



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 02:34 PM EST

PDB ID : 6XII
EMDB ID : EMD-22192
Title : Escherichia coli transcription-translation complex B (TTC-B) containing an
24 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-06-20
Resolution : 7.00 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

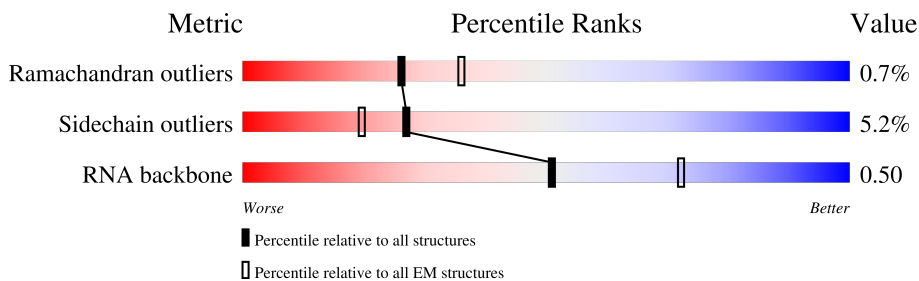
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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	103	
2	1	110	
3	2	100	
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	41	

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Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	C	75	
17	D	1542	
18	E	87	
19	F	71	
20	G	241	
21	H	557	
22	I	233	
23	J	206	
24	K	167	
25	L	135	
26	M	179	
27	N	130	
28	O	130	
29	P	103	
30	Q	129	
31	R	124	

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Mol	Chain	Length	Quality of chain
32	S	101	22% 95%
33	T	89	22% 85% 13%
34	U	82	15% 94% 6%
35	V	84	30% 93% 5%
36	W	92	33% 86% 10%
37	X	118	46% 88% 10%
38	Y	142	66% 68% 27%
39	Z	121	22% 12% 12% 75%
40	a	2904	81% 18%
41	b	85	11% 88% 11%
42	c	78	35% 94% 5%
43	d	120	8% 86% 14%
44	e	63	21% 97%
45	f	59	14% 95%
46	g	70	44% 86% 9% 6%
47	h	273	27% 93% 7%
48	i	57	19% 88% 11%
49	j	209	16% 97%
50	k	55	18% 89% 5% 5%
51	l	201	20% 93% 7%
52	m	46	11% 93% 7%
53	n	179	33% 89% 10%
54	o	65	8% 91% 8%
55	p	177	28% 97%
56	q	38	95% 5%

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Mol	Chain	Length	Quality of chain
57	r	149	
58	s	142	
59	t	123	
60	u	144	
61	v	136	
62	w	127	
63	x	117	
64	y	115	
65	z	118	

2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 276059 atoms, of which 99203 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 L21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	0	103	1655	516	839	153	145	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	1	110	1779	532	922	166	156	3	0	0

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	2	94	1557	470	811	140	134	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	3	103	1632	498	844	148	142	0	0

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	4	94	1533	479	780	137	134	3	0	0

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
6	5	23	732	225	260	87	137	23	0	0

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	31	Total	C	N	O	P	0	0
			647	289	92	235	31		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	162	Total	C	N	O	S	0	0
			1282	816	222	237	7		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AD	218	1677	1048	297	326	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AE	1337	10404	6535	1856	1963	50	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AF	82	650	396	122	131	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	C	66	1103	344	559	102	97	1	0	0

- Molecule 17 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
17	D	1524	49126	14585	16423	6003	10591	1524	0	0

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	E	86	1388	414	719	138	114	3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
19	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
20	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 21 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 22 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 23 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 24 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 25 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 26 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	M	151	2416	735	1235	227	215	4	0	0

- Molecule 27 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	N	129	2010	616	1031	173	184	6	0	0

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	O	127	2092	634	1070	206	179	3	0	0

- Molecule 29 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	P	99	1621	495	831	151	143	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	Q	117	1764	540	887	174	160	3	0	0

- Molecule 31 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	R	121	1940	580	1001	194	161	4	0	0

- Molecule 32 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	S	100	1649	499	844	164	139	3	0	0

- Molecule 33 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
33	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 34 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
34	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
35	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 36 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
36	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 37 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
37	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 38 is a protein called 50S ribosomal protein L11.

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

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 40 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
40	a	2880	92918	27587	31077	11398	19976	2880	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	b	76	1181	360	599	117	104	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	c	77	1277	388	652	129	106	2	0	0

- Molecule 43 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
43	d	120	3870	1144	1301	468	837	120	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	e	62	1032	308	531	98	94	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	f	58	936	281	488	87	78	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
46	g	66	1042	323	520	99	94	6	0	0

- Molecule 47 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
47	h	271	4236	1288	2154	423	364	7	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
48	i	56	903	269	459	94	80	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
49	j	209	3182	979	1617	288	294	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
50	k	52	890	275	464	78	73		0	0

- Molecule 51 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
51	l	201	3171	974	1619	283	290	5	0	0

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	m	46	795	228	418	90	57	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
53	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
54	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
56	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 58 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 59 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
59	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 60 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
60	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 61 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
61	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 62 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
62	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 63 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
63	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 64 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
64	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 65 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
65	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	AE	1	Total	Mg	0
			1	1	

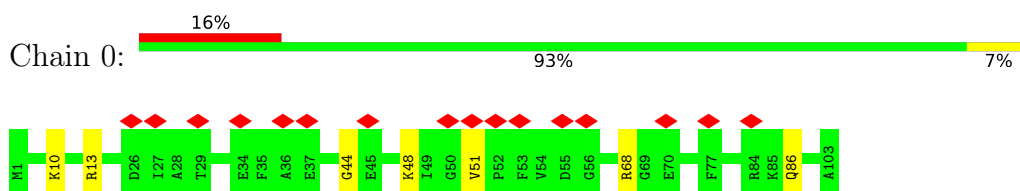
- Molecule 67 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
67	AE	2	Total 2	Zn 2	0

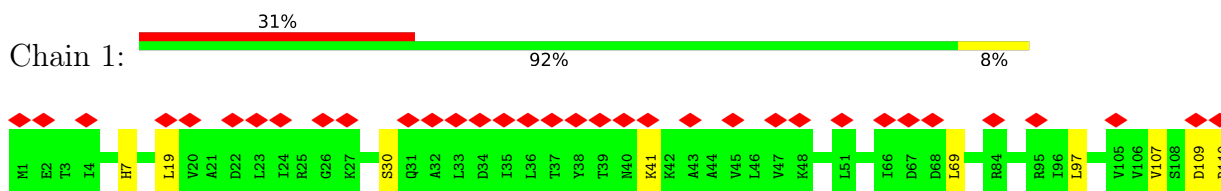
3 Residue-property plots [i](#)

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

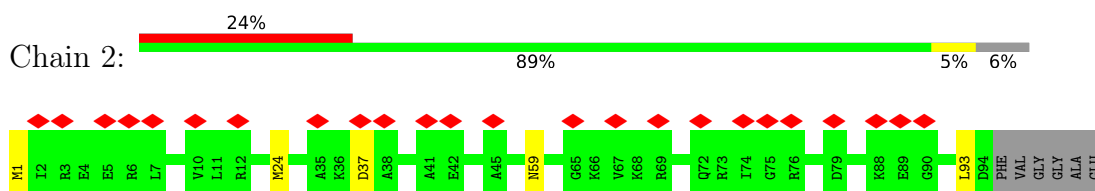
- Molecule 1: 50S ribosomal protein L21



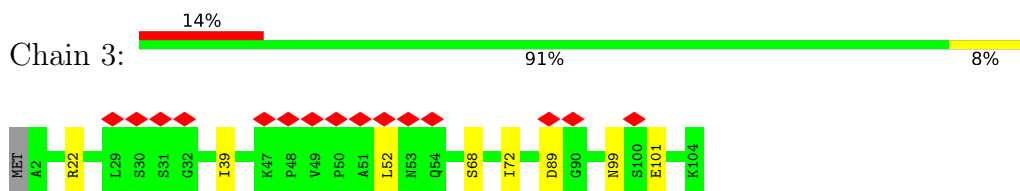
- Molecule 2: 50S ribosomal protein L22



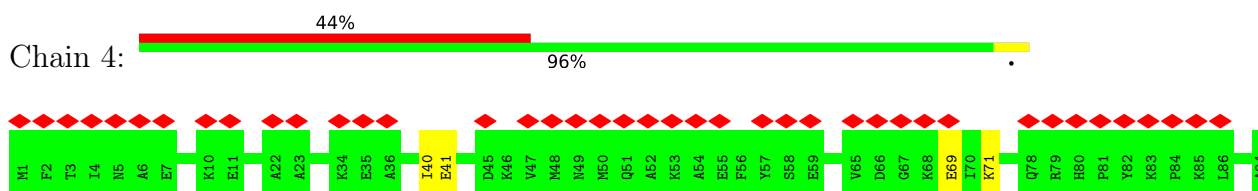
- Molecule 3: 50S ribosomal protein L23



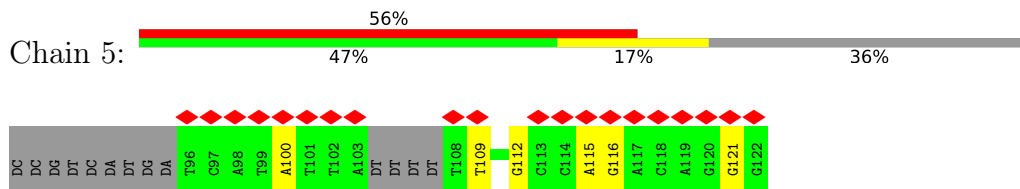
- Molecule 4: 50S ribosomal protein L24



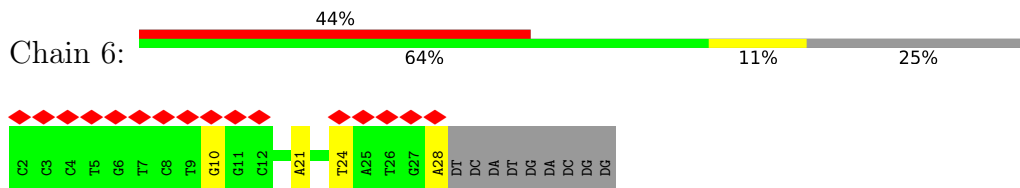
- Molecule 5: 50S ribosomal protein L25



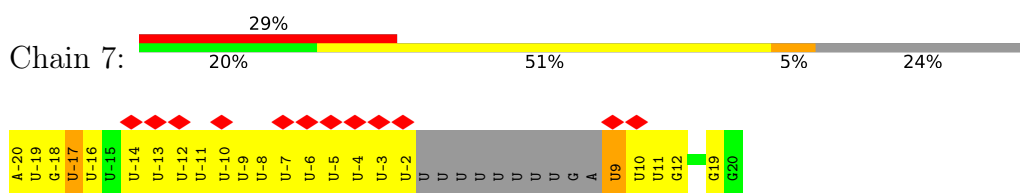
- Molecule 6: NT DNA



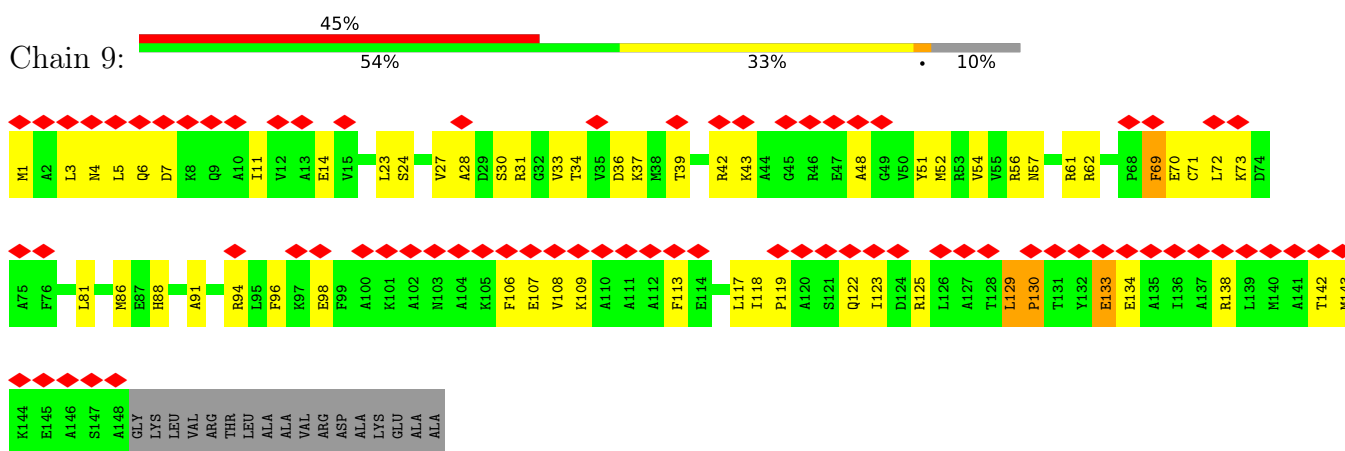
- Molecule 7: T DNA



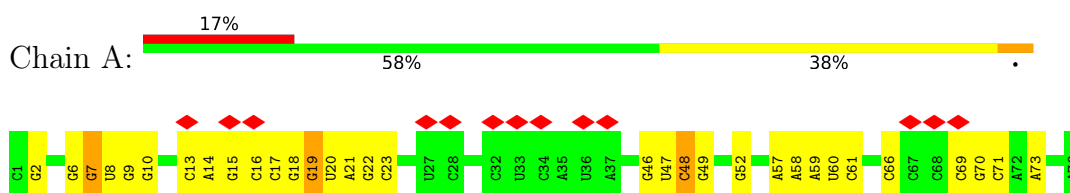
- Molecule 8: mRNA with 24 nt long spacer



- Molecule 9: 50S ribosomal protein L10

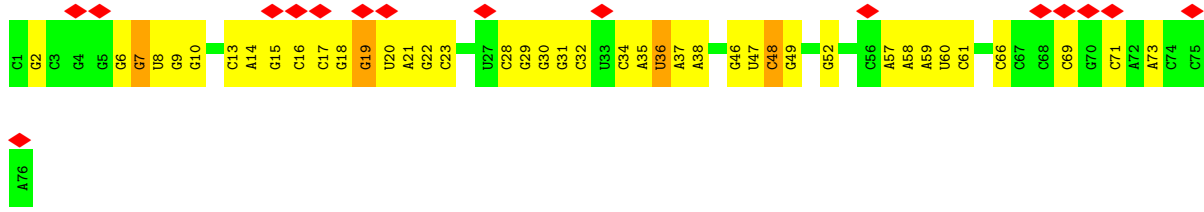


- Molecule 10: E-site and P-site tRNA (fMet)

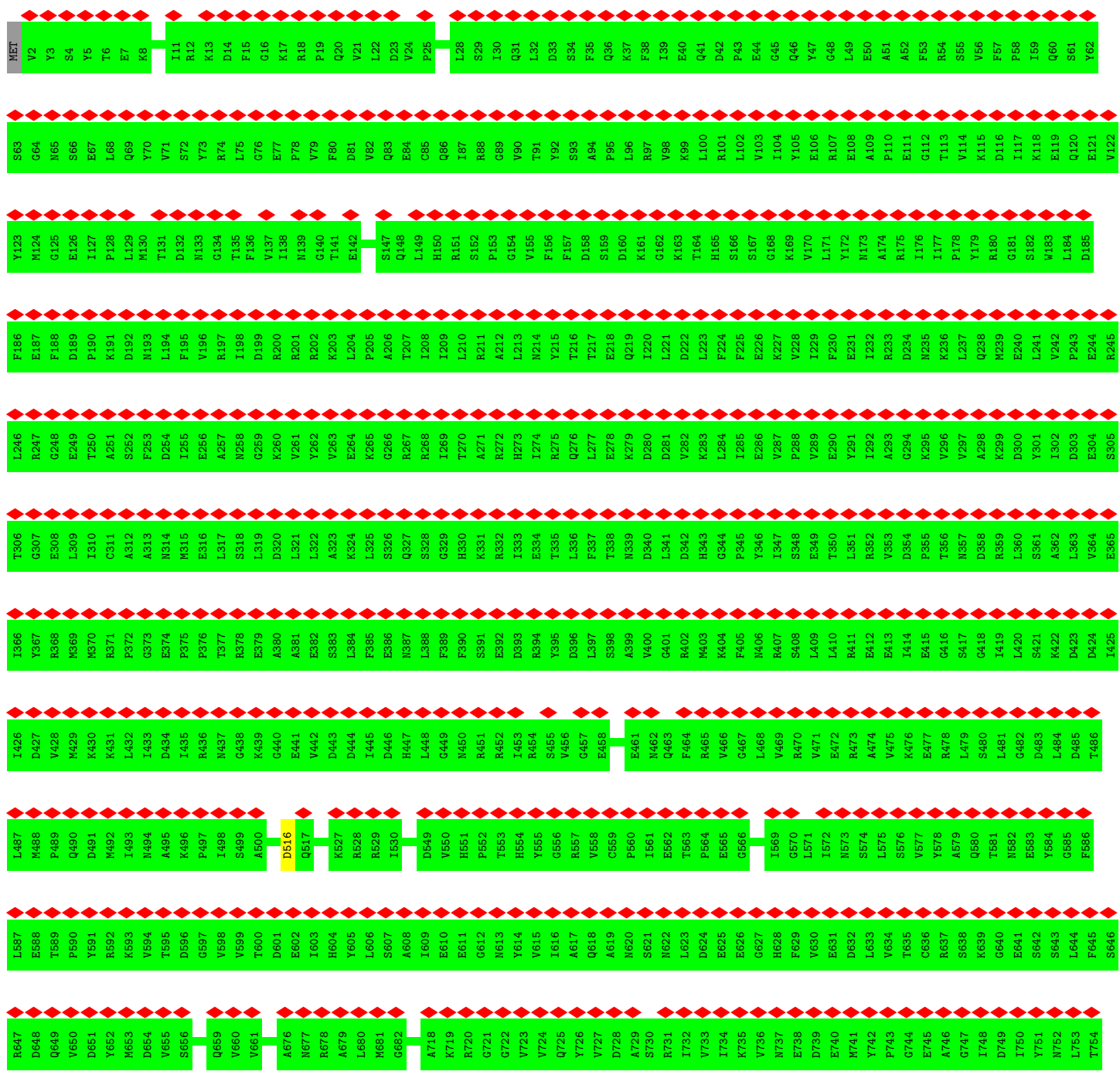
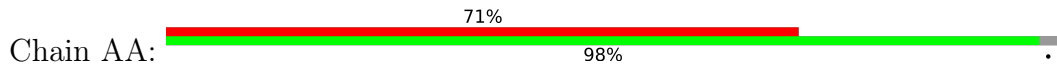


