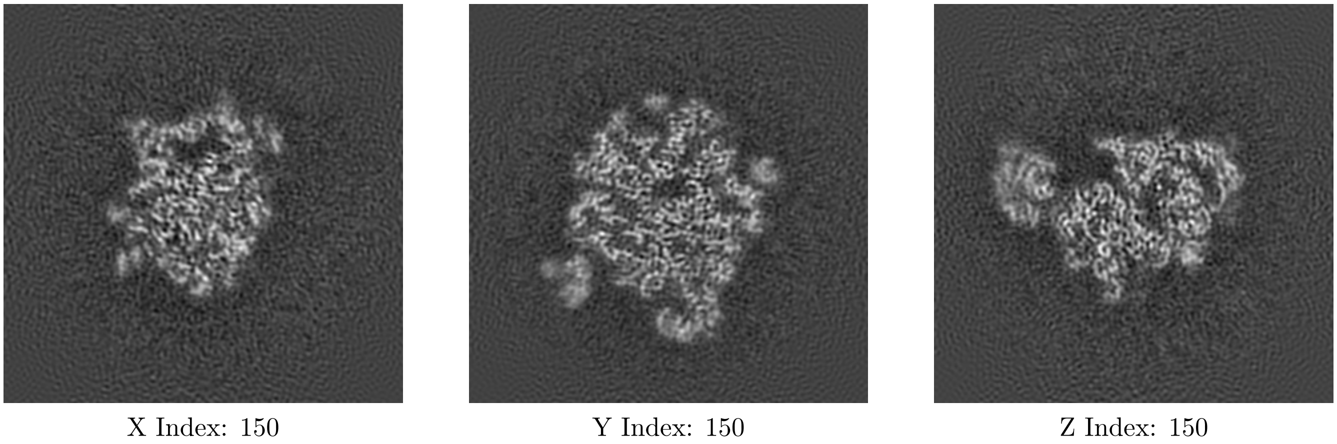
6.1.1 Primary map



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

6.2 Central slices ⓘ

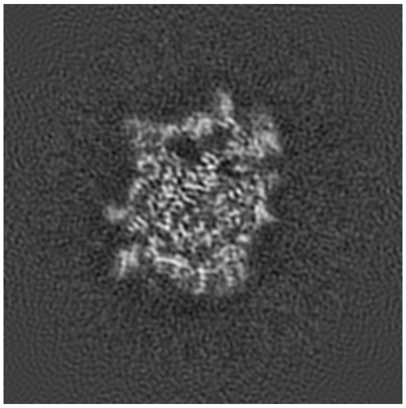
6.2.1 Primary map



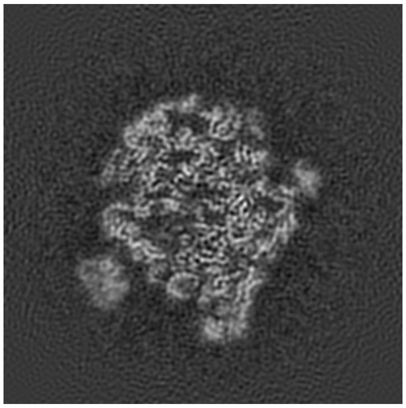
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

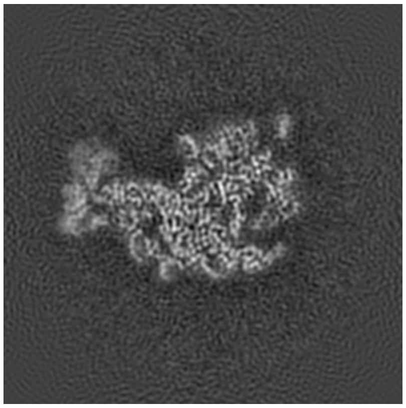
6.3.1 Primary map



X Index: 153



Y Index: 155



Z Index: 164

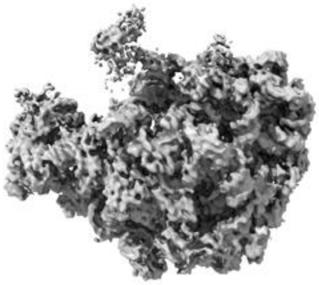
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

