



wwPDB EM Validation Summary Report ⓘ

Feb 5, 2024 – 02:06 PM EST

PDB ID : 8G38
EMDB ID : EMD-29689
Title : Time-resolved cryo-EM study of the 70S recycling by the HflX:3rd Intermediate
Authors : Bhattacharjee, S.; Brown, P.Z.; Frank, J.
Deposited on : 2023-02-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), 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) : 2.36

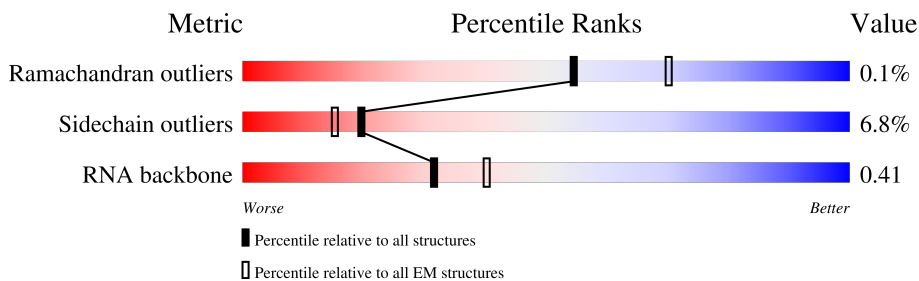
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	51	
3	2	46	
4	3	64	
5	4	38	
6	A	117	
7	B	2903	
8	C	272	

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Mol	Chain	Length	Quality of chain
9	D	209	12% 98%
10	E	201	30% 99%
11	F	178	99% 94% 6%
12	G	176	66% 95% 5%
13	J	142	16% 96%
14	K	122	20% 97%
15	L	143	20% 99%
16	M	136	12% 94% 6%
17	N	121	96% ..
18	O	116	51% 95% 5%
19	P	114	25% 93% 7%
20	Q	117	15% 97% .
21	R	103	21% 93% 7%
22	S	110	18% 95% 5%
23	T	94	26% 90% 10%
24	U	103	33% 89% 11%
25	V	94	33% 90% 10%
26	W	79	33% 92% 6% .
27	X	77	13% 96% .
28	Y	63	32% 98% .
29	Z	58	19% 95% 5%
30	w	218	88% 93% 7%
31	x	206	22% 95% 5%
32	c	205	24% 94% 6%
33	d	150	10% 95% 5%

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Mol	Chain	Length	Quality of chain
34	e	100	40% 98%
35	f	151	50% 97%
36	g	129	5% 99%
37	h	127	30% 94% 5%
38	i	98	48% 98%
39	j	117	44% 91% 9%
40	k	123	20% 98%
41	l	114	45% 90% 9%
42	m	100	15% 90% 6%
43	n	88	20% 94% 6%
44	o	82	16% 98%
45	p	80	25% 99%
46	q	55	15% 98%
47	r	79	20% 97%
48	s	85	18% 96%
49	t	51	90% 92% 8%
50	u	59	100% 93% 7%
51	v	1539	13% 61% 34% 5%
52	6	426	71% 61% 39%

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	GTP	6	501	X	-	-	-

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 144290 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 RNA chain called 5S.

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

- Molecule 7 is a RNA chain called 23S.

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

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

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

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

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called Ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	w	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	x	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 32 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 33 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 34 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	151	1182	735	227	216	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S8.

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

- Molecule 37 is a protein called 30S ribosomal protein S9.

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

- Molecule 38 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	98	787	493	150	143	1	0	0

- Molecule 39 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	j	117	877	540	174	160	3	0	0

- Molecule 40 is a protein called 30S ribosomal protein S12.

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

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	114	884	546	178	157	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 43 is a protein called 30S ribosomal protein S15.

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

- Molecule 44 is a protein called 30S ribosomal protein S16.

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

- Molecule 45 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	q	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 47 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 48 is a protein called 30S ribosomal protein S20.

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

- Molecule 49 is a protein called 30S ribosomal protein S21 (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	t	51	426	265	86	74	1	0	0

- Molecule 50 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	u	59	468	297	78	92	1	0	0

- Molecule 51 is a RNA chain called 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	v	1539	33012	14725	6052	10697	1538	0	0

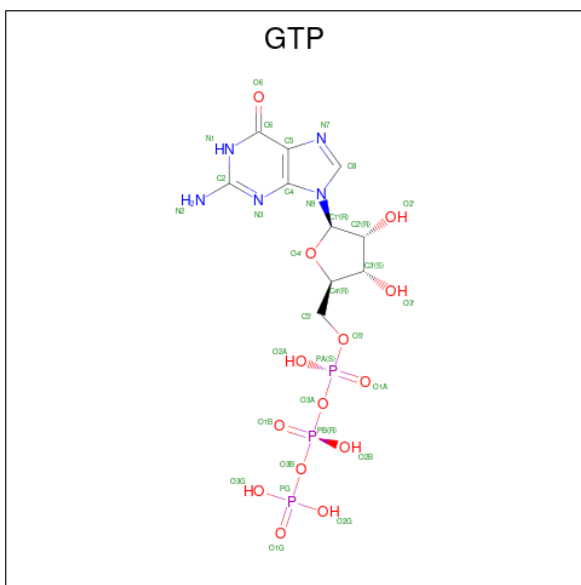
- Molecule 52 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	6	426	3403	2129	624	641	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	338	ASN	ILE	conflict	UNP C3SG37

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	6	1	32	10	5	14	3	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
54	6	1	1	1	0

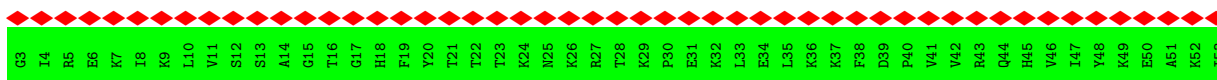
3 Residue-property plots [i](#)