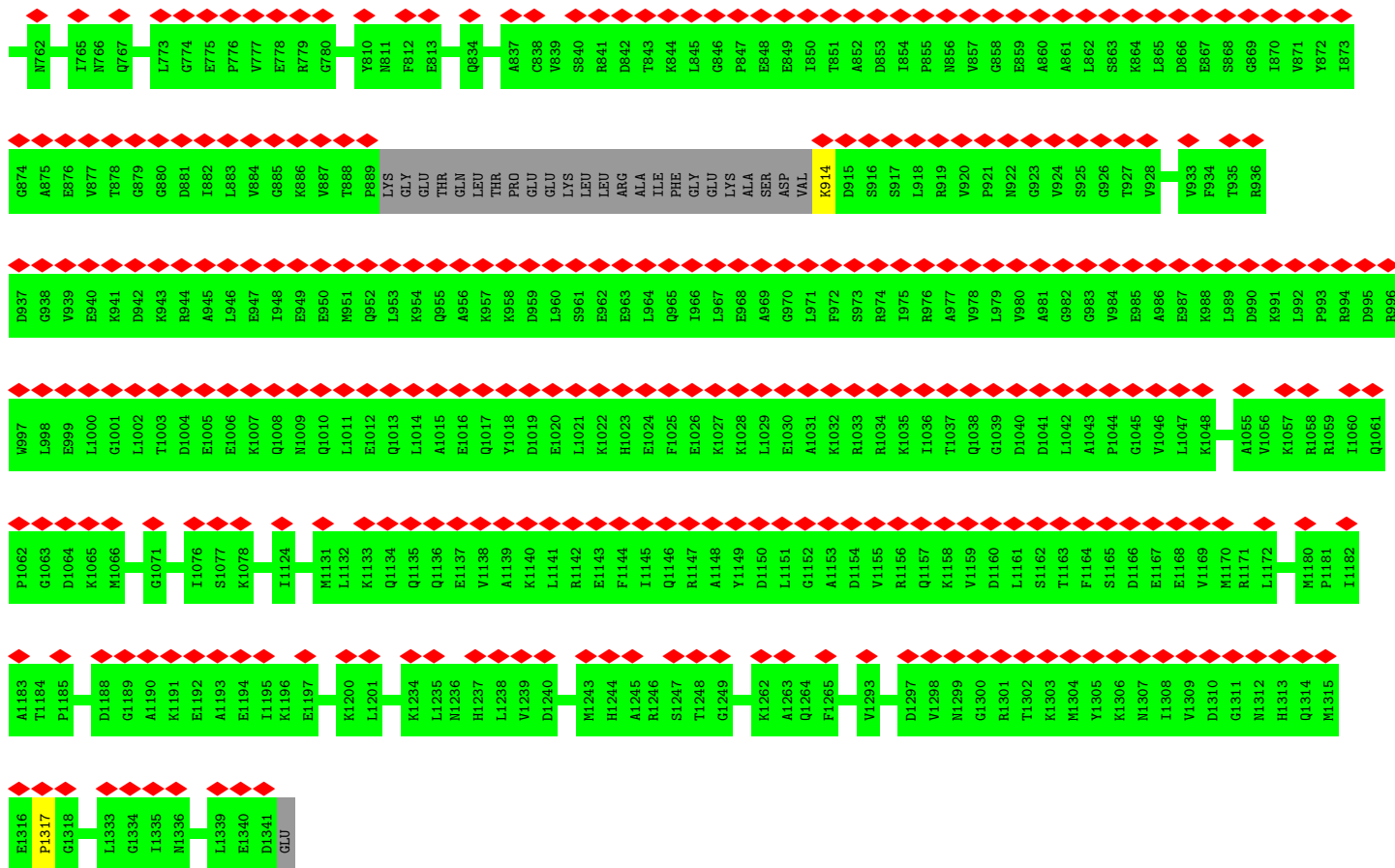
- Molecule 10: E-site and P-site tRNA (fMet)



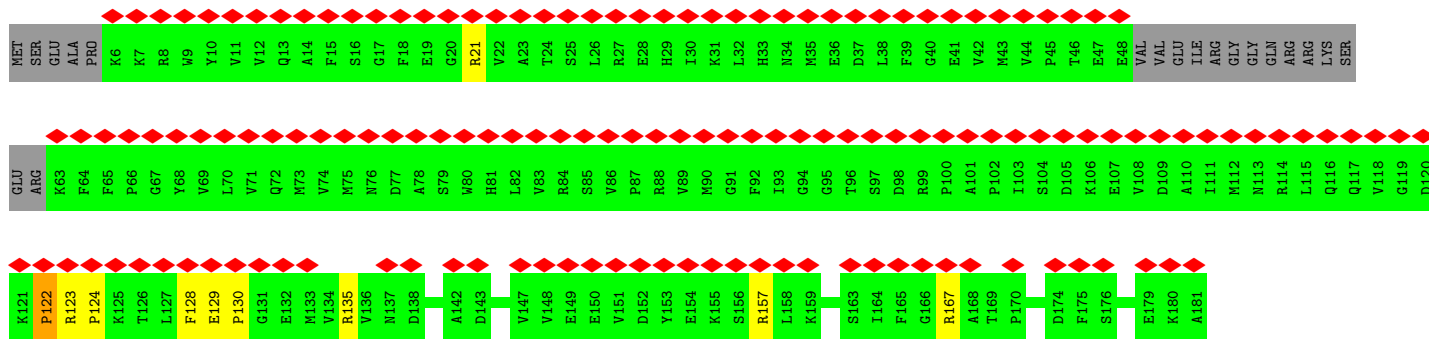
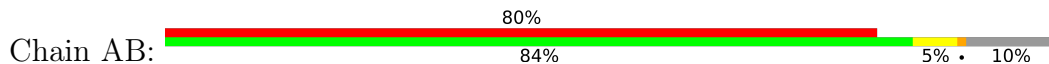


• Molecule 11: DNA-directed RNA polymerase subunit beta

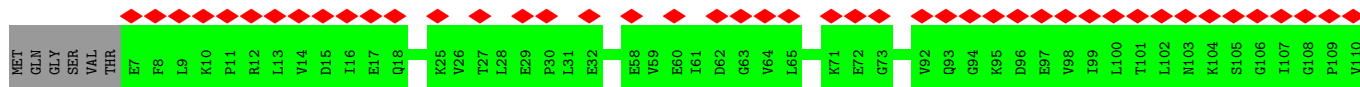


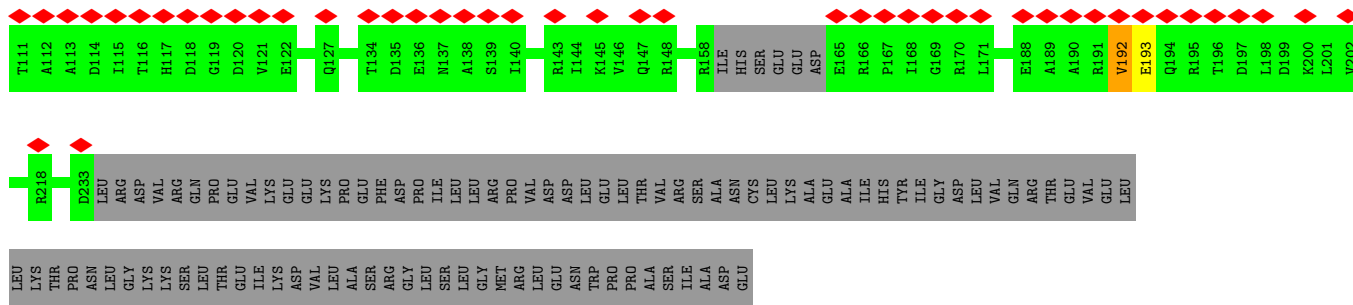


• Molecule 12: Transcription termination/antitermination protein NusG

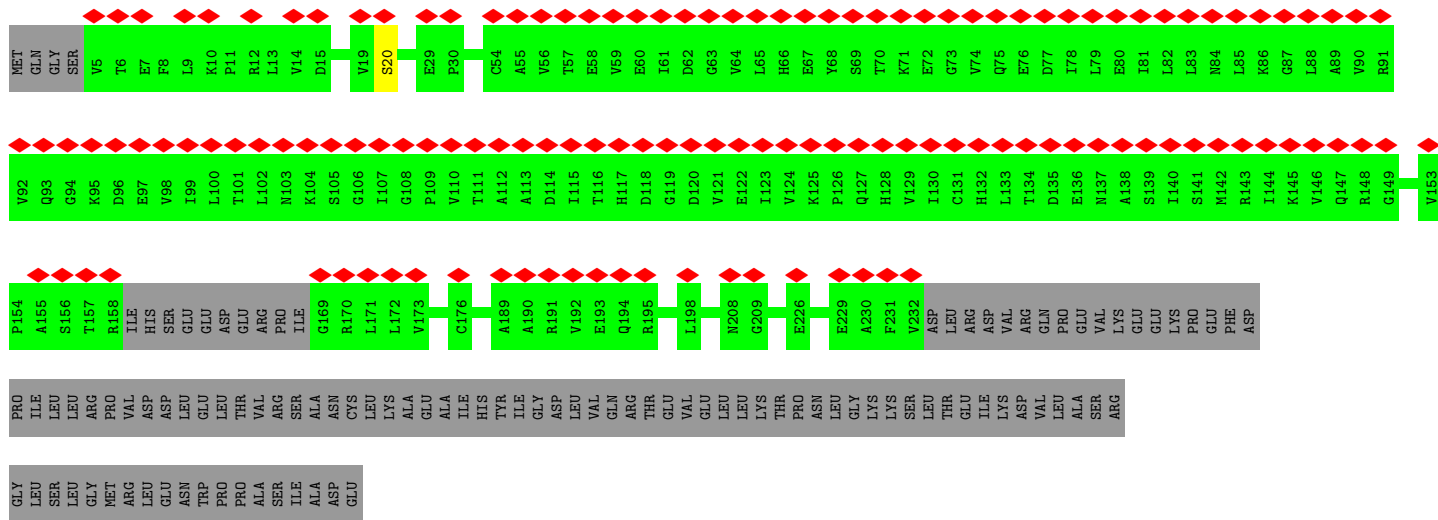
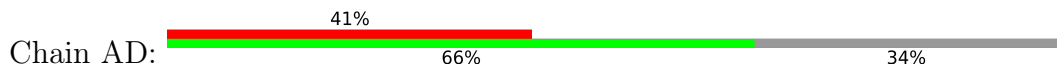


• Molecule 13: DNA-directed RNA polymerase subunit alpha

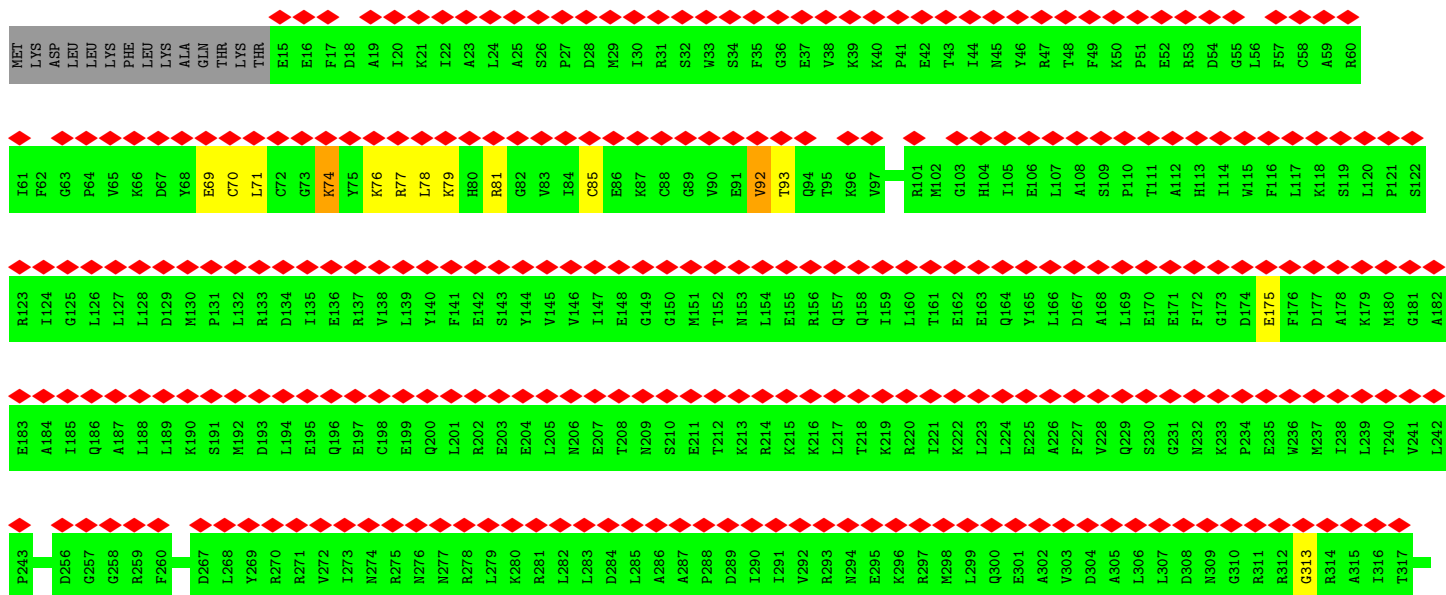


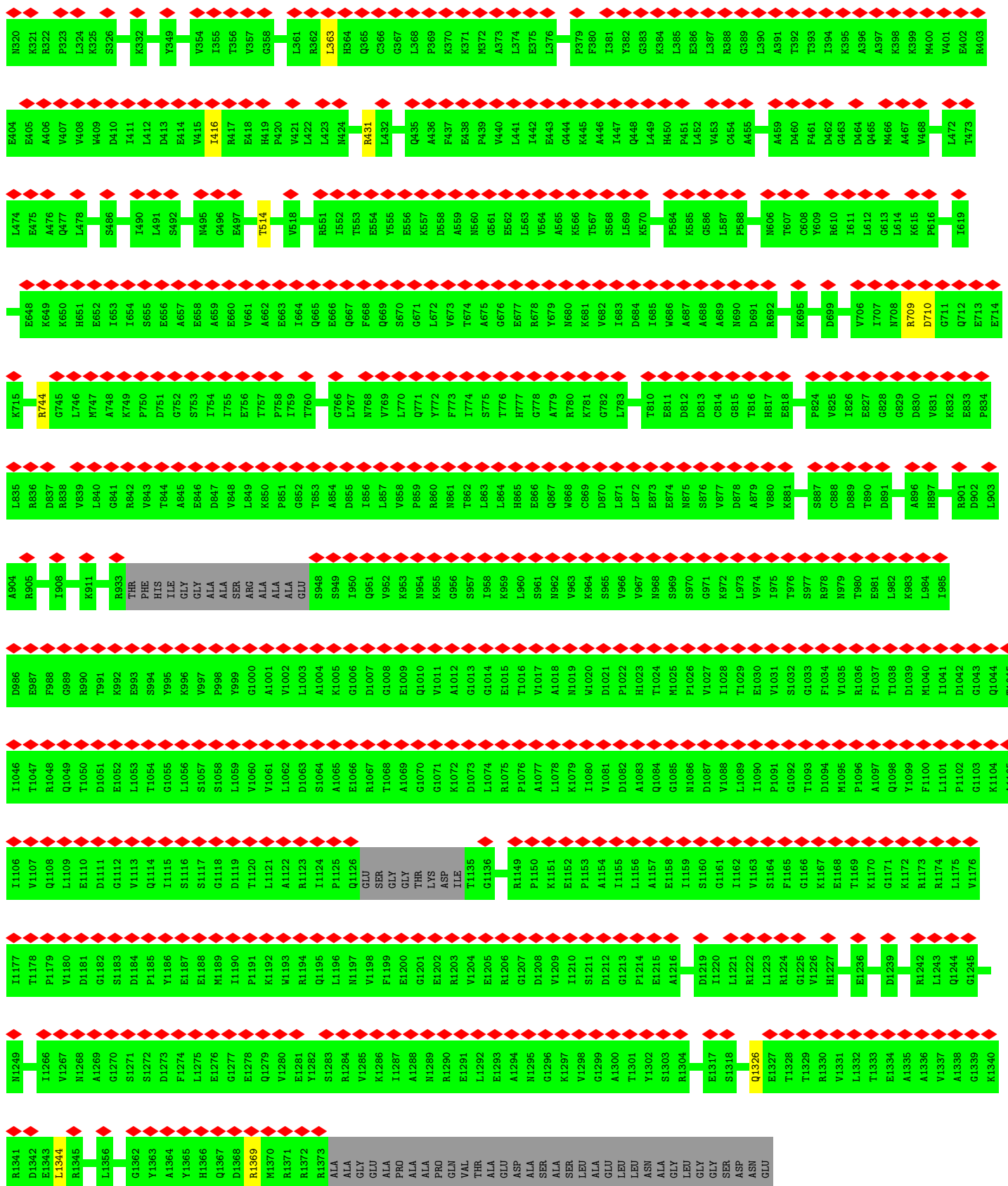


● Molecule 13: DNA-directed RNA polymerase subunit alpha

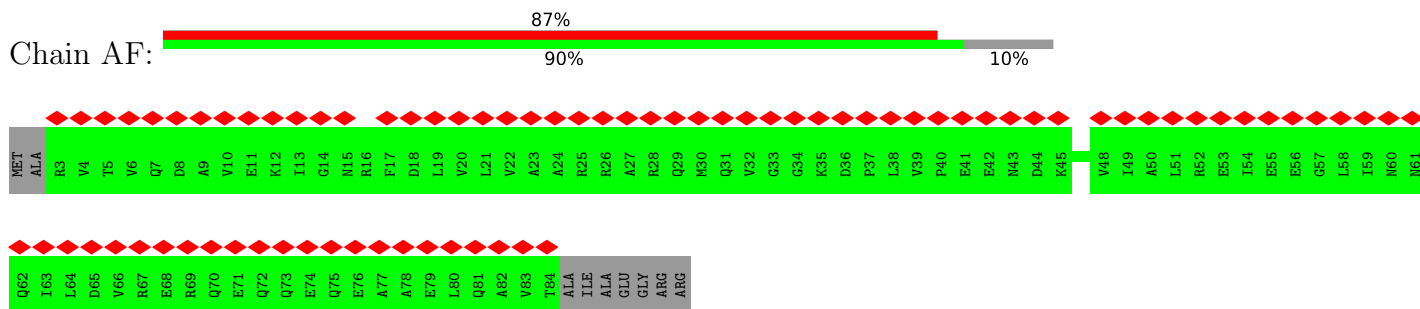


● Molecule 14: DNA-directed RNA polymerase subunit beta'

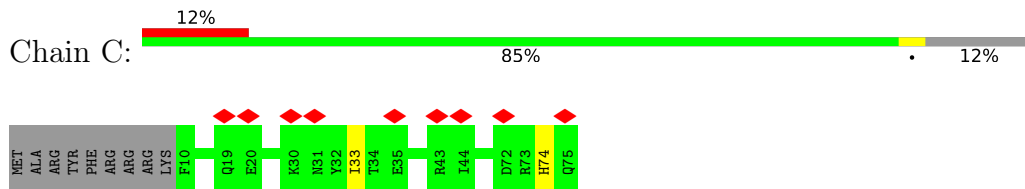




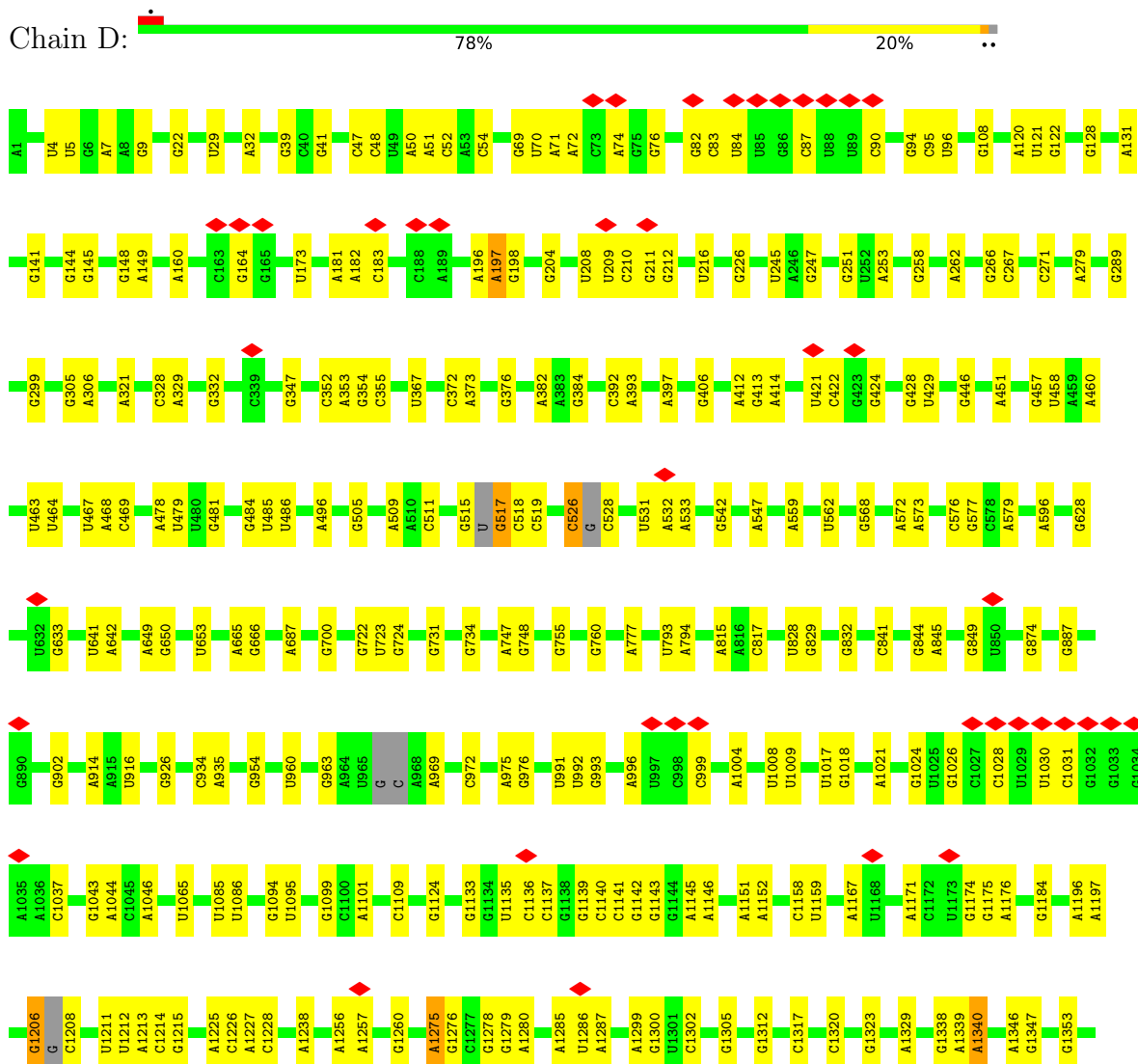
- Molecule 15: DNA-directed RNA polymerase subunit omega

