



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 07:48 PM EST

PDB ID : 6X6T
EMDB ID : EMD-22082
Title : Cryo-EM structure of an Escherichia coli coupled transcription-translational complex B1 (TTC-B1) containing an mRNA with a 24 nt long spacer, transcription factors NusA and NusG, and fMet-tRNAs at P-site and E-site
Authors : Molodtsov, V.; Ebright, R.H.; Wang, C.; Su, M.
Deposited on : 2020-05-29
Resolution : 3.20 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:

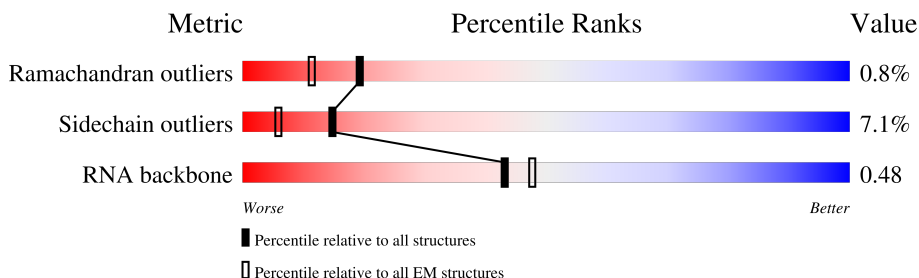
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	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	AG	495	
17	C	75	
18	D	1542	
19	E	87	
20	F	71	
21	G	241	
22	H	557	
23	I	233	
24	J	206	
25	K	167	
26	L	135	
27	M	179	
28	N	130	
29	O	130	
30	P	103	
31	Q	129	

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Mol	Chain	Length	Quality of chain
32	R	124	
33	S	101	
34	T	89	
35	U	82	
36	V	84	
37	W	92	
38	X	118	
39	Y	142	
40	Z	121	
41	a	2904	
42	b	85	
43	c	78	
44	d	120	
45	e	63	
46	f	59	
47	g	70	
48	h	273	
49	i	57	
50	j	209	
51	k	55	
52	l	201	
53	m	46	
54	n	179	
55	o	65	
56	p	177	

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Mol	Chain	Length	Quality of chain
57	q	38	<div>79%</div> <div>95%</div> <div>5%</div>
58	r	149	<div>72%</div> <div>94%</div> <div>6%</div>
59	s	142	<div>71%</div> <div>96%</div> <div>.</div>
60	t	123	<div>67%</div> <div>93%</div> <div>7%</div>
61	u	144	<div>62%</div> <div>95%</div> <div>5%</div>
62	v	136	<div>72%</div> <div>97%</div> <div>.</div>
63	w	127	<div>59%</div> <div>89%</div> <div>5%</div> <div>6%</div>
64	x	117	<div>60%</div> <div>95%</div> <div>.</div> <div>.</div>
65	y	115	<div>62%</div> <div>96%</div> <div>.</div> <div>.</div>
66	z	118	<div>63%</div> <div>96%</div> <div>.</div> <div>.</div>

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 291628 atoms, of which 109913 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
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

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

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

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

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

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

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

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

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

- Molecule 6 is a DNA chain called NT DNA.

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

- 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	33	Total	C	H	N	O	P	0	0
			784	307	97	96	251	33		

- 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	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AB	162	Total	C	H	N	O	S	0	0
			1283	816	1	222	237	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	301	Total	C	N	O	S	0	0
			2094	1296	379	413	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	299	Total	C	N	O	S	0	0
			2078	1287	378	407	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AE	1335	Total	C	H	N	O	S	0	0
			21000	6526	10612	1854	1958	50		

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
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AG	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a RNA chain called 16S rRNA.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a protein called 30S ribosomal protein S2.

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

- Molecule 22 is a protein called 30S ribosomal protein S1.

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

- Molecule 23 is a protein called 30S ribosomal protein S3.

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

- Molecule 24 is a protein called 30S ribosomal protein S4.

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

- Molecule 25 is a protein called 30S ribosomal protein S5.

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

- Molecule 26 is a protein called 30S ribosomal protein S6.

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

- Molecule 27 is a protein called 30S ribosomal protein S7.

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

- Molecule 28 is a protein called 30S ribosomal protein S8.

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

- Molecule 29 is a protein called 30S ribosomal protein S9.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S11.

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

- Molecule 32 is a protein called 30S ribosomal protein S12.

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

- Molecule 33 is a protein called 30S ribosomal protein S14.

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

- Molecule 34 is a protein called 30S ribosomal protein S15.

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

- Molecule 35 is a protein called 30S ribosomal protein S16.

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

- Molecule 36 is a protein called 30S ribosomal protein S17.

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

- Molecule 37 is a protein called 30S ribosomal protein S19.

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

- Molecule 38 is a protein called 30S ribosomal protein S13.

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

- Molecule 39 is a protein called 50S ribosomal protein L11.

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

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 41 is a RNA chain called 23S rRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

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

- Molecule 43 is a protein called 50S ribosomal protein L28.

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

- Molecule 44 is a RNA chain called 5S rRNA.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L2.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L4.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is a protein called 50S ribosomal protein L6.

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

- Molecule 57 is a protein called 50S ribosomal protein L36.

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

- Molecule 58 is a protein called 50S ribosomal protein L9.