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

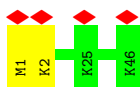
- Molecule 1: 50S ribosomal protein L32



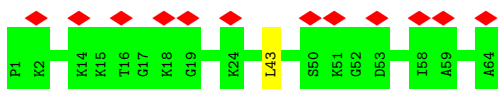
- Molecule 2: 50S ribosomal protein L33



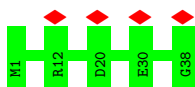
- Molecule 3: 50S ribosomal protein L34



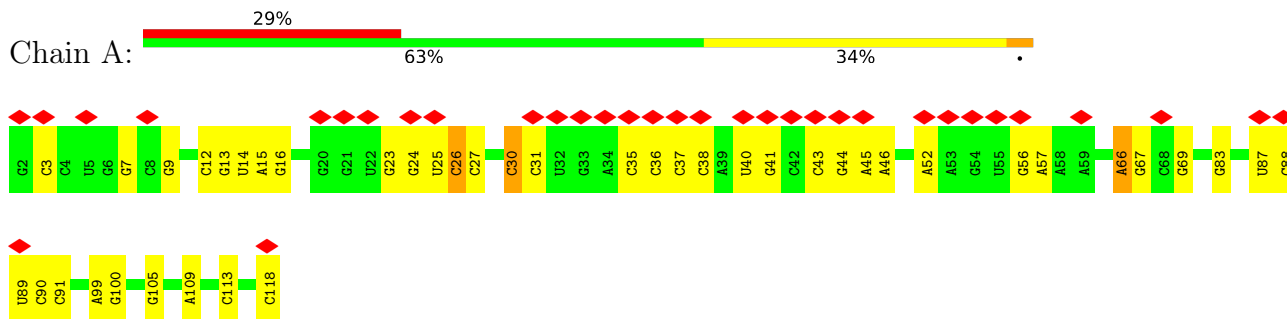
- Molecule 4: 50S ribosomal protein L35



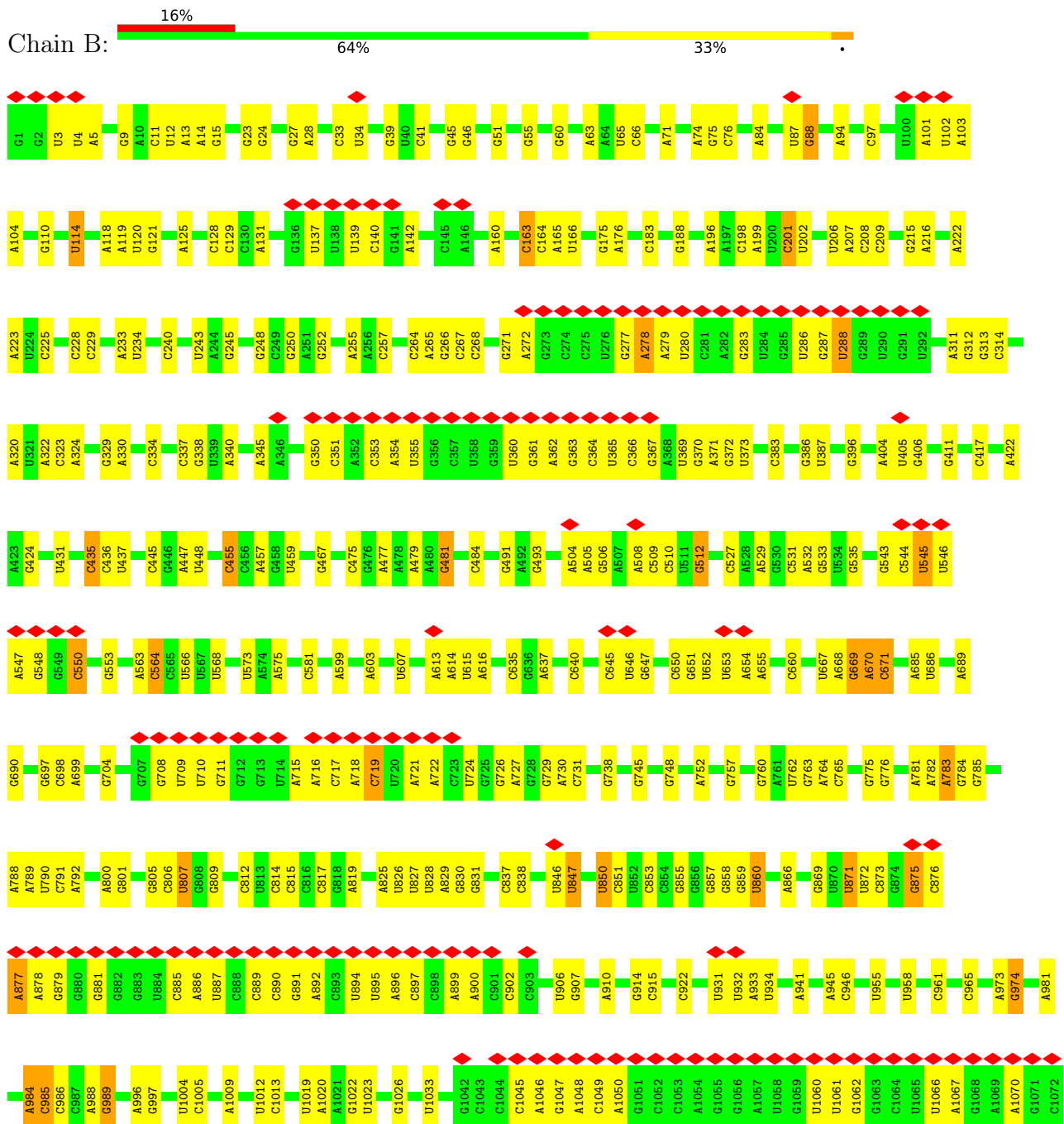
- Molecule 5: 50S ribosomal protein L36

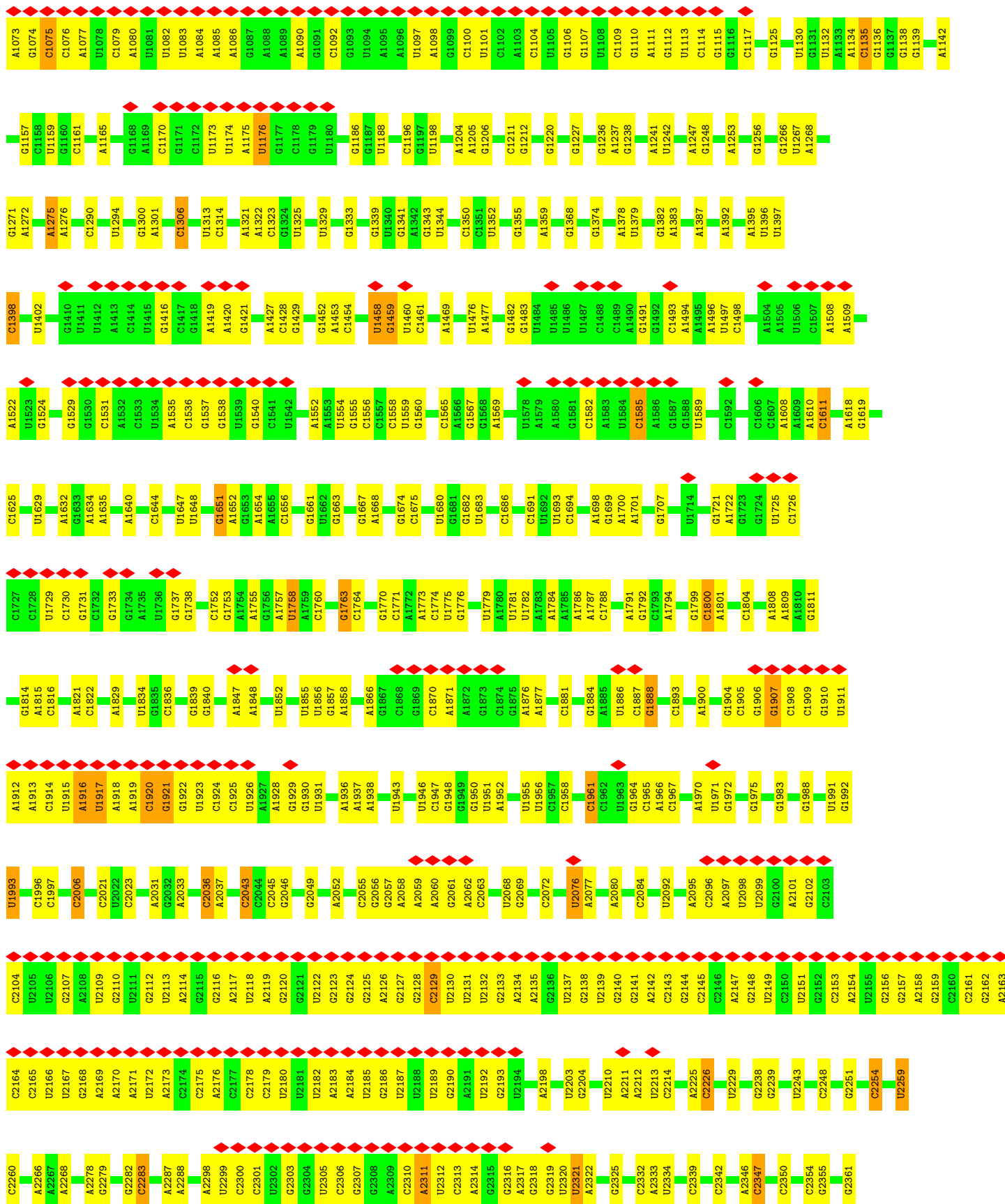


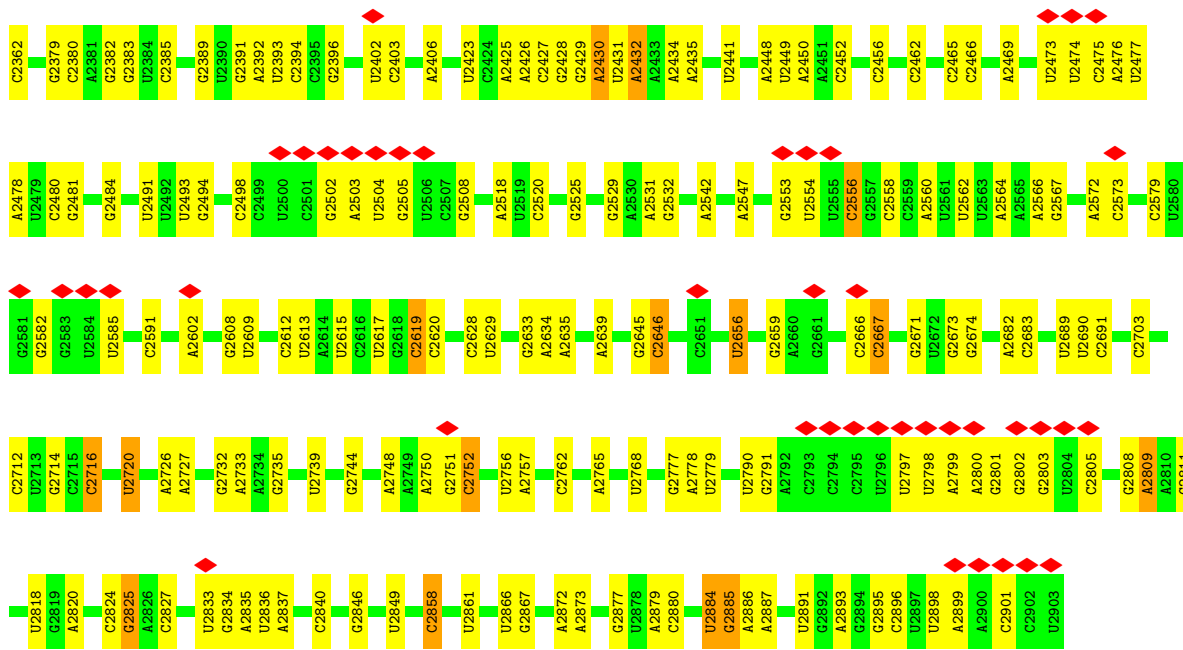
• Molecule 6: 5S



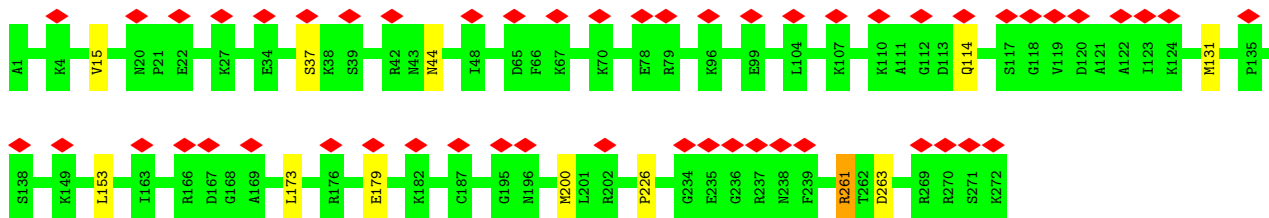
• Molecule 7: 23S



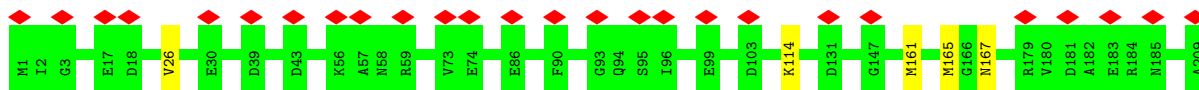




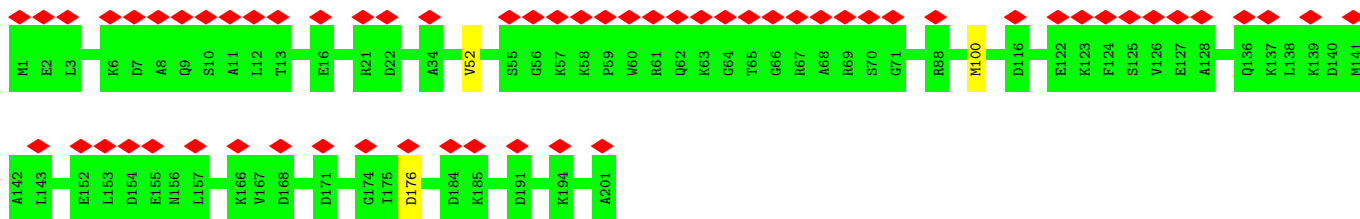
• Molecule 8: 50S ribosomal protein L2



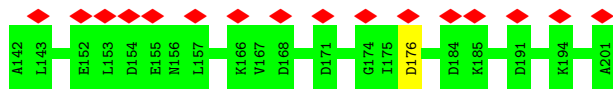
• Molecule 9: 50S ribosomal protein L3

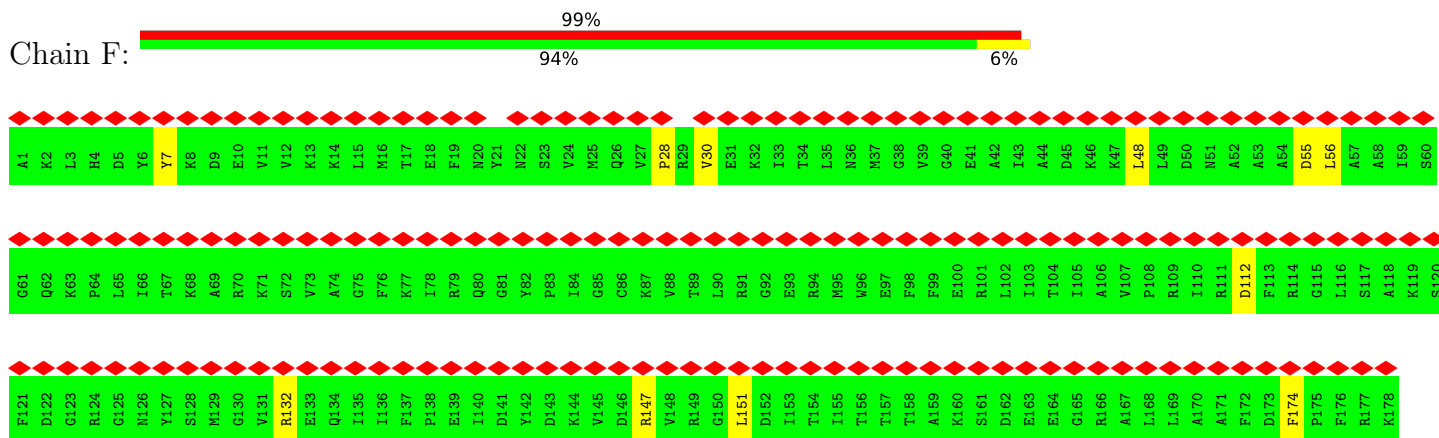


• Molecule 10: 50S ribosomal protein L4

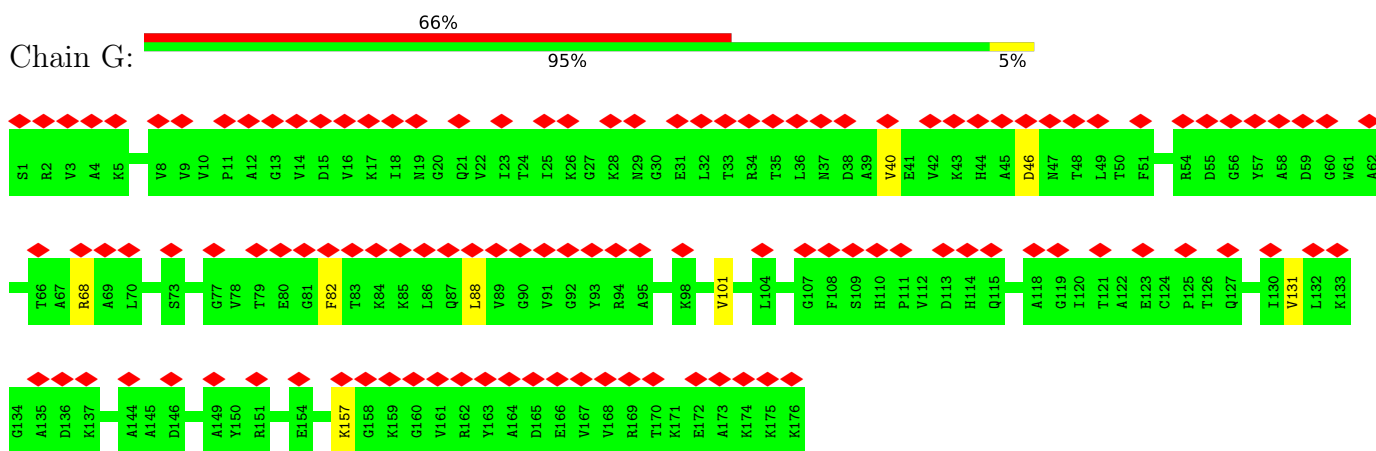


• Molecule 11: 50S ribosomal protein L5

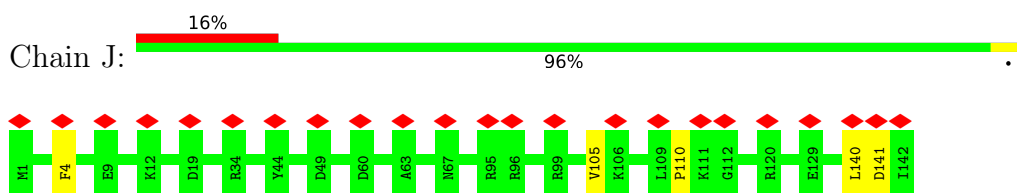




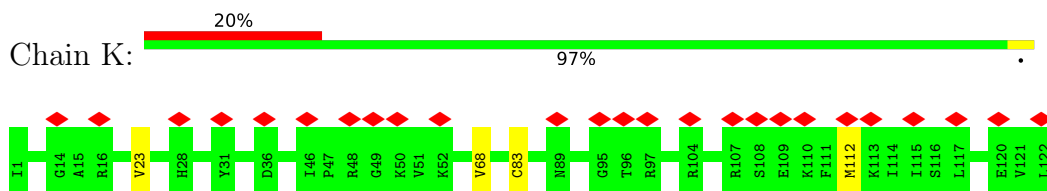
• Molecule 12: 50S ribosomal protein L6



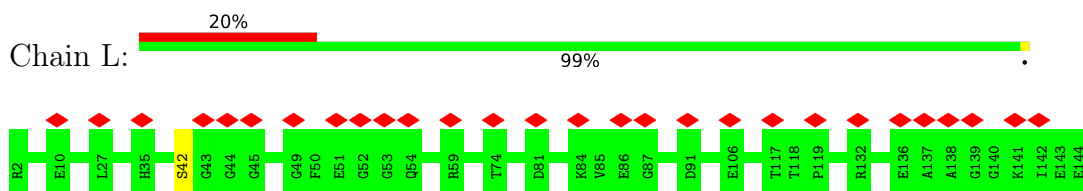
• Molecule 13: 50S ribosomal protein L13