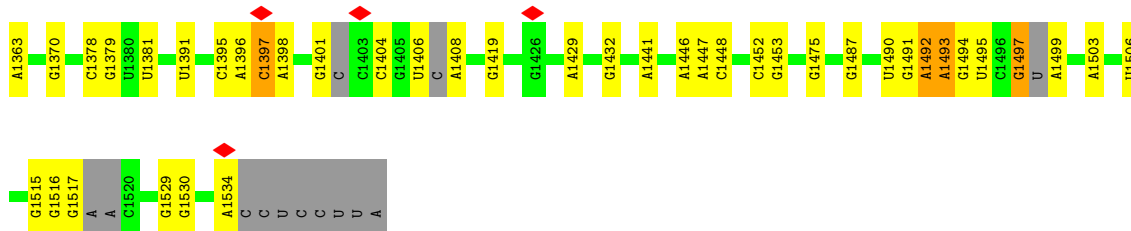


• Molecule 16: 30S ribosomal protein S18

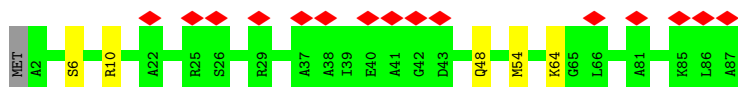


• Molecule 17: 16S rRNA

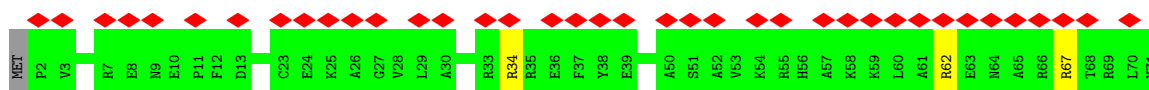
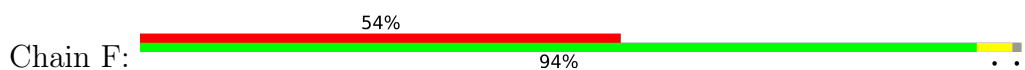




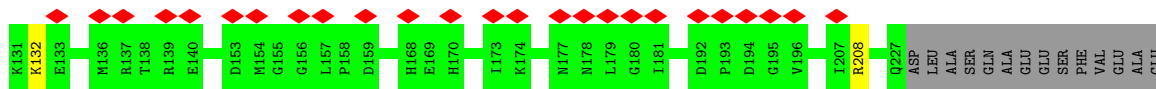
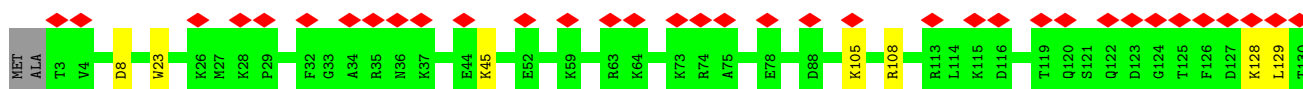
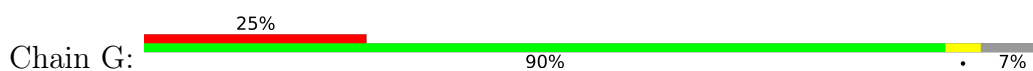
• Molecule 18: 30S ribosomal protein S20



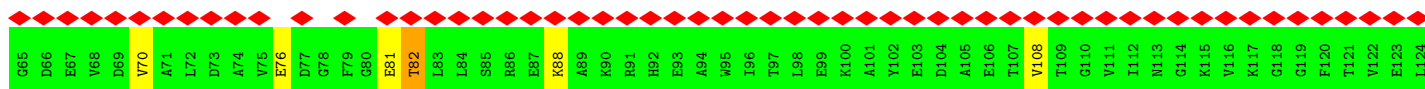
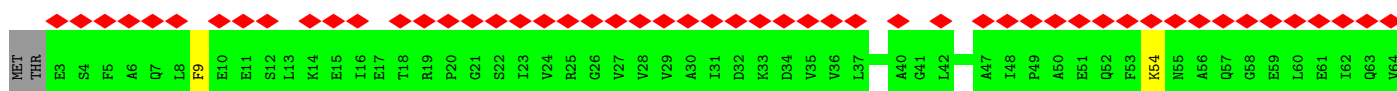
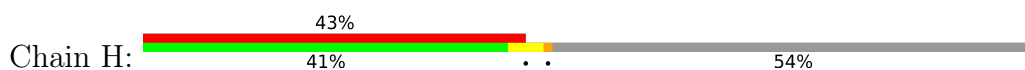
• Molecule 19: 30S ribosomal protein S21

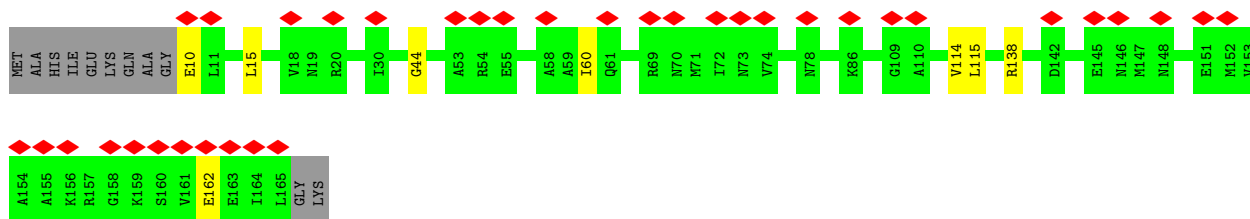


• Molecule 20: 30S ribosomal protein S2

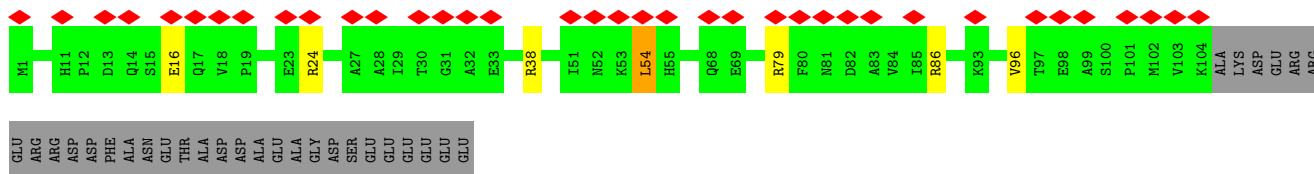


• Molecule 21: 30S ribosomal protein S1

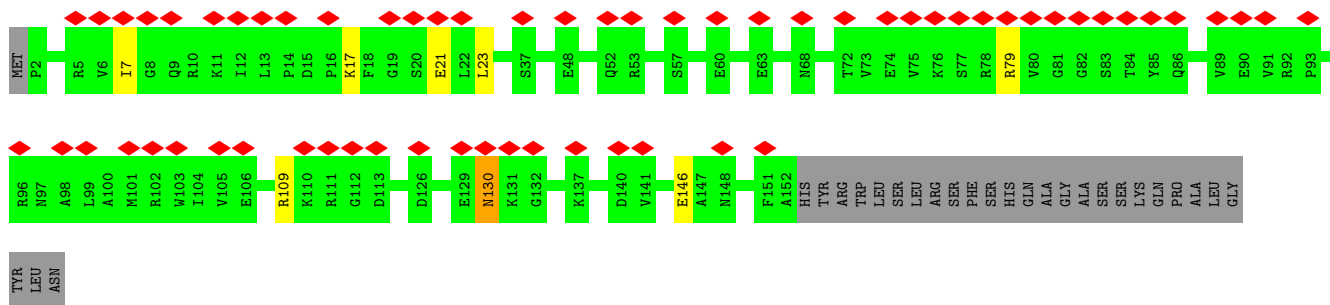
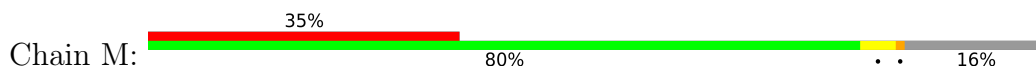




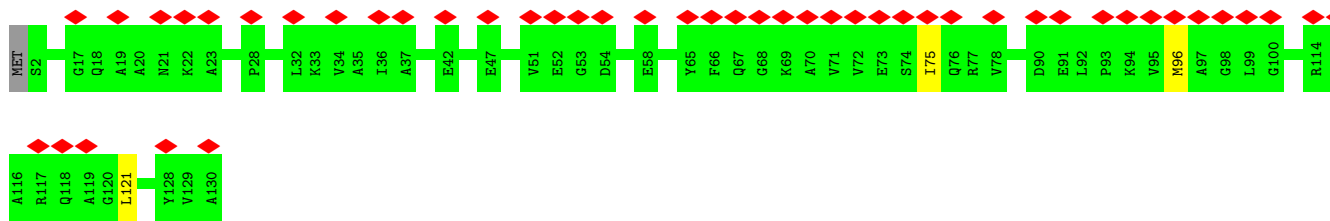
• Molecule 25: 30S ribosomal protein S6



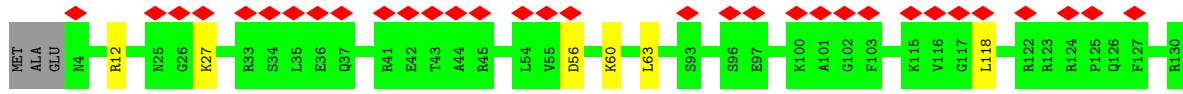
• Molecule 26: 30S ribosomal protein S7



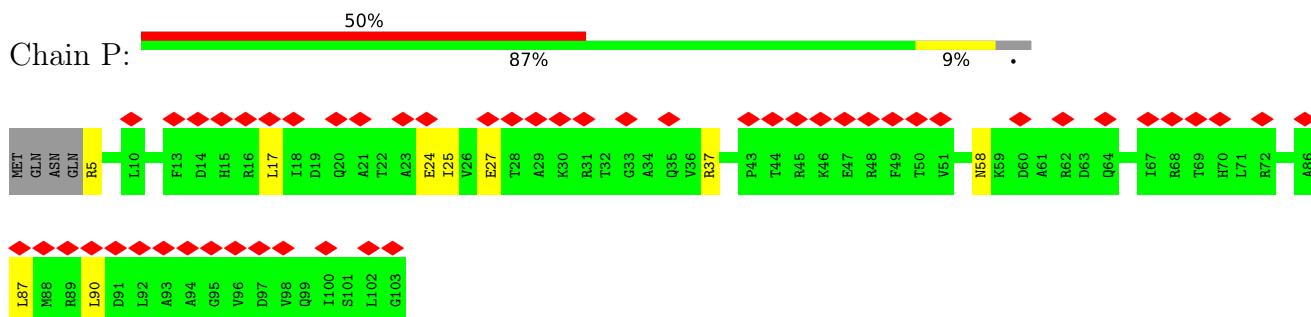
• Molecule 27: 30S ribosomal protein S8



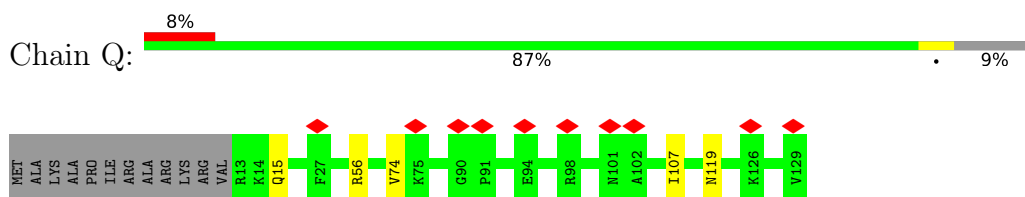
• Molecule 28: 30S ribosomal protein S9



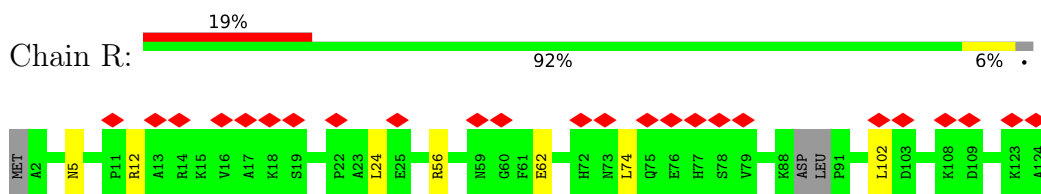
- Molecule 29: 30S ribosomal protein S10



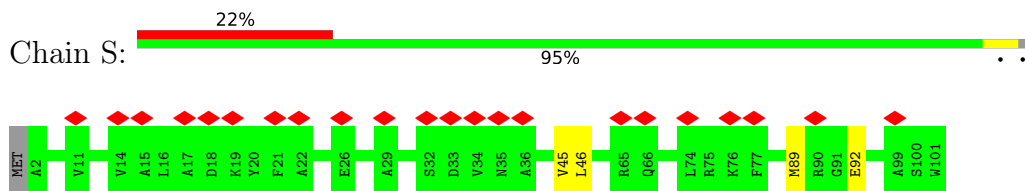
- Molecule 30: 30S ribosomal protein S11



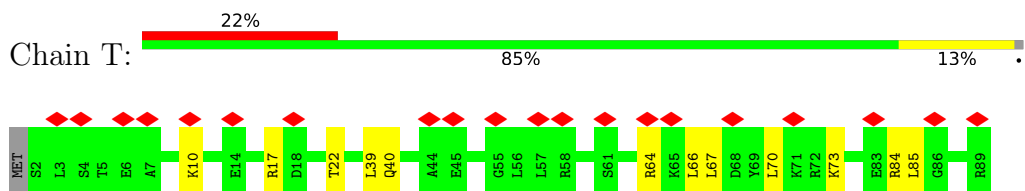
- Molecule 31: 30S ribosomal protein S12



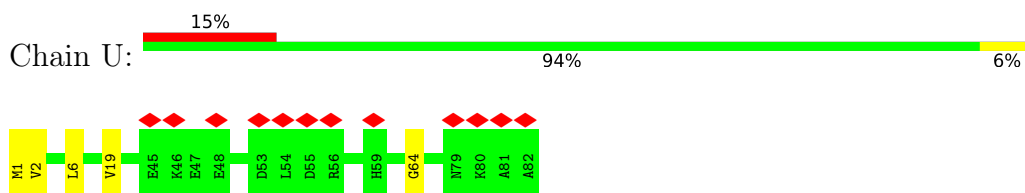
- Molecule 32: 30S ribosomal protein S14



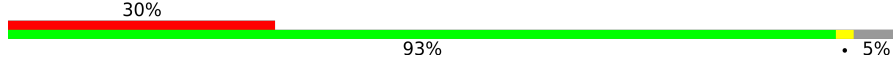
- Molecule 33: 30S ribosomal protein S15



- Molecule 34: 30S ribosomal protein S16




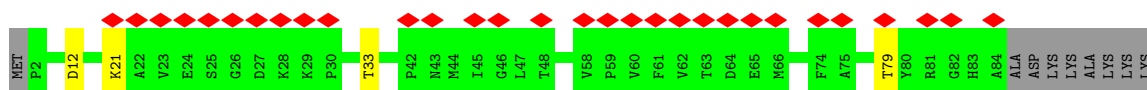
- Molecule 35: 30S ribosomal protein S17

Chain V: 




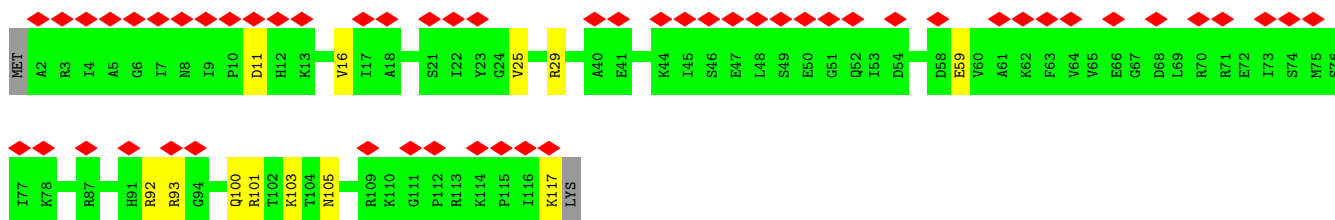
- Molecule 36: 30S ribosomal protein S19

Chain W: 



- Molecule 37: 30S ribosomal protein S13

Chain X: 



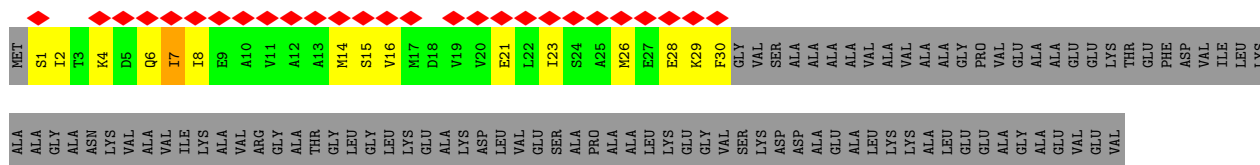
- Molecule 38: 50S ribosomal protein L11

Chain Y: 