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

- Molecule 59 is a protein called 50S ribosomal protein L13.

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

- Molecule 60 is a protein called 50S ribosomal protein L14.

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

- Molecule 61 is a protein called 50S ribosomal protein L15.

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

- Molecule 62 is a protein called 50S ribosomal protein L16.

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

- Molecule 63 is a protein called 50S ribosomal protein L17.

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

- Molecule 64 is a protein called 50S ribosomal protein L18.

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

- Molecule 65 is a protein called 50S ribosomal protein L19.

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

- Molecule 66 is a protein called 50S ribosomal protein L20.

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

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	7	1	Total 1	Mg 1	0

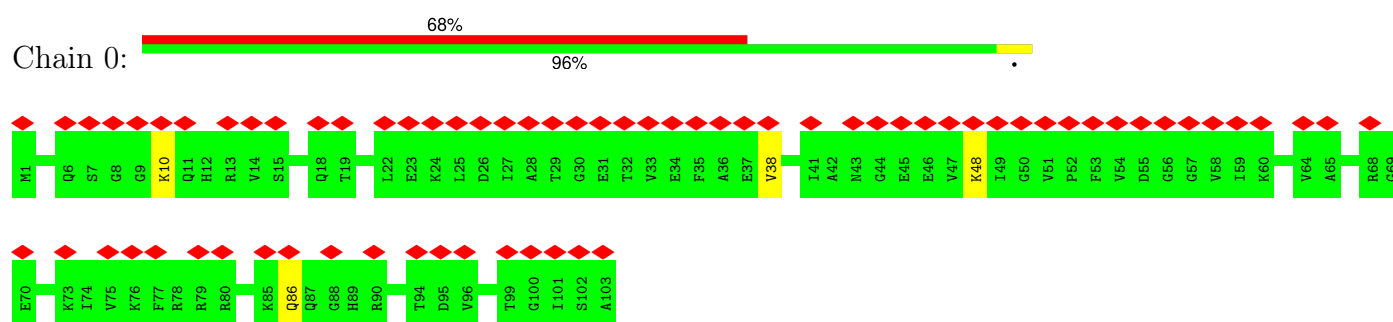
- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	AA	2	Total 2	Zn 2	0