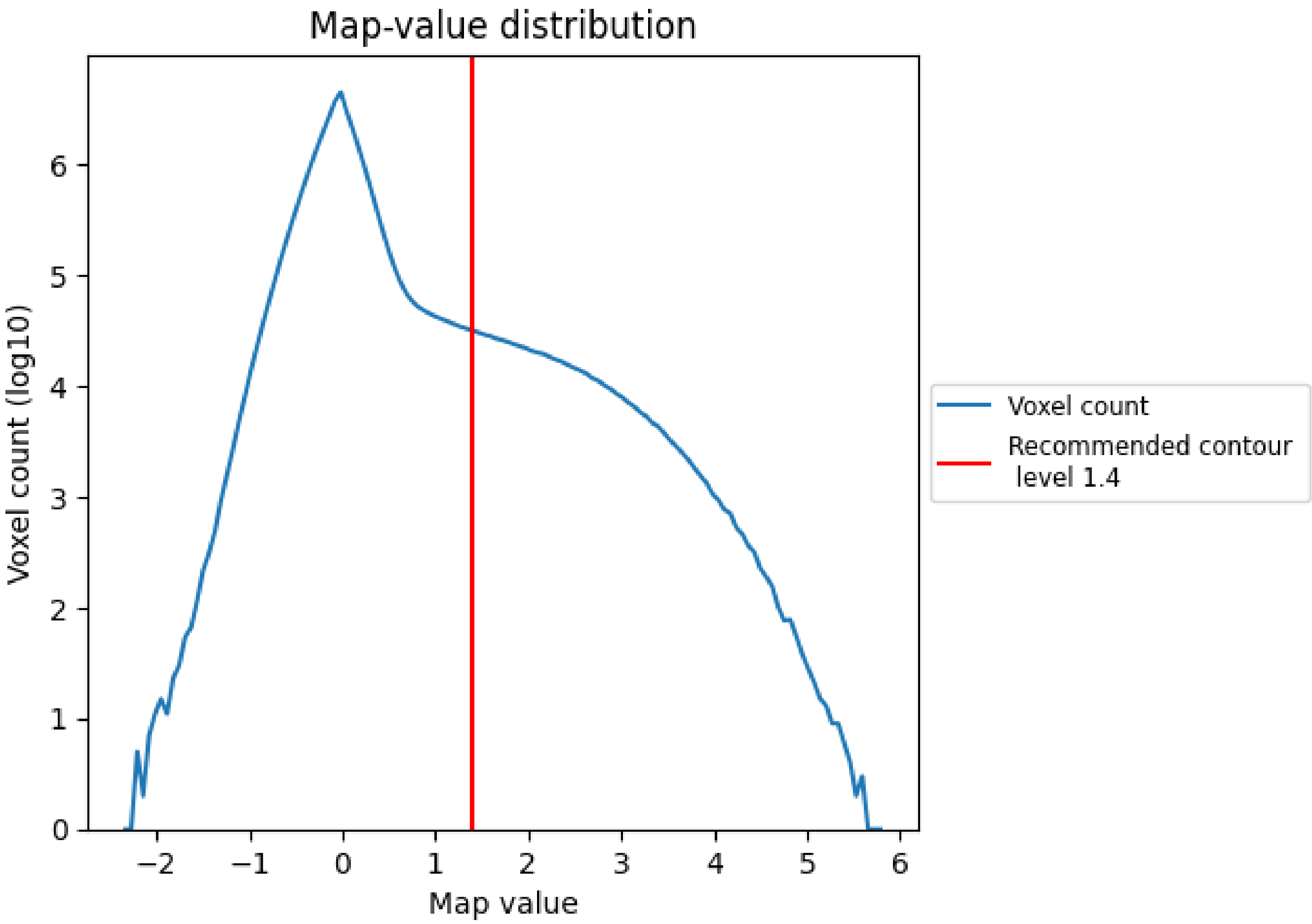
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

