



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 09:28 pm BST

PDB ID : 6GXP / pdb_00006gxp
EMDB ID : EMD-0083
Title : Cryo-EM structure of a rotated E. coli 70S ribosome in complex with RF3-GDPCP(RF3-only)
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.
Deposited on : 2018-06-27
Resolution : 4.40 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

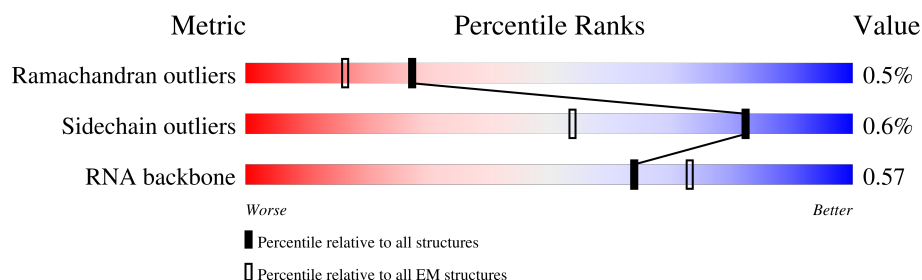
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2903	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	I	141	99% 100%
10	J	142	50% 100%
11	K	122	73% 99%
12	L	143	63% 99%
13	M	136	71% 97%
14	N	120	48% 99%
15	O	116	48% 100%
16	P	114	65% 99%
17	Q	117	45% 100%
18	R	103	57% 98%
19	S	110	71% 98%
20	T	93	53% 100%
21	U	102	52% 98%
22	V	94	46% 100%
23	W	75	68% 99%
24	X	77	56% 99%
25	Y	63	33% 100%
26	Z	58	62% 100%
27	0	56	68% 100%
28	1	50	80% 100%
29	2	46	70% 100%
30	3	64	83% 94% 5%
31	4	38	47% 97%
32	5	131	99% 98%
33	a	1539	40% 81% 17%

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Mol	Chain	Length	Quality of chain
34	b	218	94% 97% .
35	c	206	100% 99% .
36	d	205	90% 99% .
37	e	157	74% 98% ..
38	f	100	90% 96% .
39	g	151	99% 99% .
40	h	129	67% 100%
41	i	127	97% 98% ..
42	j	98	100% 100%
43	k	112	91% 96% ..
44	l	123	90% 98% .
45	m	114	98% 98% ..
46	n	101	100% 100%
47	o	88	74% 100%
48	p	82	67% 99% .
49	q	80	84% 96% .
50	r	65	89% 100%
51	s	79	100% 99% .
52	t	85	61% 100%
53	u	65	95% 98% .
54	w	529	91% 92% 6%
55	z	14	100% 93% 7%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147637 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2896	Total	C	N	O	P	0	0
			62177	27736	11444	20101	2896		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1063812051
A	1847	G	A	conflict	GB 1063812051

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1373146531

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

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

- Molecule 35 is a protein called 30S ribosomal protein S3.

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

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

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

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

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

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	112	Total	C	N	O	S	0	0
			829	511	161	154	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

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

- Molecule 45 is a protein called 30S ribosomal protein S13.

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

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 51 is a protein called 30S ribosomal protein S19.

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

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 54 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	499	Total	C	N	O	S	0	0
			3943	2498	680	745	20		

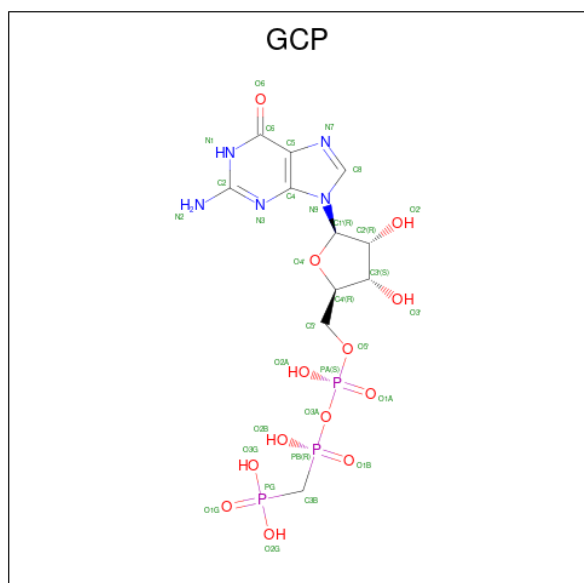
- Molecule 55 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	z	14	Total	C	N	O	0	0
			120	80	25	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP Q8WSY8

- Molecule 56 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



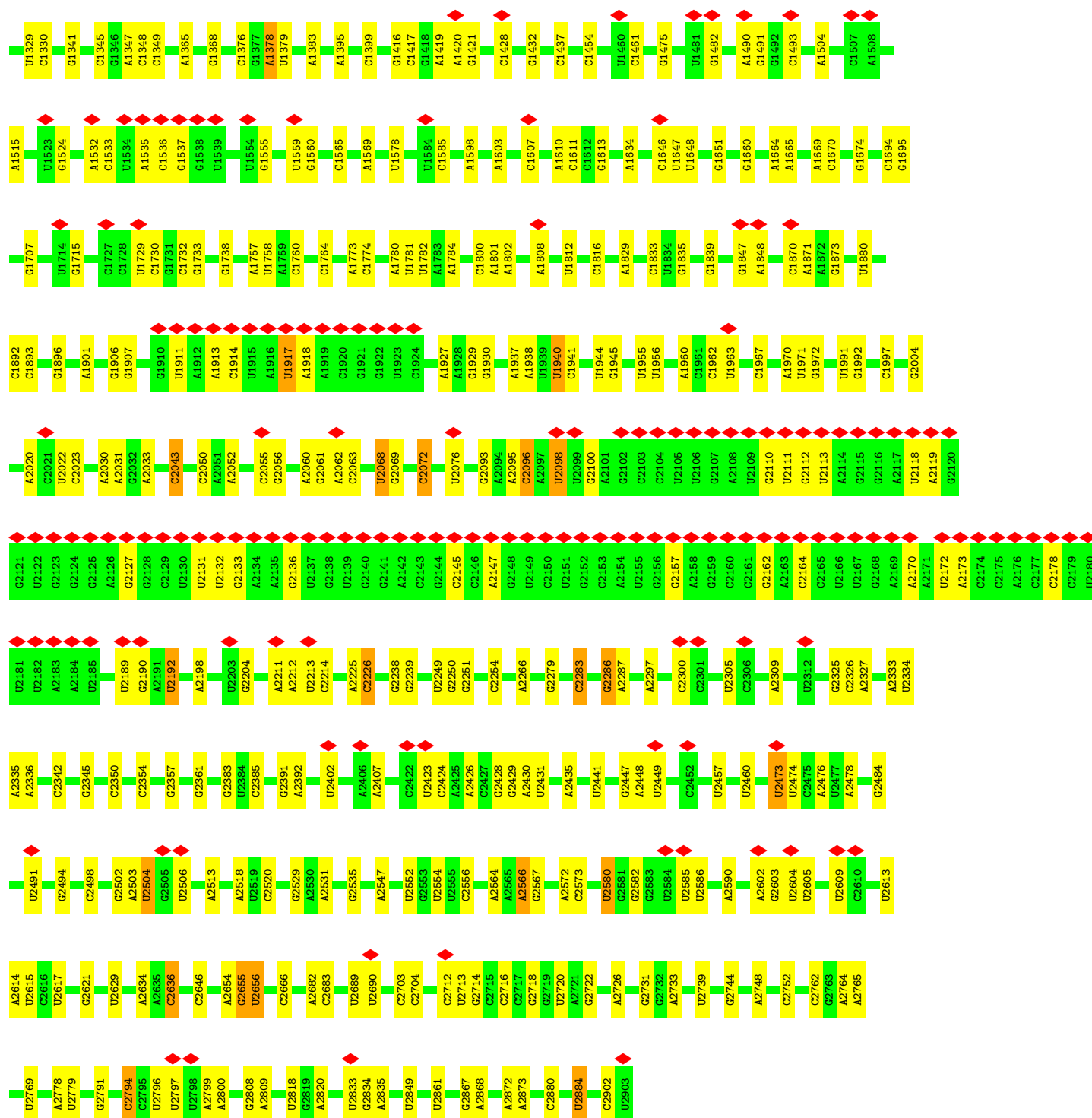
Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

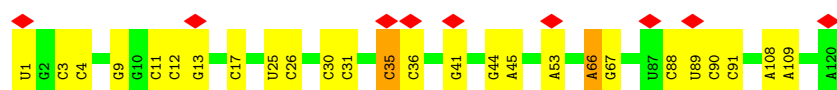
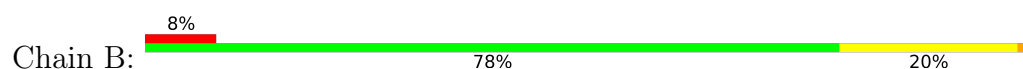
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