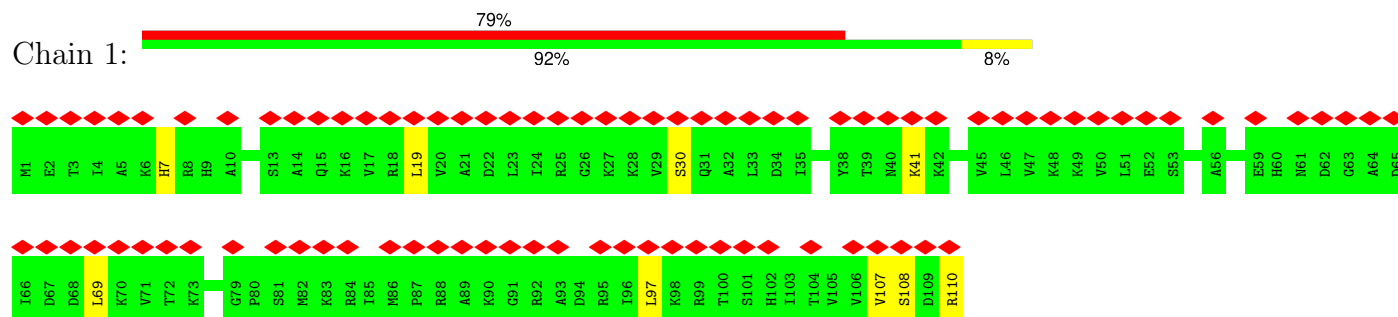
3 Residue-property plots

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

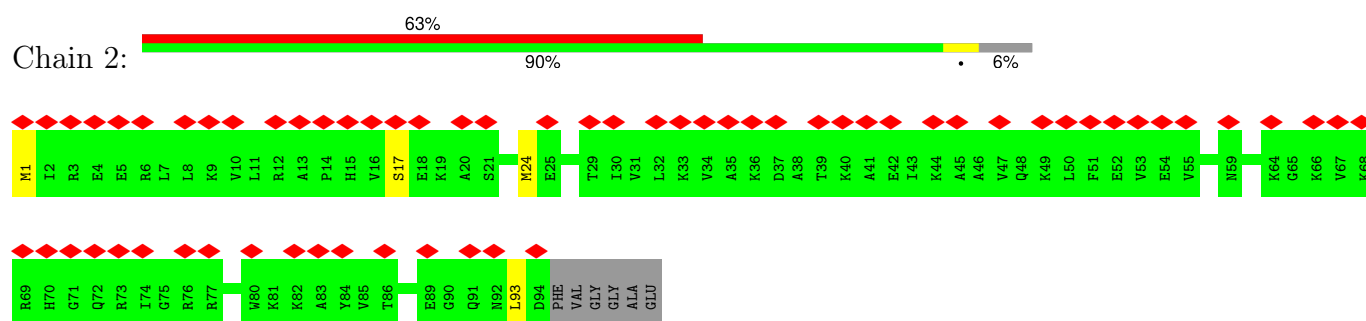
- Molecule 1: 50S ribosomal protein L21



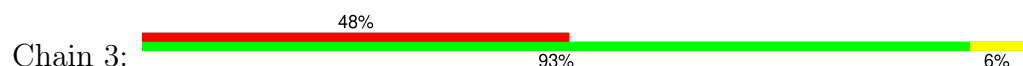
- Molecule 2: 50S ribosomal protein L22

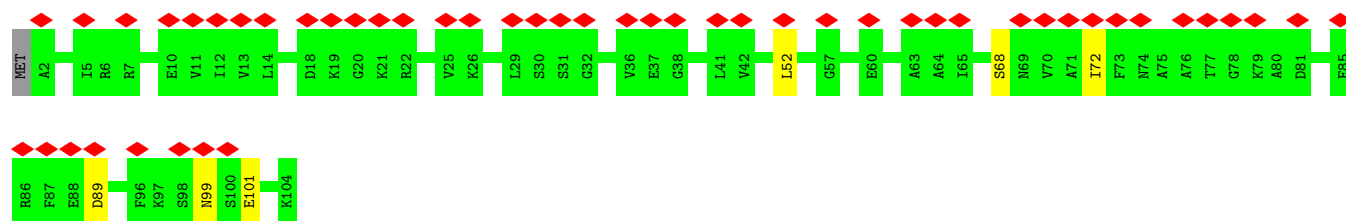


- Molecule 3: 50S ribosomal protein L23

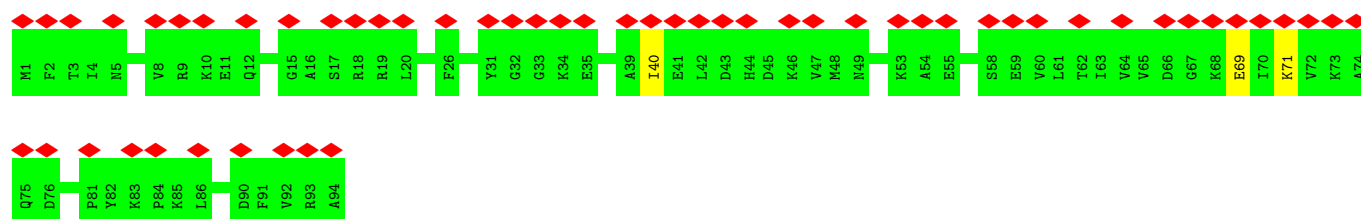


- Molecule 4: 50S ribosomal protein L24

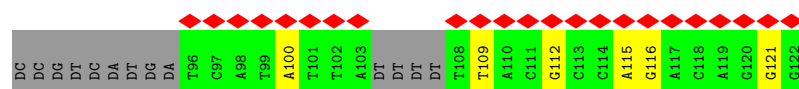




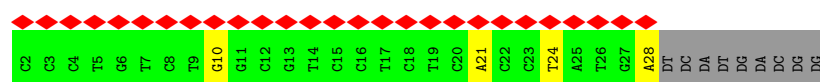
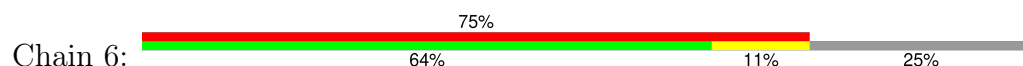
• Molecule 5: 50S ribosomal protein L25



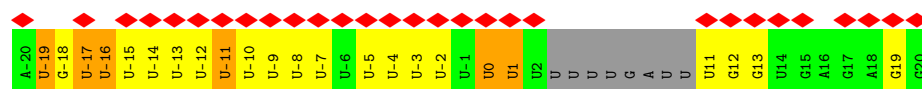
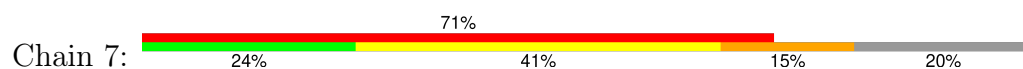
• Molecule 6: NT DNA



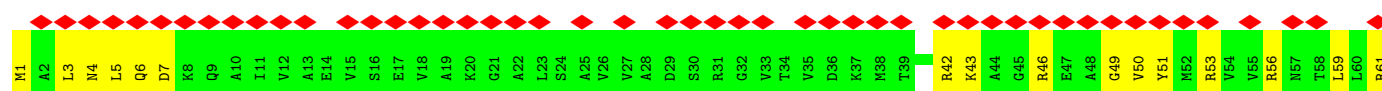
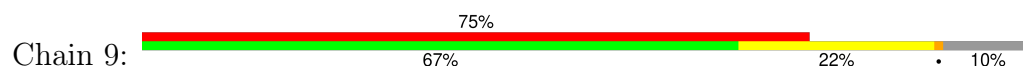
• Molecule 7: T DNA