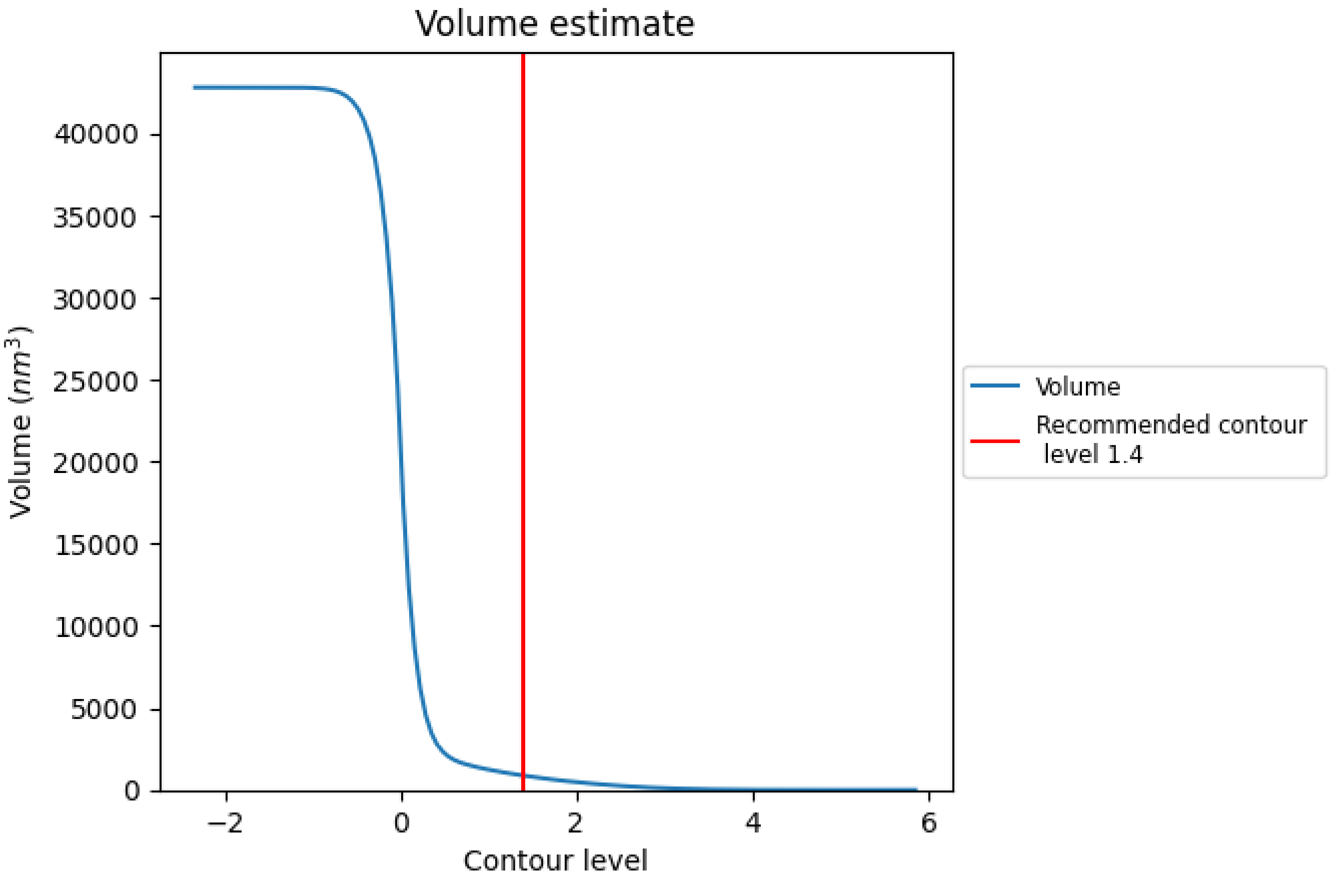
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