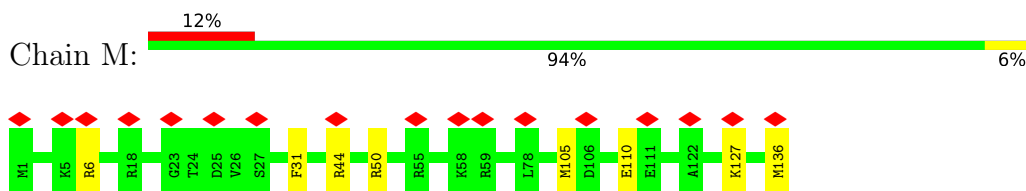
• Molecule 14: 50S ribosomal protein L14



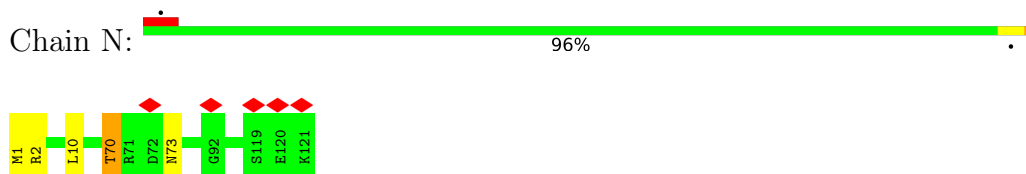
• Molecule 15: 50S ribosomal protein L15



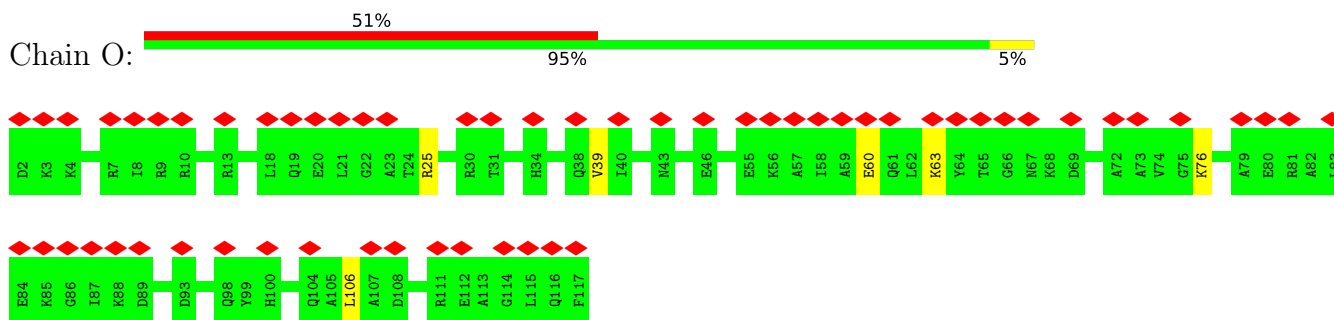
- Molecule 16: 50S ribosomal protein L16



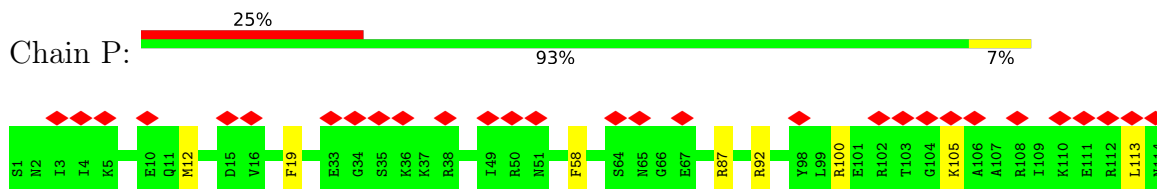
- Molecule 17: 50S ribosomal protein L17



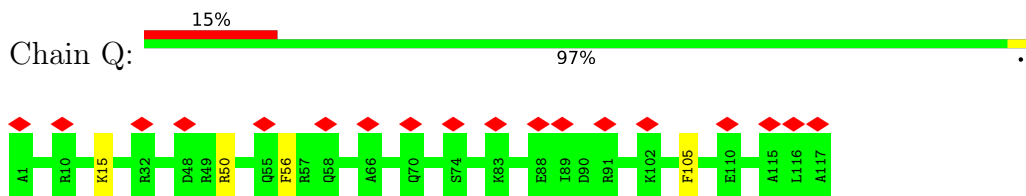
- Molecule 18: 50S ribosomal protein L18



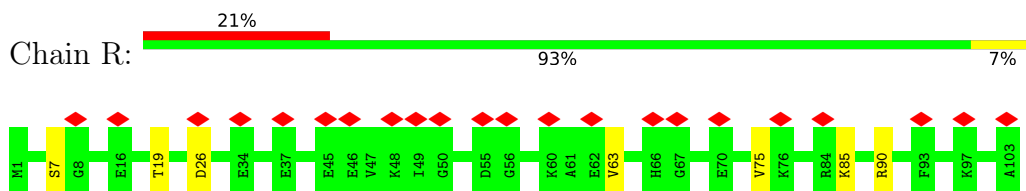
- Molecule 19: 50S ribosomal protein L19



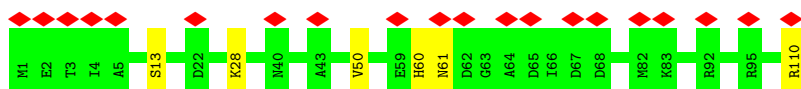
- Molecule 20: 50S ribosomal protein L20



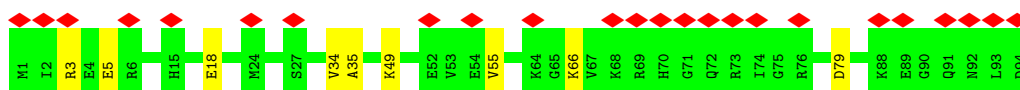
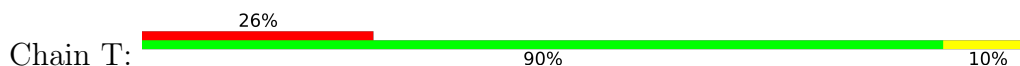
- Molecule 21: Ribosomal protein L21



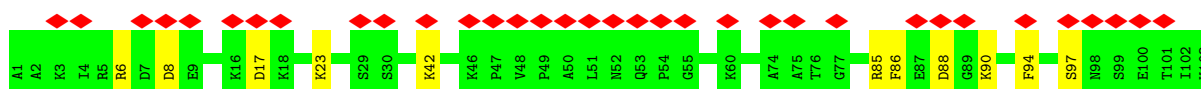
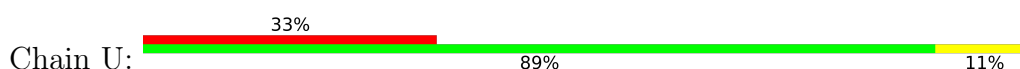
- Molecule 22: 50S ribosomal protein L22



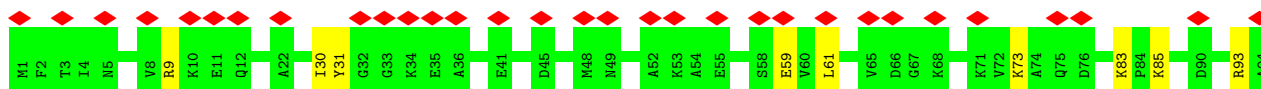
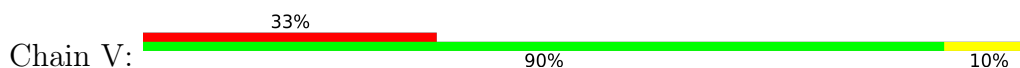
- Molecule 23: 50S ribosomal protein L23



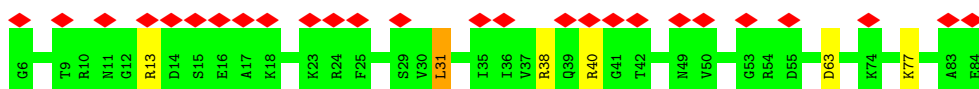
- Molecule 24: 50S ribosomal protein L24



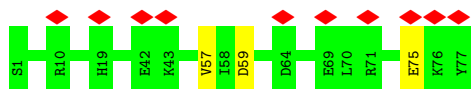
- Molecule 25: 50S ribosomal protein L25



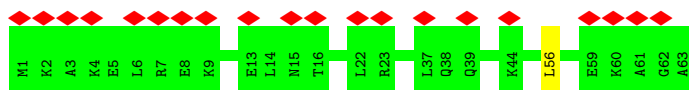
- Molecule 26: 50S ribosomal protein L27



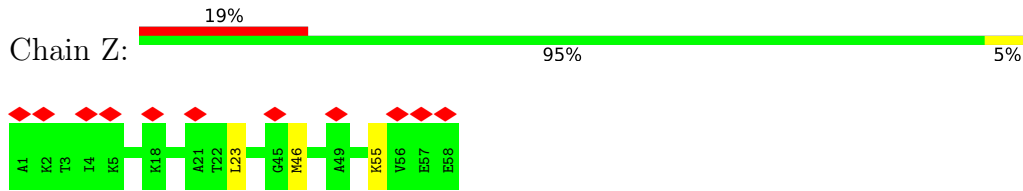
- Molecule 27: 50S ribosomal protein L28



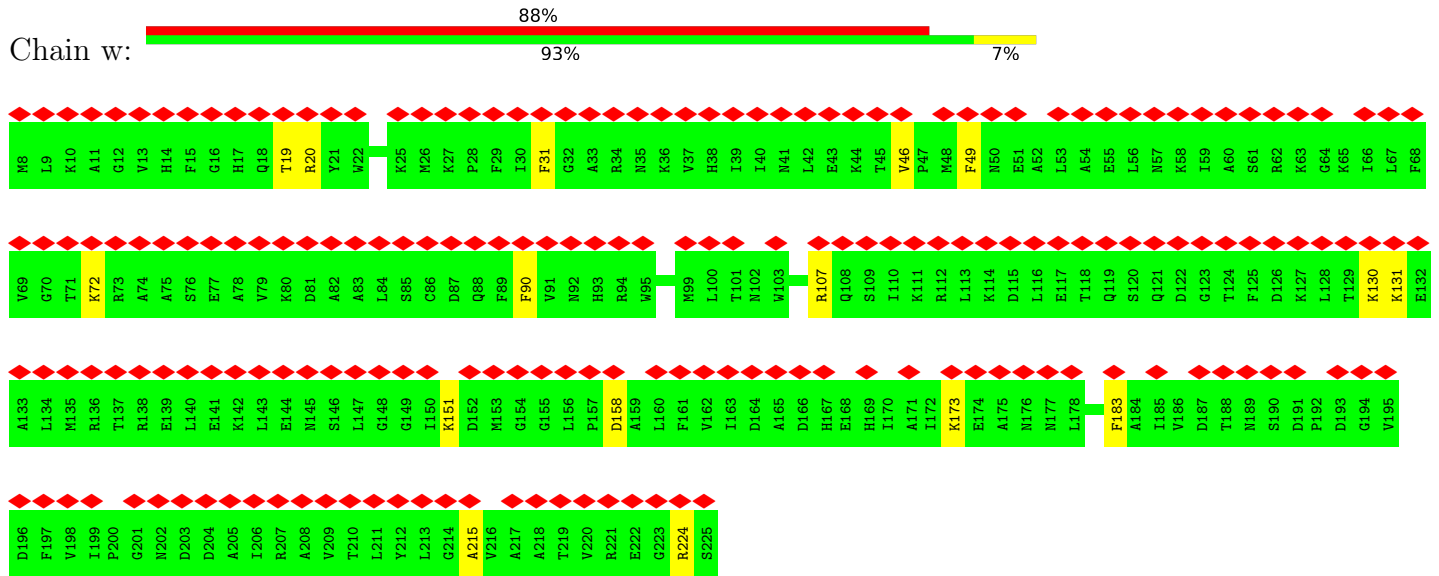
- Molecule 28: 50S ribosomal protein L29