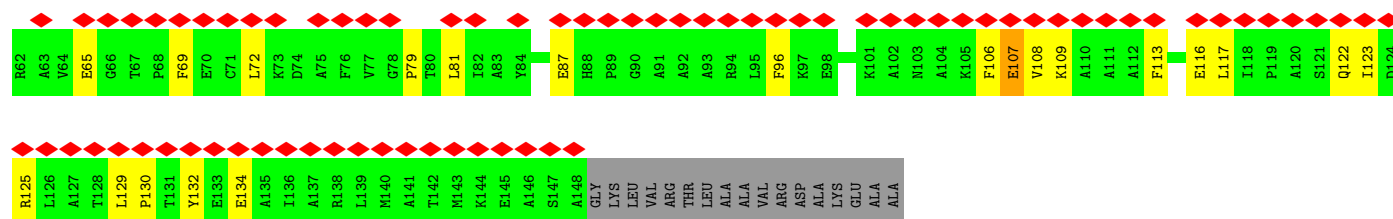


• Molecule 8: mRNA with 24 nt long spacer

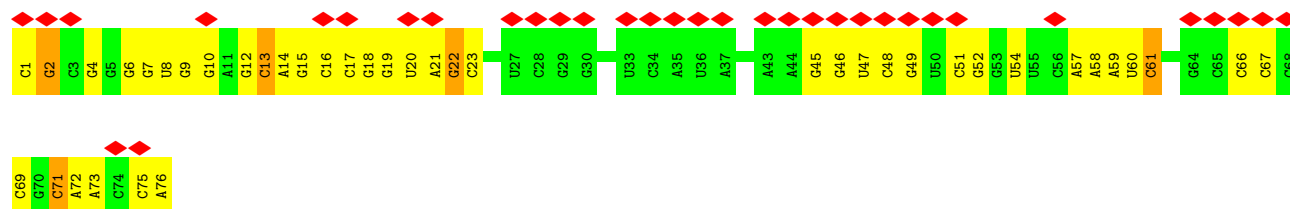


• Molecule 9: 50S ribosomal protein L10

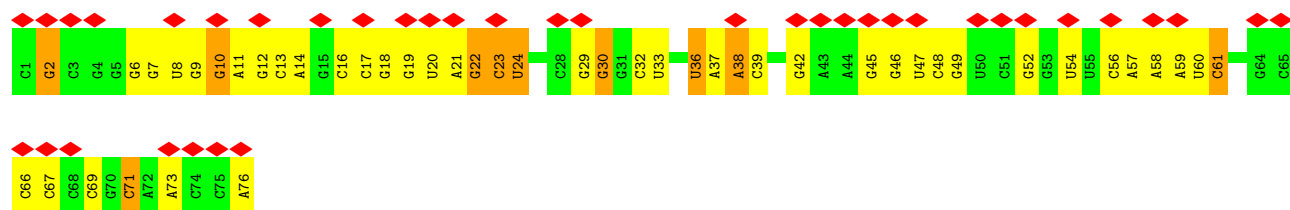




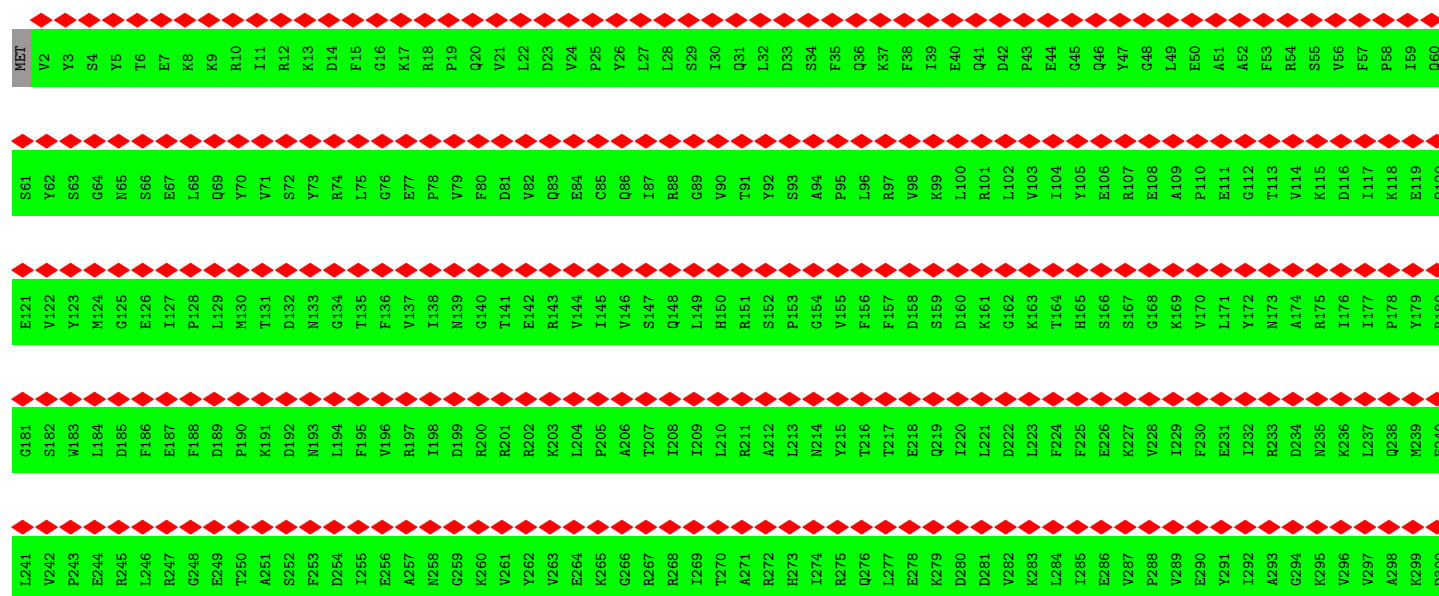
• Molecule 10: E-site and P-site tRNA (fMet)