- Molecule 39: 50S ribosomal protein L7/L12

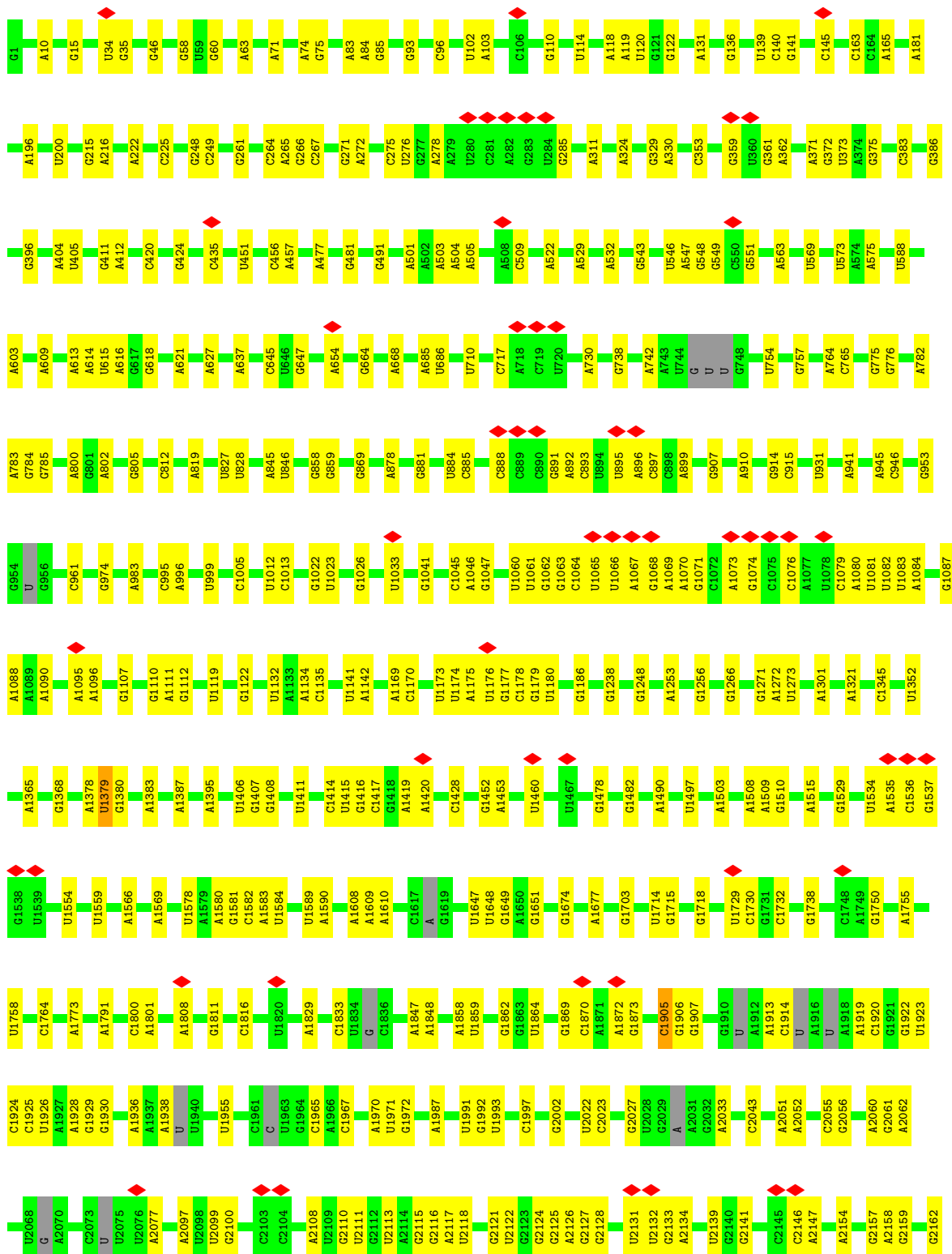
Chain Z: 

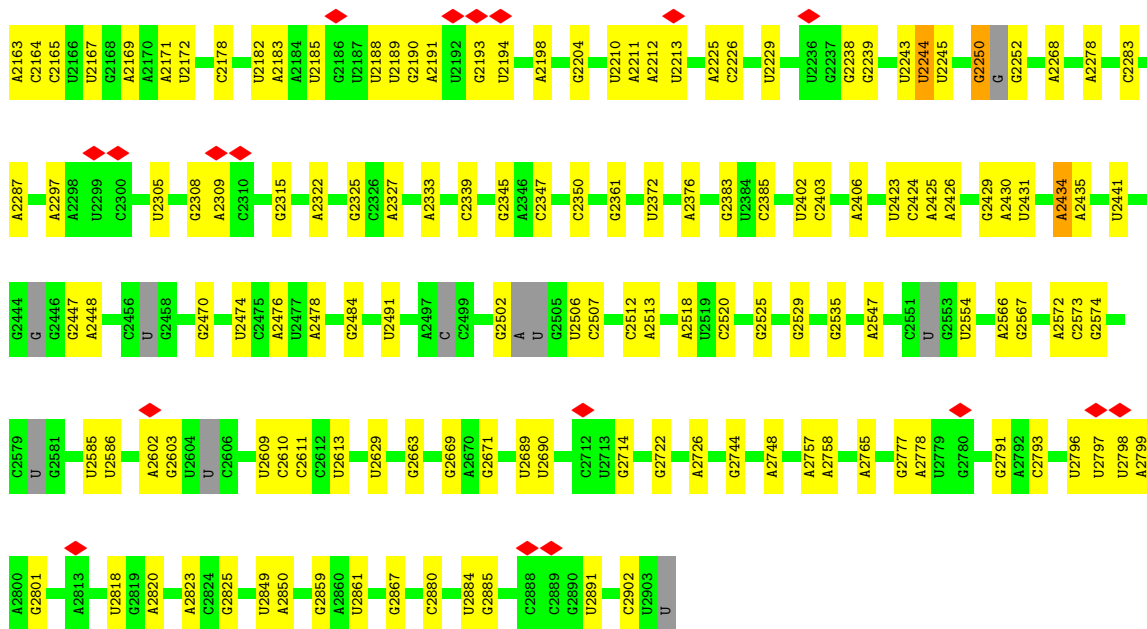


LYS

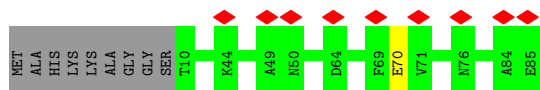
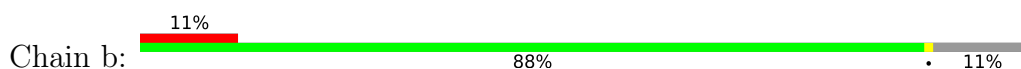
- Molecule 40: 23S rRNA

Chain a:  81% 18%

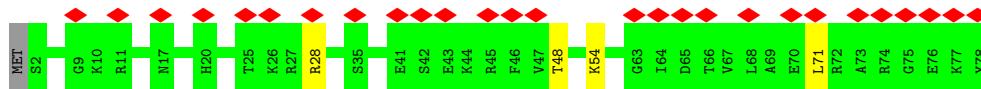
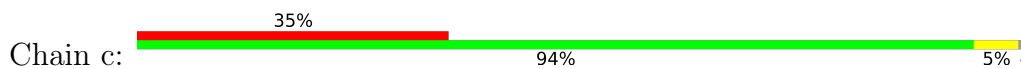




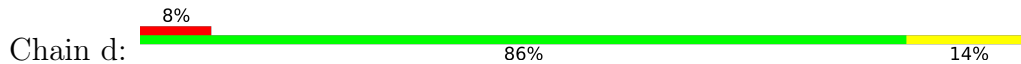
• Molecule 41: 50S ribosomal protein L27



• Molecule 42: 50S ribosomal protein L28



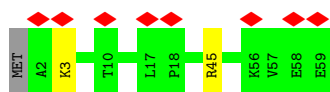
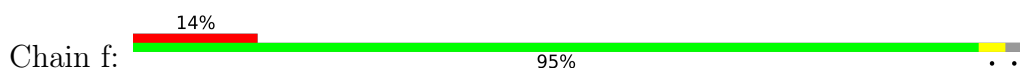
• Molecule 43: 5S rRNA



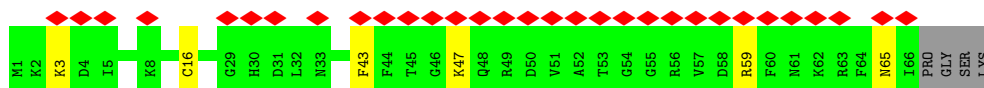
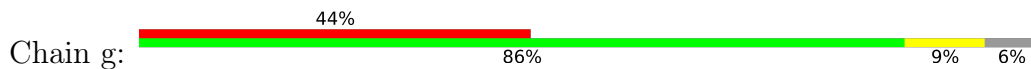
• Molecule 44: 50S ribosomal protein L29



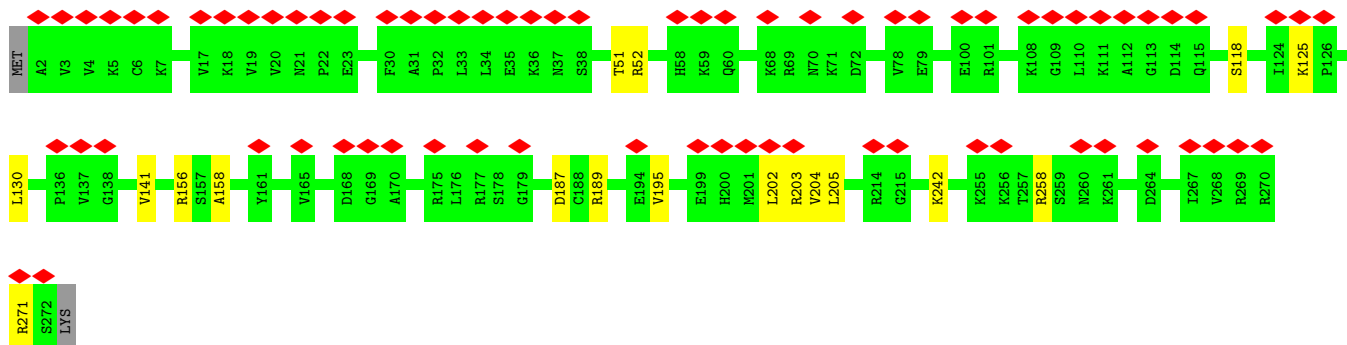
• Molecule 45: 50S ribosomal protein L30



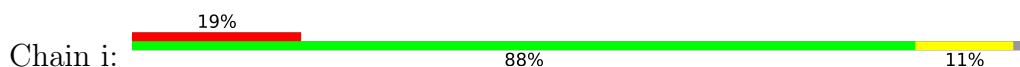
- Molecule 46: 50S ribosomal protein L31



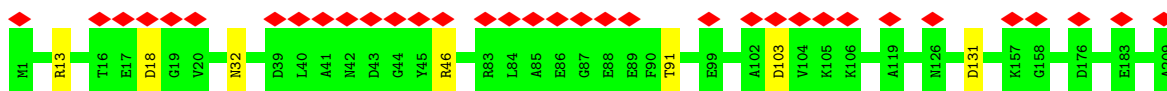
- Molecule 47: 50S ribosomal protein L2



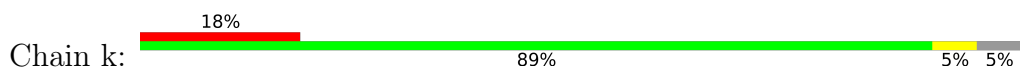
- Molecule 48: 50S ribosomal protein L32



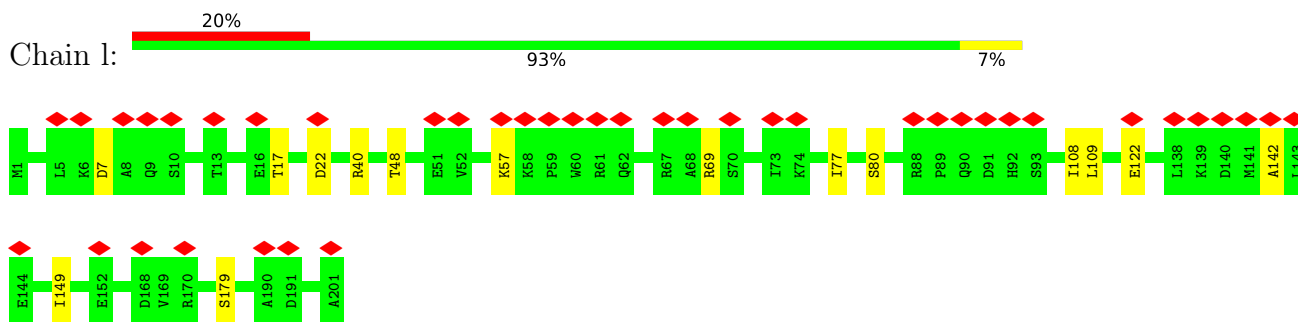
- Molecule 49: 50S ribosomal protein L3



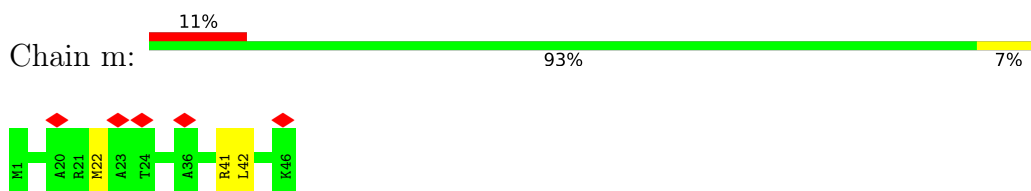
- Molecule 50: 50S ribosomal protein L33



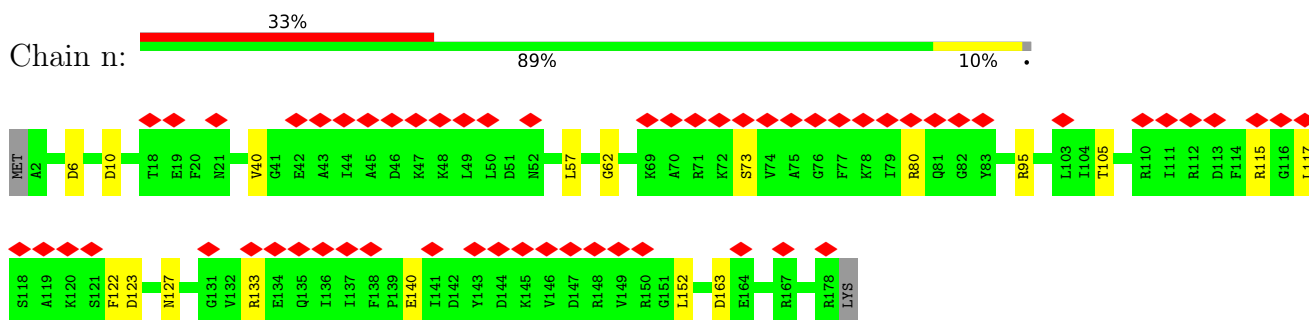
- Molecule 51: 50S ribosomal protein L4



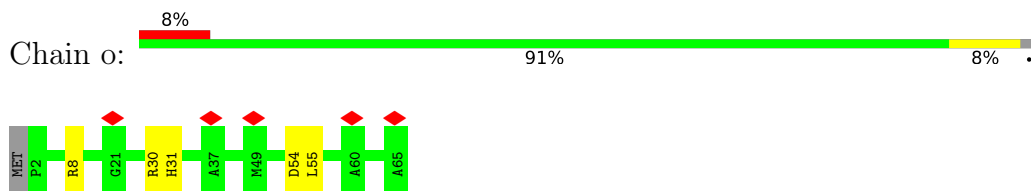
- Molecule 52: 50S ribosomal protein L34



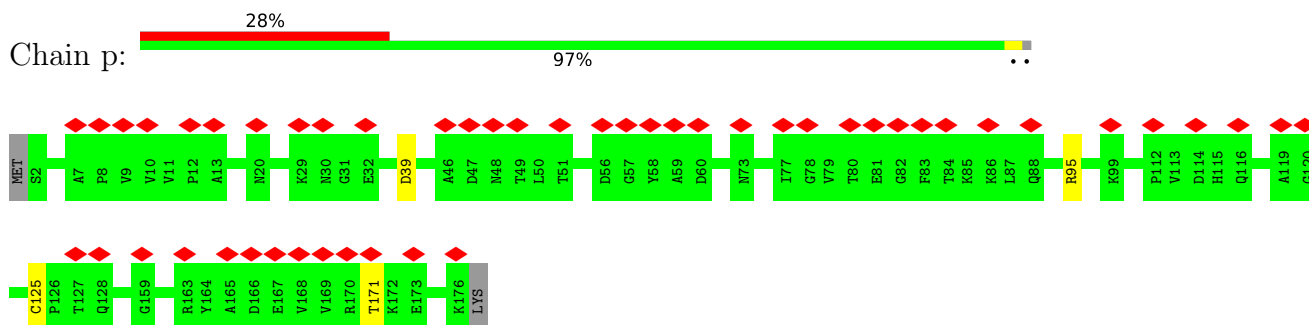
- Molecule 53: 50S ribosomal protein L5



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L6

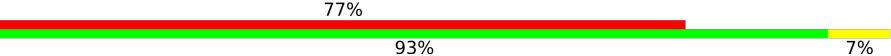


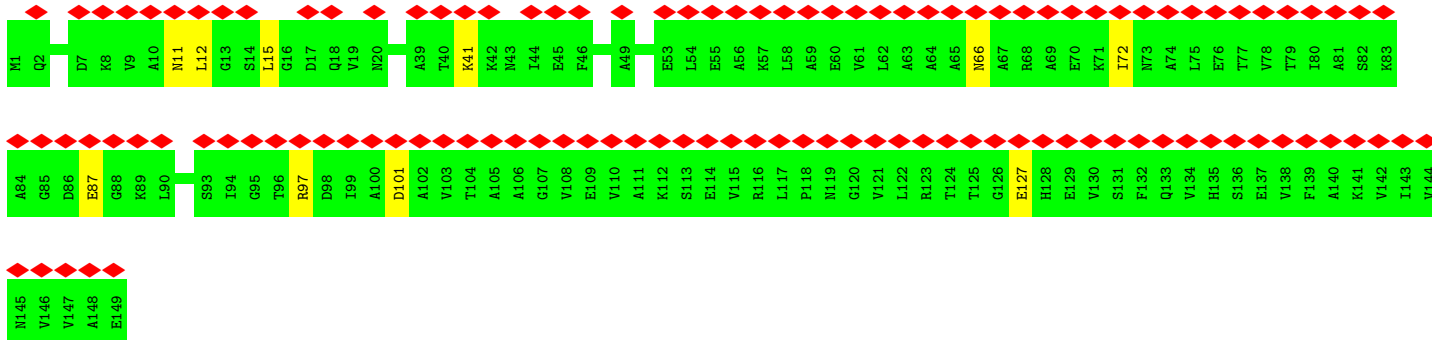
- Molecule 56: 50S ribosomal protein L36

Chain q:  95% 5%

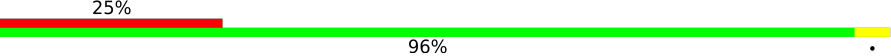


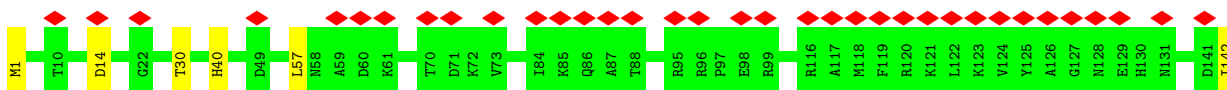
- Molecule 57: 50S ribosomal protein L9

Chain r:  77% 93% 7%

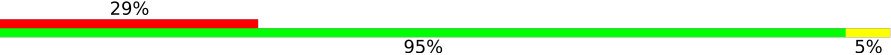


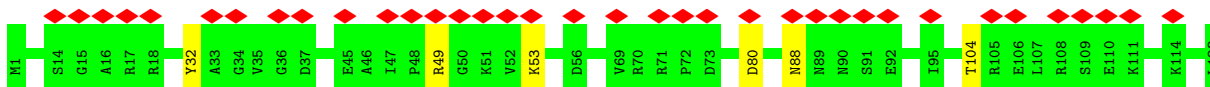
- Molecule 58: 50S ribosomal protein L13

Chain s:  25% 96%



- Molecule 59: 50S ribosomal protein L14

Chain t:  29% 95% 5%



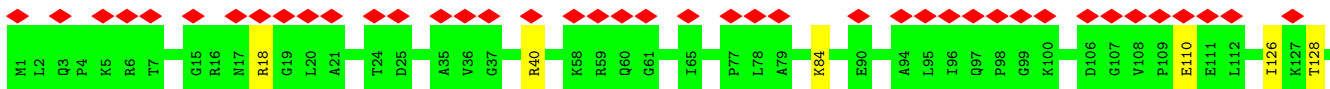
- Molecule 60: 50S ribosomal protein L15

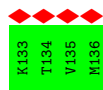
Chain u:  9% 96%



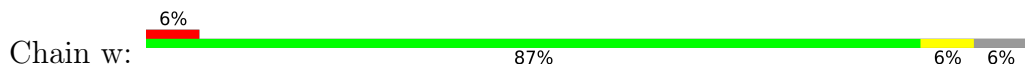
- Molecule 61: 50S ribosomal protein L16