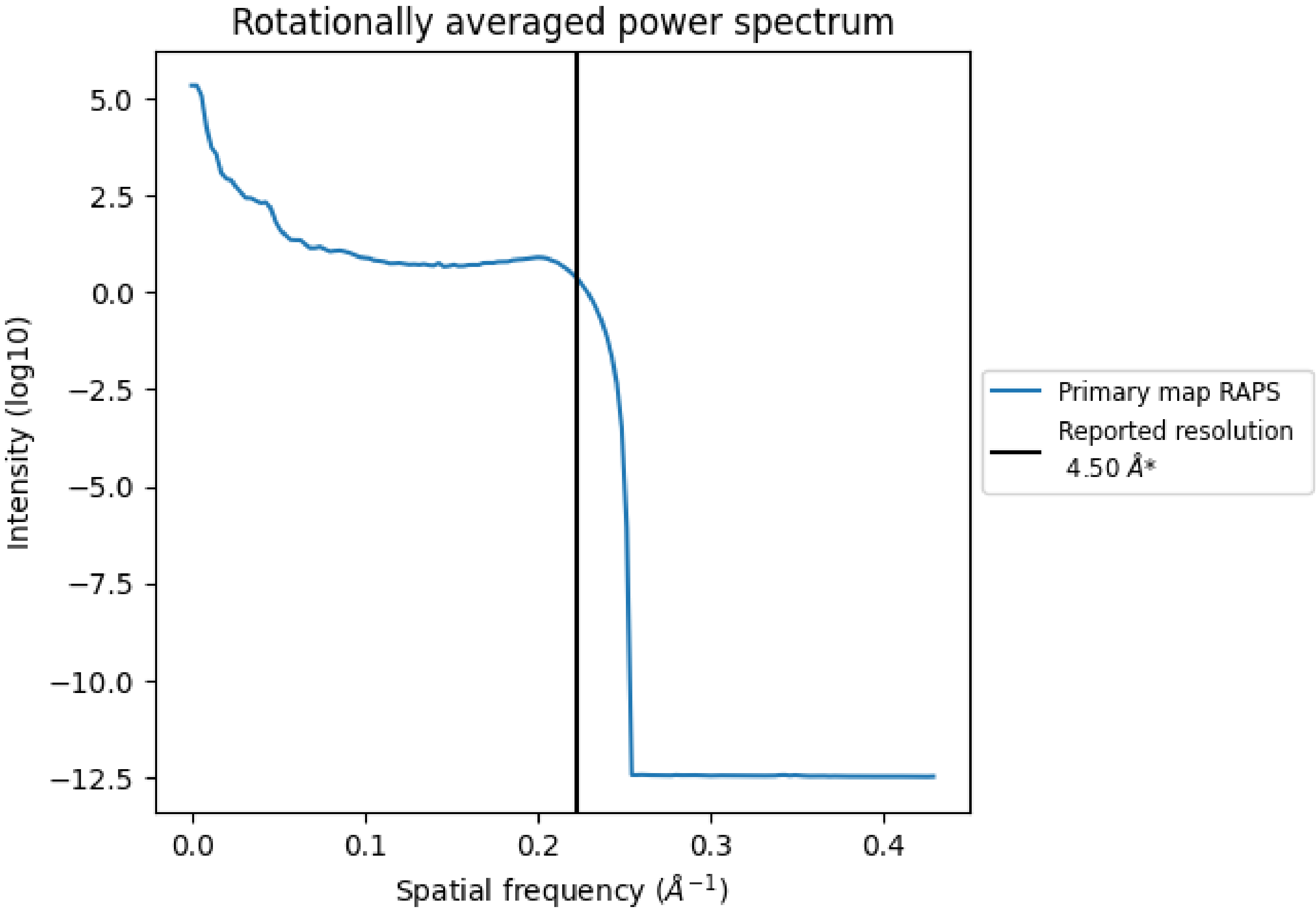
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 869 nm^3; this corresponds to an approximate mass of 785 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 0.222 Å^{-1}

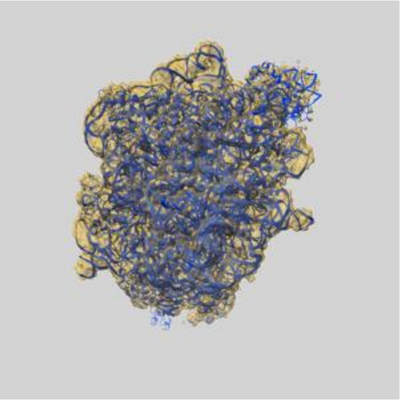
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

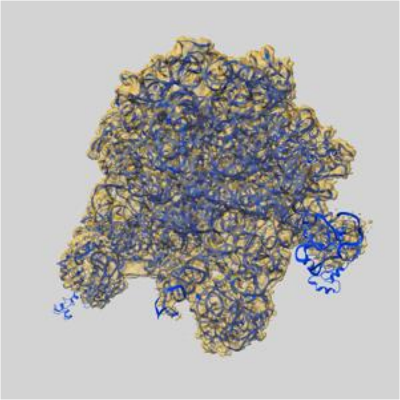
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3133 and PDB model 5ADY. Per-residue inclusion information can be found in section 3 on page 12.