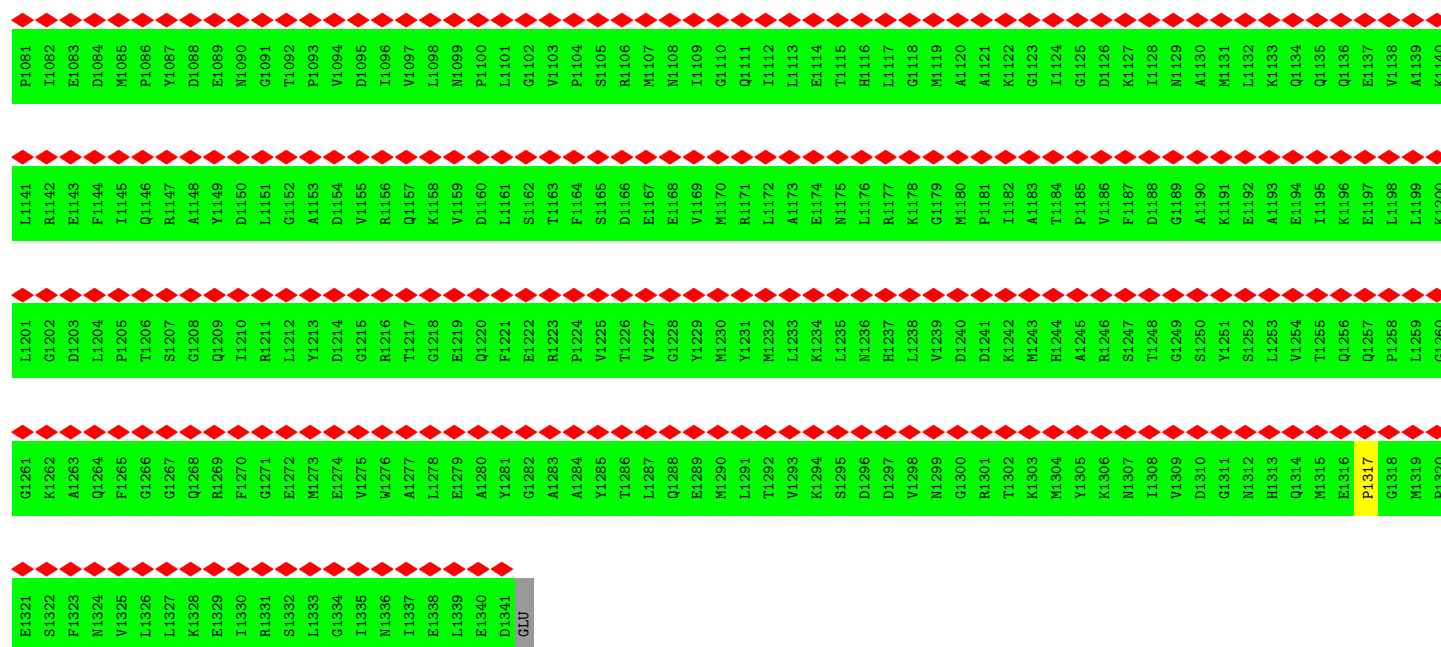
• Molecule 10: E-site and P-site tRNA (fMet)



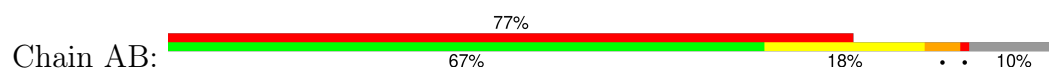
• Molecule 11: DNA-directed RNA polymerase subunit beta