Chain v:  33% 96%

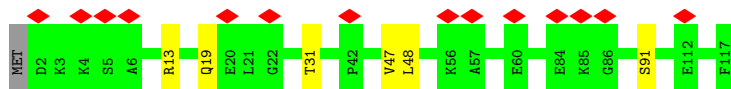




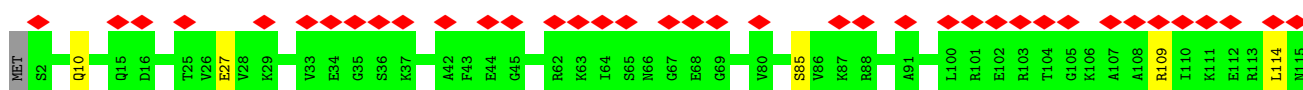
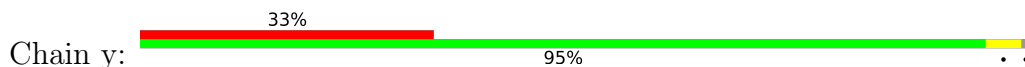
• Molecule 62: 50S ribosomal protein L17



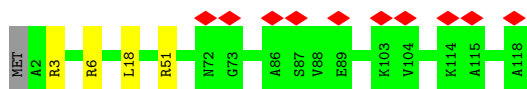
• Molecule 63: 50S ribosomal protein L18



• Molecule 64: 50S ribosomal protein L19



• Molecule 65: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00722	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/829	0.67	0/1107
2	1	0.49	0/864	0.82	0/1156
3	2	0.42	0/752	0.70	0/1005
4	3	0.35	0/796	0.66	2/1062 (0.2%)
5	4	0.40	0/766	0.68	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.59	2/717 (0.3%)	0.93	4/1110 (0.4%)
9	9	0.79	2/1131 (0.2%)	0.64	1/1524 (0.1%)
10	A	0.39	0/1810	0.75	1/2821 (0.0%)
10	B	0.46	1/1810 (0.1%)	0.86	7/2821 (0.2%)
11	AA	0.42	0/10547	0.60	1/14232 (0.0%)
12	AB	0.70	0/1310	0.68	1/1766 (0.1%)
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.36	0/1696	0.62	0/2298
14	AE	0.41	0/10561	0.63	3/14258 (0.0%)
15	AF	0.33	0/652	0.57	0/879
16	C	0.48	0/553	0.83	0/743
17	D	0.34	10/36610 (0.0%)	0.74	30/57091 (0.1%)
18	E	0.57	0/675	0.85	0/895
19	F	0.56	0/597	0.87	0/792
20	G	0.49	0/1791	0.71	0/2413
21	H	0.54	1/1746 (0.1%)	1.03	12/2382 (0.5%)
22	I	0.43	0/1663	0.71	0/2241
23	J	0.47	0/1665	0.73	0/2227
24	K	0.45	0/1165	0.75	0/1568
25	L	0.43	0/867	0.75	1/1171 (0.1%)
26	M	0.50	0/1195	0.81	0/1602
27	N	0.41	0/989	0.69	0/1326
28	O	0.43	0/1034	0.75	0/1375
29	P	0.43	0/800	0.75	0/1082
30	Q	0.40	0/893	0.70	0/1205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	R	0.35	0/952	0.74	0/1274
32	S	0.50	0/817	0.79	0/1088
33	T	0.53	0/722	0.86	0/964
34	U	0.44	0/659	0.78	0/884
35	V	0.34	0/657	0.62	0/881
36	W	0.38	0/680	0.62	0/915
37	X	0.49	0/909	0.86	0/1215
38	Y	0.67	0/1046	0.59	0/1410
39	Z	0.69	0/227	0.57	0/304
40	a	0.38	3/69247 (0.0%)	0.72	18/107985 (0.0%)
41	b	0.39	0/589	0.70	0/779
42	c	0.48	0/635	0.81	1/848 (0.1%)
43	d	0.29	0/2872	0.70	0/4478
44	e	0.53	0/502	0.83	0/667
45	f	0.45	0/452	0.78	0/605
46	g	0.43	0/531	0.68	0/709
47	h	0.39	0/2121	0.78	0/2852
48	i	0.40	0/450	0.79	0/599
49	j	0.44	0/1586	0.70	0/2134
50	k	0.35	0/433	0.65	0/576
51	l	0.46	0/1571	0.77	0/2113
52	m	0.53	0/380	0.99	0/498
53	n	0.49	0/1434	0.88	3/1926 (0.2%)
54	o	0.45	0/513	0.83	0/676
55	p	0.39	0/1333	0.67	0/1805
56	q	0.37	0/303	0.77	0/397
57	r	0.44	0/1122	0.69	0/1515
58	s	0.50	0/1152	0.75	0/1551
59	t	0.41	0/955	0.78	0/1279
60	u	0.40	0/1062	0.76	0/1413
61	v	0.47	0/1093	0.81	0/1460
62	w	0.52	0/964	0.87	0/1289
63	x	0.46	0/902	0.81	0/1209
64	y	0.41	0/929	0.73	1/1242 (0.1%)
65	z	0.60	0/960	0.91	1/1278 (0.1%)
All	All	0.41	29/190093 (0.0%)	0.73	88/280059 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	2
10	B	0	2
12	AB	0	3
13	AC	0	1
13	AD	0	1
14	AE	0	4
21	H	0	3
37	X	0	1
All	All	0	17

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.71	1.70	1.47
17	D	1516	G	O3'-P	-13.43	1.45	1.61
17	D	1339	A	O3'-P	10.56	1.73	1.61
6	5	109	DT	O3'-P	8.78	1.71	1.61
17	D	145	G	O3'-P	8.43	1.71	1.61
17	D	196	A	O3'-P	8.32	1.71	1.61
7	6	10	DG	C1'-N9	-8.25	1.35	1.47
17	D	1275	A	O3'-P	7.77	1.70	1.61
40	a	2434	A	O3'-P	7.52	1.70	1.61
21	H	169	SER	N-CA	7.51	1.61	1.46
17	D	1515	G	O3'-P	-7.25	1.52	1.61
17	D	1395	C	O3'-P	7.23	1.69	1.61
6	5	121	DG	C1'-N9	-7.21	1.37	1.47
8	7	19	G	C1'-N9	-7.20	1.36	1.46
17	D	1490	U	O3'-P	6.86	1.69	1.61
8	7	-19	U	C1'-N1	6.81	1.58	1.48
6	5	112	DG	C1'-N9	-6.67	1.38	1.47
17	D	1492	A	O3'-P	6.64	1.69	1.61
40	a	1905	C	O3'-P	6.61	1.69	1.61
40	a	2167	U	O3'-P	6.51	1.69	1.61
6	5	100	DA	C1'-N9	-6.48	1.38	1.47
7	6	21	DA	C1'-N9	-6.40	1.38	1.47
6	5	116	DG	C1'-N9	-6.14	1.38	1.47
9	9	129	LEU	C-N	6.12	1.45	1.34
6	5	115	DA	C1'-N9	-6.04	1.38	1.47
10	B	36	U	O3'-P	5.76	1.68	1.61
17	D	1397	C	O3'-P	5.73	1.68	1.61
7	6	28	DA	C1'-N9	-5.69	1.39	1.47
7	6	24	DT	C1'-N1	5.32	1.56	1.49

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1516	G	P-O3'-C3'	-19.01	96.89	119.70
17	D	1516	G	O3'-P-O5'	13.80	130.22	104.00
40	a	2252	G	N9-C1'-C2'	-10.95	99.76	114.00
17	D	1401	G	N9-C1'-C2'	-10.68	100.12	114.00
53	n	73	SER	N-CA-CB	-10.63	94.56	110.50
17	D	1499	A	N9-C1'-C2'	-10.28	100.64	114.00
17	D	528	C	N1-C1'-C2'	-10.21	100.72	114.00
21	H	169	SER	N-CA-C	9.98	137.94	111.00
17	D	1339	A	P-O3'-C3'	9.88	131.56	119.70
10	B	29	G	N9-C1'-C2'	-9.75	101.27	112.00
10	B	28	C	P-O3'-C3'	9.59	131.21	119.70
17	D	196	A	P-O3'-C3'	9.33	130.90	119.70
17	D	526	C	N1-C1'-C2'	-8.85	102.26	112.00
21	H	88	LYS	C-N-CA	8.77	143.61	121.70
40	a	2167	U	P-O3'-C3'	8.61	130.03	119.70
17	D	1208	C	N1-C1'-C2'	-8.58	102.56	112.00
17	D	1206	G	N9-C1'-C2'	-8.38	102.78	112.00
40	a	2434	A	P-O3'-C3'	8.24	129.59	119.70
9	9	130	PRO	CA-N-CD	-8.23	99.98	111.50
14	AE	710	ASP	CB-CG-OD1	8.22	125.70	118.30
17	D	1406	U	N1-C1'-C2'	-7.79	103.43	112.00
40	a	1905	C	P-O3'-C3'	7.63	128.86	119.70
17	D	1275	A	P-O3'-C3'	7.61	128.83	119.70
17	D	1492	A	P-O3'-C3'	7.55	128.76	119.70
17	D	1490	U	P-O3'-C3'	7.51	128.72	119.70
21	H	305	HIS	N-CA-C	7.45	131.12	111.00
10	B	29	G	C3'-C2'-O2'	7.37	134.68	113.30
8	7	-20	A	OP2-P-O3'	7.17	120.98	105.20
17	D	1206	G	C4'-C3'-O3'	7.16	127.33	113.00
10	B	35	A	P-O3'-C3'	7.14	128.27	119.70
17	D	1493	A	C2'-C3'-O3'	7.11	125.13	109.50
40	a	2245	U	N1-C1'-C2'	-7.07	104.22	112.00
17	D	145	G	P-O3'-C3'	7.06	128.17	119.70
17	D	1395	C	P-O3'-C3'	7.00	128.09	119.70
17	D	1516	G	OP1-P-O3'	-6.98	89.85	105.20
8	7	-20	A	O3'-P-O5'	-6.79	91.09	104.00
53	n	73	SER	CB-CA-C	6.74	122.90	110.10
17	D	1515	G	O3'-P-O5'	-6.68	91.31	104.00
17	D	1401	G	C4'-C3'-O3'	6.62	126.25	113.00
40	a	2243	U	N1-C1'-C2'	-6.59	104.75	112.00
40	a	2250	G	C4'-C3'-O3'	-6.59	95.56	109.40
40	a	1379	U	C2'-C3'-O3'	6.52	124.13	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1515	G	P-O3'-C3'	6.49	127.48	119.70
21	H	339	ARG	C-N-CA	6.47	137.87	121.70
17	D	515	G	N9-C1'-C2'	-6.42	104.94	112.00
17	D	1408	A	N9-C1'-C2'	-6.40	104.96	112.00
17	D	1497	G	N9-C1'-C2'	-6.37	104.99	112.00
10	B	34	C	P-O3'-C3'	6.37	127.34	119.70
6	5	109	DT	P-O3'-C3'	6.32	127.28	119.70
21	H	140	PRO	N-CA-CB	6.00	110.50	103.30
14	AE	363	LEU	CA-CB-CG	5.96	129.00	115.30
10	B	29	G	P-O3'-C3'	5.94	126.83	119.70
21	H	330	VAL	N-CA-C	5.91	126.97	111.00
21	H	336	ASP	CB-CA-C	-5.87	98.66	110.40
40	a	754	U	N1-C1'-C2'	5.84	121.60	114.00
21	H	132	PRO	N-CA-CB	5.79	110.25	103.30
21	H	168	VAL	C-N-CA	5.78	136.14	121.70
17	D	517	G	C5'-C4'-C3'	5.72	125.15	116.00
8	7	9	U	C2'-C3'-O3'	5.70	122.82	113.70
21	H	344	LEU	CA-CB-CG	5.66	128.31	115.30
53	n	127	ASN	CB-CA-C	5.62	121.64	110.40
40	a	2244	U	C1'-C2'-O2'	-5.61	93.77	110.60
25	L	54	LEU	CA-CB-CG	5.60	128.17	115.30
12	AB	122	PRO	N-CA-CB	5.56	109.97	103.30
14	AE	709	ARG	C-N-CA	5.50	135.46	121.70
40	a	783	A	C4'-C3'-O3'	5.45	123.90	113.00
64	y	109	ARG	NE-CZ-NH2	5.43	123.01	120.30
17	D	1397	C	P-O3'-C3'	5.35	126.12	119.70
17	D	1340	A	C5'-C4'-C3'	5.34	124.54	116.00
42	c	28	ARG	NE-CZ-NH2	-5.33	117.64	120.30
4	3	22	ARG	NE-CZ-NH1	5.33	122.96	120.30
40	a	742	A	C8-N9-C1'	-5.23	118.29	127.70
17	D	1340	A	C5'-C4'-O4'	5.21	115.36	109.10
40	a	404	A	C2'-C3'-O3'	5.21	122.03	113.70
21	H	169	SER	N-CA-CB	-5.19	102.72	110.50
40	a	2244	U	C4'-C3'-O3'	5.16	123.32	113.00
8	7	-17	U	C2'-C3'-O3'	5.12	121.89	113.70
4	3	22	ARG	NE-CZ-NH2	-5.10	117.75	120.30
11	AA	516	ASP	CB-CG-OD2	5.09	122.88	118.30
40	a	742	A	C4-N9-C1'	5.09	135.46	126.30
40	a	2252	G	C4'-C3'-O3'	5.09	123.17	113.00
17	D	197	A	C2'-C3'-O3'	5.07	121.81	113.70
10	B	48	C	N1-C1'-C2'	5.06	120.58	114.00
10	A	48	C	N1-C1'-C2'	5.04	120.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	a	1141	U	N1-C1'-C2'	5.03	120.53	114.00
21	H	332	VAL	N-CA-C	5.02	124.56	111.00
65	z	6	ARG	NE-CZ-NH2	5.02	122.81	120.30
40	a	2243	U	C4'-C3'-O3'	5.01	123.03	113.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
12	AB	135	ARG	Sidechain
12	AB	157	ARG	Sidechain
12	AB	167	ARG	Sidechain
13	AC	192	VAL	Peptide
13	AD	20	SER	Peptide
14	AE	1326	GLN	Peptide
14	AE	1344	LEU	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
10	B	19	G	Sidechain
10	B	7	G	Sidechain
21	H	274	TYR	Peptide
21	H	81	GLU	Peptide
21	H	82	THR	Peptide
37	X	100	GLN	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	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	54
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	54
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	10
11	AA	1312/1342 (98%)	1199 (91%)	112 (8%)	1 (0%)	51	86
12	AB	158/181 (87%)	142 (90%)	12 (8%)	4 (2%)	5	32
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	17	57
13	AD	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
14	AE	1331/1407 (95%)	1217 (91%)	111 (8%)	3 (0%)	47	81
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
18	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
19	F	68/71 (96%)	68 (100%)	0	0	100	100
20	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
21	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	21
22	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29	69
23	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
24	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	66
25	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	54
26	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22	63
27	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	60
28	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19	60
29	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	15	54
30	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9	42
31	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
32	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
33	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
34	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12	48
35	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
36	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	8	40
38	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	1	11
39	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	14
41	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
42	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
44	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
45	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
46	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
47	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34	72
48	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
49	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
50	k	50/55 (91%)	50 (100%)	0	0	100	100
51	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	69
52	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	14	52
54	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
56	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
58	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
59	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
60	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
61	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
62	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
63	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
64	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
65	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	57
All	All	9485/10577 (90%)	8776 (92%)	640 (7%)	69 (1%)	26	63

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS

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Mol	Chain	Res	Type
12	AB	122	PRO
21	H	139	ARG
21	H	153	GLU
21	H	169	SER
21	H	306	VAL
21	H	340	ARG
28	O	56	ASP
37	X	103	LYS
38	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
12	AB	124	PRO
14	AE	92	VAL
14	AE	175	GLU
21	H	108	VAL
21	H	309	MET
21	H	333	LEU
38	Y	93	ASN
47	h	158	ALA
51	l	142	ALA
65	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
21	H	76	GLU
21	H	142	ARG
26	M	130	ASN
29	P	58	ASN
30	Q	119	ASN
38	Y	20	SER
38	Y	64	ARG
38	Y	106	GLN
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
12	AB	123	ARG
12	AB	130	PRO
13	AC	193	GLU
21	H	82	THR

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Mol	Chain	Res	Type
22	I	80	LYS
37	X	105	ASN
38	Y	83	ALA
39	Z	21	GLU
53	n	40	VAL
9	9	28	ALA
14	AE	74	LYS
21	H	70	VAL
38	Y	22	PRO
38	Y	71	LYS
38	Y	89	SER
39	Z	7	ILE
4	3	39	ILE
13	AC	192	VAL
38	Y	62	ALA
25	L	96	VAL
38	Y	23	VAL
38	Y	100	ILE
1	0	44	GLY
24	K	44	GLY
30	Q	74	VAL
34	U	64	GLY
9	9	54	VAL
11	AA	1317	PRO
53	n	62	GLY
27	N	75	ILE

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	84/84 (100%)	78 (93%)	6 (7%)	14 39
2	1	93/93 (100%)	84 (90%)	9 (10%)	8 27
3	2	81/84 (96%)	76 (94%)	5 (6%)	18 43
4	3	84/85 (99%)	78 (93%)	6 (7%)	14 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	78/78 (100%)	74 (95%)	4 (5%)	24	48
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1135/1157 (98%)	1134 (100%)	1 (0%)	93	97
12	AB	138/158 (87%)	135 (98%)	3 (2%)	52	71
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1106 (99%)	16 (1%)	67	80
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	C	57/65 (88%)	55 (96%)	2 (4%)	36	59
18	E	65/66 (98%)	60 (92%)	5 (8%)	13	37
19	F	60/61 (98%)	57 (95%)	3 (5%)	24	49
20	G	187/199 (94%)	178 (95%)	9 (5%)	25	50
21	H	137/461 (30%)	128 (93%)	9 (7%)	16	41
22	I	171/190 (90%)	165 (96%)	6 (4%)	36	59
23	J	172/173 (99%)	165 (96%)	7 (4%)	30	55
24	K	119/126 (94%)	112 (94%)	7 (6%)	19	45
25	L	91/116 (78%)	85 (93%)	6 (7%)	16	41
26	M	124/147 (84%)	116 (94%)	8 (6%)	17	42
27	N	104/105 (99%)	102 (98%)	2 (2%)	57	75
28	O	105/107 (98%)	100 (95%)	5 (5%)	25	50
29	P	86/90 (96%)	78 (91%)	8 (9%)	9	28
30	Q	90/99 (91%)	87 (97%)	3 (3%)	38	61
31	R	101/104 (97%)	94 (93%)	7 (7%)	15	40
32	S	83/84 (99%)	79 (95%)	4 (5%)	25	50
33	T	76/77 (99%)	64 (84%)	12 (16%)	2	13
34	U	65/65 (100%)	61 (94%)	4 (6%)	18	43
35	V	74/78 (95%)	72 (97%)	2 (3%)	44	65
36	W	72/79 (91%)	68 (94%)	4 (6%)	21	46
37	X	94/96 (98%)	85 (90%)	9 (10%)	8	27
38	Y	109/110 (99%)	72 (66%)	37 (34%)	0	1
39	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	b	58/63 (92%)	57 (98%)	1 (2%)	60	78
42	c	67/68 (98%)	64 (96%)	3 (4%)	27	52
44	e	54/55 (98%)	53 (98%)	1 (2%)	57	75
45	f	48/49 (98%)	46 (96%)	2 (4%)	30	54
46	g	59/62 (95%)	53 (90%)	6 (10%)	7	25
47	h	216/218 (99%)	199 (92%)	17 (8%)	12	35
48	i	47/48 (98%)	41 (87%)	6 (13%)	4	18
49	j	164/164 (100%)	157 (96%)	7 (4%)	29	53
50	k	47/49 (96%)	44 (94%)	3 (6%)	17	42
51	l	165/165 (100%)	151 (92%)	14 (8%)	10	33
52	m	38/38 (100%)	35 (92%)	3 (8%)	12	35
53	n	148/150 (99%)	134 (90%)	14 (10%)	8	27
54	o	51/52 (98%)	46 (90%)	5 (10%)	8	26
55	p	136/138 (99%)	132 (97%)	4 (3%)	42	64
56	q	34/34 (100%)	32 (94%)	2 (6%)	19	45
57	r	114/114 (100%)	104 (91%)	10 (9%)	10	31
58	s	116/116 (100%)	110 (95%)	6 (5%)	23	48
59	t	104/104 (100%)	98 (94%)	6 (6%)	20	45
60	u	103/103 (100%)	97 (94%)	6 (6%)	20	45
61	v	109/109 (100%)	103 (94%)	6 (6%)	21	47
62	w	99/103 (96%)	91 (92%)	8 (8%)	11	35
63	x	86/87 (99%)	80 (93%)	6 (7%)	15	40
64	y	99/100 (99%)	95 (96%)	4 (4%)	31	55
65	z	89/90 (99%)	87 (98%)	2 (2%)	52	71
All	All	7887/8739 (90%)	7475 (95%)	412 (5%)	27	48