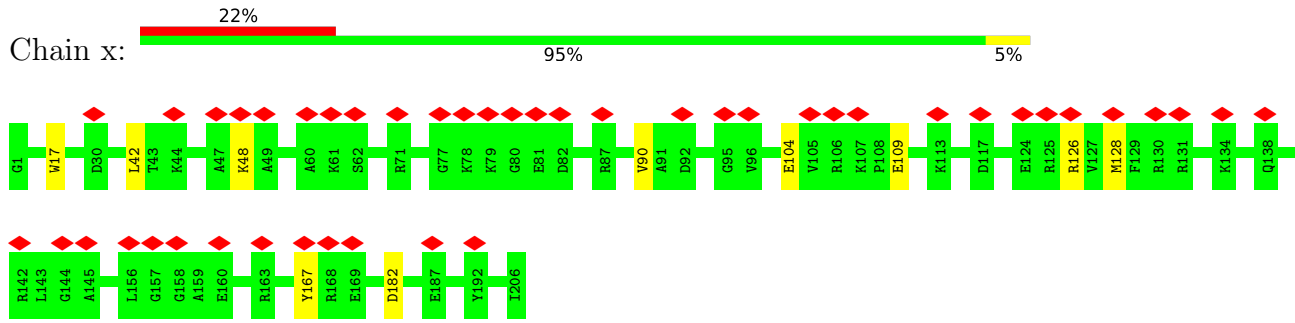
• Molecule 29: 50S ribosomal protein L30



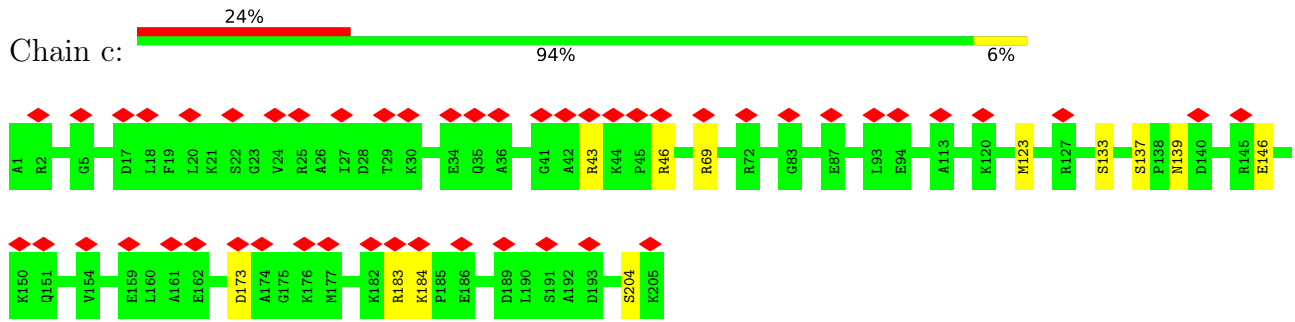
• Molecule 30: 30S ribosomal protein S2



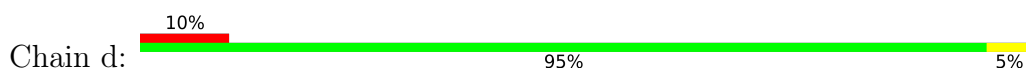
• Molecule 31: 30S ribosomal protein S3



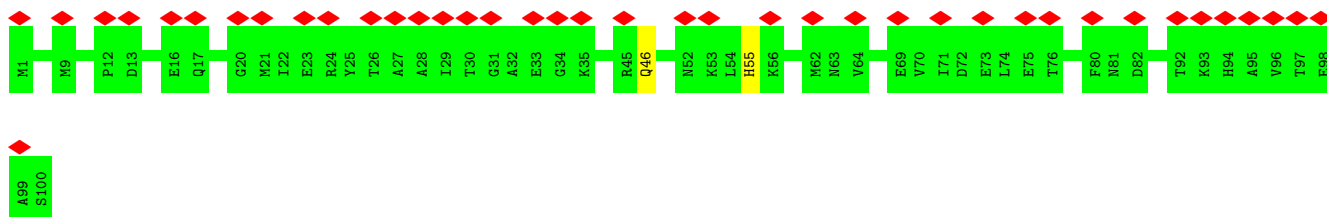
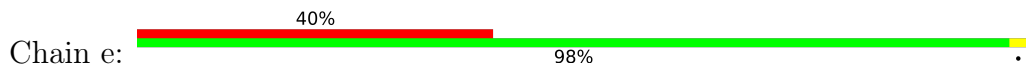
• Molecule 32: 30S ribosomal protein S4



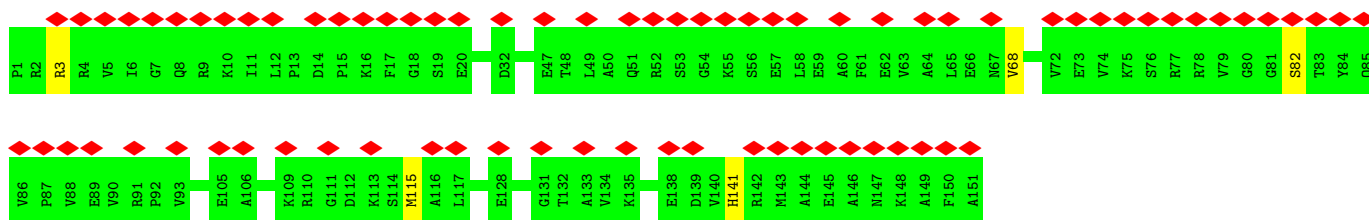
• Molecule 33: 30S ribosomal protein S5



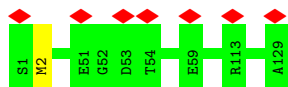
- Molecule 34: 30S ribosomal protein S6, non-modified isoform



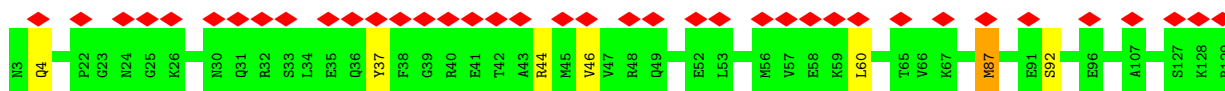
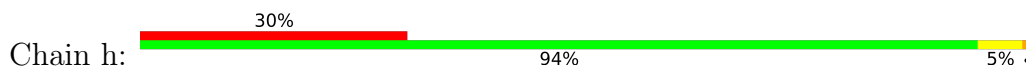
- Molecule 35: 30S ribosomal protein S7



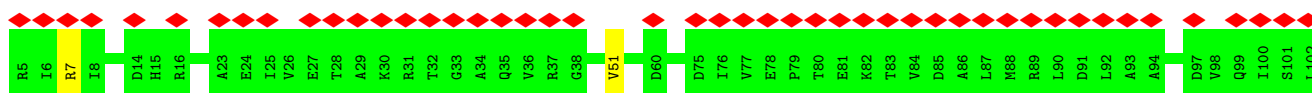
- Molecule 36: 30S ribosomal protein S8



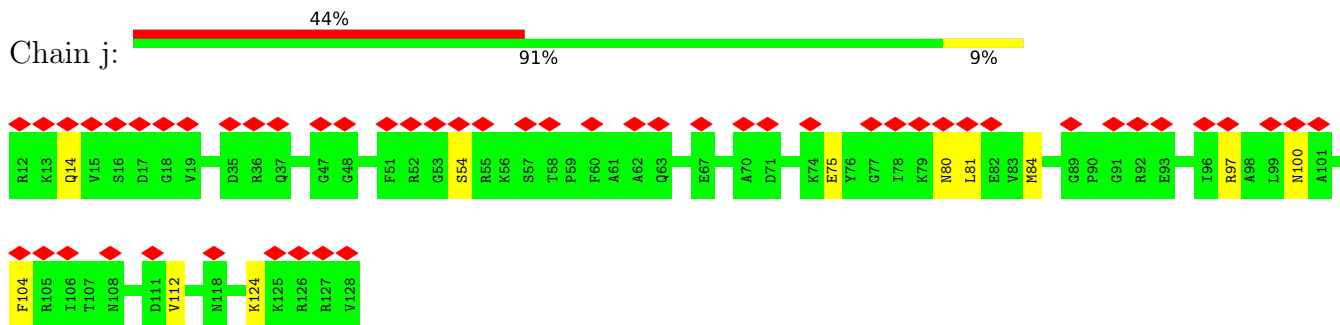
- Molecule 37: 30S ribosomal protein S9



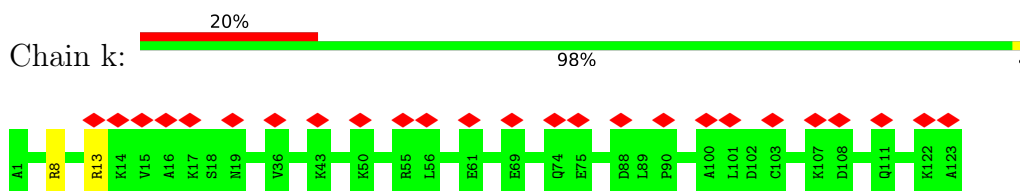
- Molecule 38: 30S ribosomal protein S10



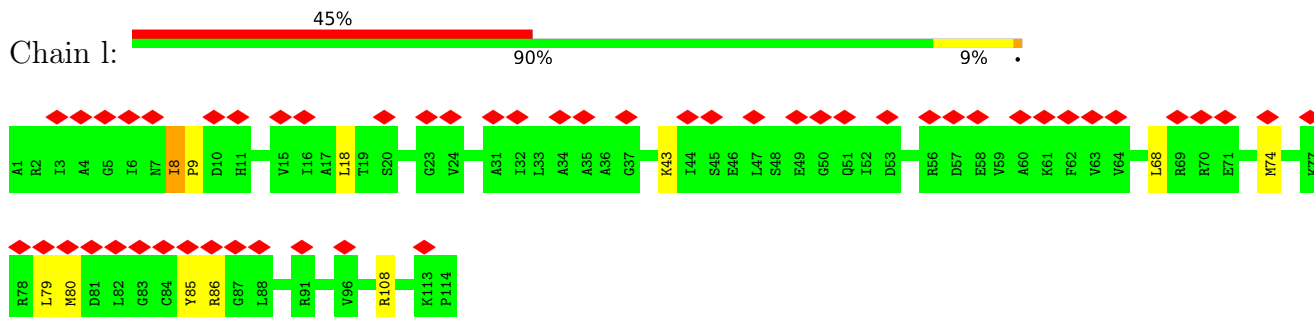
- Molecule 39: 30S ribosomal protein S11



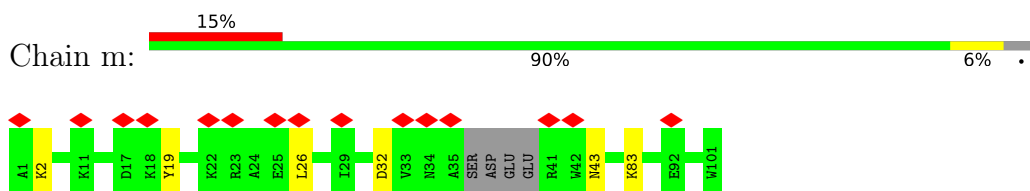
- Molecule 40: 30S ribosomal protein S12



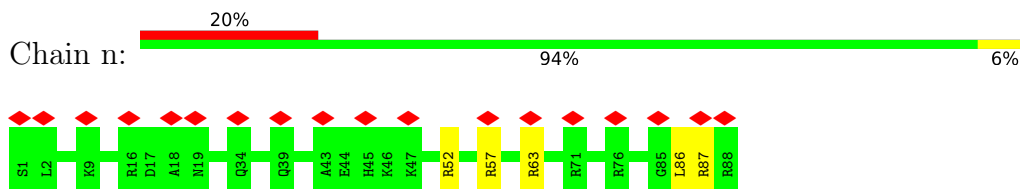
- Molecule 41: 30S ribosomal protein S13



- Molecule 42: 30S ribosomal protein S14

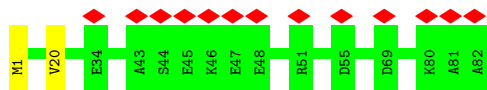


- Molecule 43: 30S ribosomal protein S15

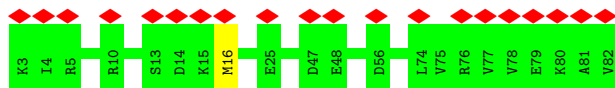


- Molecule 44: 30S ribosomal protein S16

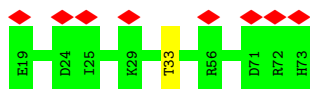




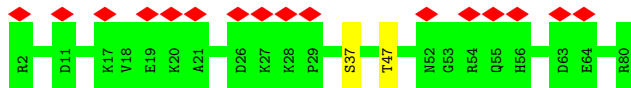
- Molecule 45: 30S ribosomal protein S17



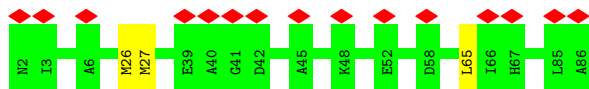
- Molecule 46: 30S ribosomal protein S18



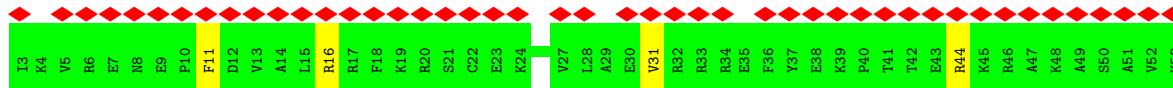
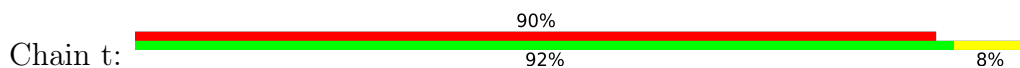
- Molecule 47: 30S ribosomal protein S19