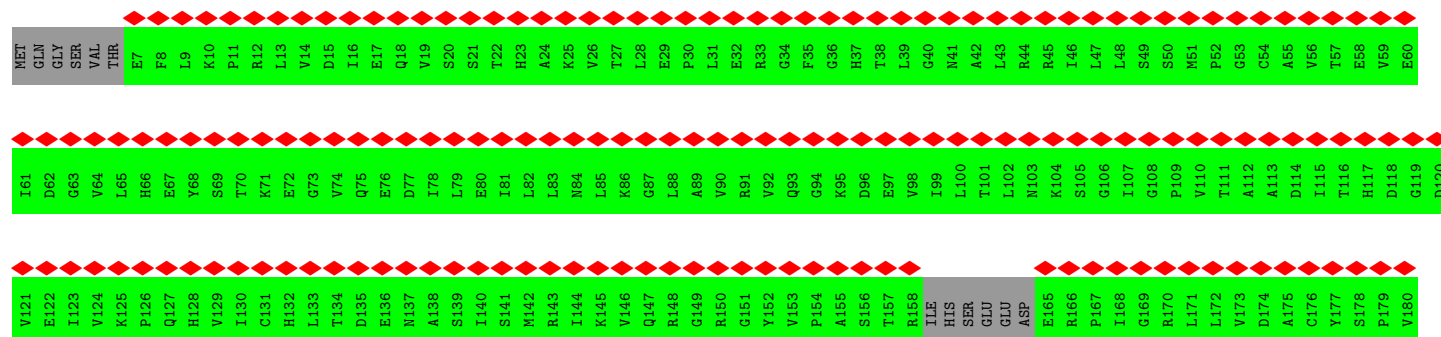
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H1023	E963	T843	L783	V723	V663	I603	A543	D483	D423	L363	D303
E1024	L964	K844	A784	V724	G664	H604	G544	L484	D424	V364	E304
F1025	Q965	L845	D785	V725	A665	Y605	F545	D485	I425	E365	S305
E1026	L966	G846	G786	V726	S666	L606	E546	T486	I426	I366	T306
K1027	L967	P847	P787	V727	L667	S607	V547	L487	D427	Y367	G307
K1028	E968	E848	S788	D728	T668	A608	R548	M488	V428	R368	E308
L1029	K969	E849	T789	A729	P669	I609	D549	P489	M429	M369	L309
E1030	A910	T850	D790	S730	F670	E610	V550	Q490	K430	M370	I310
A1031	L971	T851	L791	R731	L671	E611	H551	D491	K431	R371	C311
K1032	F972	A852	G792	I732	E672	G612	P552	M492	L432	P372	A312
R1033	S973	D853	E793	V733	H673	N613	T553	I493	I433	G373	A313
R1034	R974	T854	L794	I734	D674	Y614	H554	M494	D434	E374	N314
K1035	I975	P855	A795	K735	D675	V615	Y555	A495	I435	P375	M315
I1036	R976	N856	L796	V736	A676	I616	G556	K496	R436	P376	E316
T1037	S977	V857	G797	N737	N677	A617	R557	P497	N437	T377	L317
Q1038	V978	G858	Q798	E738	R678	Q618	V558	I498	G438	R378	S318
G1039	L979	E859	N799	D739	A679	A619	C559	S499	K439	E379	L319
D1040	V980	A860	M800	E740	L680	N620	P560	A500	G440	A380	D320
D1041	A981	A861	R801	M741	M681	S621	I561	A501	E441	A381	L321
L1042	G982	L862	V802	Y742	G682	L623	E562	V502	D442	E382	L322
A1043	G983	S863	A803	P743	A683	L623	T563	K503	D443	S383	A323
P1044	V984	K864	F804	G744	N684	D624	P564	E504	I444	L384	K324
E985	E985	L865	M805	E745	M685	E625	E565	F505	I445	F385	L325
V1046	G986	D866	P806	A746	Q686	E626	G566	F506	D446	S386	S326
L1047	E987	E867	M807	G747	R687	G627	P567	G507	H447	N387	Q327
K1048	K988	S868	N808	I748	Q688	H628	N568	S508	L448	L388	S328
I1049	R989	G869	G809	D749	A689	F629	I569	S509	G449	F389	G329
V1050	D990	T870	Y810	I750	V690	V630	G570	Q510	N450	F390	H330
K1051	V991	V871	N811	Y751	P691	E631	L571	L511	R451	S391	K331
V1052	L992	H872	F812	T52	T692	D632	I572	S512	R452	E392	L332
Y1053	P993	L873	E813	L753	L693	L633	N573	Q513	I453	D393	L333
L1054	R994	G874	D814	T754	R694	V634	S574	F514	R454	R394	E334
A1055	D995	A875	S815	K755	A695	T635	L575	M515	S455	Y395	T335
V1056	R996	E876	T816	Y756	D696	C636	S576	D516	V456	D396	L336
K1057	V997	V877	L817	T757	K697	R637	V577	Q517	G457	L397	F337
R1058	L998	T878	V818	R758	P698	S638	V578	N518	E458	S398	T338
I1059	E999	G879	S819	S759	L699	K639	A579	N519	M459	A399	N339
I1060	L1000	G880	E820	N760	V700	G640	Q580	P520	A460	V400	D340
Q1061	G1001	D881	R821	Q761	G701	E641	T581	L521	E461	G401	L341
P1062	L1002	L882	V822	T762	T702	S642	N582	S522	N462	R402	D342
G1063	T1003	L883	E823	T763	G703	S643	E583	E523	Q463	M403	H343
D1064	D1004	V884	Q824	C764	M704	L644	Y584	I524	F464	K404	G344
A1065	E1005	G885	E825	I765	E705	F645	G585	T525	R465	F405	P345
M1066	E1006	K886	D826	N766	R706	S646	F586	H526	V466	N406	Y346
A1067	K1007	V887	R827	Q767	A707	R647	L587	K527	G467	R407	I347
Q1068	Q1008	T888	F828	M768	V708	D648	E588	R528	L468	S408	S348
R1069	N1009	P889	T829	P769	A709	Q649	T589	R529	V469	S409	E349
H1070	Q1010	K890	T830	C770	V710	V650	P590	I530	R470	L409	T350
G1071	L1011	G891	R831	V771	D711	D651	Y591	S531	V471	R411	L351
N1072	E1012	E892	H832	T772	S712	Y652	R592	A532	E472	E412	R352
K1073	Q1013	T893	L833	L773	G713	M653	K593	L533	R473	E413	V353
G1074	L1014	D894	Q834	G774	V714	D654	Y594	G534	A474	I414	D354
V1075	A1015	L895	E835	E775	T715	V655	T595	P535	V475	E415	P355
I1076	E1016	T896	L836	P776	A716	S656	D596	G536	K476	G416	T356
S1077	Q1017	P897	A837	V777	V717	T657	G597	G537	E477	S417	N357
K1078	Y1018	E898	C838	E778	A718	Q658	V598	L538	R478	G418	D358
I1079	D1019	E899	V839	R779	K719	Q659	V599	T539	L479	I419	R359
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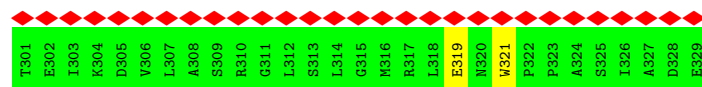
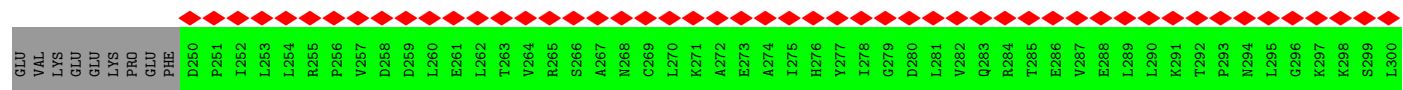
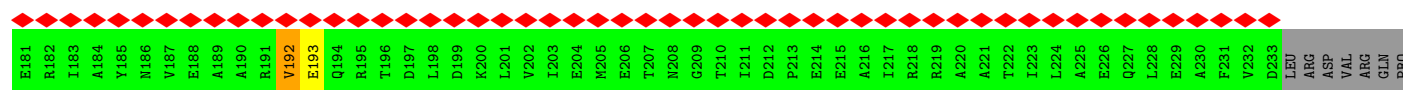