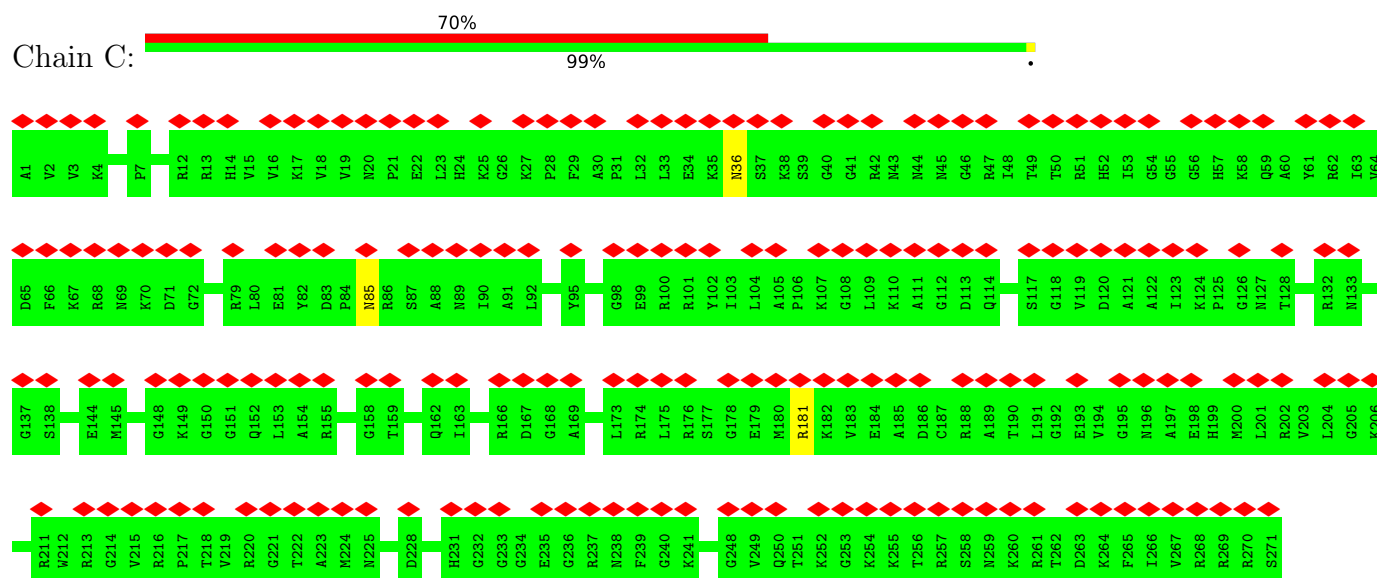




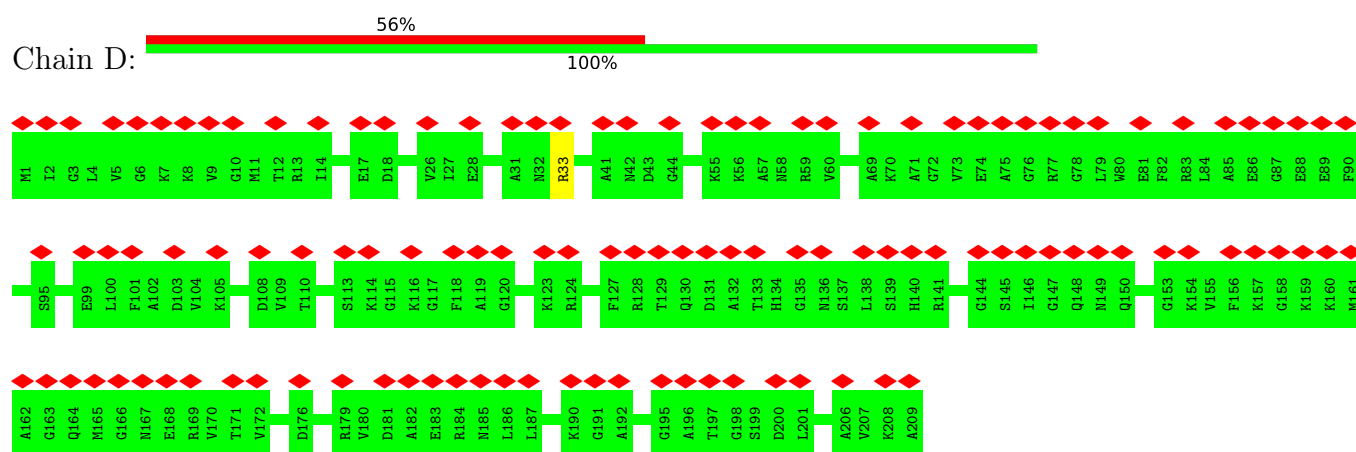
• Molecule 2: 5S ribosomal RNA



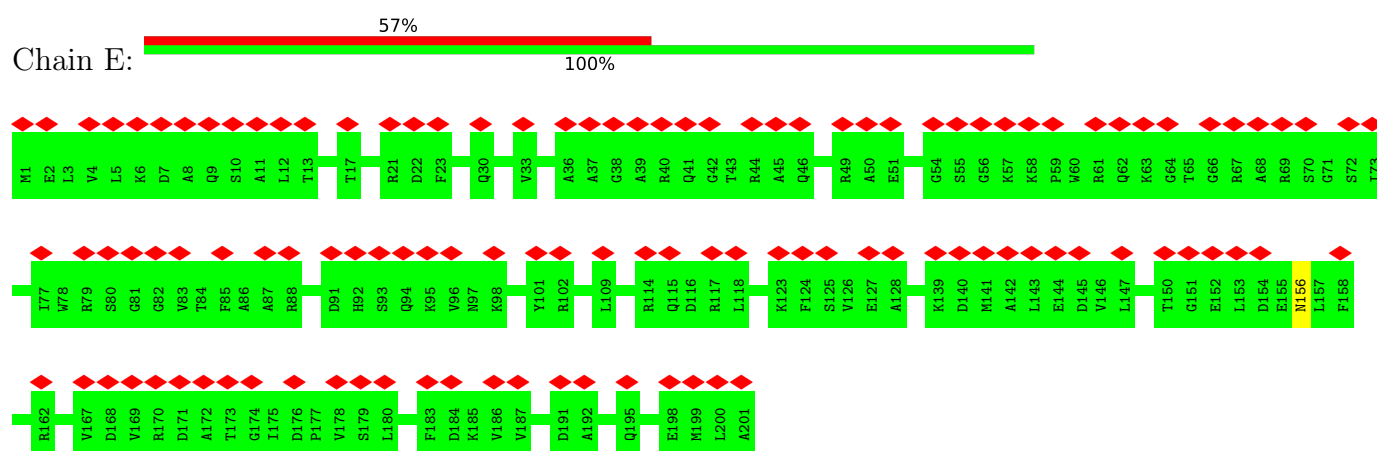
- Molecule 3: 50S ribosomal protein L2



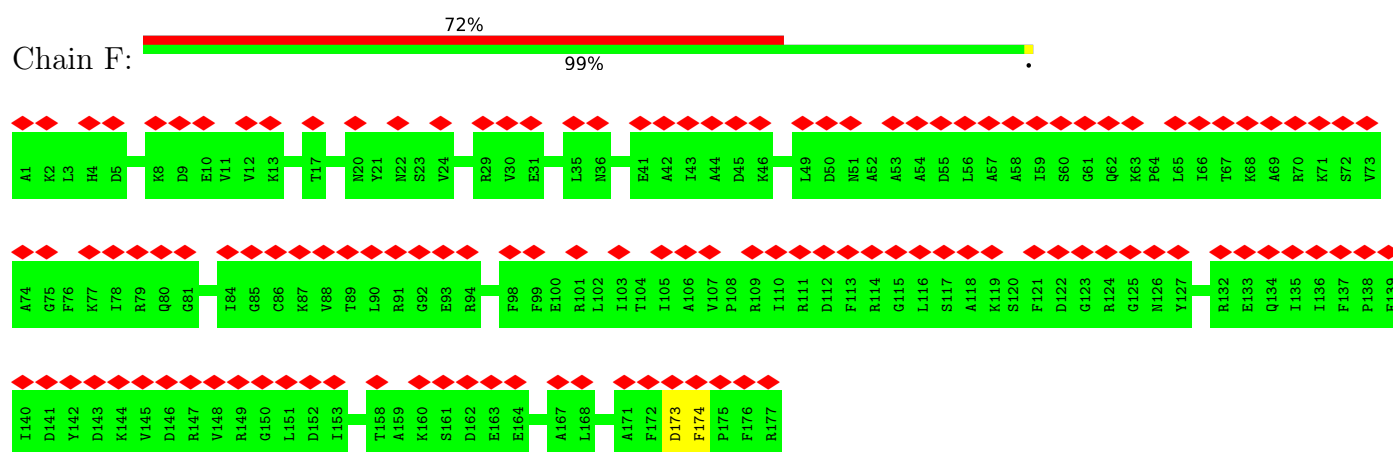
- Molecule 4: 50S ribosomal protein L3



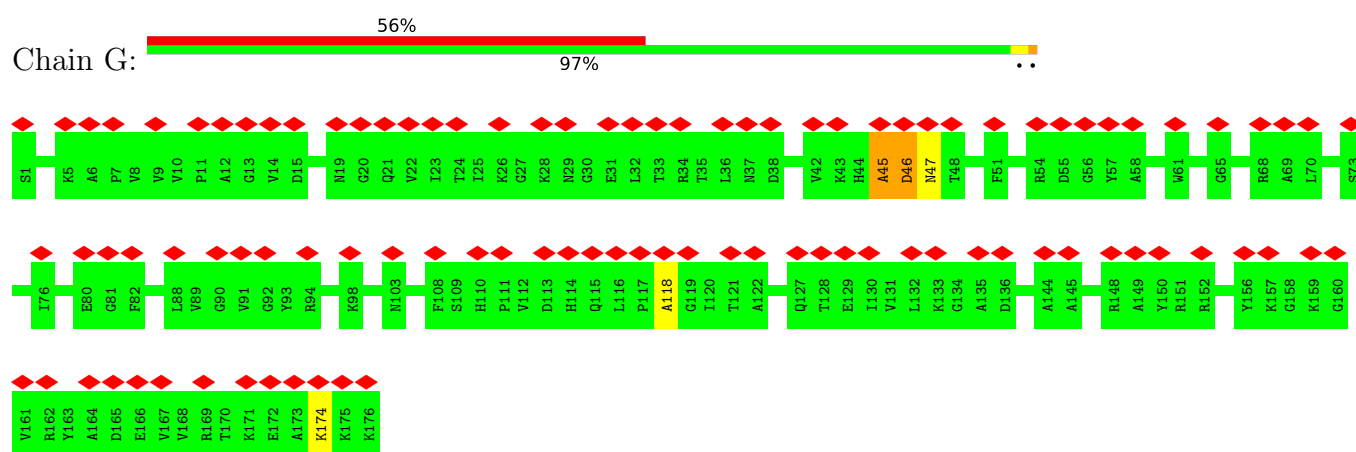
- Molecule 5: 50S ribosomal protein L4



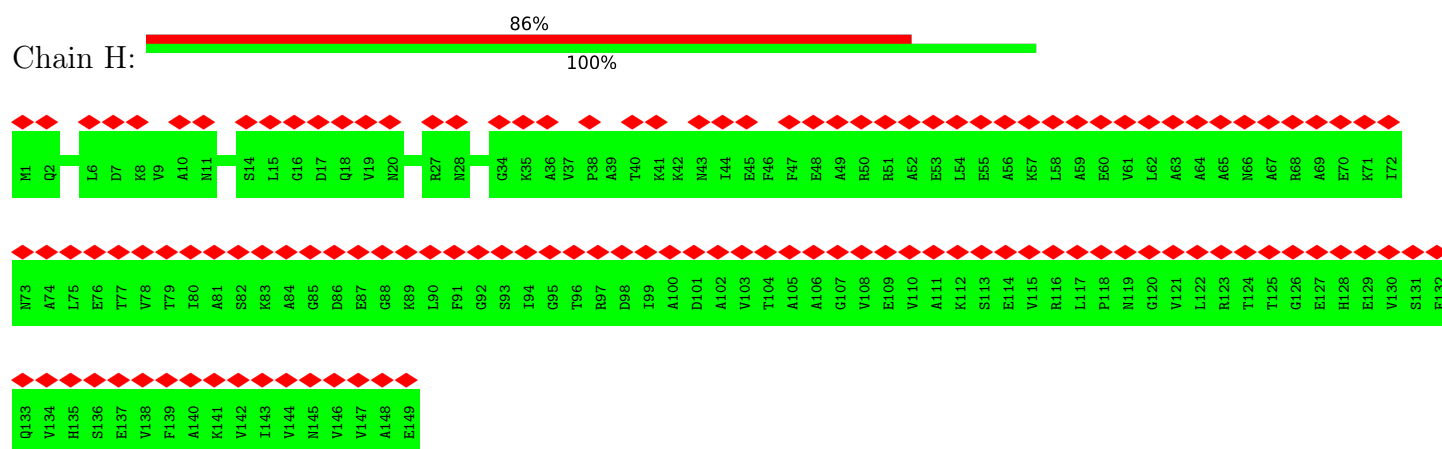
- Molecule 6: 50S ribosomal protein L5



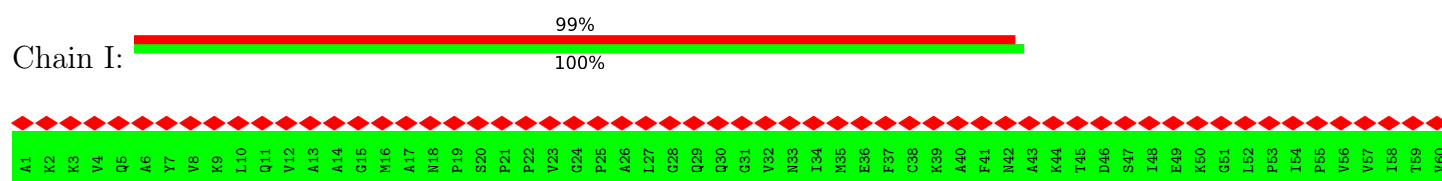
• Molecule 7: 50S ribosomal protein L6

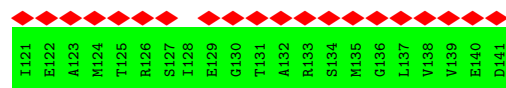
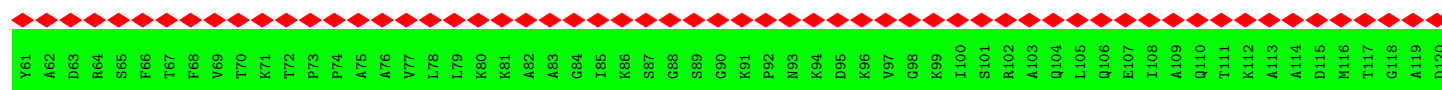


• Molecule 8: 50S ribosomal protein L9

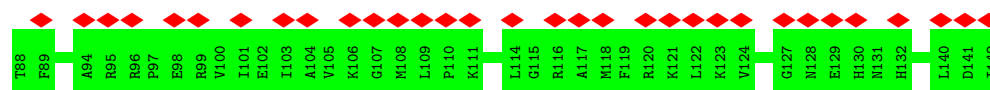
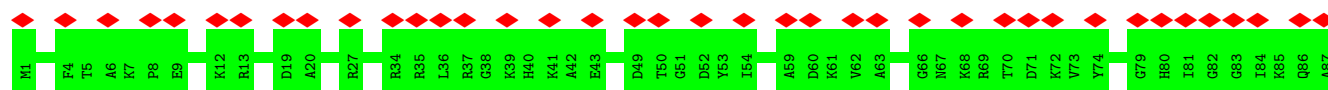


• Molecule 9: 50S ribosomal protein L11

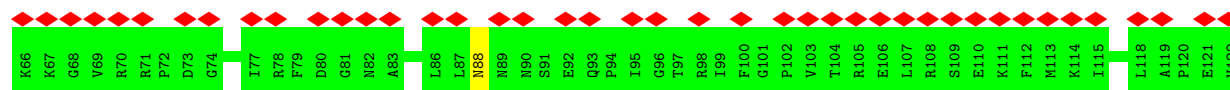
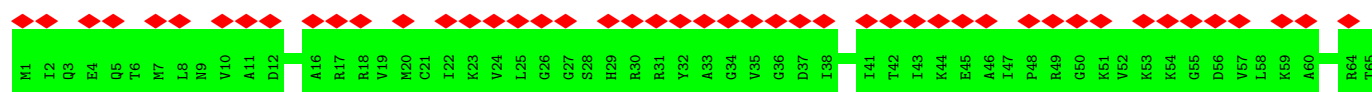
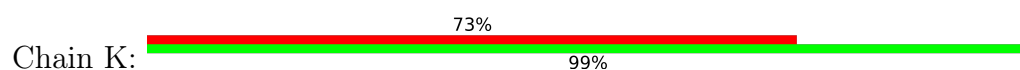




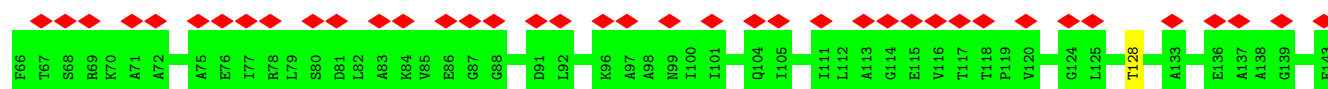
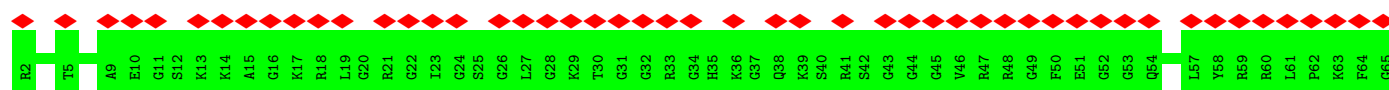
• Molecule 10: 50S ribosomal protein L13



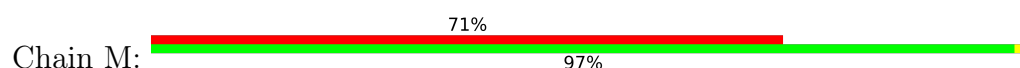
• Molecule 11: 50S ribosomal protein L14

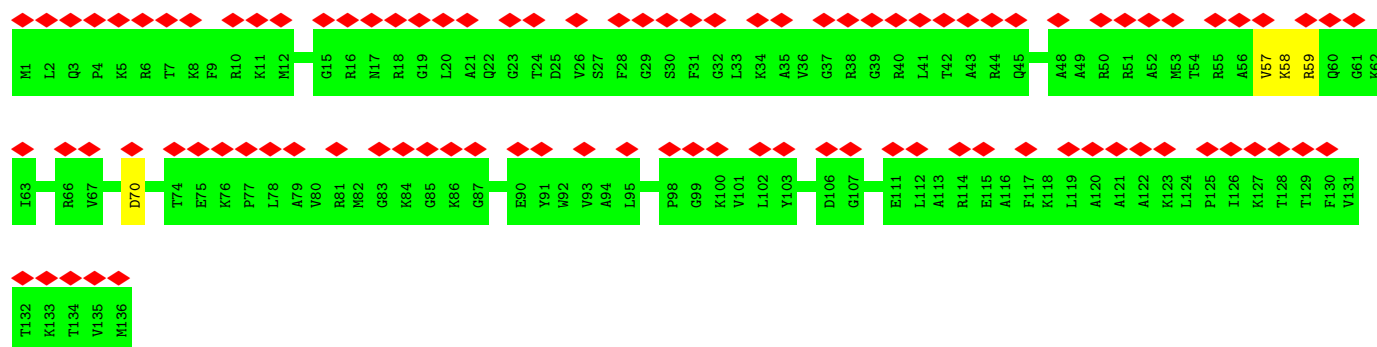


• Molecule 12: 50S ribosomal protein L15



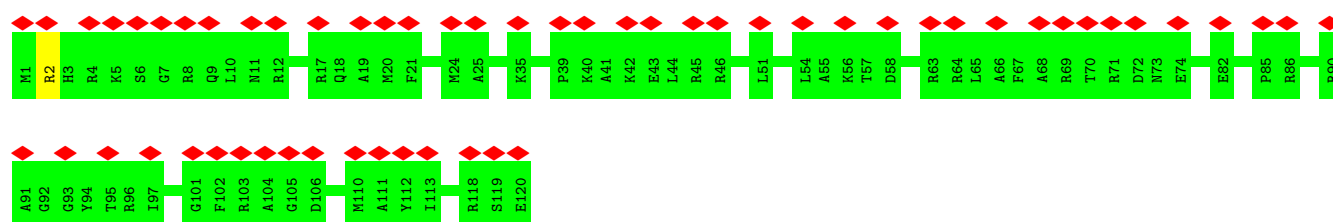
• Molecule 13: 50S ribosomal protein L16





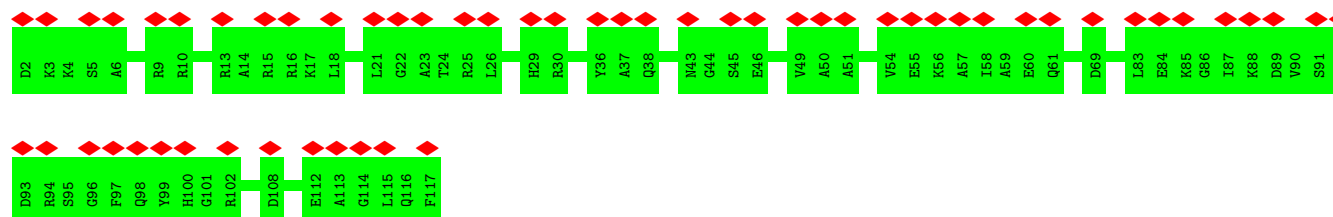
- Molecule 14: 50S ribosomal protein L17

Chain N: 48% 99% .