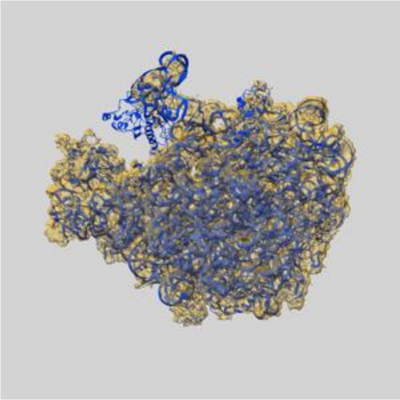
9.1 Map-model overlay ⓘ



X



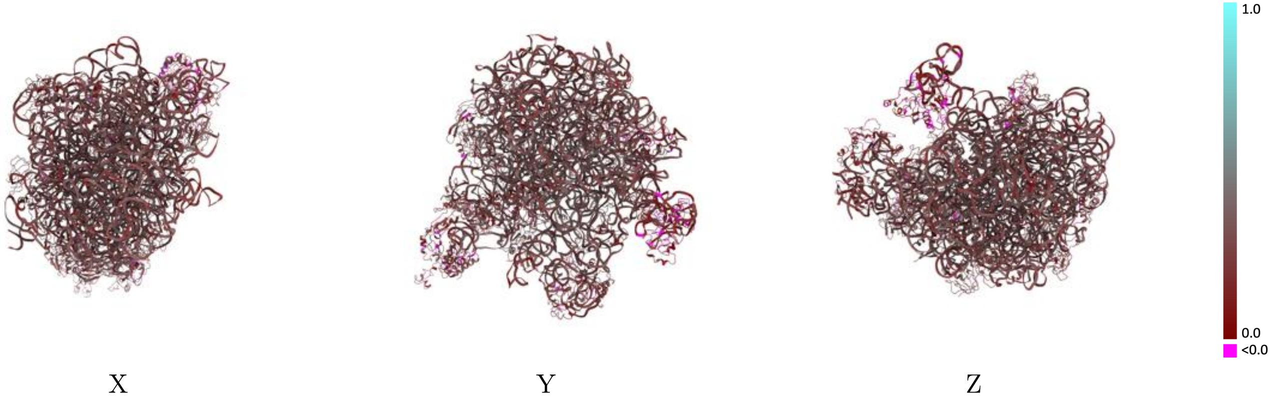
Y



Z

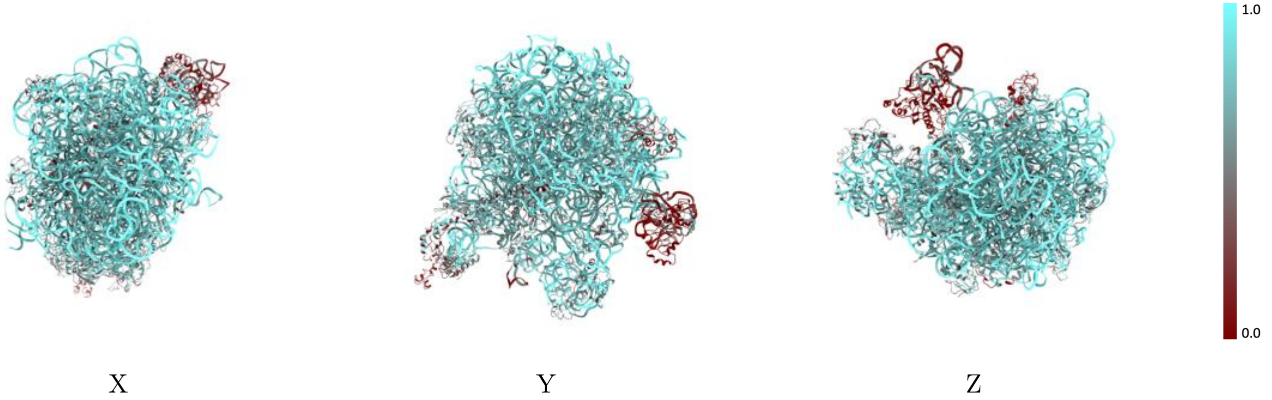
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