All (412) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	13	ARG
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG

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Mol	Chain	Res	Type
1	0	86	GLN
2	1	7	HIS
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	109	ASP
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	59	ASN
3	2	93	LEU
4	3	52	LEU
4	3	68	SER
4	3	72	ILE
4	3	89	ASP
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	41	GLU
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	30	SER
9	9	31	ARG
9	9	34	THR
9	9	36	ASP
9	9	37	LYS
9	9	39	THR

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Mol	Chain	Res	Type
9	9	42	ARG
9	9	43	LYS
9	9	51	TYR
9	9	52	MET
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	62	ARG
9	9	69	PHE
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR
9	9	143	MET
11	AA	914	LYS
12	AB	21	ARG
12	AB	128	PHE
12	AB	129	GLU
14	AE	69	GLU
14	AE	70	CYS
14	AE	71	LEU
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	79	LYS

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Mol	Chain	Res	Type
14	AE	81	ARG
14	AE	85	CYS
14	AE	92	VAL
14	AE	93	THR
14	AE	431	ARG
14	AE	514	THR
14	AE	744	ARG
14	AE	1369	ARG
16	C	33	ILE
16	C	74	HIS
18	E	6	SER
18	E	10	ARG
18	E	48	GLN
18	E	54	MET
18	E	64	LYS
19	F	34	ARG
19	F	62	ARG
19	F	67	ARG
20	G	8	ASP
20	G	23	TRP
20	G	45	LYS
20	G	105	LYS
20	G	108	ARG
20	G	128	LYS
20	G	129	LEU
20	G	132	LYS
20	G	208	ARG
21	H	9	PHE
21	H	54	LYS
21	H	273	ARG
21	H	305	HIS
21	H	336	ASP
21	H	337	GLU
21	H	338	GLU
21	H	339	ARG
21	H	340	ARG
22	I	14	ILE
22	I	75	ILE
22	I	89	LYS
22	I	164	ARG
22	I	185	ASN
22	I	200	VAL

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Mol	Chain	Res	Type
23	J	47	ARG
23	J	48	LEU
23	J	95	GLU
23	J	104	ARG
23	J	116	GLN
23	J	138	SER
23	J	143	VAL
24	K	10	GLU
24	K	15	LEU
24	K	60	ILE
24	K	114	VAL
24	K	115	LEU
24	K	138	ARG
24	K	162	GLU
25	L	16	GLU
25	L	24	ARG
25	L	38	ARG
25	L	54	LEU
25	L	79	ARG
25	L	86	ARG
26	M	7	ILE
26	M	17	LYS
26	M	21	GLU
26	M	23	LEU
26	M	79	ARG
26	M	109	ARG
26	M	130	ASN
26	M	146	GLU
27	N	96	MET
27	N	121	LEU
28	O	12	ARG
28	O	27	LYS
28	O	60	LYS
28	O	63	LEU
28	O	118	LEU
29	P	5	ARG
29	P	17	LEU
29	P	24	GLU
29	P	25	ILE
29	P	27	GLU
29	P	37	ARG
29	P	87	LEU

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Mol	Chain	Res	Type
29	P	90	LEU
30	Q	15	GLN
30	Q	56	ARG
30	Q	107	ILE
31	R	5	ASN
31	R	12	ARG
31	R	24	LEU
31	R	56	ARG
31	R	62	GLU
31	R	74	LEU
31	R	102	LEU
32	S	45	VAL
32	S	46	LEU
32	S	89	MET
32	S	92	GLU
33	T	10	LYS
33	T	17	ARG
33	T	22	THR
33	T	39	LEU
33	T	40	GLN
33	T	64	ARG
33	T	66	LEU
33	T	67	LEU
33	T	70	LEU
33	T	73	LYS
33	T	84	ARG
33	T	85	LEU
34	U	1	MET
34	U	2	VAL
34	U	6	LEU
34	U	19	VAL
35	V	75	LEU
35	V	81	LYS
36	W	12	ASP
36	W	21	LYS
36	W	33	THR
36	W	79	THR
37	X	11	ASP
37	X	16	VAL
37	X	25	VAL
37	X	29	ARG
37	X	59	GLU

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Mol	Chain	Res	Type
37	X	92	ARG
37	X	93	ARG
37	X	101	ARG
37	X	117	LYS
38	Y	9	LYS
38	Y	10	LEU
38	Y	16	MET
38	Y	23	VAL
38	Y	27	LEU
38	Y	30	GLN
38	Y	36	GLU
38	Y	44	LYS
38	Y	48	ILE
38	Y	50	LYS
38	Y	58	ILE
38	Y	60	VAL
38	Y	61	TYR
38	Y	64	ARG
38	Y	65	SER
38	Y	67	THR
38	Y	71	LYS
38	Y	78	LEU
38	Y	80	LYS
38	Y	81	LYS
38	Y	91	LYS
38	Y	94	LYS
38	Y	95	ASP
38	Y	99	LYS
38	Y	100	ILE
38	Y	101	SER
38	Y	102	ARG
38	Y	104	GLN
38	Y	108	ILE
38	Y	112	LYS
38	Y	116	MET
38	Y	120	ASP
38	Y	124	MET
38	Y	125	THR
38	Y	126	ARG
38	Y	133	ARG
38	Y	135	MET
39	Z	1	SER

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Mol	Chain	Res	Type
39	Z	2	ILE
39	Z	4	LYS
39	Z	6	GLN
39	Z	7	ILE
39	Z	8	ILE
39	Z	14	MET
39	Z	15	SER
39	Z	16	VAL
39	Z	23	ILE
39	Z	26	MET
39	Z	28	GLU
39	Z	29	LYS
39	Z	30	PHE
41	b	70	GLU
42	c	48	THR
42	c	54	LYS
42	c	71	LEU
44	e	58	ASN
45	f	3	LYS
45	f	45	ARG
46	g	3	LYS
46	g	16	CYS
46	g	43	PHE
46	g	47	LYS
46	g	59	ARG
46	g	65	ASN
47	h	51	THR
47	h	52	ARG
47	h	118	SER
47	h	125	LYS
47	h	130	LEU
47	h	141	VAL
47	h	156	ARG
47	h	187	ASP
47	h	189	ARG
47	h	195	VAL
47	h	202	LEU
47	h	203	ARG
47	h	204	VAL
47	h	205	LEU
47	h	242	LYS
47	h	258	ARG

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Mol	Chain	Res	Type
47	h	271	ARG
48	i	9	THR
48	i	12	LYS
48	i	26	THR
48	i	27	SER
48	i	29	SER
48	i	40	ARG
49	j	13	ARG
49	j	18	ASP
49	j	32	ASN
49	j	46	ARG
49	j	91	THR
49	j	103	ASP
49	j	131	ASP
50	k	5	ILE
50	k	24	THR
50	k	26	ASN
51	l	7	ASP
51	l	17	THR
51	l	22	ASP
51	l	40	ARG
51	l	48	THR
51	l	57	LYS
51	l	69	ARG
51	l	77	ILE
51	l	80	SER
51	l	108	ILE
51	l	109	LEU
51	l	122	GLU
51	l	149	ILE
51	l	179	SER
52	m	22	MET
52	m	41	ARG
52	m	42	LEU
53	n	6	ASP
53	n	10	ASP
53	n	57	LEU
53	n	80	ARG
53	n	95	ARG
53	n	105	THR
53	n	115	ARG
53	n	117	LEU

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Mol	Chain	Res	Type
53	n	122	PHE
53	n	123	ASP
53	n	133	ARG
53	n	140	GLU
53	n	152	LEU
53	n	163	ASP
54	o	8	ARG
54	o	30	ARG
54	o	31	HIS
54	o	54	ASP
54	o	55	LEU
55	p	39	ASP
55	p	95	ARG
55	p	125	CYS
55	p	171	THR
56	q	3	VAL
56	q	26	ILE
57	r	11	ASN
57	r	12	LEU
57	r	15	LEU
57	r	41	LYS
57	r	66	ASN
57	r	72	ILE
57	r	87	GLU
57	r	97	ARG
57	r	101	ASP
57	r	127	GLU
58	s	1	MET
58	s	14	ASP
58	s	30	THR
58	s	40	HIS
58	s	57	LEU
58	s	142	ILE
59	t	32	TYR
59	t	49	ARG
59	t	53	LYS
59	t	80	ASP
59	t	88	ASN
59	t	104	THR
60	u	5	THR
60	u	27	LEU
60	u	48	ARG

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Mol	Chain	Res	Type
60	u	59	ARG
60	u	76	GLU
60	u	78	ARG
61	v	18	ARG
61	v	40	ARG
61	v	84	LYS
61	v	110	GLU
61	v	126	ILE
61	v	128	THR
62	w	2	ARG
62	w	20	MET
62	w	24	MET
62	w	51	LEU
62	w	63	ARG
62	w	65	LEU
62	w	69	ARG
62	w	95	THR
63	x	13	ARG
63	x	19	GLN
63	x	31	THR
63	x	47	VAL
63	x	48	LEU
63	x	91	SER
64	y	10	GLN
64	y	27	GLU
64	y	85	SER
64	y	114	LEU
65	z	18	LEU
65	z	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
9	9	103	ASN
11	AA	69	GLN
11	AA	150	HIS
11	AA	314	ASN
11	AA	554	HIS
11	AA	580	GLN
11	AA	604	HIS
11	AA	688	GLN
11	AA	1268	GLN

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Mol	Chain	Res	Type
11	AA	1313	HIS
13	AC	147	GLN
13	AD	66	HIS
13	AD	84	ASN
13	AD	117	HIS
13	AD	227	GLN
14	AE	157	GLN
14	AE	450	HIS
14	AE	777	HIS
14	AE	805	GLN
14	AE	910	ASN
14	AE	1108	GLN
14	AE	1326	GLN
14	AE	1367	GLN
20	G	18	HIS
24	K	70	ASN
37	X	105	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
17	D	1515/1542 (98%)	289 (19%)	35 (2%)
40	a	2859/2904 (98%)	531 (18%)	0
43	d	119/120 (99%)	17 (14%)	0
8	7	30/41 (73%)	19 (63%)	5 (16%)
All	All	4673/4759 (98%)	920 (19%)	52 (1%)

All (920) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-18	G
8	7	-17	U
8	7	-16	U
8	7	-14	U
8	7	-13	U
8	7	-12	U
8	7	-11	U
8	7	-10	U
8	7	-9	U

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Mol	Chain	Res	Type
8	7	-8	U
8	7	-7	U
8	7	-6	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U
8	7	10	U
8	7	11	U
8	7	12	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G

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Mol	Chain	Res	Type
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
17	D	4	U
17	D	5	U
17	D	9	G
17	D	22	G
17	D	29	U
17	D	32	A
17	D	39	G
17	D	41	G
17	D	47	C
17	D	48	C

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Mol	Chain	Res	Type
17	D	50	A
17	D	51	A
17	D	52	C
17	D	54	C
17	D	69	G
17	D	70	U
17	D	71	A
17	D	72	A
17	D	74	A
17	D	76	G
17	D	82	G
17	D	83	C
17	D	84	U
17	D	87	C
17	D	90	C
17	D	94	G
17	D	95	C
17	D	96	U
17	D	108	G
17	D	120	A
17	D	122	G
17	D	128	G
17	D	131	A
17	D	141	G
17	D	144	G
17	D	148	G
17	D	149	A
17	D	160	A
17	D	164	G
17	D	173	U
17	D	181	A
17	D	182	A
17	D	197	A
17	D	198	G
17	D	204	G
17	D	208	U
17	D	209	U
17	D	210	C
17	D	211	G
17	D	212	G
17	D	216	U
17	D	226	G

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Mol	Chain	Res	Type
17	D	245	U
17	D	247	G
17	D	251	G
17	D	253	A
17	D	258	G
17	D	262	A
17	D	266	G
17	D	267	C
17	D	271	C
17	D	279	A
17	D	289	G
17	D	299	G
17	D	306	A
17	D	321	A
17	D	328	C
17	D	329	A
17	D	332	G
17	D	347	G
17	D	352	C
17	D	353	A
17	D	354	G
17	D	355	C
17	D	367	U
17	D	372	C
17	D	373	A
17	D	376	G
17	D	382	A
17	D	384	G
17	D	392	C
17	D	393	A
17	D	397	A
17	D	406	G
17	D	412	A
17	D	413	G
17	D	414	A
17	D	421	U
17	D	422	C
17	D	424	G
17	D	429	U
17	D	446	G
17	D	451	A
17	D	457	G

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Mol	Chain	Res	Type
17	D	458	U
17	D	460	A
17	D	463	U
17	D	464	U
17	D	467	U
17	D	468	A
17	D	469	C
17	D	478	A
17	D	479	U
17	D	481	G
17	D	484	G
17	D	485	U
17	D	486	U
17	D	505	G
17	D	509	A
17	D	511	C
17	D	518	C
17	D	519	C
17	D	526	C
17	D	531	U
17	D	532	A
17	D	533	A
17	D	542	G
17	D	547	A
17	D	559	A
17	D	562	U
17	D	568	G
17	D	572	A
17	D	573	A
17	D	576	C
17	D	577	G
17	D	579	A
17	D	596	A
17	D	628	G
17	D	633	G
17	D	642	A
17	D	649	A
17	D	650	G
17	D	653	U
17	D	665	A
17	D	666	G
17	D	687	A

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Mol	Chain	Res	Type
17	D	700	G
17	D	723	U
17	D	724	G
17	D	731	G
17	D	734	G
17	D	747	A
17	D	748	G
17	D	755	G
17	D	760	G
17	D	777	A
17	D	793	U
17	D	794	A
17	D	815	A
17	D	817	C
17	D	828	U
17	D	829	G
17	D	832	G
17	D	841	C
17	D	844	G
17	D	845	A
17	D	849	G
17	D	874	G
17	D	887	G
17	D	902	G
17	D	914	A
17	D	916	U
17	D	926	G
17	D	934	C
17	D	935	A
17	D	954	G
17	D	960	U
17	D	963	G
17	D	969	A
17	D	972	C
17	D	975	A
17	D	976	G
17	D	991	U
17	D	992	U
17	D	993	G
17	D	996	A
17	D	999	C
17	D	1004	A

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Mol	Chain	Res	Type
17	D	1008	U
17	D	1009	U
17	D	1017	U
17	D	1018	G
17	D	1021	A
17	D	1024	G
17	D	1026	G
17	D	1028	C
17	D	1030	U
17	D	1031	C
17	D	1037	C
17	D	1043	G
17	D	1044	A
17	D	1046	A
17	D	1065	U
17	D	1085	U
17	D	1086	U
17	D	1094	G
17	D	1095	U
17	D	1099	G
17	D	1101	A
17	D	1124	G
17	D	1133	G
17	D	1135	U
17	D	1136	C
17	D	1137	C
17	D	1139	G
17	D	1140	C
17	D	1141	C
17	D	1142	G
17	D	1143	G
17	D	1145	A
17	D	1146	A
17	D	1151	A
17	D	1152	A
17	D	1158	C
17	D	1159	U
17	D	1167	A
17	D	1171	A
17	D	1174	G
17	D	1175	G
17	D	1176	A

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Mol	Chain	Res	Type
17	D	1184	G
17	D	1196	A
17	D	1197	A
17	D	1206	G
17	D	1211	U
17	D	1212	U
17	D	1213	A
17	D	1214	C
17	D	1215	G
17	D	1226	C
17	D	1227	A
17	D	1228	C
17	D	1238	A
17	D	1256	A
17	D	1257	A
17	D	1260	G
17	D	1275	A
17	D	1276	G
17	D	1278	G
17	D	1279	G
17	D	1280	A
17	D	1285	A
17	D	1286	U
17	D	1287	A
17	D	1299	A
17	D	1300	G
17	D	1302	C
17	D	1305	G
17	D	1312	G
17	D	1317	C
17	D	1320	C
17	D	1323	G
17	D	1329	A
17	D	1338	G
17	D	1340	A
17	D	1346	A
17	D	1347	G
17	D	1353	G
17	D	1363	A
17	D	1370	G
17	D	1378	C
17	D	1379	G

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Mol	Chain	Res	Type
17	D	1381	U
17	D	1391	U
17	D	1396	A
17	D	1397	C
17	D	1398	A
17	D	1404	C
17	D	1419	G
17	D	1429	A
17	D	1441	A
17	D	1446	A
17	D	1447	A
17	D	1448	C
17	D	1452	C
17	D	1453	G
17	D	1475	G
17	D	1487	G
17	D	1492	A
17	D	1493	A
17	D	1494	G
17	D	1495	U
17	D	1497	G
17	D	1503	A
17	D	1506	U
17	D	1517	G
17	D	1529	G
17	D	1530	G
17	D	1534	A
40	a	10	A
40	a	15	G
40	a	34	U
40	a	35	G
40	a	46	G
40	a	58	G
40	a	60	G
40	a	63	A
40	a	71	A
40	a	74	A
40	a	75	G
40	a	83	A
40	a	84	A
40	a	85	G
40	a	93	G

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Mol	Chain	Res	Type
40	a	96	C
40	a	102	U
40	a	103	A
40	a	110	G
40	a	114	U
40	a	118	A
40	a	119	A
40	a	120	U
40	a	122	G
40	a	131	A
40	a	136	G
40	a	139	U
40	a	140	C
40	a	141	G
40	a	145	C
40	a	163	C
40	a	165	A
40	a	181	A
40	a	196	A
40	a	200	U
40	a	215	G
40	a	216	A
40	a	222	A
40	a	225	C
40	a	248	G
40	a	249	C
40	a	261	G
40	a	264	C
40	a	265	A
40	a	266	G
40	a	267	C
40	a	271	G
40	a	272	A
40	a	275	C
40	a	276	U
40	a	278	A
40	a	285	G
40	a	311	A
40	a	324	A
40	a	329	G
40	a	330	A
40	a	353	C

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Mol	Chain	Res	Type
40	a	359	G
40	a	361	G
40	a	362	A
40	a	371	A
40	a	372	G
40	a	373	U
40	a	375	G
40	a	383	C
40	a	386	G
40	a	396	G
40	a	405	U
40	a	411	G
40	a	412	A
40	a	420	C
40	a	424	G
40	a	435	C
40	a	451	U
40	a	456	C
40	a	457	A
40	a	477	A
40	a	481	G
40	a	491	G
40	a	501	A
40	a	503	A
40	a	504	A
40	a	505	A
40	a	509	C
40	a	522	A
40	a	529	A
40	a	532	A
40	a	543	G
40	a	546	U
40	a	547	A
40	a	548	G
40	a	549	G
40	a	551	G
40	a	563	A
40	a	569	U
40	a	573	U
40	a	575	A
40	a	588	U
40	a	603	A