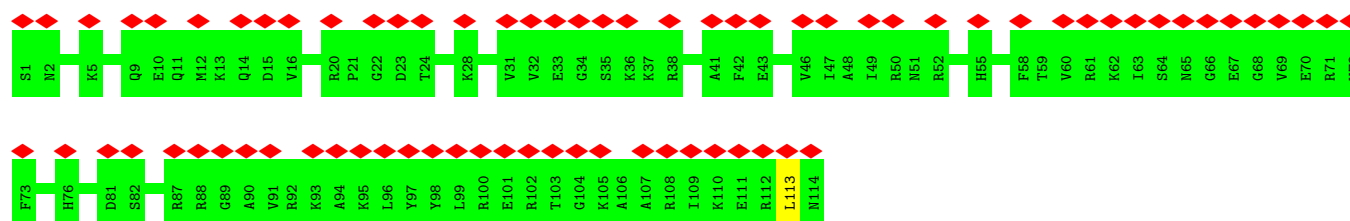
- Molecule 15: 50S ribosomal protein L18

Chain O: 48% 100% .



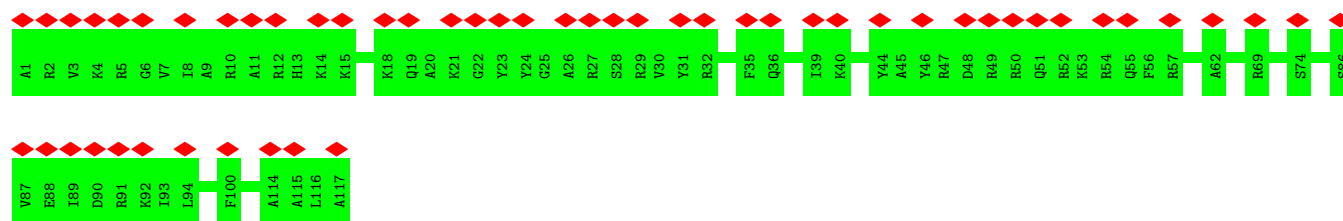
- Molecule 16: 50S ribosomal protein L19

Chain P: 65% 99% .

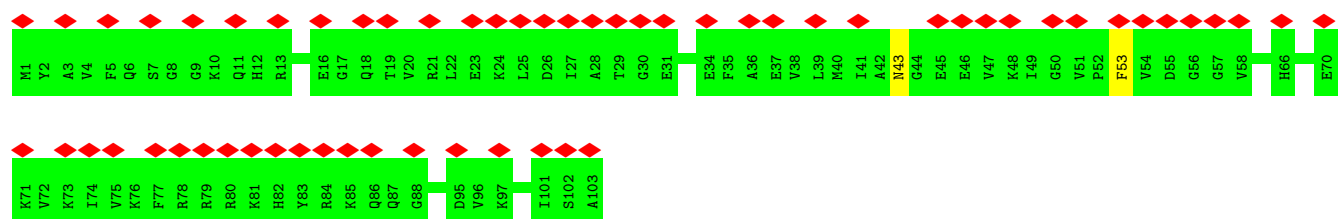


- Molecule 17: 50S ribosomal protein L20

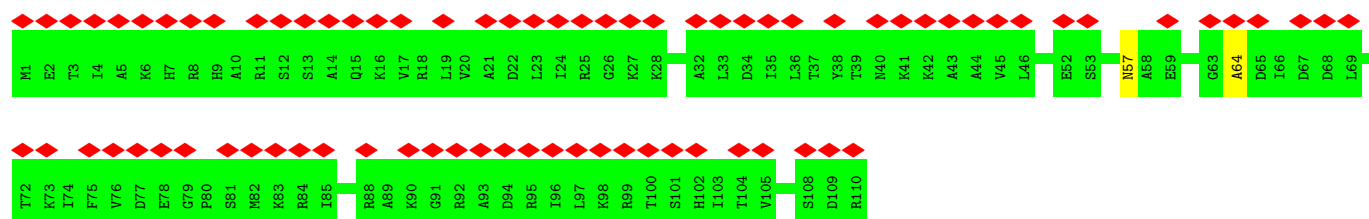
Chain Q: 45% 100% .



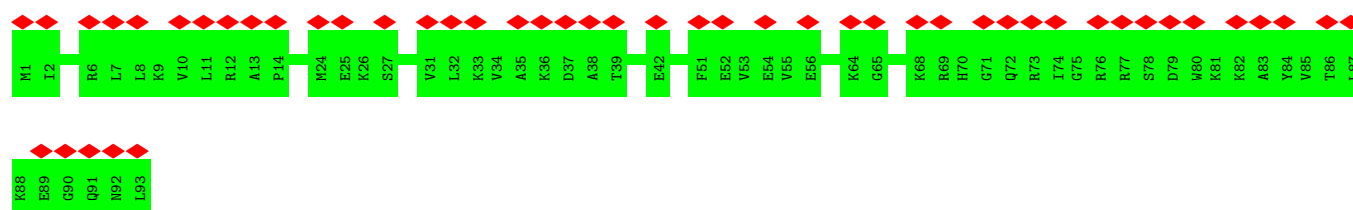
• Molecule 18: 50S ribosomal protein L21



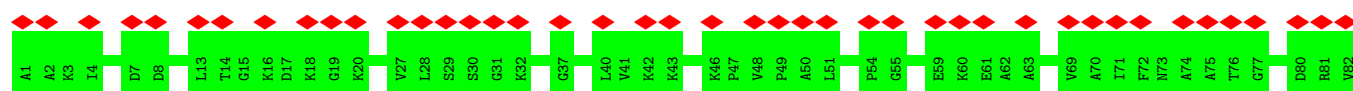
• Molecule 19: 50S ribosomal protein L22



• Molecule 20: 50S ribosomal protein L23

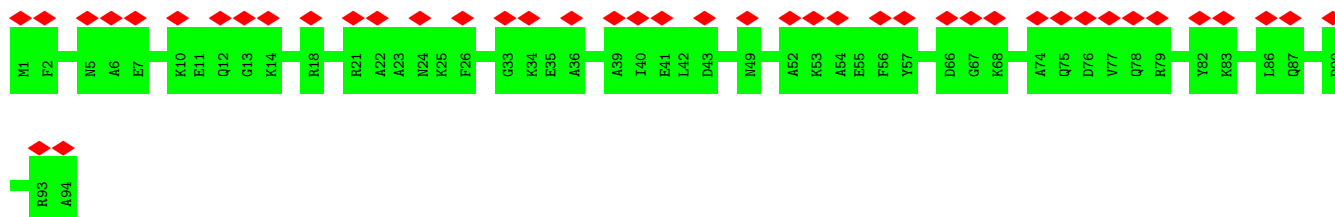


• Molecule 21: 50S ribosomal protein L24

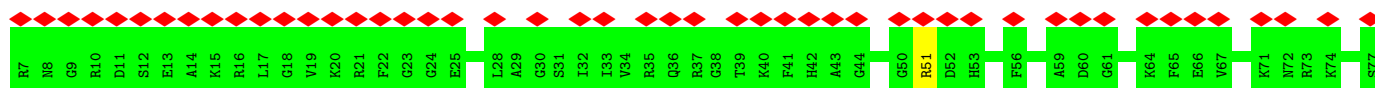




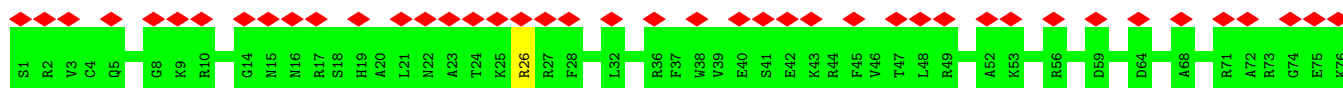
- Molecule 22: 50S ribosomal protein L25



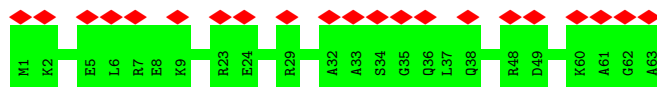
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

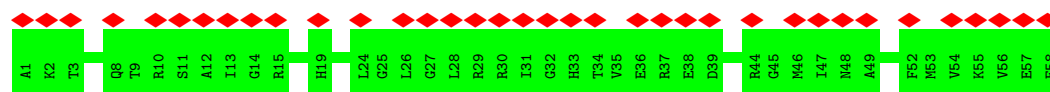


- Molecule 25: 50S ribosomal protein L29

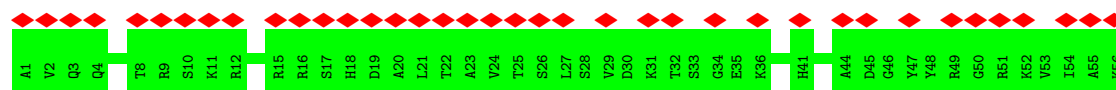


- Molecule 26: 50S ribosomal protein L30





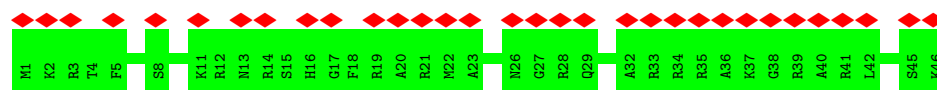
- Molecule 27: 50S ribosomal protein L32



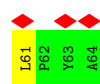
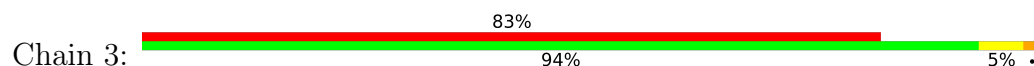
- Molecule 28: 50S ribosomal protein L33



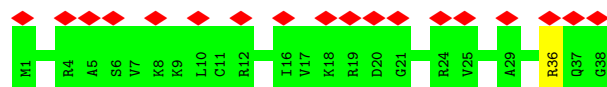
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

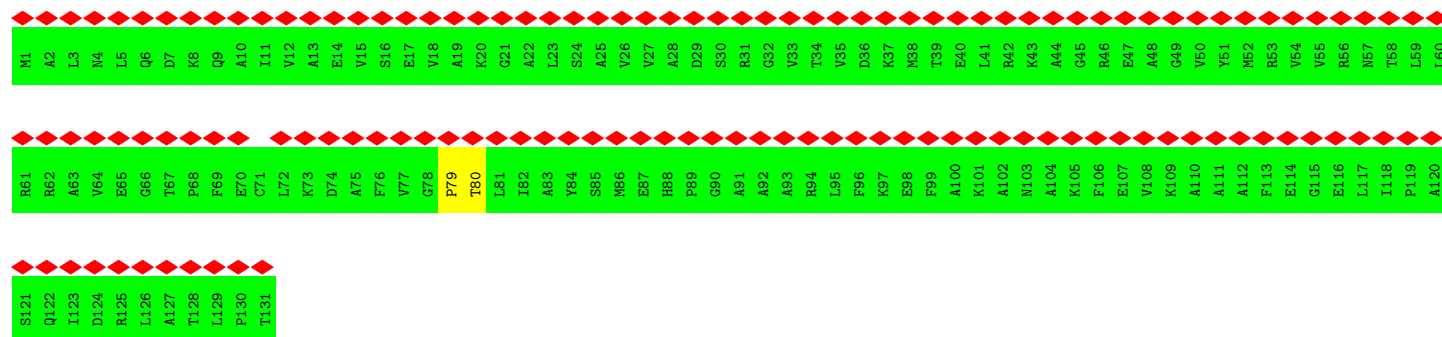


- Molecule 31: 50S ribosomal protein L36

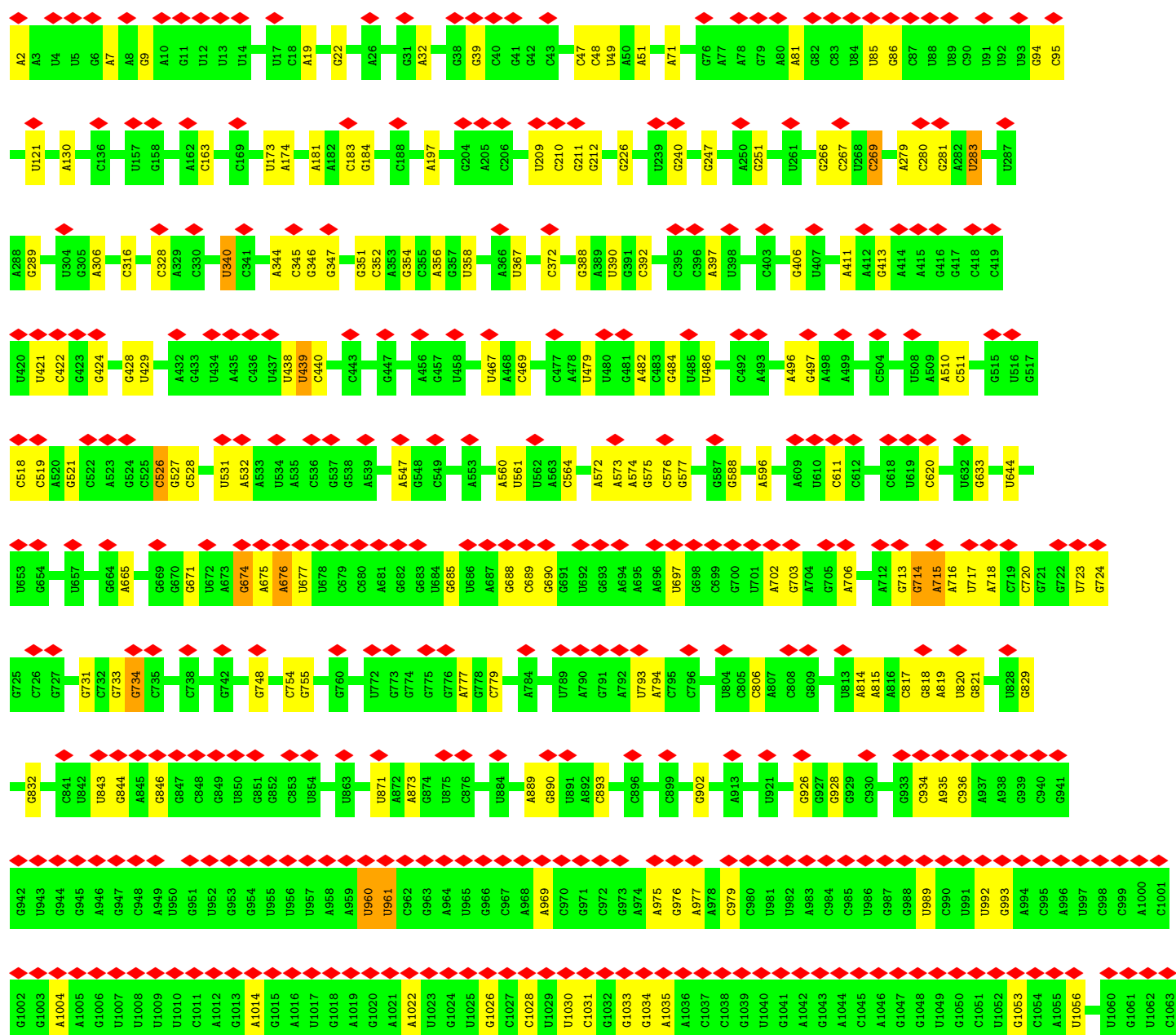
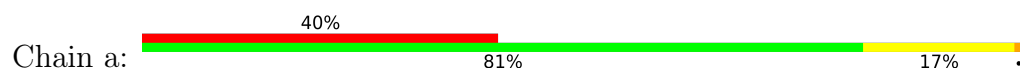