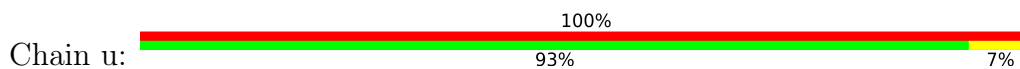
- Molecule 48: 30S ribosomal protein S20



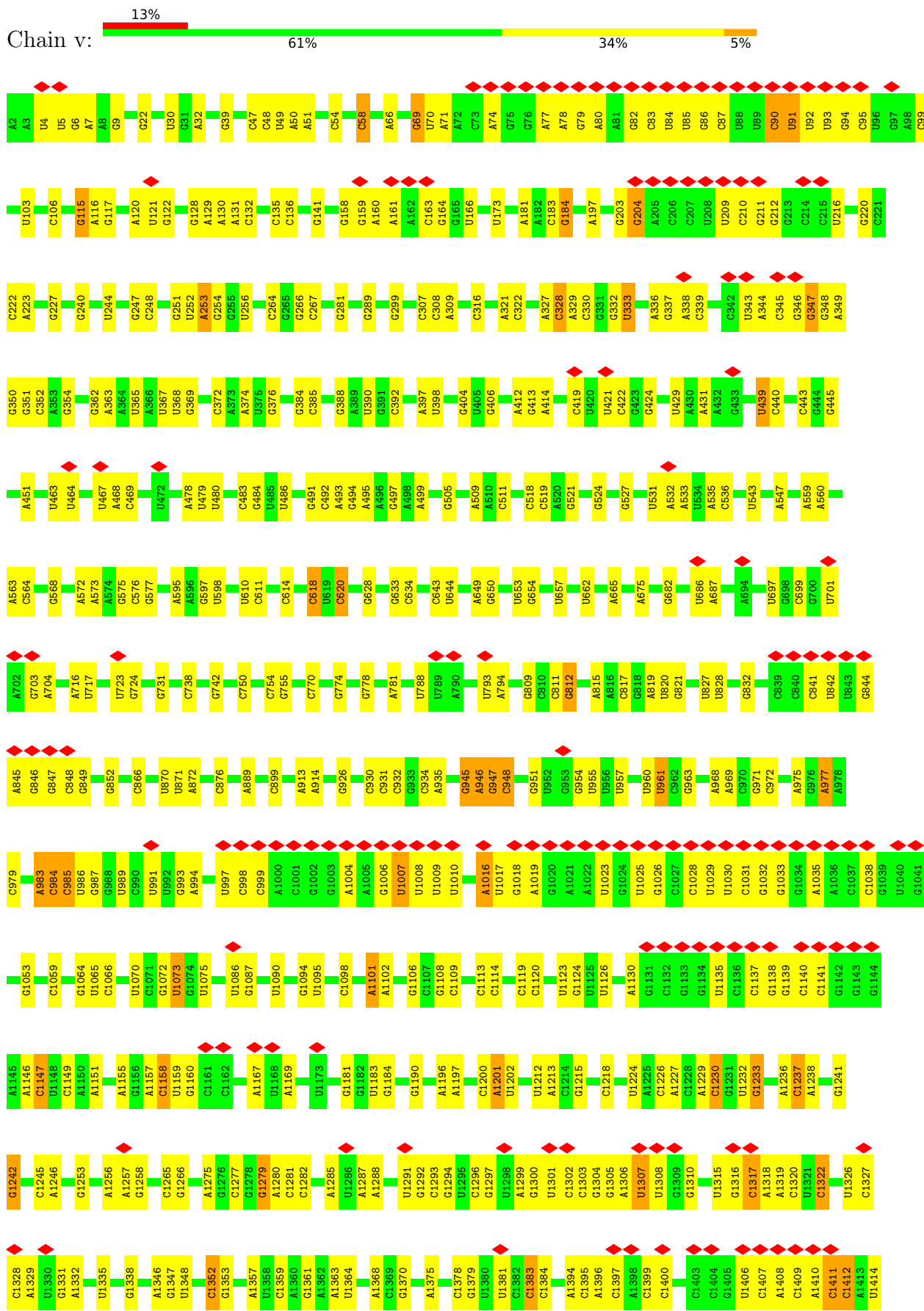
- Molecule 49: 30S ribosomal protein S21 (Fragment)

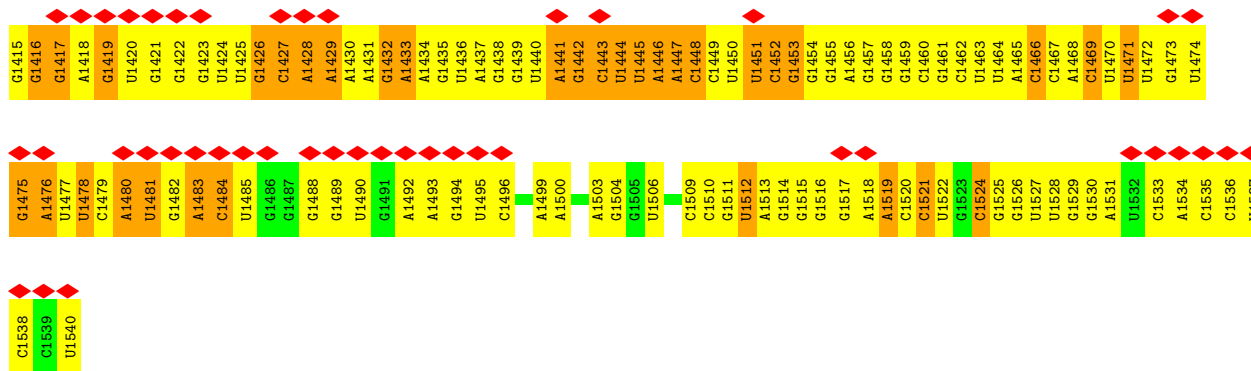


- Molecule 50: Transcription termination/antitermination protein NusG

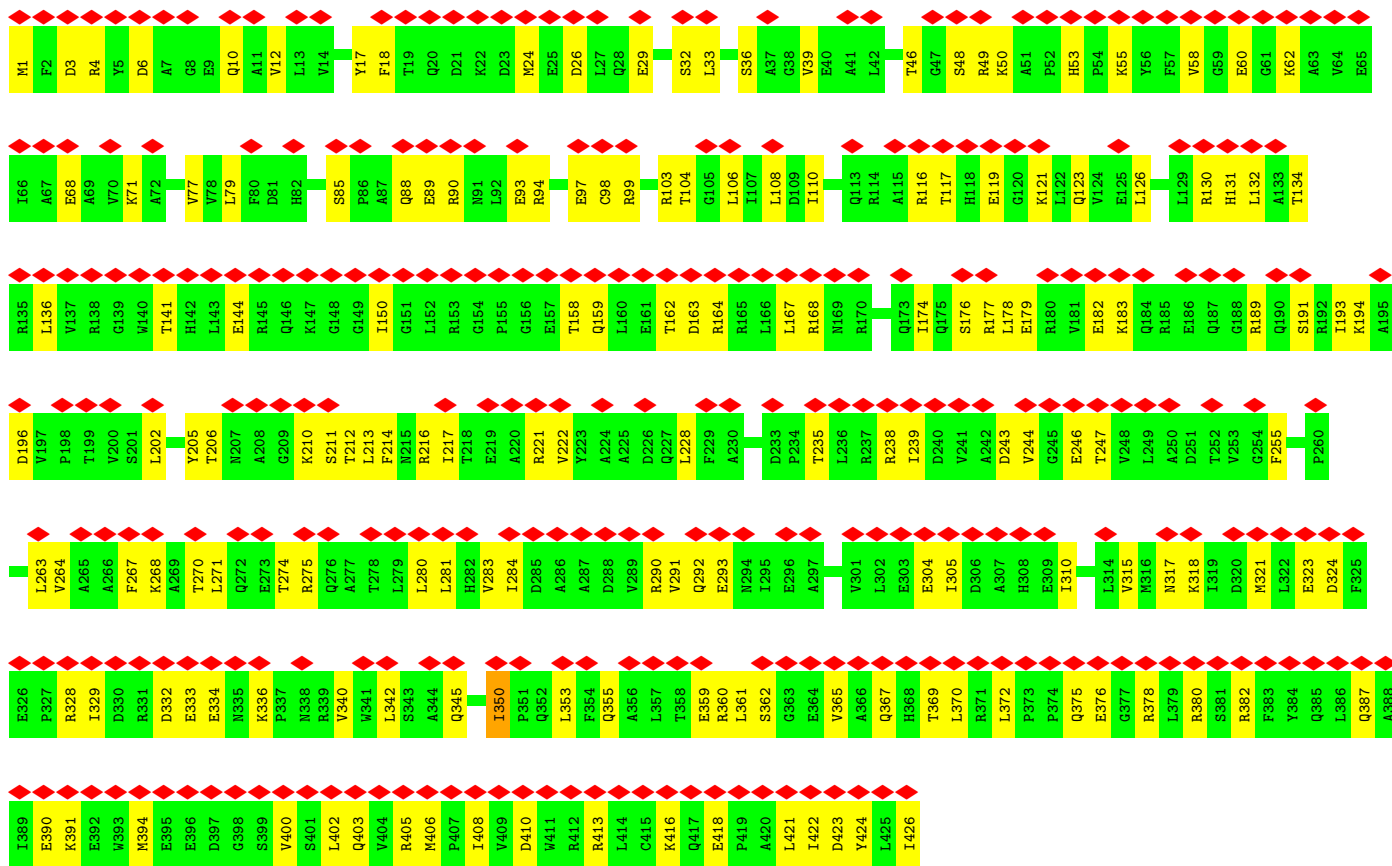


- Molecule 51: 16S





• Molecule 52: GTPase Hfx



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113038	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.404	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.163	Depositor
Map size (\AA)	348.60202, 348.60202, 348.60202	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0253, 1.0253, 1.0253	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.44	0/450	0.70	0/599
2	1	0.27	0/417	0.55	0/556
3	2	0.37	0/380	0.67	0/498
4	3	0.38	0/513	0.78	1/676 (0.1%)
5	4	0.32	0/303	0.66	0/397
6	A	0.56	0/2800	1.18	22/4367 (0.5%)
7	B	0.73	13/69795 (0.0%)	1.15	420/108884 (0.4%)
8	C	0.49	1/2122 (0.0%)	0.77	7/2854 (0.2%)
9	D	0.47	0/1586	0.75	4/2134 (0.2%)
10	E	0.47	1/1571 (0.1%)	0.70	2/2113 (0.1%)
11	F	0.52	2/1444 (0.1%)	0.83	4/1937 (0.2%)
12	G	0.41	0/1343	0.76	5/1816 (0.3%)
13	J	0.48	0/1152	0.70	2/1551 (0.1%)
14	K	0.52	2/940 (0.2%)	0.75	0/1260
15	L	0.41	0/1054	0.70	0/1403
16	M	0.44	0/1093	0.71	1/1460 (0.1%)
17	N	0.46	0/974	0.74	1/1303 (0.1%)
18	O	0.45	1/902 (0.1%)	0.72	1/1209 (0.1%)
19	P	0.49	0/929	0.87	4/1242 (0.3%)
20	Q	0.45	0/960	0.62	0/1278
21	R	0.60	2/829 (0.2%)	0.74	1/1107 (0.1%)
22	S	0.41	1/864 (0.1%)	0.66	1/1156 (0.1%)
23	T	0.65	2/745 (0.3%)	0.75	0/996
24	U	0.43	0/788	0.73	1/1053 (0.1%)
25	V	0.52	0/766	0.80	4/1025 (0.4%)
26	W	0.50	0/603	0.79	1/797 (0.1%)
27	X	0.39	0/635	0.73	2/848 (0.2%)
28	Y	0.40	0/510	0.82	1/677 (0.1%)
29	Z	0.40	0/453	0.89	2/605 (0.3%)
30	w	0.40	1/1736 (0.1%)	0.71	4/2338 (0.2%)
31	x	0.55	1/1652 (0.1%)	0.86	7/2225 (0.3%)
32	c	0.45	0/1664	0.70	2/2225 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.49	1/1119 (0.1%)	0.74	3/1504 (0.2%)
34	e	0.44	0/836	0.80	0/1128
35	f	0.45	0/1196	0.69	1/1602 (0.1%)
36	g	0.48	0/989	0.67	0/1326
37	h	0.47	1/1034 (0.1%)	0.88	3/1375 (0.2%)
38	i	0.46	1/797 (0.1%)	0.74	1/1077 (0.1%)
39	j	0.52	3/893 (0.3%)	0.77	1/1205 (0.1%)
40	k	0.42	0/969	0.73	0/1300
41	l	1.38	2/893 (0.2%)	1.37	10/1193 (0.8%)
42	m	0.41	0/785	0.72	1/1043 (0.1%)
43	n	0.37	0/722	0.68	1/964 (0.1%)
44	o	0.48	1/659 (0.2%)	0.71	1/884 (0.1%)
45	p	0.37	0/658	0.73	1/881 (0.1%)
46	q	0.41	0/463	0.71	1/621 (0.2%)
47	r	0.42	0/653	0.69	0/877
48	s	0.42	0/671	0.66	1/888 (0.1%)
49	t	0.42	0/431	0.85	1/570 (0.2%)
50	u	0.29	0/477	0.55	0/642
51	v	0.74	1/36963 (0.0%)	1.20	312/57662 (0.5%)
52	6	0.61	0/3456	0.75	0/4675
All	All	0.67	37/156637 (0.0%)	1.07	838/234006 (0.4%)