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Mol	Chain	Res	Type
40	a	609	A
40	a	613	A
40	a	614	A
40	a	615	U
40	a	616	A
40	a	618	G
40	a	621	A
40	a	627	A
40	a	637	A
40	a	645	C
40	a	647	G
40	a	654	A
40	a	664	G
40	a	668	A
40	a	685	A
40	a	686	U
40	a	710	U
40	a	717	C
40	a	730	A
40	a	738	G
40	a	757	G
40	a	764	A
40	a	765	C
40	a	775	G
40	a	776	G
40	a	782	A
40	a	784	G
40	a	785	G
40	a	800	A
40	a	802	A
40	a	805	G
40	a	812	C
40	a	819	A
40	a	827	U
40	a	828	U
40	a	845	A
40	a	846	U
40	a	858	G
40	a	859	G
40	a	869	G
40	a	878	A
40	a	881	G

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Mol	Chain	Res	Type
40	a	884	U
40	a	885	C
40	a	888	C
40	a	891	G
40	a	892	A
40	a	893	C
40	a	895	U
40	a	896	A
40	a	897	C
40	a	899	A
40	a	907	G
40	a	910	A
40	a	914	G
40	a	915	C
40	a	931	U
40	a	941	A
40	a	945	A
40	a	946	C
40	a	953	G
40	a	961	C
40	a	974	G
40	a	983	A
40	a	995	C
40	a	996	A
40	a	999	U
40	a	1005	C
40	a	1012	U
40	a	1013	C
40	a	1022	G
40	a	1023	U
40	a	1026	G
40	a	1033	U
40	a	1041	G
40	a	1045	C
40	a	1046	A
40	a	1047	G
40	a	1060	U
40	a	1061	U
40	a	1062	G
40	a	1063	G
40	a	1064	C
40	a	1065	U

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Mol	Chain	Res	Type
40	a	1066	U
40	a	1067	A
40	a	1068	G
40	a	1069	A
40	a	1070	A
40	a	1071	G
40	a	1073	A
40	a	1074	G
40	a	1076	C
40	a	1079	C
40	a	1080	A
40	a	1081	U
40	a	1082	U
40	a	1083	U
40	a	1084	A
40	a	1087	G
40	a	1088	A
40	a	1090	A
40	a	1095	A
40	a	1096	A
40	a	1107	G
40	a	1110	G
40	a	1111	A
40	a	1112	G
40	a	1119	U
40	a	1122	G
40	a	1132	U
40	a	1134	A
40	a	1135	C
40	a	1142	A
40	a	1169	A
40	a	1170	C
40	a	1173	U
40	a	1174	U
40	a	1175	A
40	a	1176	U
40	a	1177	G
40	a	1178	C
40	a	1179	G
40	a	1180	U
40	a	1186	G
40	a	1238	G

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Mol	Chain	Res	Type
40	a	1248	G
40	a	1253	A
40	a	1256	G
40	a	1266	G
40	a	1271	G
40	a	1272	A
40	a	1273	U
40	a	1301	A
40	a	1321	A
40	a	1345	C
40	a	1352	U
40	a	1365	A
40	a	1368	G
40	a	1378	A
40	a	1379	U
40	a	1380	G
40	a	1383	A
40	a	1387	A
40	a	1395	A
40	a	1406	U
40	a	1407	G
40	a	1408	G
40	a	1411	U
40	a	1414	C
40	a	1415	U
40	a	1416	G
40	a	1417	C
40	a	1419	A
40	a	1420	A
40	a	1428	C
40	a	1452	G
40	a	1453	A
40	a	1460	U
40	a	1478	G
40	a	1482	G
40	a	1490	A
40	a	1497	U
40	a	1503	A
40	a	1508	A
40	a	1509	A
40	a	1510	G
40	a	1515	A

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Mol	Chain	Res	Type
40	a	1529	G
40	a	1534	U
40	a	1535	A
40	a	1536	C
40	a	1537	G
40	a	1554	U
40	a	1559	U
40	a	1566	A
40	a	1569	A
40	a	1578	U
40	a	1580	A
40	a	1581	G
40	a	1582	C
40	a	1583	A
40	a	1584	U
40	a	1589	U
40	a	1590	A
40	a	1608	A
40	a	1609	A
40	a	1610	A
40	a	1647	U
40	a	1648	U
40	a	1649	G
40	a	1651	G
40	a	1674	G
40	a	1677	A
40	a	1703	G
40	a	1714	U
40	a	1715	G
40	a	1718	G
40	a	1729	U
40	a	1730	C
40	a	1732	C
40	a	1738	G
40	a	1750	G
40	a	1755	A
40	a	1758	U
40	a	1764	C
40	a	1773	A
40	a	1791	A
40	a	1800	C
40	a	1801	A

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Mol	Chain	Res	Type
40	a	1808	A
40	a	1811	G
40	a	1816	C
40	a	1829	A
40	a	1833	C
40	a	1847	A
40	a	1848	A
40	a	1858	A
40	a	1859	U
40	a	1862	G
40	a	1864	U
40	a	1869	G
40	a	1870	C
40	a	1872	A
40	a	1873	G
40	a	1905	C
40	a	1906	G
40	a	1907	G
40	a	1913	A
40	a	1914	C
40	a	1919	A
40	a	1920	C
40	a	1922	G
40	a	1923	U
40	a	1924	C
40	a	1925	C
40	a	1926	U
40	a	1928	A
40	a	1929	G
40	a	1930	G
40	a	1936	A
40	a	1938	A
40	a	1955	U
40	a	1965	C
40	a	1967	C
40	a	1970	A
40	a	1971	U
40	a	1972	G
40	a	1987	A
40	a	1991	U
40	a	1992	G
40	a	1993	U

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Mol	Chain	Res	Type
40	a	1997	C
40	a	2002	G
40	a	2022	U
40	a	2023	C
40	a	2027	G
40	a	2033	A
40	a	2043	C
40	a	2051	A
40	a	2052	A
40	a	2055	C
40	a	2056	G
40	a	2060	A
40	a	2061	G
40	a	2062	A
40	a	2077	A
40	a	2097	A
40	a	2099	U
40	a	2100	G
40	a	2108	A
40	a	2110	G
40	a	2111	U
40	a	2113	U
40	a	2115	G
40	a	2116	G
40	a	2117	A
40	a	2118	U
40	a	2121	G
40	a	2122	U
40	a	2124	G
40	a	2125	G
40	a	2126	A
40	a	2127	G
40	a	2128	G
40	a	2131	U
40	a	2132	U
40	a	2133	G
40	a	2134	A
40	a	2139	U
40	a	2141	G
40	a	2146	C
40	a	2147	A
40	a	2154	A

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Mol	Chain	Res	Type
40	a	2157	G
40	a	2158	A
40	a	2159	G
40	a	2162	G
40	a	2163	A
40	a	2164	C
40	a	2165	C
40	a	2169	A
40	a	2171	A
40	a	2172	U
40	a	2178	C
40	a	2182	U
40	a	2183	A
40	a	2185	U
40	a	2188	U
40	a	2189	U
40	a	2190	G
40	a	2191	A
40	a	2193	G
40	a	2194	U
40	a	2198	A
40	a	2204	G
40	a	2210	U
40	a	2211	A
40	a	2212	A
40	a	2213	U
40	a	2225	A
40	a	2226	C
40	a	2229	U
40	a	2238	G
40	a	2239	G
40	a	2244	U
40	a	2250	G
40	a	2268	A
40	a	2278	A
40	a	2283	C
40	a	2287	A
40	a	2297	A
40	a	2305	U
40	a	2308	G
40	a	2309	A
40	a	2315	G

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Mol	Chain	Res	Type
40	a	2322	A
40	a	2325	G
40	a	2327	A
40	a	2333	A
40	a	2339	C
40	a	2345	G
40	a	2347	C
40	a	2350	C
40	a	2361	G
40	a	2372	U
40	a	2376	A
40	a	2383	G
40	a	2385	C
40	a	2402	U
40	a	2403	C
40	a	2406	A
40	a	2423	U
40	a	2424	C
40	a	2425	A
40	a	2426	A
40	a	2429	G
40	a	2430	A
40	a	2431	U
40	a	2434	A
40	a	2435	A
40	a	2441	U
40	a	2447	G
40	a	2448	A
40	a	2470	G
40	a	2474	U
40	a	2476	A
40	a	2478	A
40	a	2484	G
40	a	2491	U
40	a	2502	G
40	a	2506	U
40	a	2507	C
40	a	2512	C
40	a	2513	A
40	a	2518	A
40	a	2520	C
40	a	2525	G

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Mol	Chain	Res	Type
40	a	2529	G
40	a	2535	G
40	a	2547	A
40	a	2554	U
40	a	2566	A
40	a	2567	G
40	a	2572	A
40	a	2573	C
40	a	2574	G
40	a	2585	U
40	a	2586	U
40	a	2602	A
40	a	2603	G
40	a	2609	U
40	a	2610	C
40	a	2611	C
40	a	2613	U
40	a	2629	U
40	a	2663	G
40	a	2669	G
40	a	2671	G
40	a	2689	U
40	a	2690	U
40	a	2714	G
40	a	2722	G
40	a	2726	A
40	a	2744	G
40	a	2748	A
40	a	2757	A
40	a	2758	A
40	a	2765	A
40	a	2777	G
40	a	2778	A
40	a	2791	G
40	a	2793	C
40	a	2796	U
40	a	2797	U
40	a	2798	U
40	a	2799	A
40	a	2801	G
40	a	2818	U
40	a	2820	A

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Mol	Chain	Res	Type
40	a	2823	A
40	a	2825	G
40	a	2849	U
40	a	2850	A
40	a	2859	G
40	a	2861	U
40	a	2867	G
40	a	2880	C
40	a	2884	U
40	a	2885	G
40	a	2891	U
40	a	2902	C
43	d	2	G
43	d	9	G
43	d	13	G
43	d	16	G
43	d	17	C
43	d	35	C
43	d	36	C
43	d	45	A
43	d	51	G
43	d	56	G
43	d	64	G
43	d	66	A
43	d	88	C
43	d	89	U
43	d	90	C
43	d	99	A
43	d	109	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-17	U
8	7	-14	U
8	7	-11	U
8	7	-3	U
8	7	9	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G

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Mol	Chain	Res	Type
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A
10	B	60	U
17	D	7	A
17	D	70	U
17	D	121	U
17	D	181	A
17	D	183	C
17	D	197	A
17	D	209	U
17	D	305	G
17	D	328	C
17	D	428	G
17	D	496	A
17	D	517	G
17	D	531	U
17	D	532	A
17	D	562	U
17	D	641	U
17	D	722	G
17	D	793	U
17	D	991	U
17	D	992	U
17	D	1109	C
17	D	1145	A
17	D	1196	A
17	D	1211	U
17	D	1212	U
17	D	1213	A
17	D	1214	C
17	D	1225	A
17	D	1299	A
17	D	1396	A
17	D	1432	G
17	D	1447	A
17	D	1491	G
17	D	1492	A

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Mol	Chain	Res	Type
17	D	1493	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

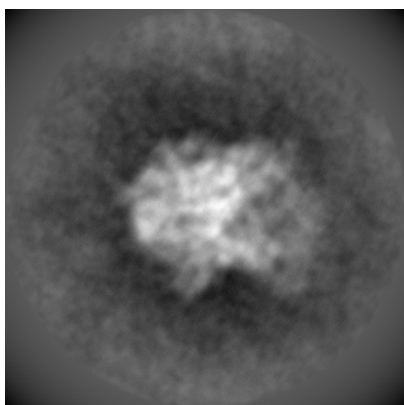
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22192. These allow visual inspection of the internal detail of the map and identification of artifacts.

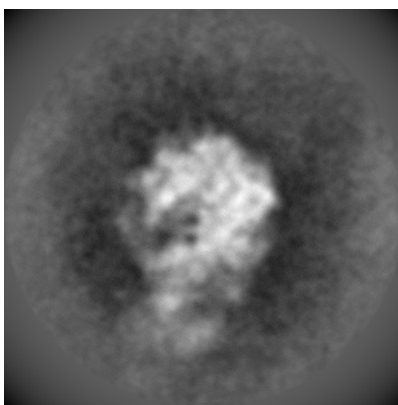
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

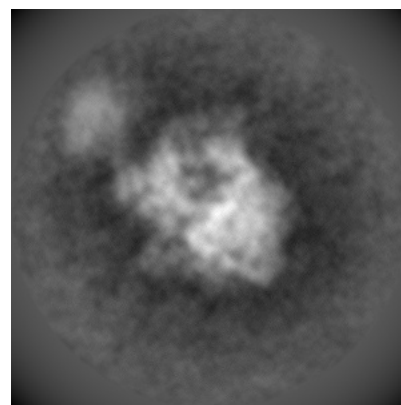
6.1.1 Primary map



X



Y

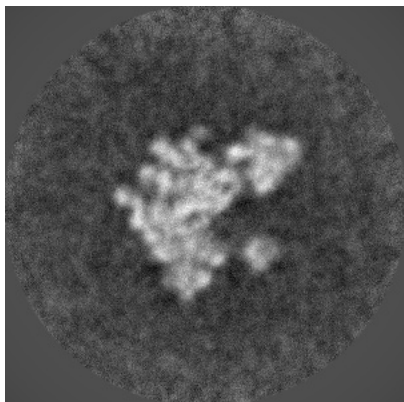


Z

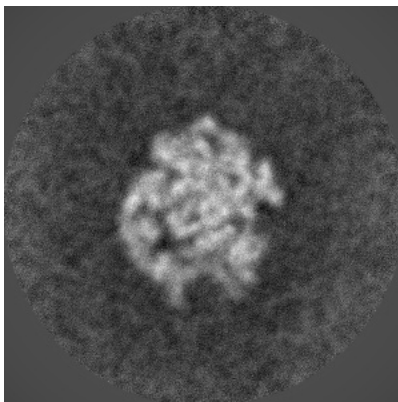
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

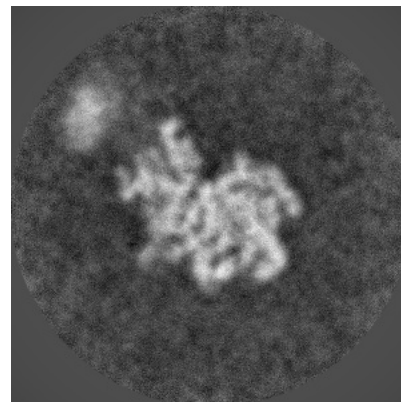
6.2.1 Primary map



X Index: 256



Y Index: 256

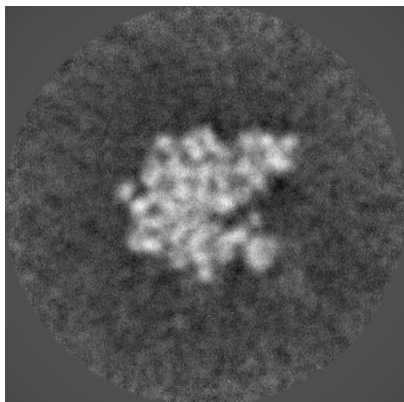


Z Index: 256

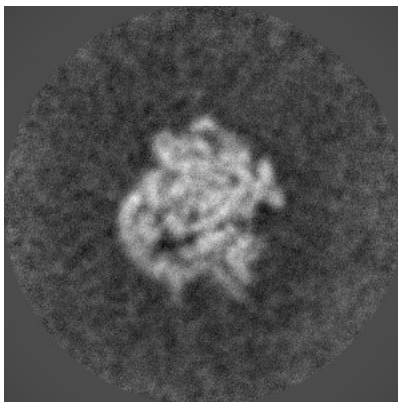
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

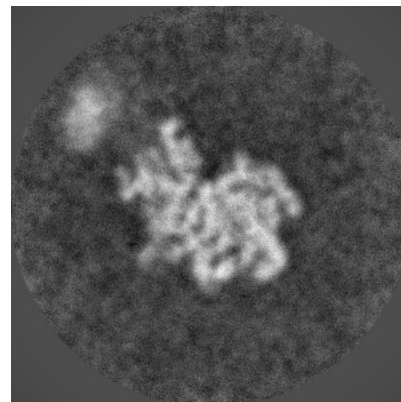
6.3.1 Primary map



X Index: 271



Y Index: 252

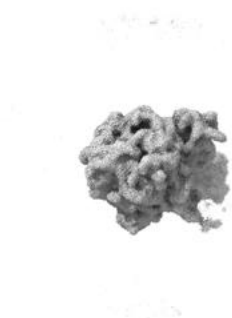


Z Index: 256

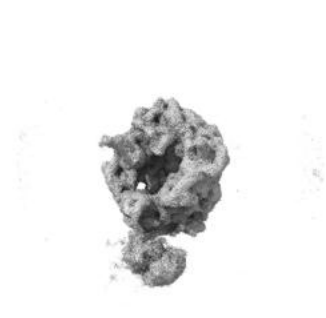
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

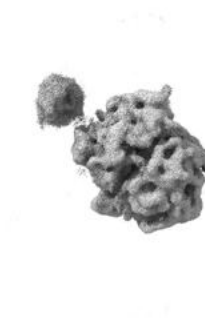
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00722. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