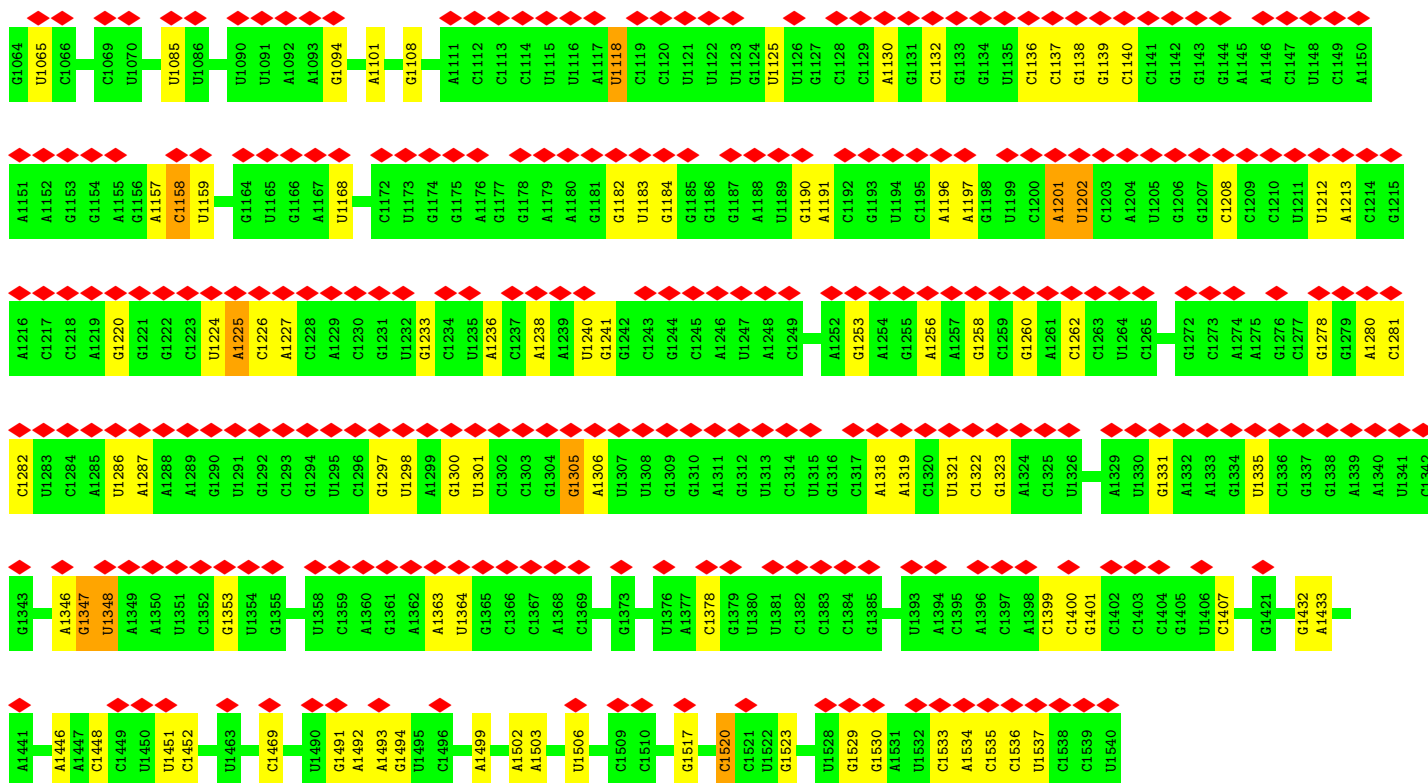
- Molecule 32: 50S ribosomal protein L10