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
8	C	0	1
23	T	0	1
26	W	0	1
41	l	0	1
All	All	0	4

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	l	9	PRO	CG-CD	-33.73	0.39	1.50
41	l	9	PRO	CB-CG	17.60	2.38	1.50
8	C	179	GLU	CD-OE1	-10.36	1.14	1.25
31	x	109	GLU	CD-OE1	-9.88	1.14	1.25
23	T	5	GLU	CG-CD	-8.54	1.39	1.51

The worst 5 of 838 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	l	9	PRO	CB-CG-CD	-27.25	0.24	106.50
7	B	1799	G	N7-C8-N9	21.88	124.04	113.10
7	B	137	U	N3-C2-O2	-18.79	109.05	122.20
51	v	932	C	OP1-P-OP2	-18.60	91.70	119.60
7	B	807	U	C4-C5-C6	17.46	130.18	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	C	261	ARG	Sidechain
23	T	34	VAL	Peptide
26	W	38	ARG	Sidechain
41	l	8	ILE	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
2	1	49/51 (96%)	49 (100%)	0	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
5	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	C	270/272 (99%)	265 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
10	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
11	F	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
12	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
13	J	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	61
14	K	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
15	L	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
16	M	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
17	N	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	19	58
18	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
19	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
20	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
21	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	S	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
23	T	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	14	51
24	U	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
25	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
26	W	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
27	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
28	Y	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	w	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
31	x	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
32	c	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
33	d	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
34	e	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
35	f	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
36	g	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
37	h	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
38	i	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
39	j	115/117 (98%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
41	l	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
42	m	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
43	n	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
44	o	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
45	p	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
46	q	53/55 (96%)	53 (100%)	0	0	100	100
47	r	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
48	s	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
49	t	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
50	u	57/59 (97%)	57 (100%)	0	0	100	100
52	6	424/426 (100%)	411 (97%)	12 (3%)	1 (0%)	47	79
All	All	5822/5926 (98%)	5619 (96%)	199 (3%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	N	70	THR
23	T	35	ALA
52	6	350	ILE
13	J	110	PRO

5.3.2 Protein sidechains [i](#)

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	47/47 (100%)	44 (94%)	3 (6%)	17	52
2	1	45/46 (98%)	45 (100%)	0	100	100
3	2	38/38 (100%)	36 (95%)	2 (5%)	22	58
4	3	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	34/34 (100%)	34 (100%)	0	100	100
8	C	216/217 (100%)	211 (98%)	5 (2%)	50	78
9	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
10	E	165/165 (100%)	165 (100%)	0	100	100
11	F	149/149 (100%)	141 (95%)	8 (5%)	22	58
12	G	137/137 (100%)	134 (98%)	3 (2%)	52	79
13	J	116/116 (100%)	114 (98%)	2 (2%)	60	83
14	K	102/103 (99%)	100 (98%)	2 (2%)	55	80
15	L	102/102 (100%)	101 (99%)	1 (1%)	76	90
16	M	109/109 (100%)	102 (94%)	7 (6%)	17	52
17	N	100/101 (99%)	96 (96%)	4 (4%)	31	66
18	O	86/86 (100%)	82 (95%)	4 (5%)	26	62
19	P	99/99 (100%)	94 (95%)	5 (5%)	24	60
20	Q	89/89 (100%)	85 (96%)	4 (4%)	27	63
21	R	84/84 (100%)	80 (95%)	4 (5%)	25	61
22	S	93/93 (100%)	89 (96%)	4 (4%)	29	64
23	T	80/81 (99%)	75 (94%)	5 (6%)	18	52
24	U	83/84 (99%)	73 (88%)	10 (12%)	5	22
25	V	78/78 (100%)	73 (94%)	5 (6%)	17	52
26	W	59/59 (100%)	54 (92%)	5 (8%)	10	38
27	X	67/67 (100%)	66 (98%)	1 (2%)	65	85
28	Y	55/55 (100%)	55 (100%)	0	100	100
29	Z	48/48 (100%)	47 (98%)	1 (2%)	53	79
30	w	180/180 (100%)	168 (93%)	12 (7%)	16	50
31	x	170/170 (100%)	165 (97%)	5 (3%)	42	74
32	c	172/172 (100%)	162 (94%)	10 (6%)	20	55
33	d	113/113 (100%)	108 (96%)	5 (4%)	28	64
34	e	87/87 (100%)	85 (98%)	2 (2%)	50	78
35	f	124/124 (100%)	120 (97%)	4 (3%)	39	71
36	g	104/104 (100%)	103 (99%)	1 (1%)	76	90
37	h	105/105 (100%)	100 (95%)	5 (5%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	i	86/86 (100%)	85 (99%)	1 (1%)	71	88
39	j	90/90 (100%)	81 (90%)	9 (10%)	7	30
40	k	103/103 (100%)	101 (98%)	2 (2%)	57	81
41	l	92/92 (100%)	88 (96%)	4 (4%)	29	64
42	m	79/83 (95%)	74 (94%)	5 (6%)	18	52
43	n	76/76 (100%)	72 (95%)	4 (5%)	22	58
44	o	65/65 (100%)	65 (100%)	0	100	100
45	p	74/74 (100%)	74 (100%)	0	100	100
46	q	48/48 (100%)	48 (100%)	0	100	100
47	r	70/70 (100%)	68 (97%)	2 (3%)	42	74
48	s	65/65 (100%)	63 (97%)	2 (3%)	40	72
49	t	44/44 (100%)	41 (93%)	3 (7%)	16	49
50	u	52/52 (100%)	48 (92%)	4 (8%)	13	44
52	6	364/364 (100%)	198 (54%)	166 (46%)	0	0
All	All	4859/4869 (100%)	4527 (93%)	332 (7%)	19	49

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	6	177	ARG
52	6	324	ASP
52	6	193	ILE
52	6	247	THR
52	6	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
38	i	58	ASN
52	6	299	ASN
40	k	58	ASN
52	6	345	GLN
52	6	10	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	v	1538/1539 (99%)	476 (30%)	0
6	A	116/117 (99%)	38 (32%)	2 (1%)
7	B	2901/2903 (99%)	888 (30%)	10 (0%)
All	All	4555/4559 (99%)	1402 (30%)	12 (0%)

5 of 1402 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	3	C
6	A	7	G
6	A	9	G
6	A	12	C
6	A	13	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	B	1905	C
7	B	2147	A
7	B	2808	G
7	B	2282	G
7	B	278	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GTP	6	501	-	26,34,34	1.02	2 (7%)	32,54,54	0.98	2 (6%)

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	GTP	6	501	-	1/1/7/7	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	6	501	GTP	C5-C6	-2.76	1.41	1.47
53	6	501	GTP	C8-N7	-2.23	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	6	501	GTP	PA-O3A-PB	-2.70	123.55	132.83
53	6	501	GTP	PB-O3B-PG	-2.17	125.36	132.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	6	501	GTP	C4'

5 of 6 torsion outliers are listed below:

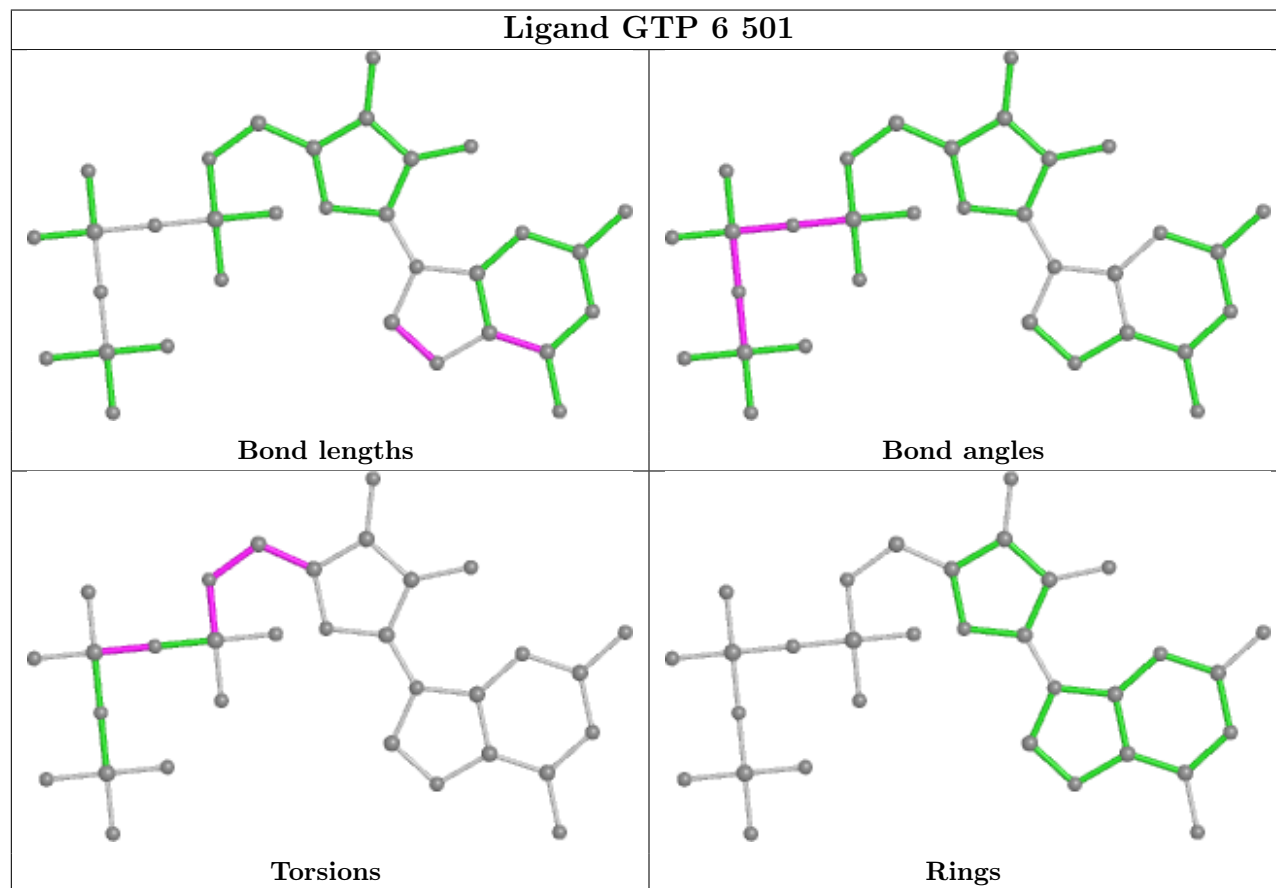
Mol	Chain	Res	Type	Atoms
53	6	501	GTP	C5'-O5'-PA-O3A
53	6	501	GTP	C5'-O5'-PA-O2A
53	6	501	GTP	O4'-C4'-C5'-O5'
53	6	501	GTP	C3'-C4'-C5'-O5'
53	6	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1902:C	O3'	1903:G	P	3.18

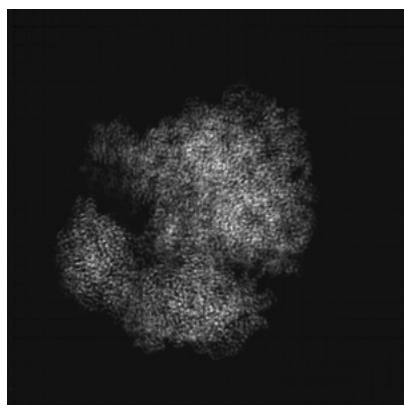
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29689. These allow visual inspection of the internal detail of the map and identification of artifacts.