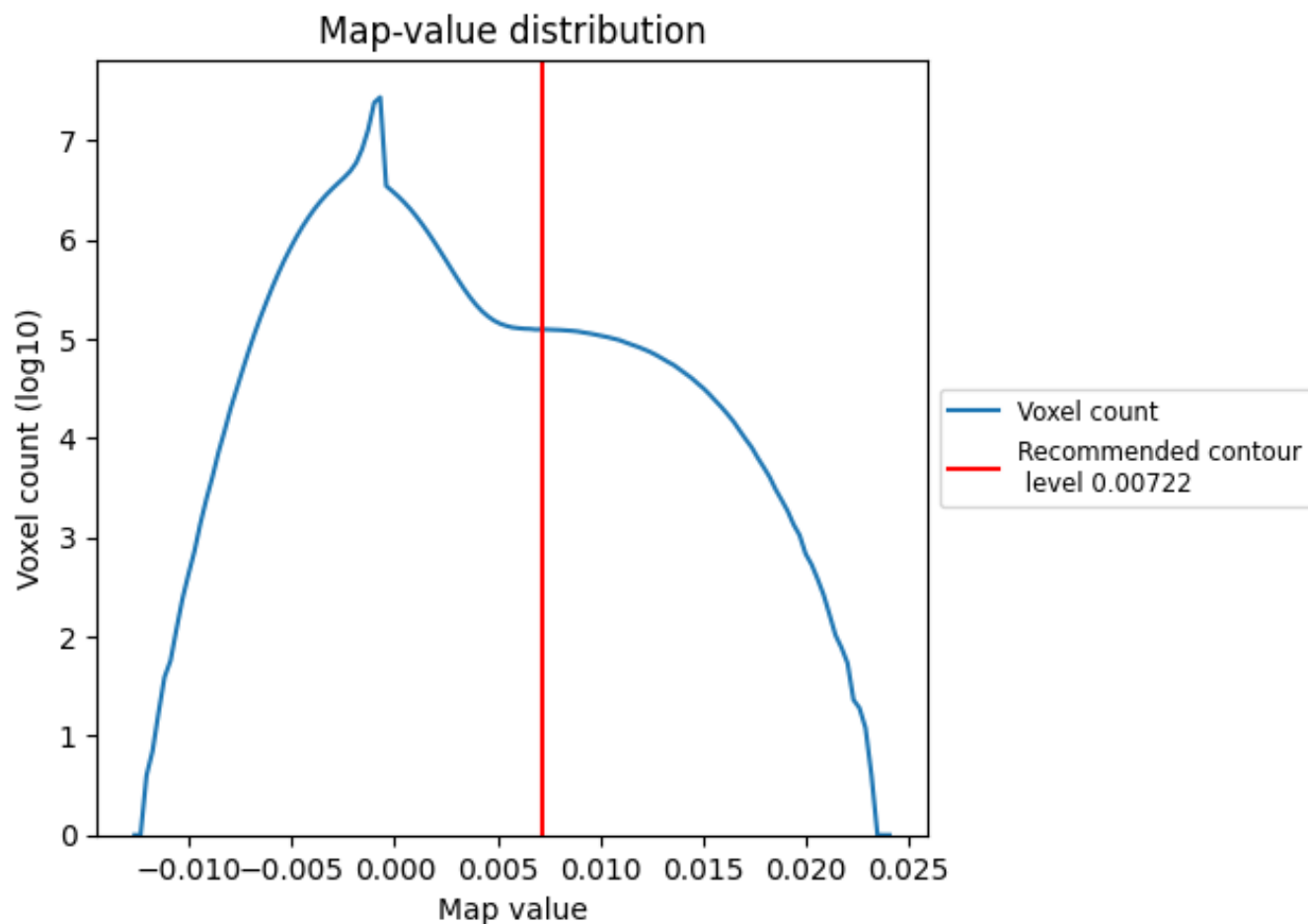
6.5 Mask visualisation

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

7 Map analysis [i](#)

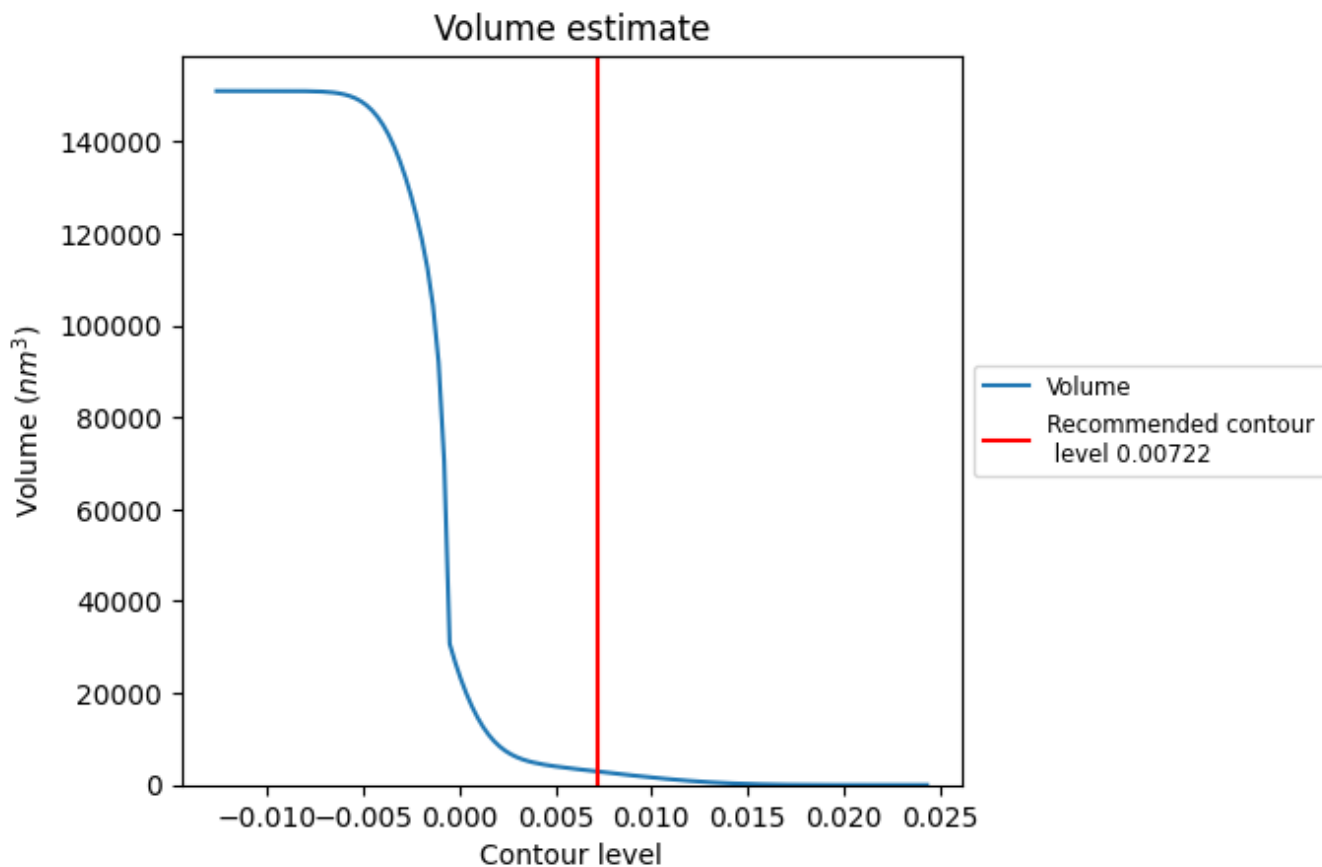
This section contains the results of statistical analysis of the map.

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.

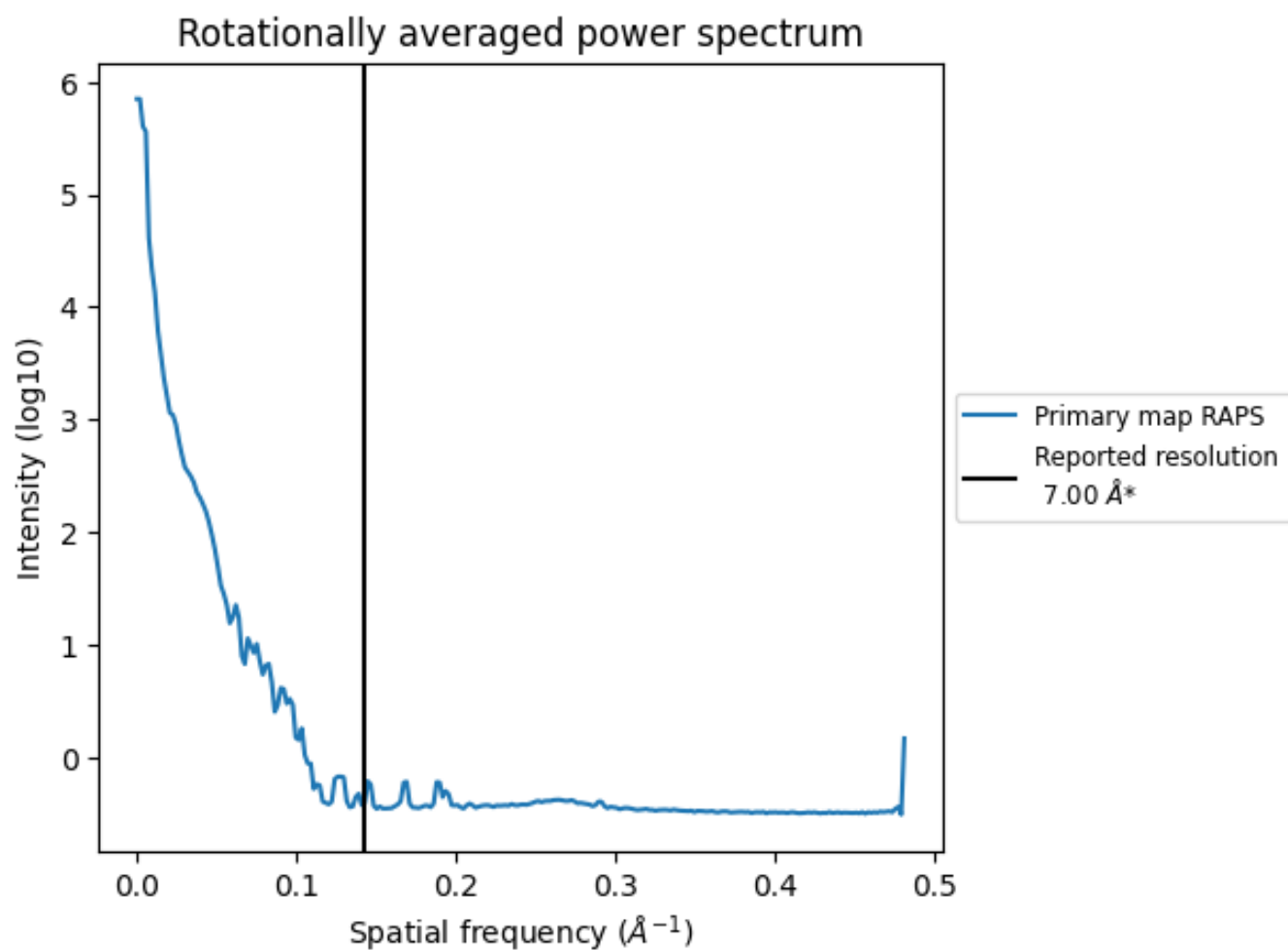
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2921 nm^3 ; this corresponds to an approximate mass of 2639 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 0.143 Å⁻¹

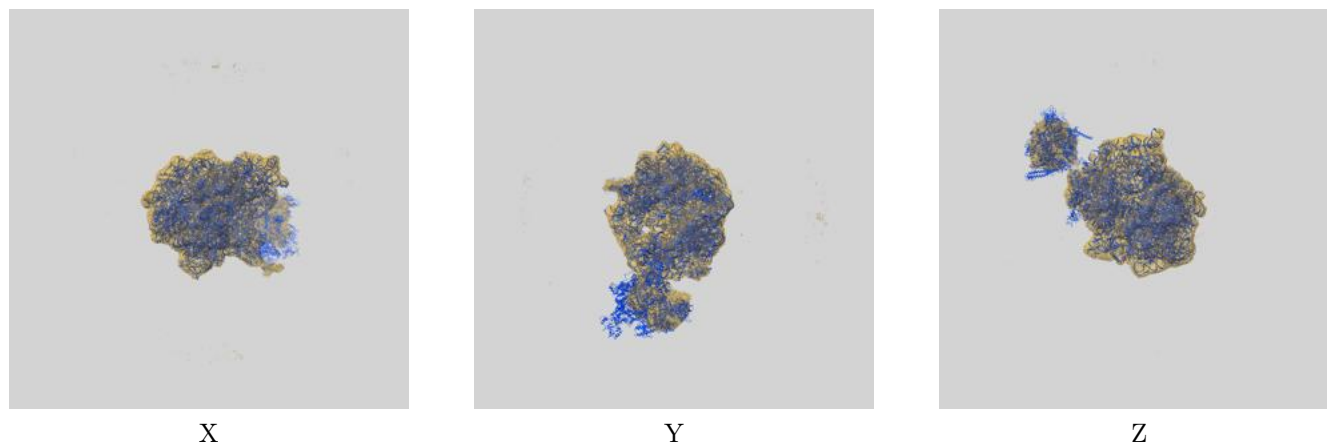
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

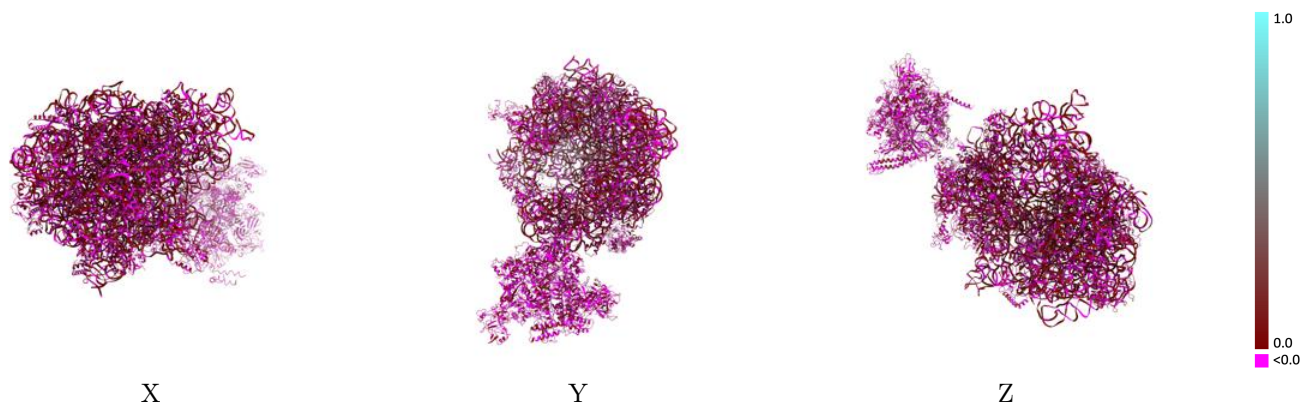
This section contains information regarding the fit between EMDB map EMD-22192 and PDB model 6XII. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



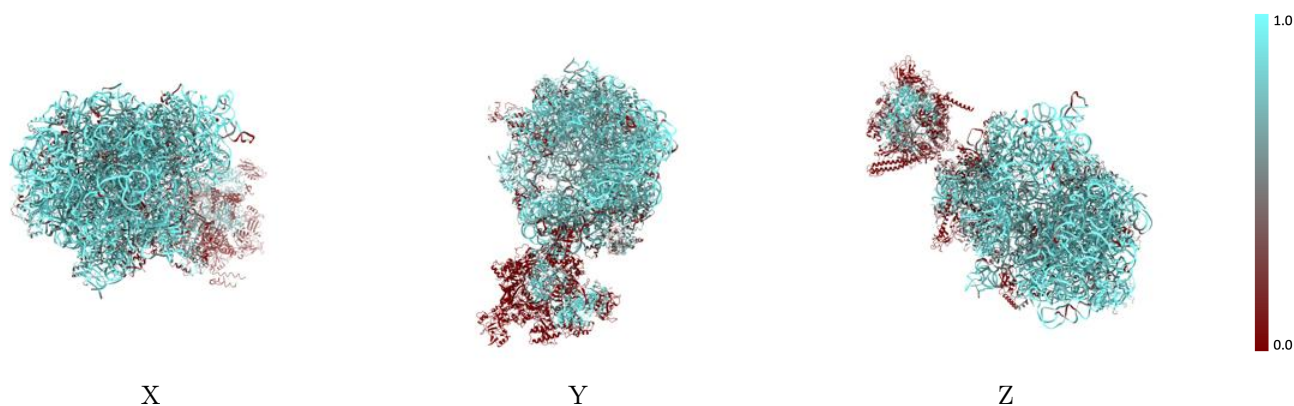
The images above show the 3D surface view of the map at the recommended contour level 0.00722 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



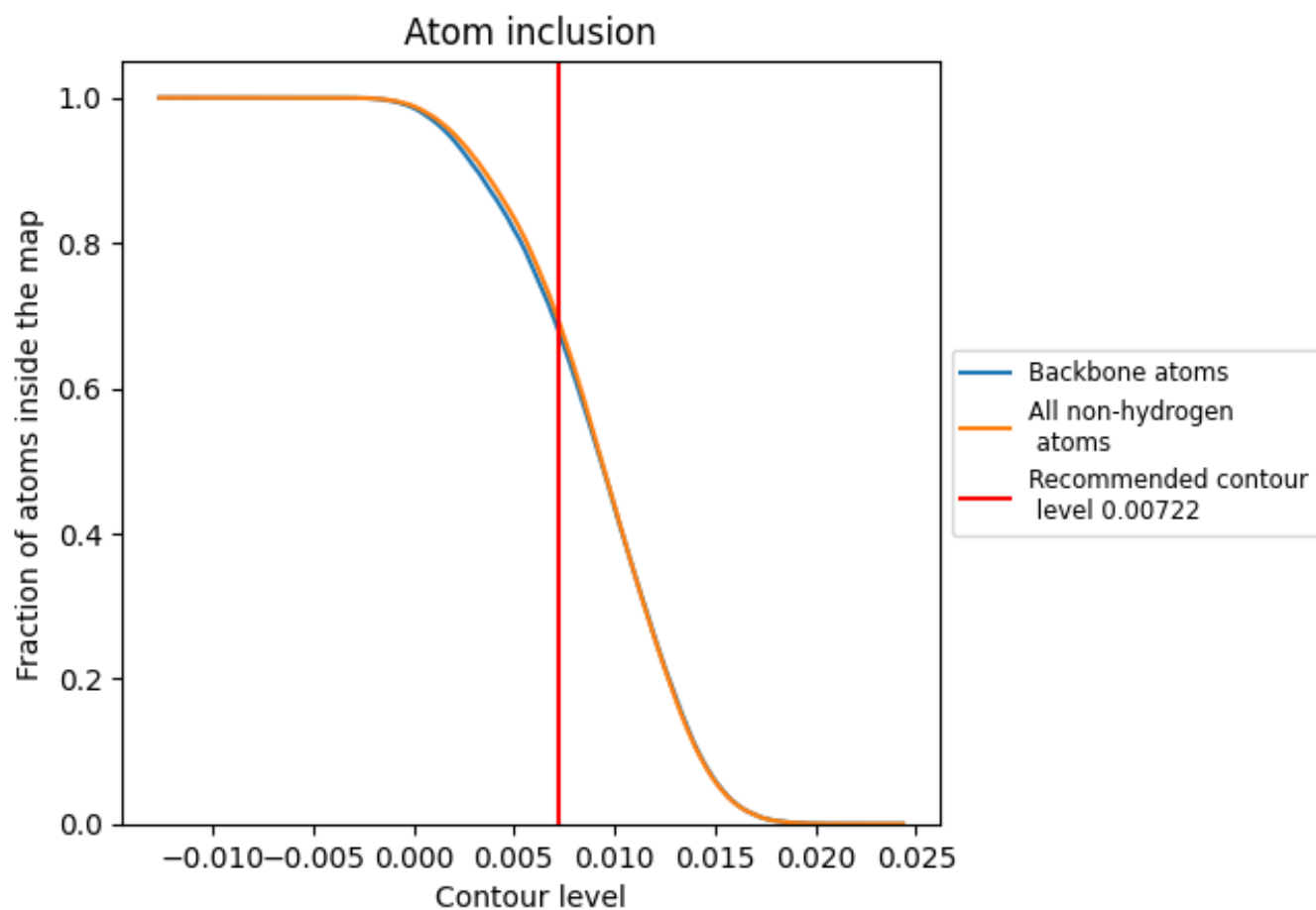
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00722).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



































































The table lists the average atom inclusion at the recommended contour level (0.00722) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6934	 0.0360
0	 0.7779	 0.0240
1	 0.6459	 0.0250
2	 0.6699	 0.0120
3	 0.8222	 0.0080
4	 0.5149	 0.0320
5	 0.0975	 -0.0420
6	 0.3875	 -0.0060
7	 0.5549	 0.0240
9	 0.4561	 0.0150
A	 0.6889	 0.0340
AA	 0.2595	 -0.0040
AB	 0.0996	 0.0060
AC	 0.5427	 0.0130
AD	 0.3719	 0.0040
AE	 0.2890	 0.0030
AF	 0.0457	 -0.0100
B	 0.6969	 0.0220
C	 0.7763	 0.0220
D	 0.9036	 0.0550
E	 0.7661	 0.0090
F	 0.4436	 0.0480
G	 0.6437	 0.0490
H	 0.0841	 0.0280
I	 0.3881	 0.0420
J	 0.6157	 0.0240
K	 0.6885	 0.0440
L	 0.5816	 0.0360
M	 0.5044	 0.0340
N	 0.5813	 0.0450
O	 0.6588	 0.0100
P	 0.4353	 -0.0010
Q	 0.8464	 0.0310
R	 0.7171	 0.0280
S	 0.7003	 0.0420



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Chain	Atom inclusion	Q-score
T	 0.7275	 0.0610
U	 0.8006	 0.0190
V	 0.6361	 -0.0130
W	 0.6136	 0.0220
X	 0.4482	 0.0240
Y	 0.2945	 0.0360
Z	 0.1233	 0.0250
a	 0.9080	 0.0500
b	 0.7633	 0.0440
c	 0.5874	 0.0040
d	 0.8641	 0.0470
e	 0.7955	 -0.0020
f	 0.7982	 0.0610
g	 0.4384	 0.0450
h	 0.6657	 0.0050
i	 0.7547	 0.0250
j	 0.7666	 0.0090
k	 0.7584	 0.0630
l	 0.7112	 0.0140
m	 0.8704	 -0.0210
n	 0.6293	 0.0490
o	 0.8411	 0.0120
p	 0.6496	 0.0340
q	 0.9178	 0.0210
r	 0.2318	 0.0310
s	 0.6609	 0.0180
t	 0.6645	 0.0480
u	 0.8369	 -0.0050
v	 0.5998	 0.0340
w	 0.8291	 0.0070
x	 0.8401	 0.0250
y	 0.6216	 0.0260
z	 0.8678	 0.0300