• Molecule 33: 16S ribosomal RNA



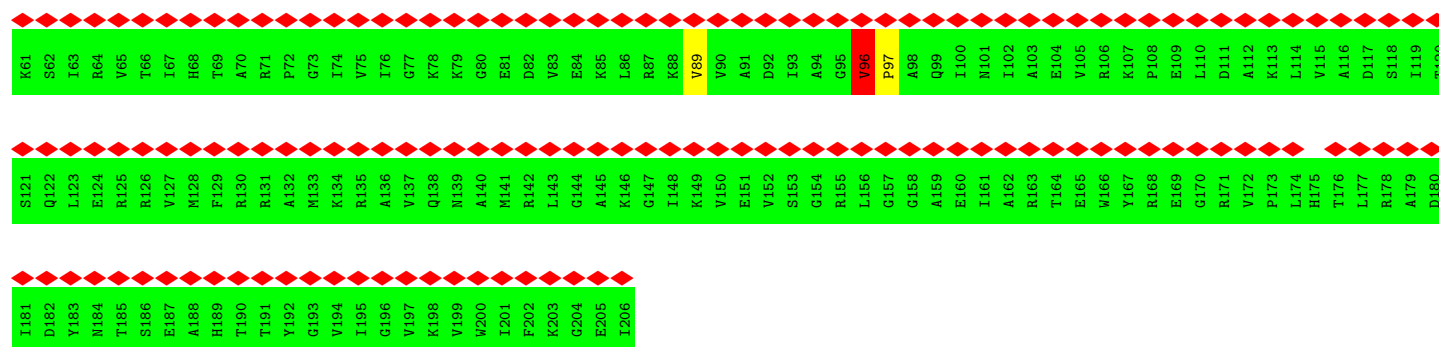


• Molecule 34: 30S ribosomal protein S2

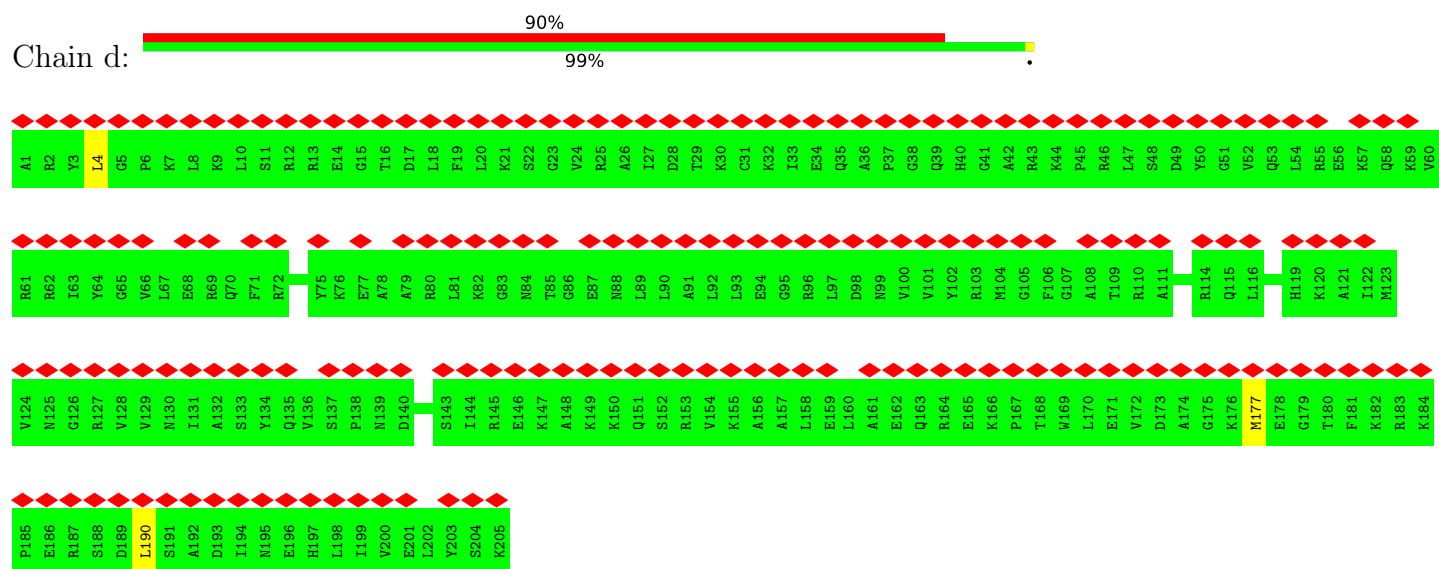


• Molecule 35: 30S ribosomal protein S3

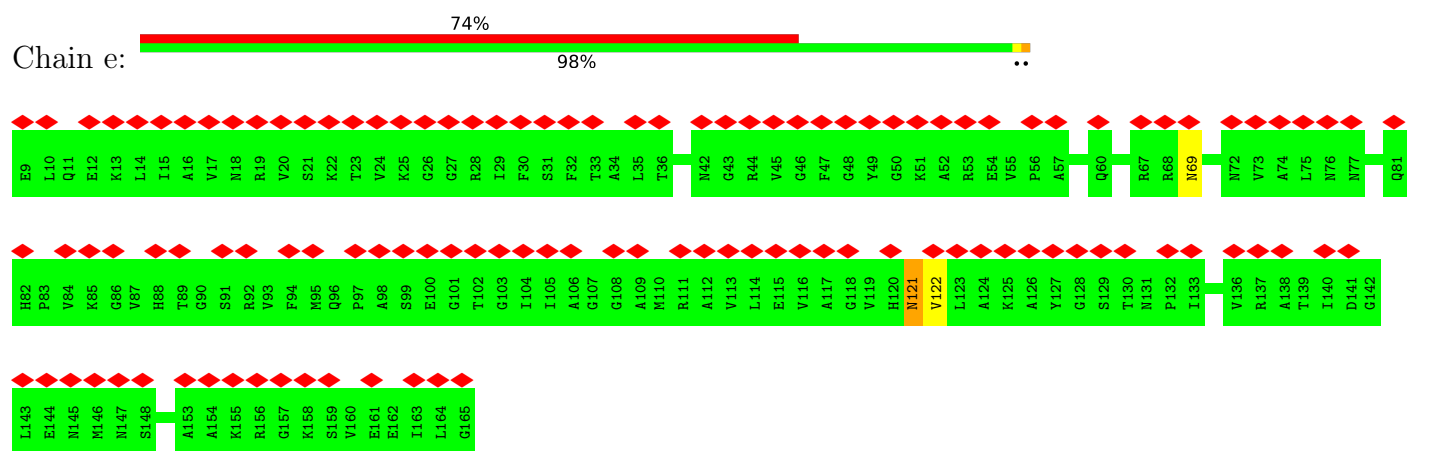




• Molecule 36: 30S ribosomal protein S4



• Molecule 37: 30S ribosomal protein S5

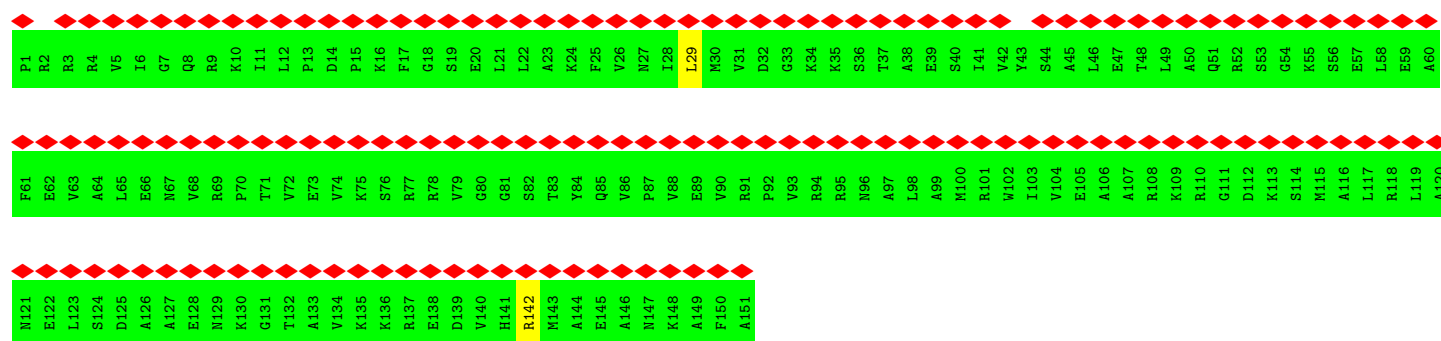


• Molecule 38: 30S ribosomal protein S6

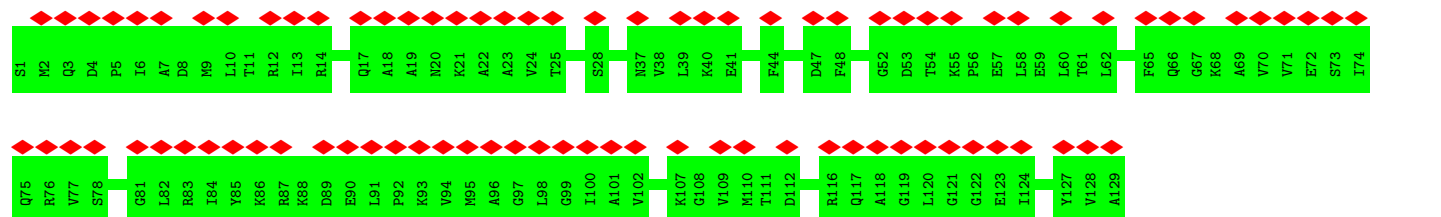




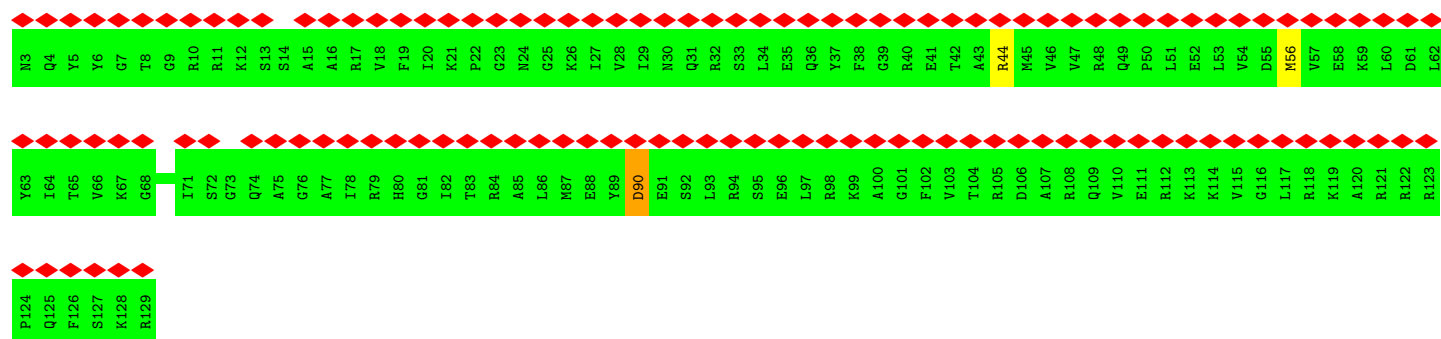
• Molecule 39: 30S ribosomal protein S7



• Molecule 40: 30S ribosomal protein S8



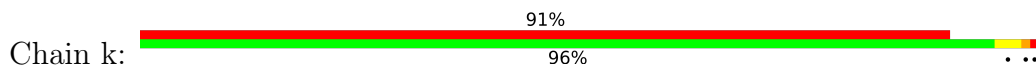
• Molecule 41: 30S ribosomal protein S9



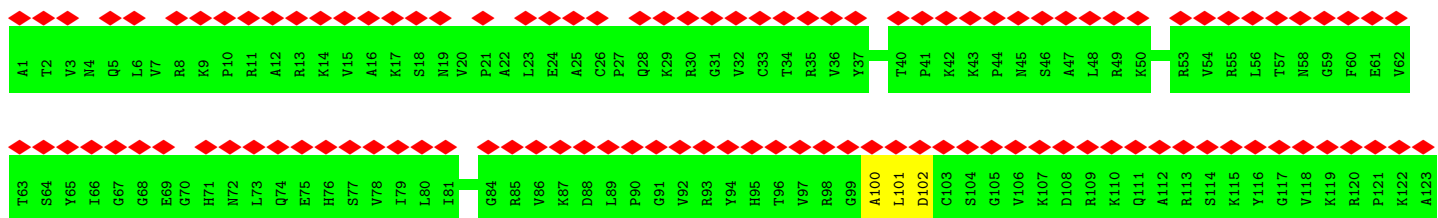
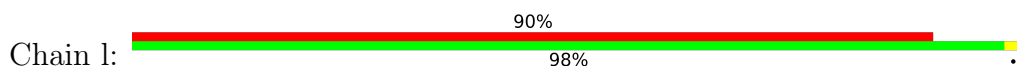
• Molecule 42: 30S ribosomal protein S10



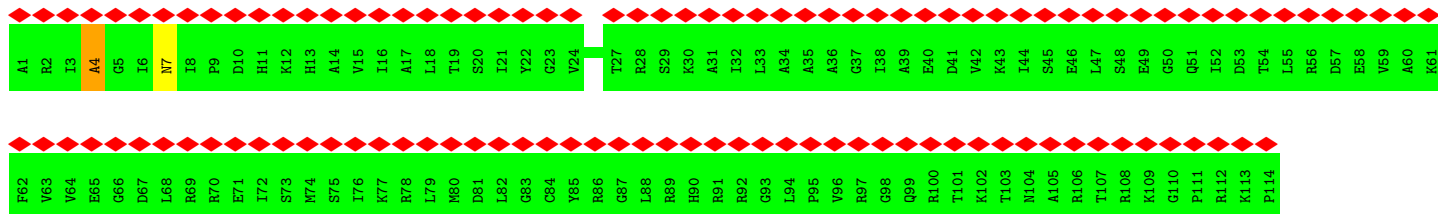
• Molecule 43: 30S ribosomal protein S11



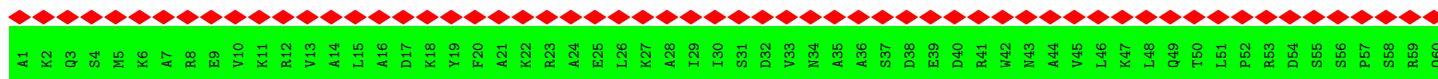
• Molecule 44: 30S ribosomal protein S12

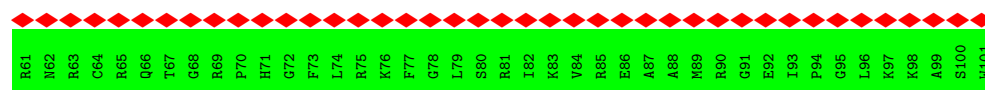


• Molecule 45: 30S ribosomal protein S13

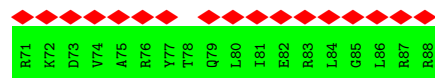
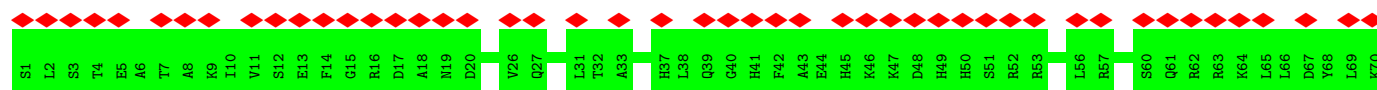
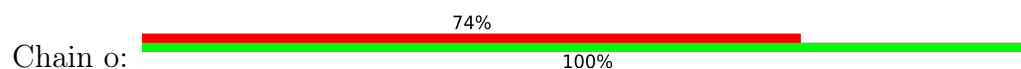


• Molecule 46: 30S ribosomal protein S14

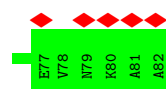
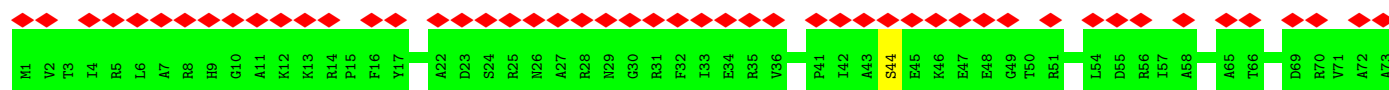




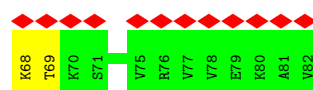
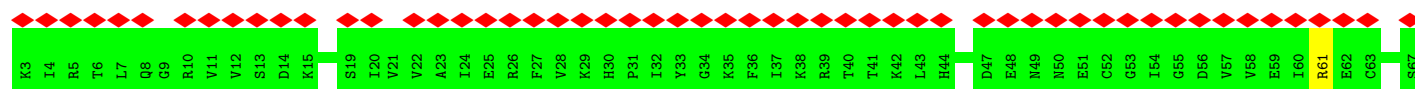
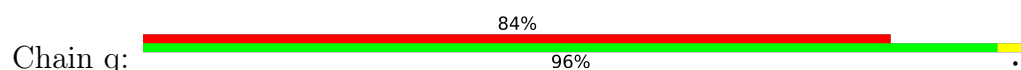
- Molecule 47: 30S ribosomal protein S15



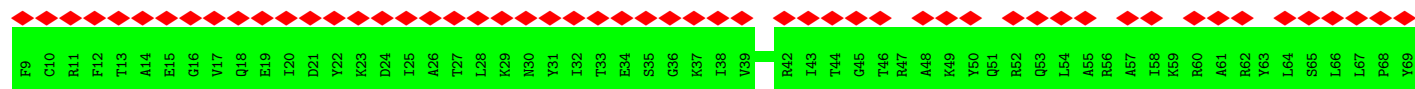
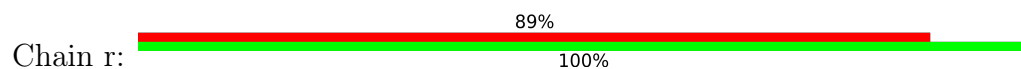
- Molecule 48: 30S ribosomal protein S16



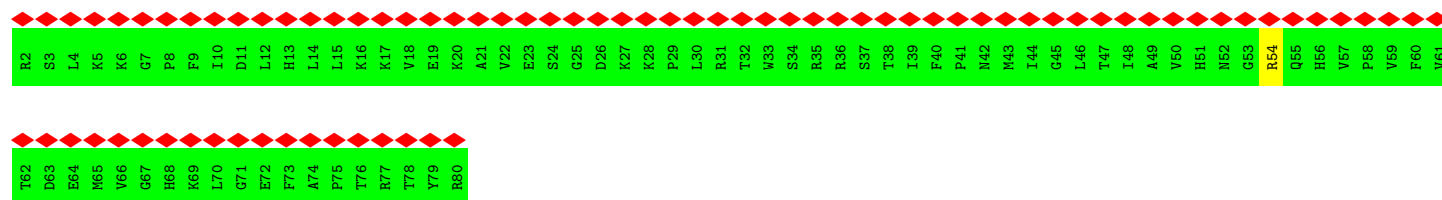
- Molecule 49: 30S ribosomal protein S17



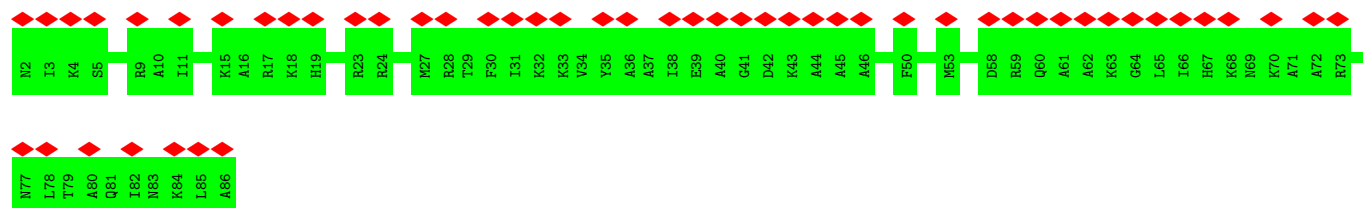
- Molecule 50: 30S ribosomal protein S18



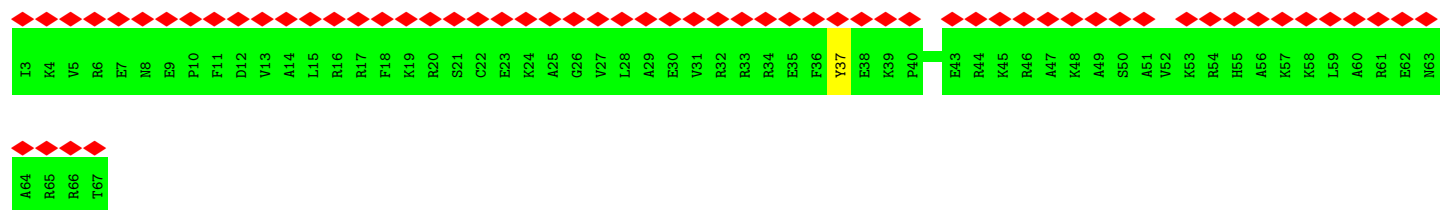
- Molecule 51: 30S ribosomal protein S19



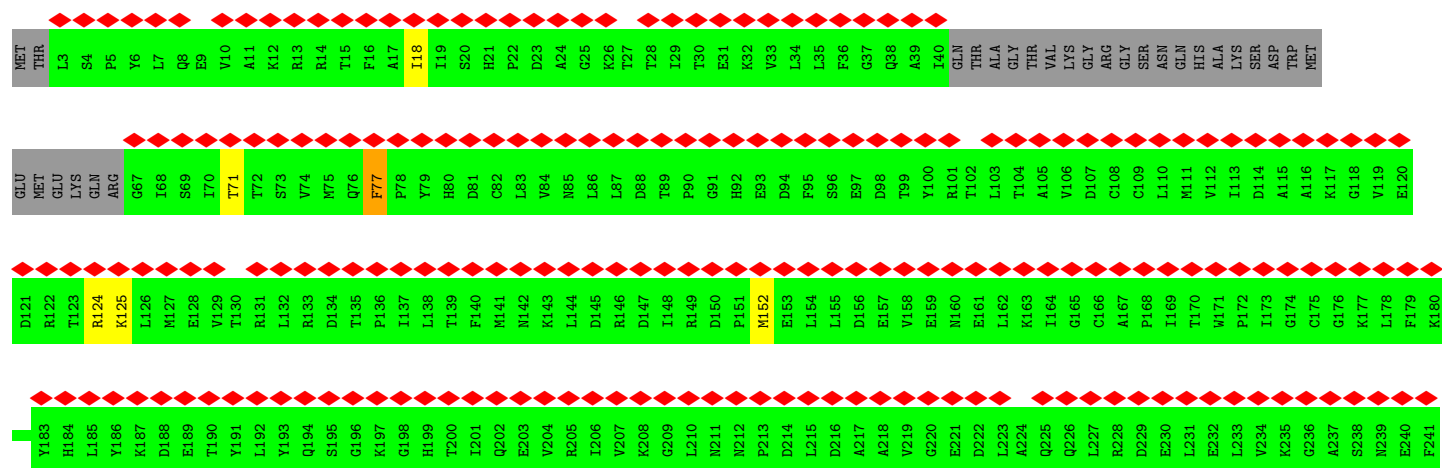
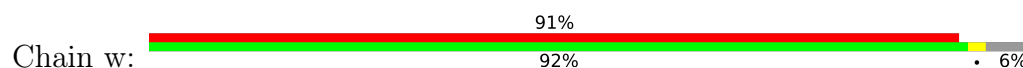
• Molecule 52: 30S ribosomal protein S20