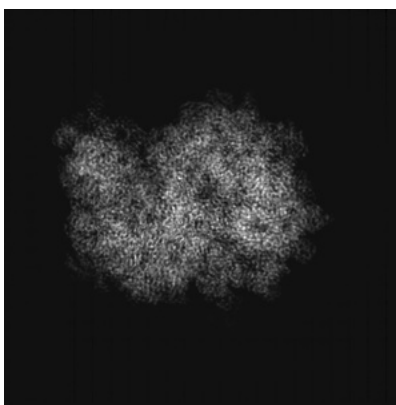
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

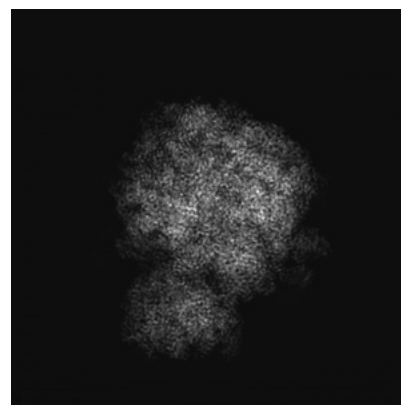
6.1.1 Primary map



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: 170



Y Index: 170



Z Index: 170

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: 157



Y Index: 164

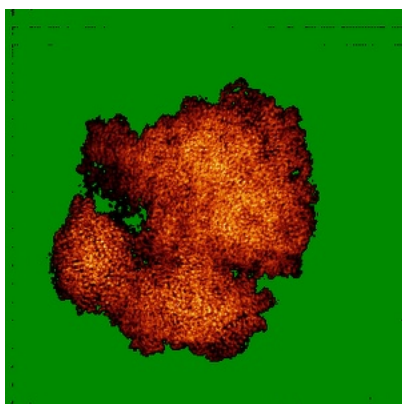


Z Index: 144

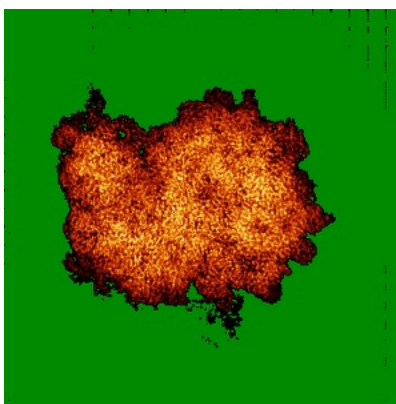
The images above show the largest variance slices of the map in three orthogonal directions.

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

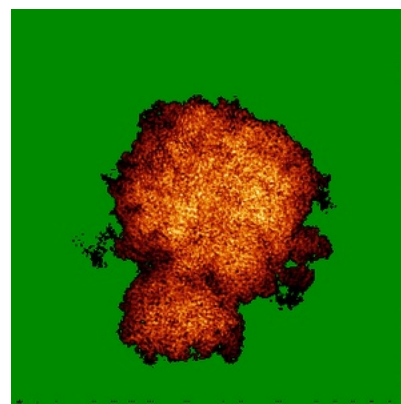
6.4.1 Primary map



X



Y

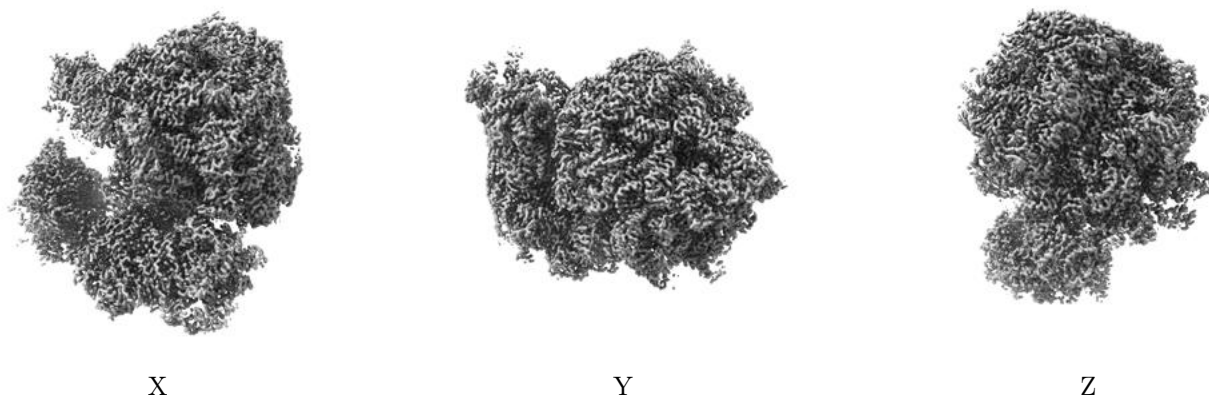


Z

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 0.163. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

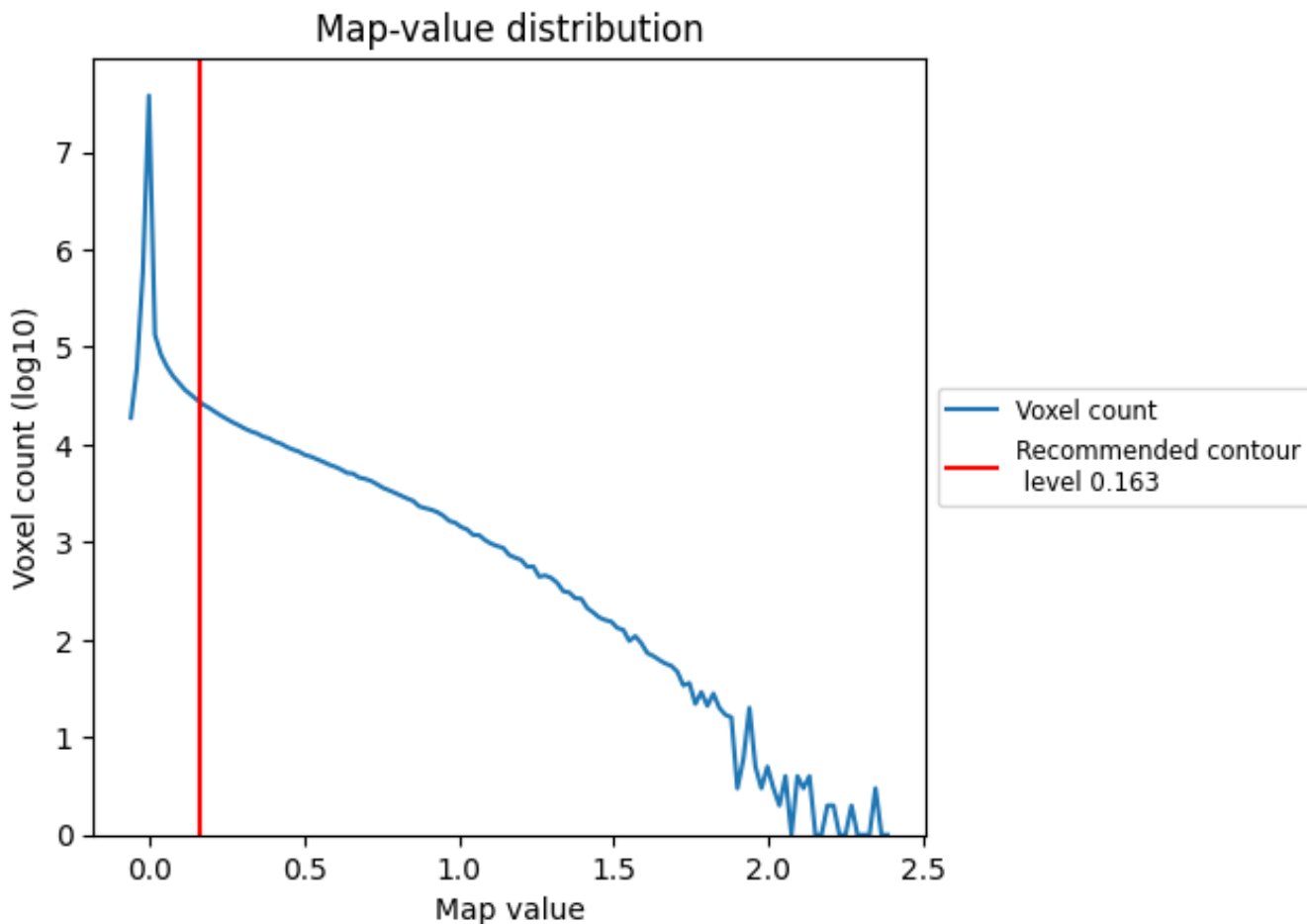
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

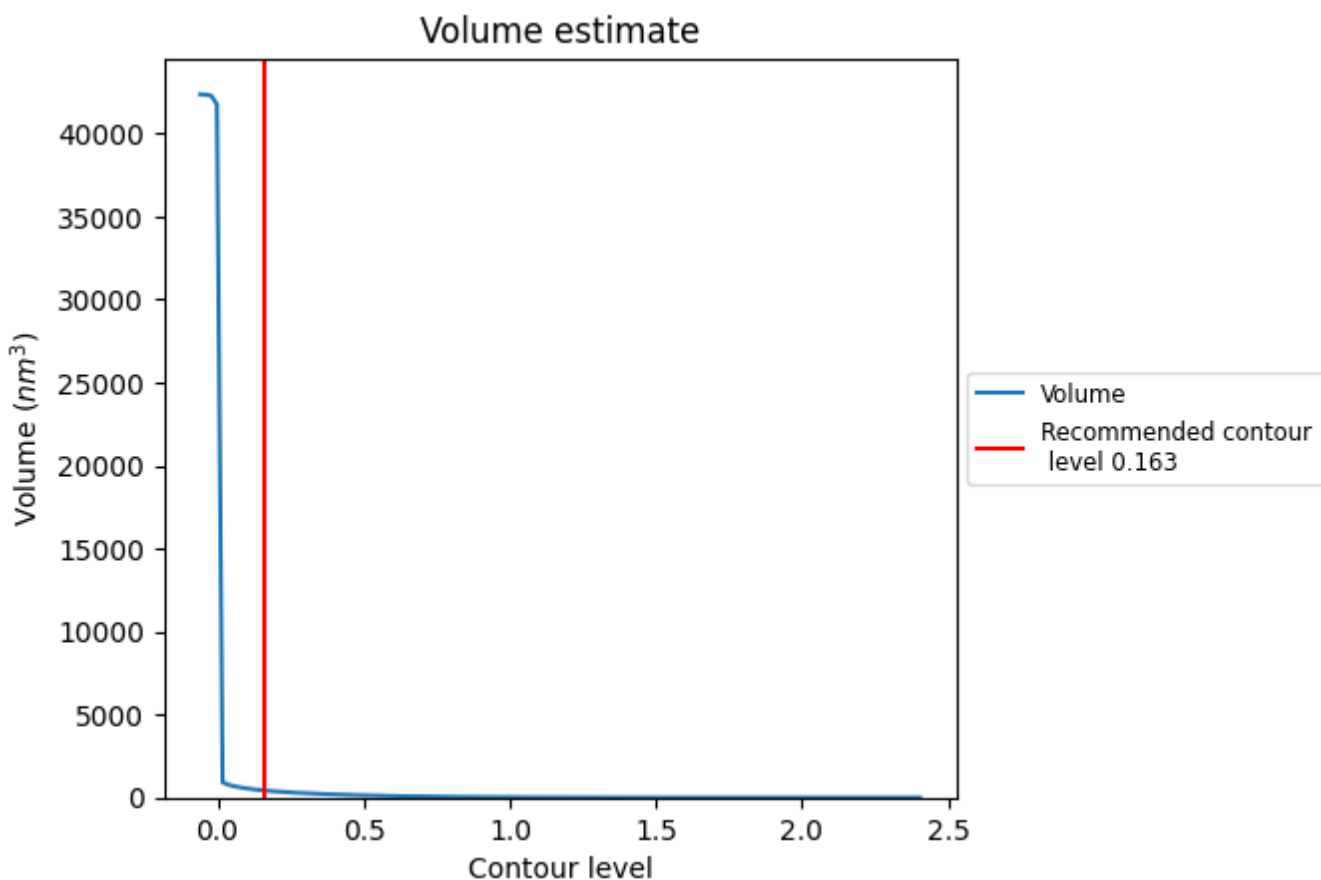
This section contains the results of statistical analysis of the map.

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.