• Molecule 12: Transcription termination/antitermination protein NusG

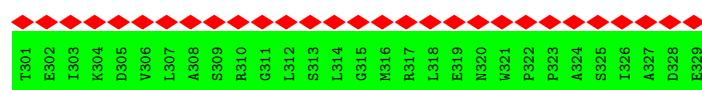
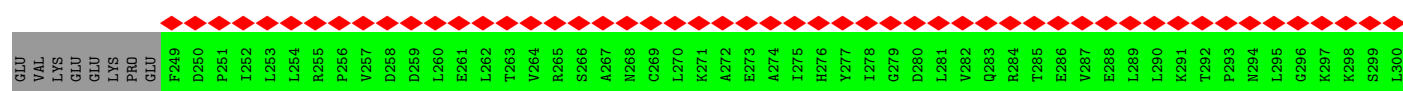
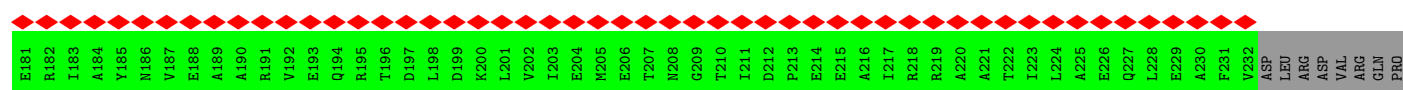
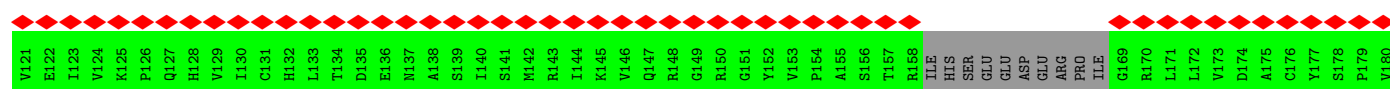
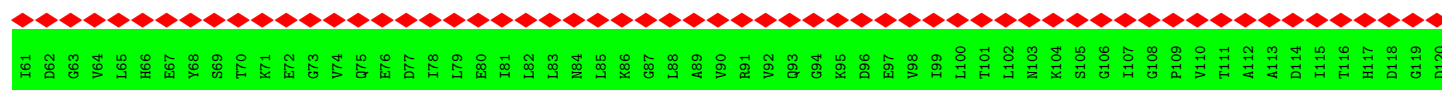


• Molecule 13: DNA-directed RNA polymerase subunit alpha

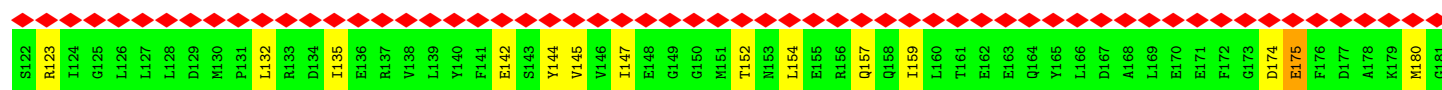
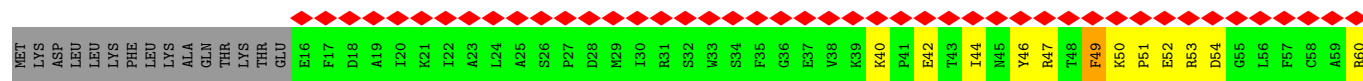
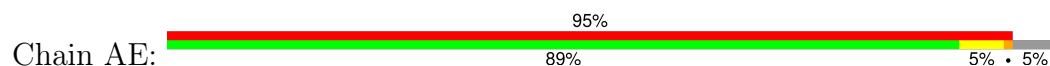