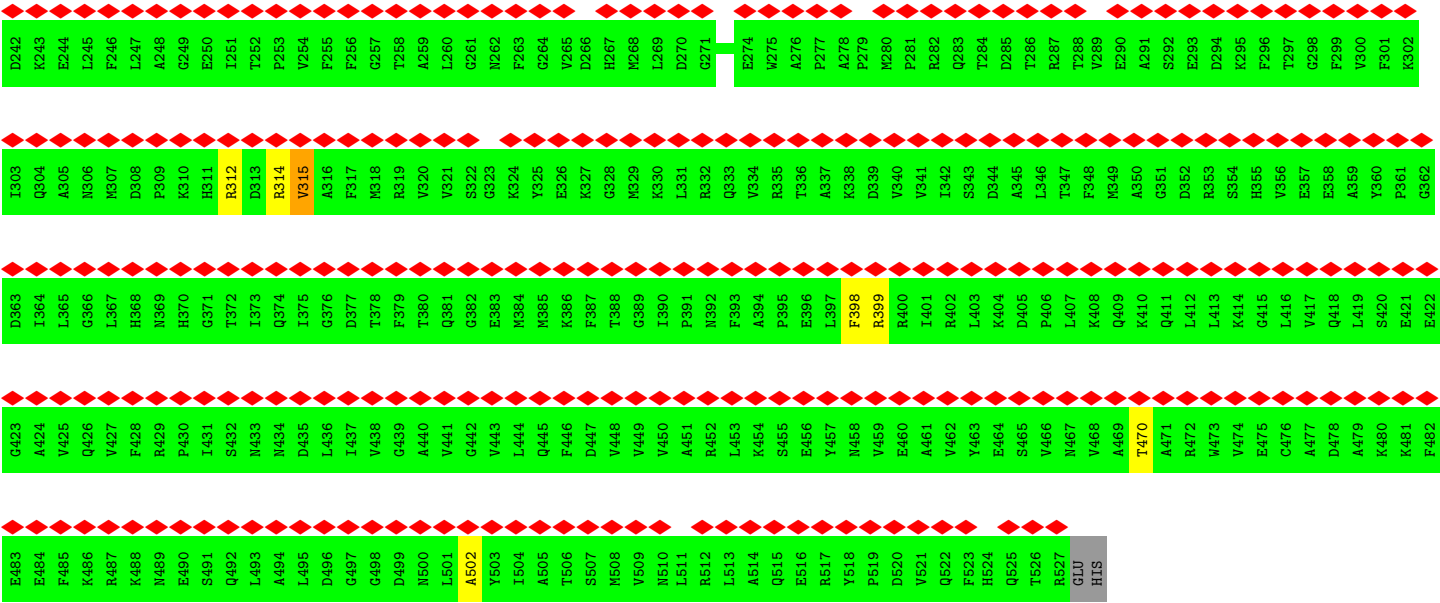


• Molecule 53: 30S ribosomal protein S21

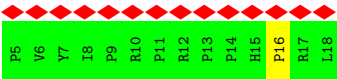
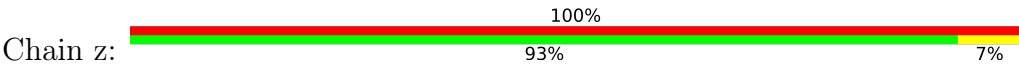


• Molecule 54: Peptide chain release factor RF3





● Molecule 55: Apidaecin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.061, 1.061, 1.061	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.29	1/69638 (0.0%)	1.00	229/108636 (0.2%)
2	B	0.38	1/2876 (0.0%)	1.16	31/4483 (0.7%)
3	C	0.25	0/2121	0.51	0/2852
4	D	0.26	0/1586	0.50	0/2134
5	E	0.25	0/1571	0.46	0/2113
6	F	0.28	0/1434	0.55	0/1926
7	G	0.26	0/1343	0.52	1/1816 (0.1%)
8	H	0.26	0/1122	0.47	0/1515
9	I	0.29	0/1046	0.55	0/1410
10	J	0.25	0/1152	0.46	0/1551
11	K	0.28	0/947	0.54	0/1268
12	L	0.27	0/1054	0.53	0/1403
13	M	0.28	0/1093	0.58	1/1460 (0.1%)
14	N	0.26	0/973	0.52	0/1301
15	O	0.26	0/902	0.46	0/1209
16	P	0.25	0/929	0.51	1/1242 (0.1%)
17	Q	0.26	0/960	0.46	0/1278
18	R	0.26	0/829	0.51	0/1107
19	S	0.24	0/864	0.49	0/1156
20	T	0.26	0/744	0.53	0/994
21	U	0.30	0/787	0.55	0/1051
22	V	0.25	0/766	0.48	0/1025
23	W	0.26	0/582	0.42	0/769
24	X	0.24	0/635	0.46	0/848
25	Y	0.23	0/510	0.47	0/677
26	Z	0.24	0/453	0.50	0/605
27	0	0.23	0/450	0.46	0/599
28	1	0.26	0/416	0.50	0/554
29	2	0.24	0/380	0.44	0/498
30	3	0.25	0/513	0.64	2/676 (0.3%)
31	4	0.30	0/303	0.75	2/397 (0.5%)
32	5	0.30	0/1001	0.63	0/1350

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.31	5/36965 (0.0%)	1.01	101/57658 (0.2%)
34	b	0.28	0/1735	0.55	0/2338
35	c	0.26	0/1651	0.51	1/2225 (0.0%)
36	d	0.26	0/1665	0.54	2/2227 (0.1%)
37	e	0.27	0/1154	0.58	0/1554
38	f	0.31	0/835	0.62	0/1128
39	g	0.27	0/1195	0.54	0/1602
40	h	0.27	0/989	0.56	0/1326
41	i	0.27	0/1034	0.58	0/1375
42	j	0.27	0/796	0.61	0/1077
43	k	0.48	3/845 (0.4%)	0.71	3/1145 (0.3%)
44	l	0.28	0/969	0.59	0/1300
45	m	0.28	0/892	0.57	0/1193
46	n	0.24	0/811	0.50	0/1081
47	o	0.24	0/722	0.52	0/964
48	p	0.26	0/659	0.51	0/884
49	q	0.28	0/657	0.58	0/881
50	r	0.25	0/511	0.52	0/689
51	s	0.27	0/652	0.51	0/877
52	t	0.28	0/671	0.48	0/888
53	u	0.31	0/500	0.62	0/668
54	w	0.29	0/4016	0.61	3/5428 (0.1%)
55	z	0.26	0/127	0.48	0/175
All	All	0.29	10/160031 (0.0%)	0.90	377/238586 (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	F	0	2
7	G	0	3
11	K	0	1
13	M	0	1
18	R	0	1
21	U	0	1
30	3	0	1
32	5	0	1
34	b	0	2
37	e	0	1
38	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	g	0	1
41	i	0	2
44	l	0	1
45	m	0	1
48	p	0	1
49	q	0	1
54	w	0	3
All	All	0	26

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-10.61	1.48	1.61
2	B	1	U	OP3-P	-10.57	1.48	1.61
33	a	2	A	OP3-P	-10.56	1.48	1.61
33	a	716	A	C1'-N9	7.29	1.59	1.48
33	a	715	A	C5-C6	-6.55	1.35	1.41

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	715	A	N1-C6-N6	16.59	128.55	118.60
33	a	715	A	C5-C6-N6	-12.93	113.36	123.70
33	a	715	A	C5-N7-C8	-12.41	97.69	103.90
33	a	715	A	C4-C5-N7	12.12	116.76	110.70
33	a	715	A	N7-C8-N9	11.91	119.76	113.80

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	173	ASP	Peptide
6	F	174	PHE	Peptide
7	G	118	ALA	Peptide
7	G	45	ALA	Peptide
7	G	46	ASP	Peptide

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 ⓘ

5.3.1 Protein backbone ⓘ

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	
3	C	269/271 (99%)	260 (97%)	9 (3%)	0	100	100
4	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	162 (93%)	13 (7%)	0	100	100
7	G	174/176 (99%)	162 (93%)	9 (5%)	3 (2%)	7	36
8	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
9	I	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
12	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	19	56
13	M	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	39
14	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
19	S	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	14	50
20	T	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	13	48
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
24	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
25	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
26	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	55 (89%)	5 (8%)	2 (3%)	3	22
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	101 (78%)	27 (21%)	1 (1%)	16	53
34	b	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	25	63
35	c	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	13	48
36	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
37	e	155/157 (99%)	142 (92%)	11 (7%)	2 (1%)	10	42
38	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	6	32
39	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
40	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
41	i	125/127 (98%)	109 (87%)	15 (12%)	1 (1%)	16	53
42	j	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
43	k	110/112 (98%)	96 (87%)	12 (11%)	2 (2%)	7	34
44	l	121/123 (98%)	96 (79%)	23 (19%)	2 (2%)	7	36
45	m	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	14	50
46	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
47	o	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
48	p	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
49	q	78/80 (98%)	65 (83%)	12 (15%)	1 (1%)	10	42
50	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
51	s	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
52	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
53	u	63/65 (97%)	49 (78%)	13 (21%)	1 (2%)	8	37
54	w	495/529 (94%)	432 (87%)	59 (12%)	4 (1%)	16	53
55	z	12/14 (86%)	11 (92%)	0	1 (8%)	0	9
All	All	6286/6422 (98%)	5731 (91%)	524 (8%)	31 (0%)	27	63

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP

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Mol	Chain	Res	Type
13	M	58	LYS
30	3	31	ILE
35	c	96	VAL
38	f	53	LYS

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	
3	C	216/216 (100%)	213 (99%)	3 (1%)	62	76
4	D	164/164 (100%)	163 (99%)	1 (1%)	84	88
5	E	165/165 (100%)	164 (99%)	1 (1%)	84	88
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	102 (100%)	0	100	100
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	100/100 (100%)	99 (99%)	1 (1%)	73	81
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	83 (99%)	1 (1%)	67	79
19	S	93/93 (100%)	92 (99%)	1 (1%)	70	80
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	57/57 (100%)	56 (98%)	1 (2%)	54	71
24	X	67/67 (100%)	66 (98%)	1 (2%)	60	75
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
29	2	38/38 (100%)	38 (100%)	0	100	100
30	3	51/51 (100%)	51 (100%)	0	100	100
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
34	b	180/180 (100%)	177 (98%)	3 (2%)	56	72
35	c	170/170 (100%)	168 (99%)	2 (1%)	67	79
36	d	172/172 (100%)	171 (99%)	1 (1%)	84	88
37	e	114/119 (96%)	113 (99%)	1 (1%)	75	83
38	f	87/87 (100%)	87 (100%)	0	100	100
39	g	124/124 (100%)	123 (99%)	1 (1%)	79	85
40	h	104/104 (100%)	104 (100%)	0	100	100
41	i	105/105 (100%)	104 (99%)	1 (1%)	73	81
42	j	86/86 (100%)	86 (100%)	0	100	100
43	k	85/85 (100%)	82 (96%)	3 (4%)	31	52
44	l	103/103 (100%)	103 (100%)	0	100	100
45	m	92/92 (100%)	91 (99%)	1 (1%)	70	80
46	n	79/83 (95%)	79 (100%)	0	100	100
47	o	76/76 (100%)	76 (100%)	0	100	100
48	p	65/65 (100%)	65 (100%)	0	100	100
49	q	74/74 (100%)	73 (99%)	1 (1%)	62	76
50	r	48/56 (86%)	48 (100%)	0	100	100
51	s	70/70 (100%)	69 (99%)	1 (1%)	62	76
52	t	65/65 (100%)	65 (100%)	0	100	100
53	u	44/55 (80%)	44 (100%)	0	100	100
54	w	427/453 (94%)	422 (99%)	5 (1%)	67	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5201/5255 (99%)	5171 (99%)	30 (1%)	82	88

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	c	96	VAL
54	w	125	LYS
39	g	142	ARG
54	w	312	ARG
51	s	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
40	h	75	GLN
45	m	99	GLN
55	z	15	HIS
41	i	36	GLN
43	k	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	538 (18%)	29 (1%)
2	B	119/120 (99%)	15 (12%)	2 (1%)
33	a	1536/1539 (99%)	251 (16%)	0
All	All	4548/4562 (99%)	804 (17%)	31 (0%)

5 of 804 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	U
1	A	2655	G
1	A	1378	A
2	B	66	A
1	A	2333	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 oligosaccharides 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
56	GCP	w	601	54	27,34,34	1.49	4 (14%)	34,54,54	2.04	6 (17%)

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
56	GCP	w	601	54	-	5/15/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	601	GCP	PB-O3A	5.63	1.64	1.58
56	w	601	GCP	C6-N1	3.08	1.38	1.33
56	w	601	GCP	PB-O2B	-2.23	1.51	1.56
56	w	601	GCP	C5-C6	2.03	1.44	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	601	GCP	C5-C6-N1	-8.41	111.93	123.43
56	w	601	GCP	C2-N1-C6	5.87	125.26	115.93
56	w	601	GCP	N3-C2-N1	-2.81	123.47	127.22
56	w	601	GCP	PB-O3A-PA	-2.66	124.14	132.56
56	w	601	GCP	C4-C5-C6	-2.56	118.36	120.80

There are no chirality outliers.

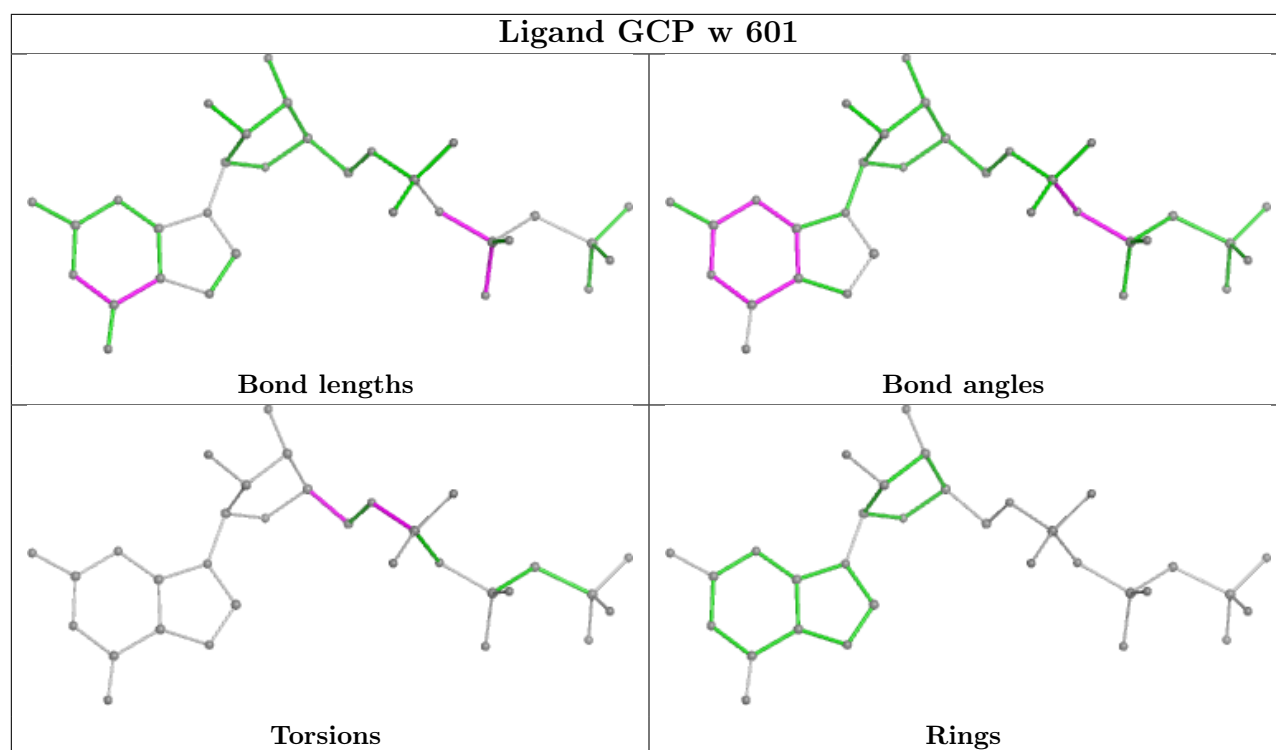
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	601	GCP	C5'-O5'-PA-O3A
56	w	601	GCP	O4'-C4'-C5'-O5'
56	w	601	GCP	C3'-C4'-C5'-O5'
56	w	601	GCP	C5'-O5'-PA-O1A
56	w	601	GCP	C5'-O5'-PA-O2A

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
33	a	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2179:C	O3'	2180:U	P	3.63
1	a	917:G	O3'	918:A	P	3.57
1	a	1394:A	O3'	1395:C	P	3.30

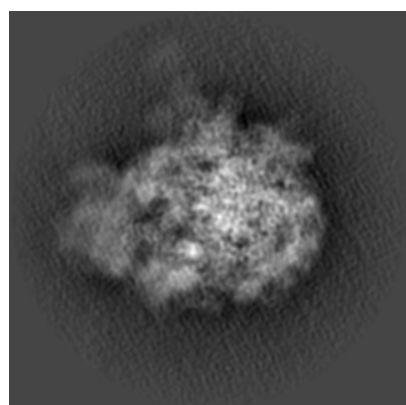
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0083. These allow visual inspection of the internal detail of the map and identification of artifacts.