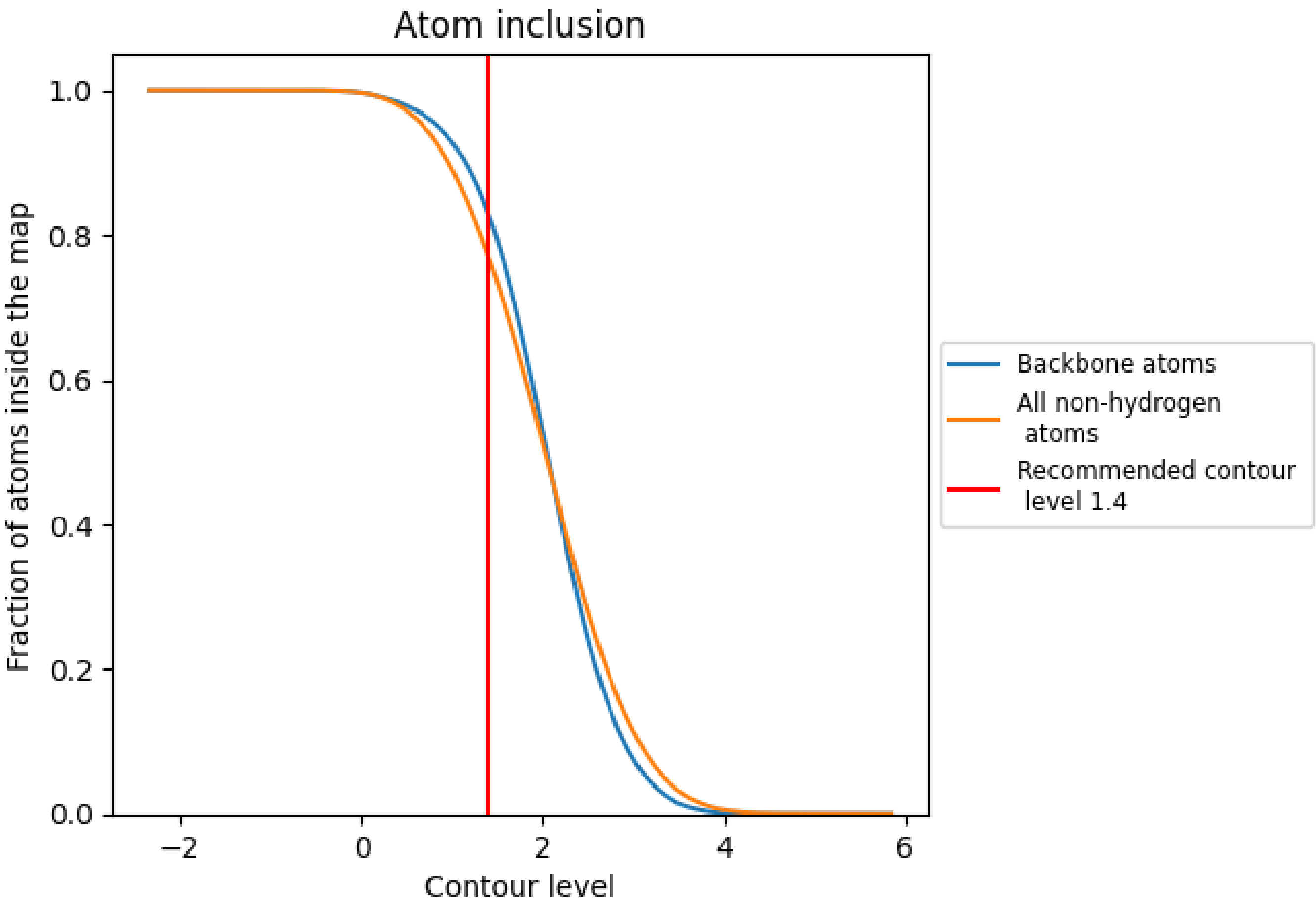
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (1.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 77% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7713	0.2890
0	0.6659	0.2990
1	0.5423	0.2310
2	0.6254	0.2920
3	0.6354	0.3150
4	0.6233	0.2650
5	0.0556	0.1520
6	0.5357	0.2530
7	0.2292	0.2080
A	0.8954	0.2860
B	0.8722	0.3020
C	0.6842	0.2940
D	0.6632	0.2870
E	0.5539	0.2820
F	0.5944	0.2280
G	0.6168	0.2780
H	0.2263	0.2040
I	0.4873	0.2160
J	0.6164	0.2920
K	0.6413	0.2870
L	0.6683	0.3000
M	0.6612	0.3040
N	0.6869	0.2840
O	0.6964	0.2500
P	0.6329	0.2850
Q	0.6762	0.2910
R	0.6688	0.2970
S	0.6304	0.2850
T	0.6584	0.2900
U	0.6471	0.2460
V	0.6301	0.2810
W	0.6190	0.2700
X	0.6290	0.2970
Y	0.6620	0.2380
Z	0.6156	0.3110