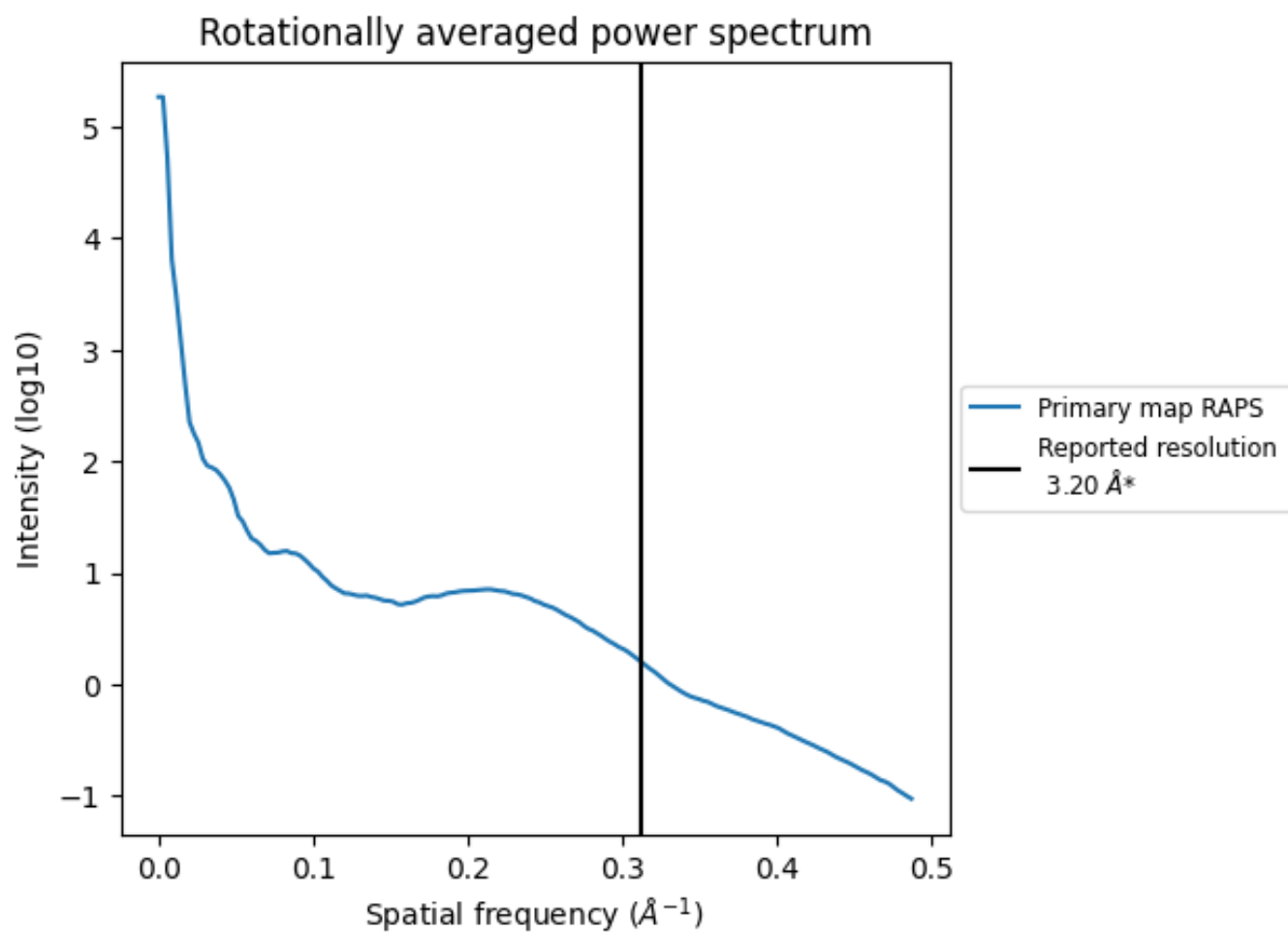
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 424 nm³; this corresponds to an approximate mass of 383 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

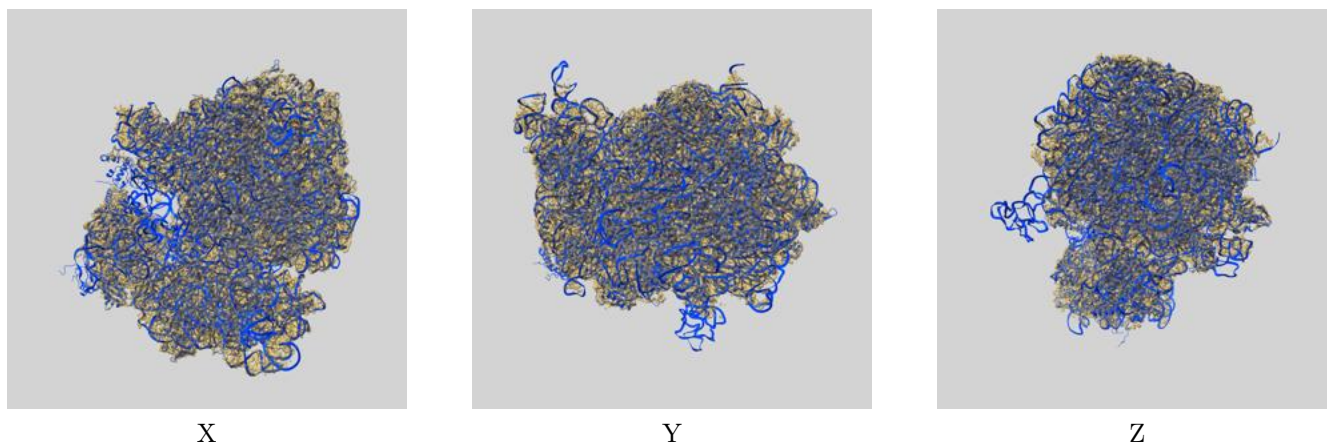
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

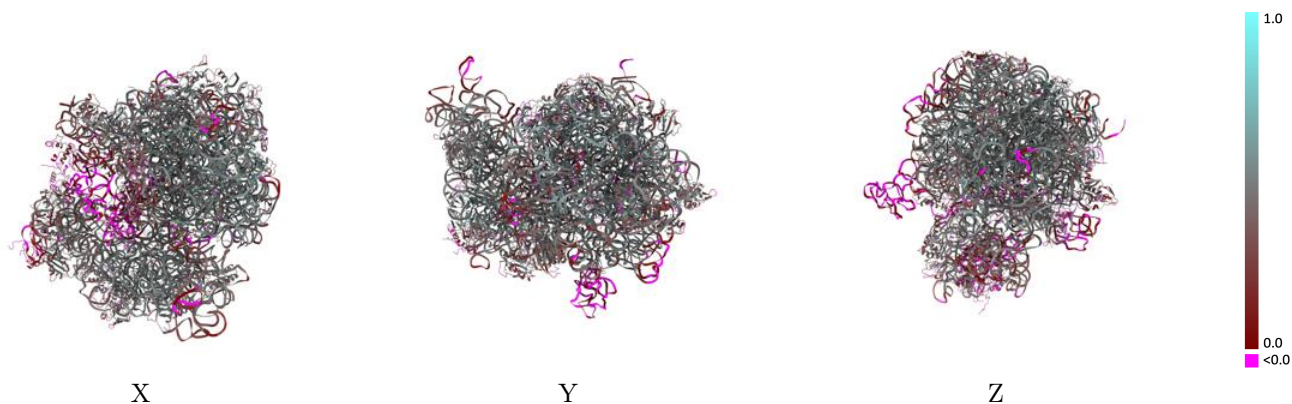
This section contains information regarding the fit between EMDB map EMD-29689 and PDB model 8G38. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



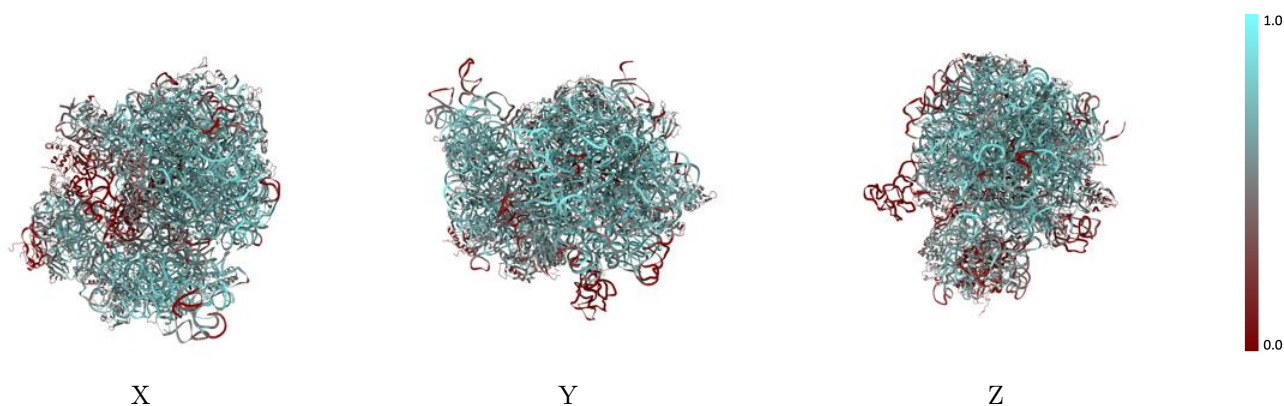
The images above show the 3D surface view of the map at the recommended contour level 0.163 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



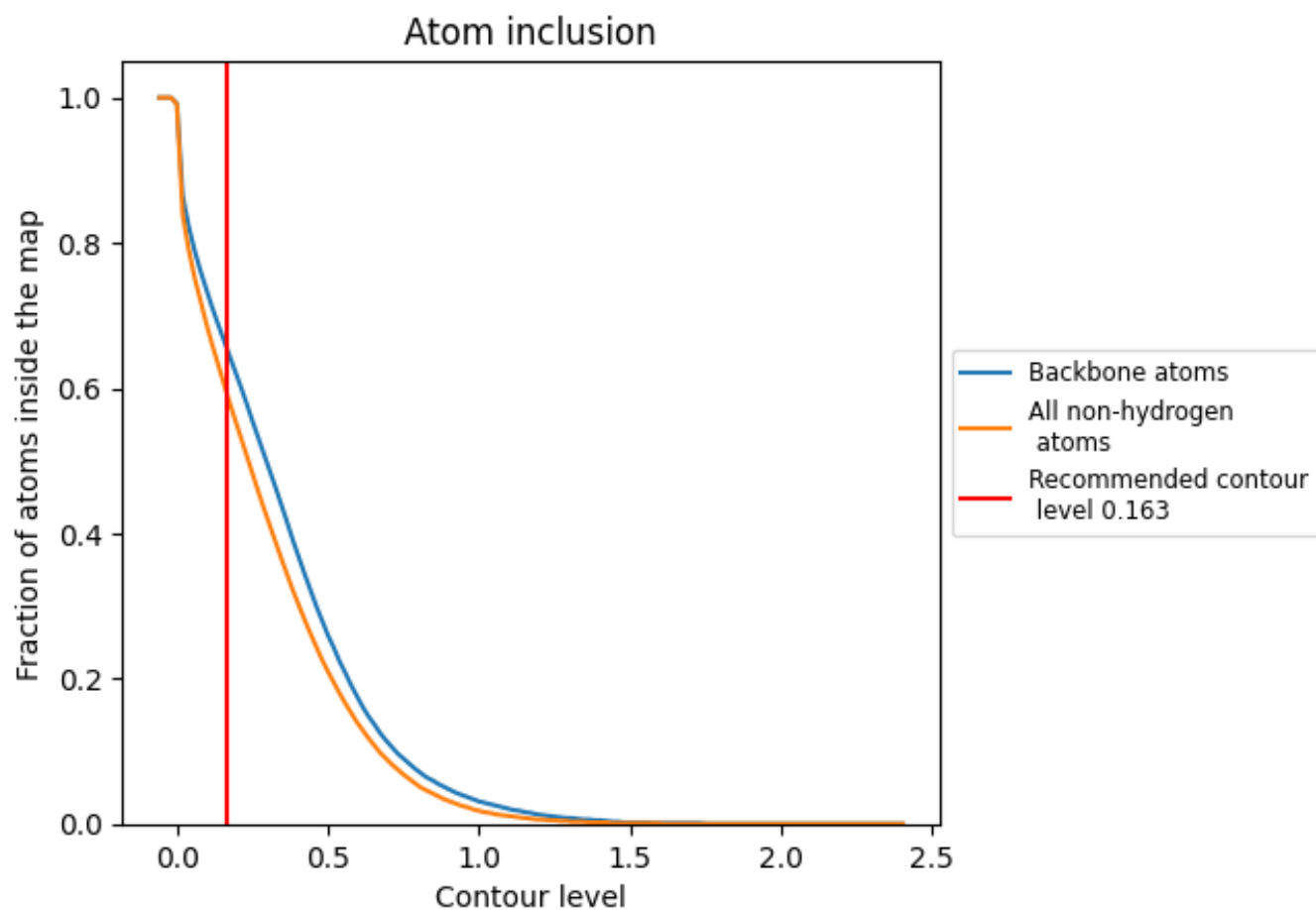
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.163).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.163) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5930	 0.4000
0	 0.6330	 0.4750
1	 0.0030	 0.0490
2	 0.6840	 0.5190
3	 0.5600	 0.4680
4	 0.6100	 0.4640
6	 0.2470	 0.1070
A	 0.5240	 0.3620
B	 0.6480	 0.4230
C	 0.5790	 0.4530
D	 0.6260	 0.4760
E	 0.5140	 0.4070
F	 0.0410	 0.0690
G	 0.3100	 0.2630
J	 0.6130	 0.4530
K	 0.5750	 0.4350
L	 0.5540	 0.4410
M	 0.6090	 0.4710
N	 0.7090	 0.5200
O	 0.4110	 0.3230
P	 0.5440	 0.3970
Q	 0.6160	 0.4540
R	 0.5710	 0.4340
S	 0.6090	 0.4480
T	 0.5450	 0.3940
U	 0.4730	 0.3710
V	 0.5030	 0.3930
W	 0.5030	 0.3390
X	 0.6120	 0.4550
Y	 0.4870	 0.3420
Z	 0.5790	 0.4460
c	 0.5570	 0.3910
d	 0.6090	 0.4690
e	 0.4500	 0.3470
f	 0.4100	 0.3250



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Chain	Atom inclusion	Q-score
g	 0.6610	 0.5100
h	 0.5120	 0.3440
i	 0.4320	 0.3350
j	 0.4370	 0.3390
k	 0.5730	 0.4600
l	 0.4240	 0.2320
m	 0.6220	 0.4360
n	 0.5750	 0.4310
o	 0.6350	 0.4590
p	 0.5320	 0.4100
q	 0.5900	 0.4400
r	 0.5510	 0.3790
s	 0.6120	 0.4540
t	 0.1230	 0.1430
u	 0.0000	 -0.0130
v	 0.6470	 0.4170
w	 0.1530	 0.1640
x	 0.5830	 0.4430