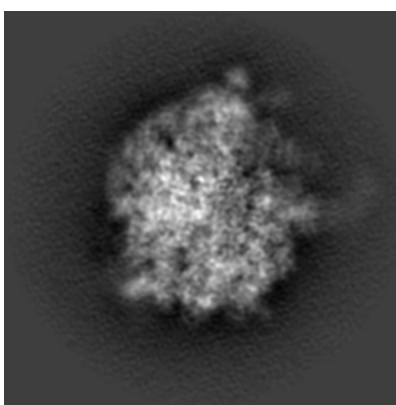
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

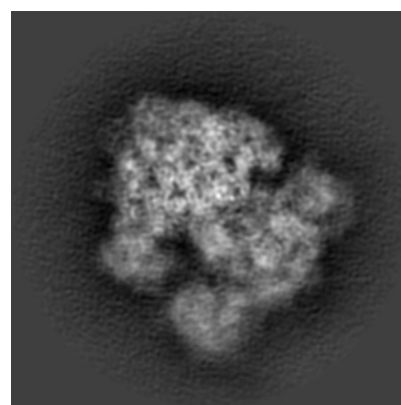
6.1.1 Primary map



X



Y

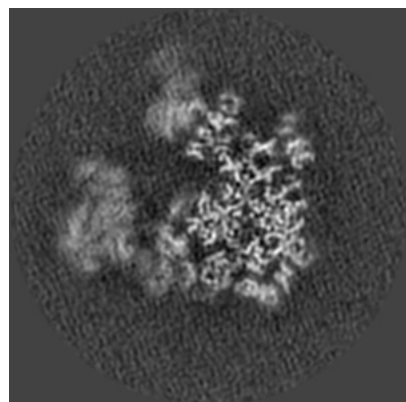


Z

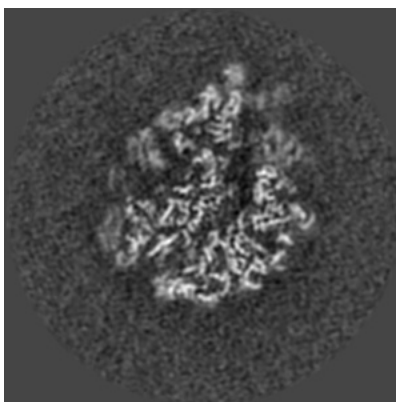
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

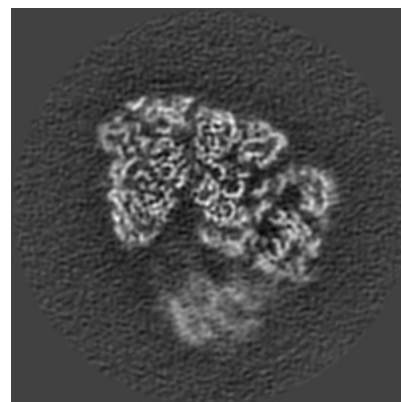
6.2.1 Primary map



X Index: 180



Y Index: 180

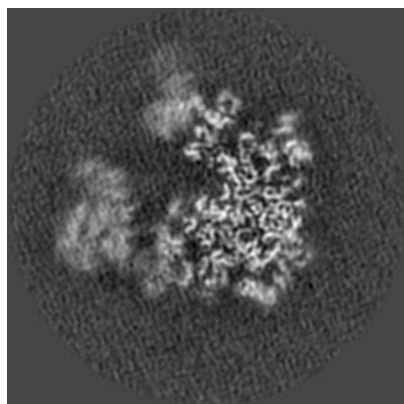


Z Index: 180

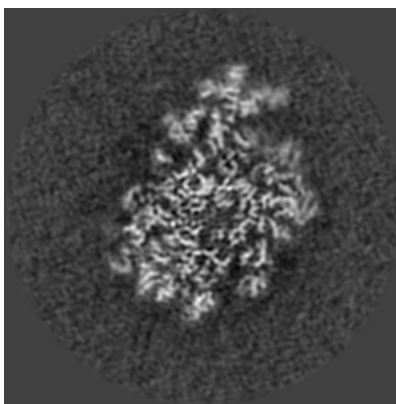
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

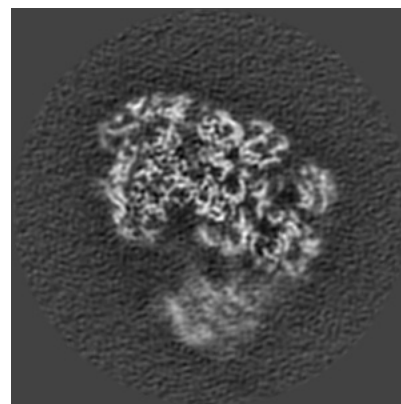
6.3.1 Primary map



X Index: 178



Y Index: 191

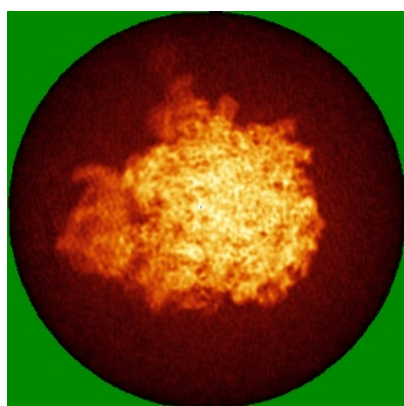


Z Index: 177

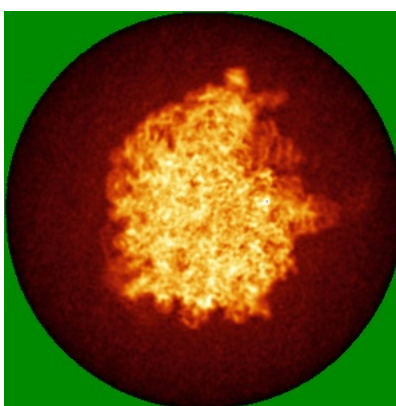
The images above show the largest variance slices of the map in three orthogonal directions.

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

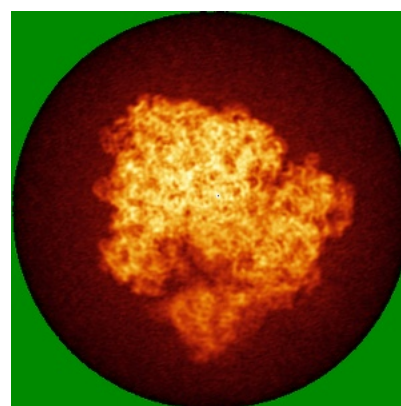
6.4.1 Primary map



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

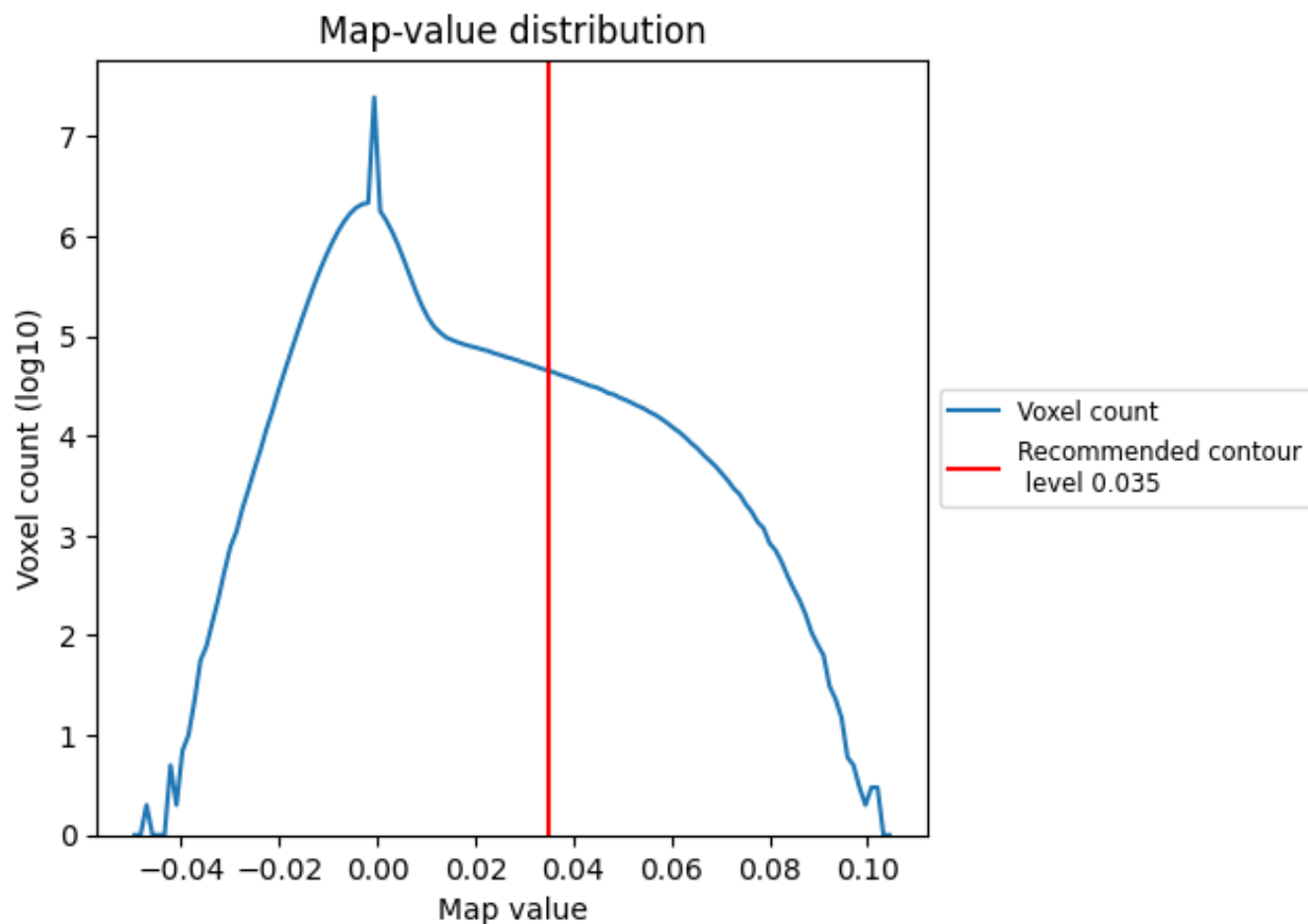
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

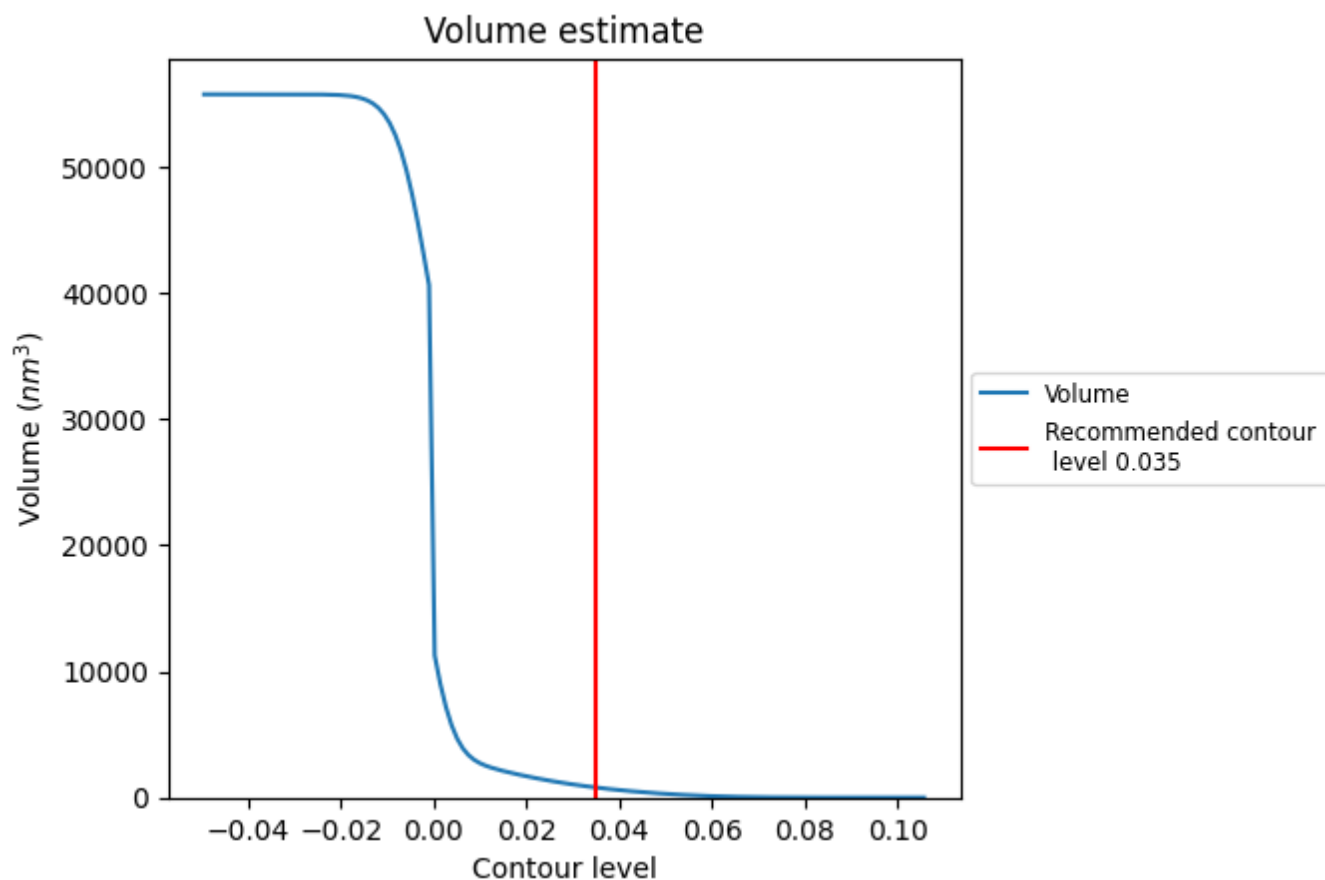
This section contains the results of statistical analysis of the map.

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.

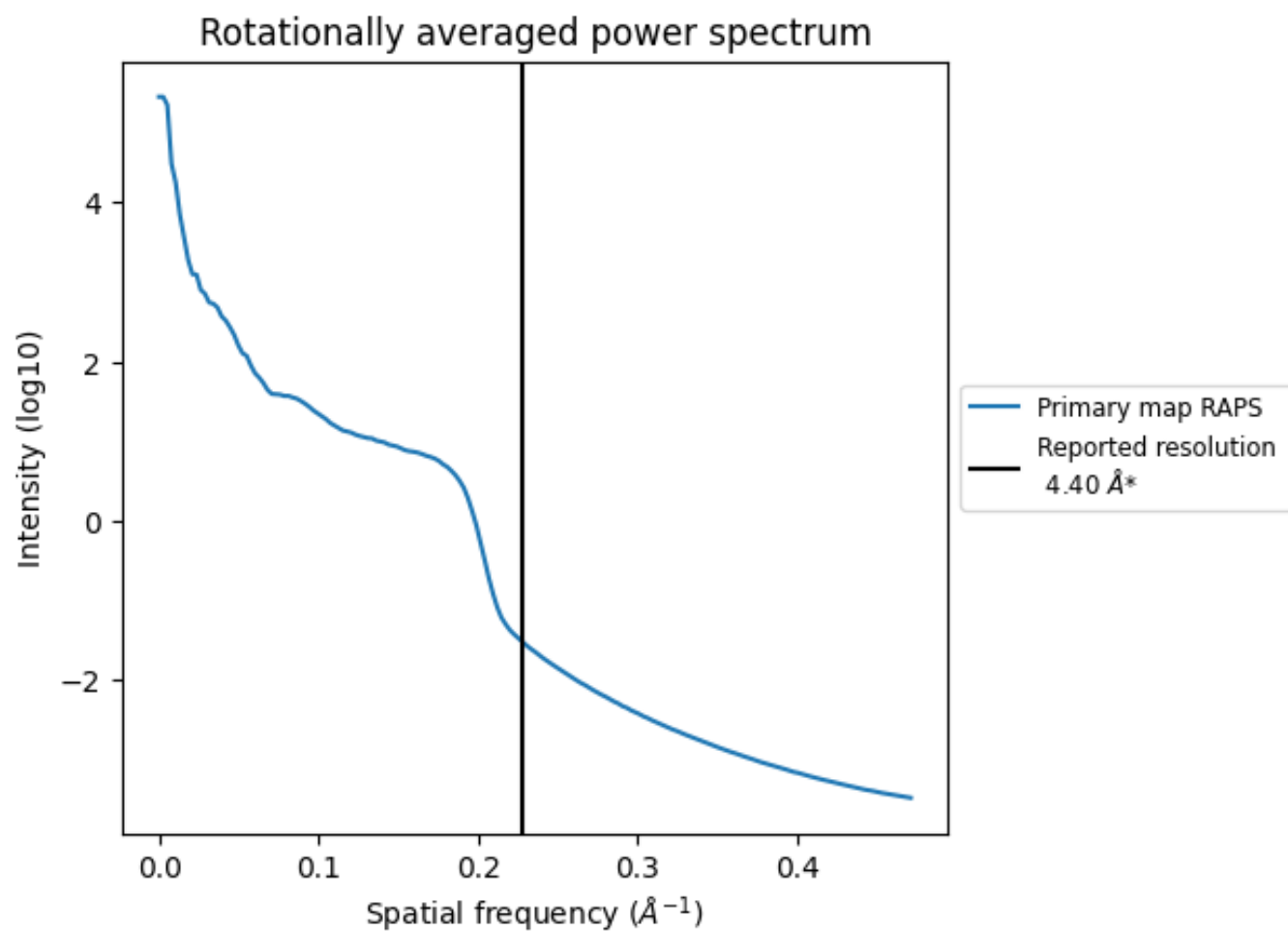
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 796 nm³; this corresponds to an approximate mass of 719 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 0.227 Å⁻¹

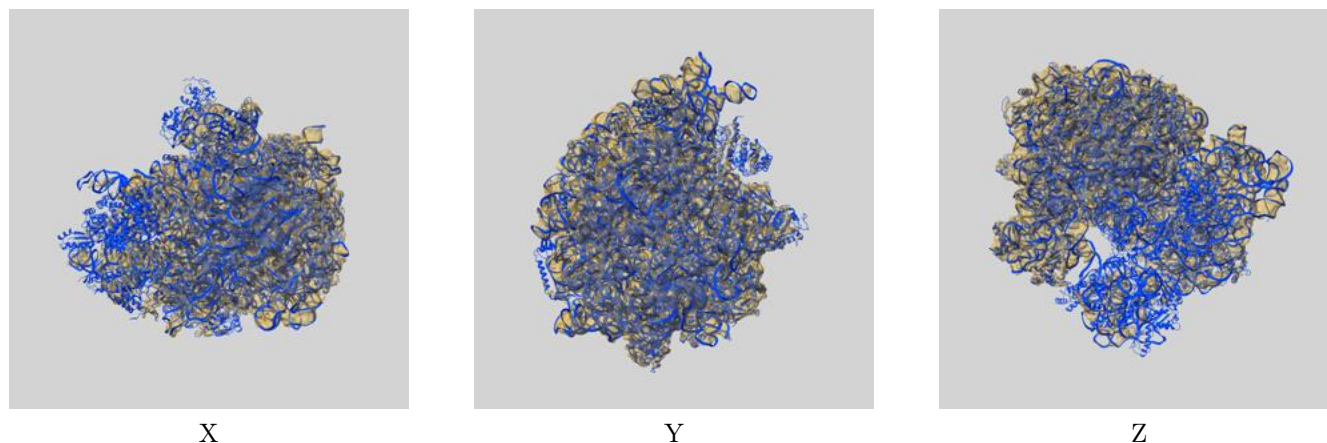
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

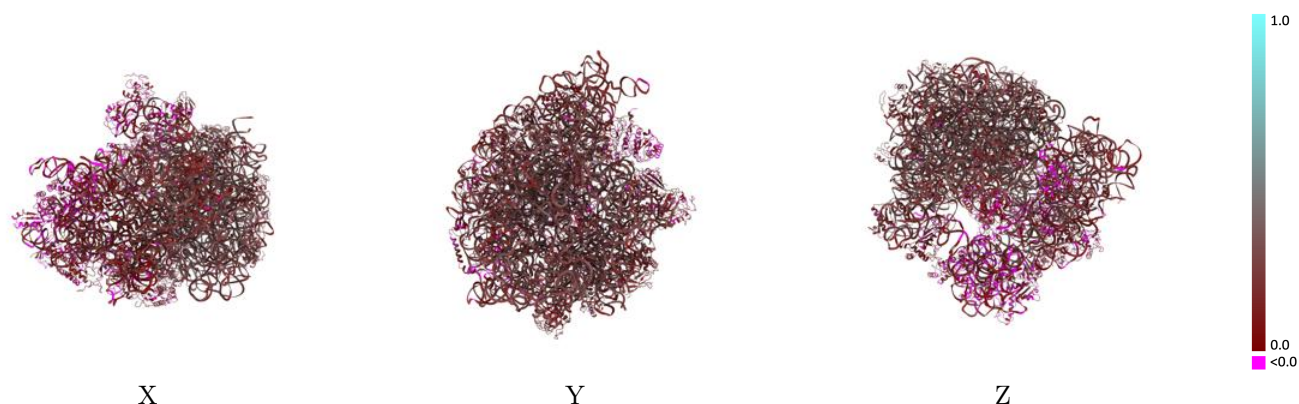
This section contains information regarding the fit between EMDB map EMD-0083 and PDB model 6GXP. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



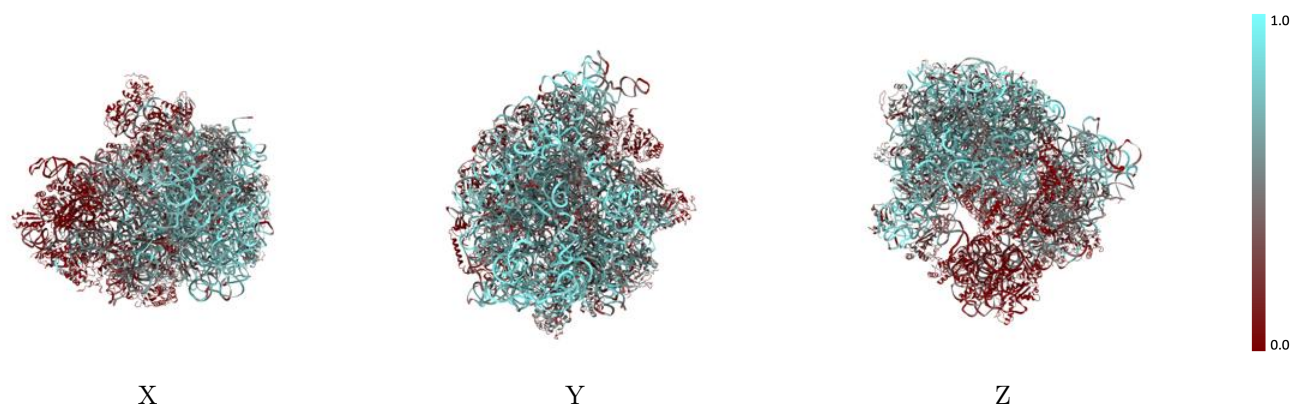
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



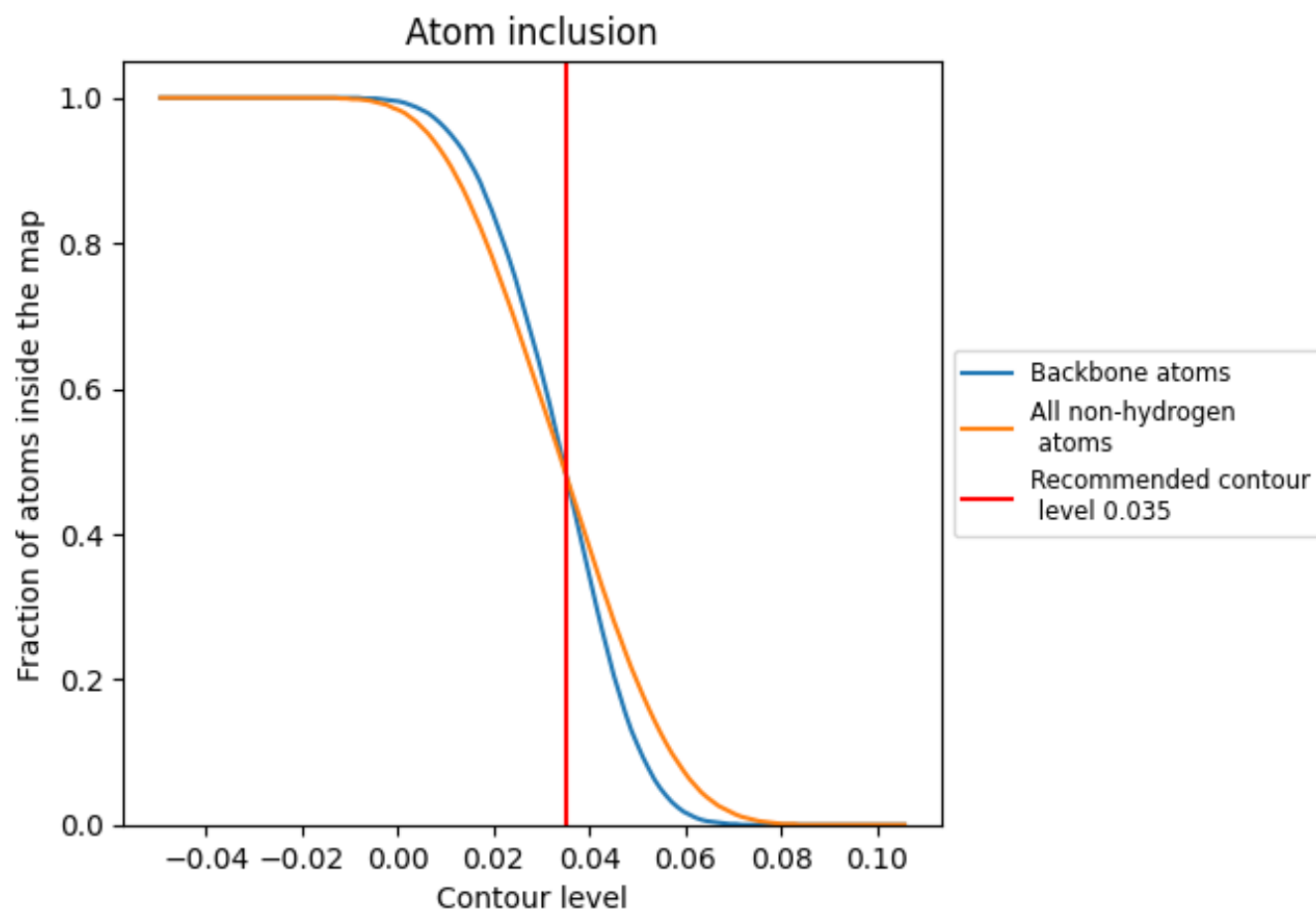
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4830	 0.2170
0	 0.3410	 0.2290
1	 0.2200	 0.2250
2	 0.3210	 0.2210
3	 0.2830	 0.2480
4	 0.4110	 0.2270
5	 0.0150	 0.0770
A	 0.6990	 0.2770
B	 0.7480	 0.2680
C	 0.3090	 0.2440
D	 0.3600	 0.2550
E	 0.3510	 0.2170
F	 0.2720	 0.1680
G	 0.3450	 0.2280
H	 0.1270	 0.1480
I	 0.0100	 0.0470
J	 0.3900	 0.2540
K	 0.2790	 0.2510
L	 0.3340	 0.2360
M	 0.3020	 0.2480
N	 0.4250	 0.2210
O	 0.4280	 0.1970
P	 0.3450	 0.2430
Q	 0.4100	 0.1970
R	 0.3580	 0.2410
S	 0.2850	 0.2160
T	 0.3850	 0.2220
U	 0.3740	 0.2140
V	 0.3890	 0.2280
W	 0.2950	 0.2390
X	 0.3640	 0.2330
Y	 0.4690	 0.1850
Z	 0.3410	 0.2180
a	 0.4480	 0.1710
b	 0.0970	 0.1530



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Chain	Atom inclusion	Q-score
c	 0.0150	 0.0900
d	 0.1240	 0.1300
e	 0.2490	 0.1620
f	 0.1030	 0.1410
g	 0.0250	 0.0770
h	 0.3010	 0.1970
i	 0.0370	 0.0690
j	 0.0000	 0.0360
k	 0.0990	 0.1440
l	 0.1070	 0.1770
m	 0.0180	 0.0690
n	 0.0080	 0.0340
o	 0.2550	 0.1740
p	 0.3010	 0.2010
q	 0.2230	 0.1840
r	 0.1360	 0.1790
s	 0.0000	 0.0140
t	 0.3690	 0.1720
u	 0.0590	 0.1400
w	 0.0480	 0.0930
z	 0.0710	 0.1890