• Molecule 13: DNA-directed RNA polymerase subunit alpha



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



N962	D902	R842	G782	I722	A662	S602	A542	A482	L422	R362	A302	L242	A182
V963	L903	V843	L783	Y723	E663	K003	S543	L483	L423	L363	V303	P243	E183
K964	A904	T844	A784	M724	I664	M604	I664	M484	N424	H364	D304	V244	A184
S965	R905	A845	D785	M725	Q665	L005	H545	M485	R425	Q365	A305	L245	I185
V966	G906	E846	T786	A726	E666	N606	A546	S486	A426	C366	L306	P246	Q186
V967	H907	D847	A787	D727	Q667	T007	R547	T487	P427	G367	L307	P247	A187
N968	I908	V848	L788	S728	F668	C608	V548	M488	T428	L368	D308	D248	L188
S969	T909	R789	K789	G729	Q669	Y009	K549	M489	L429	P369	N309	L249	L189
N970	N910	K850	T790	A730	S670	R610	V550	R610	H430	K370	R250	R250	K190
G971	K911	P851	A791	R731	G671	I611	R551	L491	R431	K371	R311	P251	S191
K972	G912	G852	T792	G732	L672	L612	L552	S492	L432	M372	R312	L252	M192
L973	E913	T853	S793	S733	V673	G613	T553	P493	G433	A373	G313	V253	D193
V974	A914	A854	G794	A734	T674	L614	E554	A494	I434	L374	R194	P254	L194
I975	T915	D855	Y795	A735	A675	K615	V555	M495	Q435	E375	A315	L255	E195
T976	G916	L856	L796	Q736	G676	P616	E556	G496	A436	L376	I316	A256	Q196
S977	V917	L857	T797	I737	E677	T617	K557	E497	F437	F377	T317	G257	E197
R978	I918	V858	R798	R738	R678	V618	D558	P498	E438	K378	G318	G258	C198
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L982	S922	T862	D802	G742	V682	D622	E562	P502	I442	Y382	R322	T262	R202
K983	I923	L863	V603	M743	I683	Q623	L563	S503	E443	G383	P323	S263	E203
G924	G924	L864	A804	R744	D684	I624	V564	D504	G444	K384	L324	E204	E204
I985	E925	H865	Q805	G745	I685	M625	A565	D505	K445	L385	K325	L265	L205
D986	P926	E866	D806	L746	M686	Y626	K566	V506	A446	E386	S326	N266	N206
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F988	T928	N868	V808	A748	A688	G628	S568	L508	Q448	R388	A328	L268	T208
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K992	L872	N872	D812	G752	R692	A632	T572	V512	L452	T392	V272	T212	T212
E993	E973	D873	D813	S753	V693	A633	T573	M513	V453	T393	G333	I273	K213
S994	E874	C814	C814	I754	S694	R634	V574	T514	C454	I394	K334	N274	R214
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V997	W877	H817	H817	T757	M697	A637	A577	C517	Y457	A397	R337	N277	L217
Y999	D878	E818	E818	P758	M698	S638	L578	V518	N458	K398	F338	R278	T218
G1000	A879	G819	G819	L759	D699	V639	L579	N519	A459	K399	R339	L279	K219
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A1001	K881	M821	M821	A761	L701	I641	M681	K521	F461	V401	N341	R281	I221
V1002	V882	M822	M822	T762	Q702	D642	L582	G522	D462	E402	L342	L282	K222
L1003	R883	T923	T923	F763	T703	D643	V683	E523	Q463	R403	L343	L283	L223
A1004	S884	P824	E704	R764	E704	M644	M524	G524	D464	E404	G344	D284	L224
K1005	V885	V825	V825	E765	T705	V645	K585	M525	Q465	E405	K345	L285	E225
G1006	V886	I826	I826	G766	V706	I646	G586	V526	M466	A406	R346	A286	A226
D1007	S887	E827	E827	L767	I707	P647	L587	L527	A467	V407	V347	A287	F227
G1008	C888	G828	G828	N768	N708	E648	P588	T528	V468	V408	D348	V228	V228
E1009	V952	D889	G829	V769	R709	K649	Y589	G529	H469	W409	Y349	D289	Q229
Q1010	K953	T890	D830	L770	D710	K650	S590	P530	V470	D410	S350	L290	S230
V1011	D891	V831	V831	Q771	G711	H651	T591	K531	P471	I411	G351	I291	G231
A1012	K955	F892	K832	Y772	Q712	E652	V592	E532	L472	D412	R352	V292	N232
G1013	G956	G993	E833	F773	E713	I653	N593	A533	T473	D413	S353	R293	K233
G1014	S957	V894	P834	I774	E714	I654	Q594	E534	L474	E414	V354	R294	P234
E1015	C958	C995	L835	S775	K715	S655	A595	R535	E475	V415	I355	E295	E235
T1016	K959	A896	R836	T776	Q716	E656	L596	L536	A476	I416	T356	K296	W236
V1017	H897	D837	D837	H777	V717	A657	G597	V537	Q477	R417	V357	R297	M237
A1018	C998	R838	R838	G778	S718	E658	K598	R538	L478	E418	G357	M298	I238
N1019	Y899	V839	V839	A779	F719	A659	K599	S539	E479	H419	P359	L299	L239
W1020	G900	L840	L840	R780	N720	E660	T600	G540	A480	Y360	Q300	T240	T240
D1021	R901	C841	C841	K781	S721	V661	A601	L541	R481	W421	E301	F201	V241

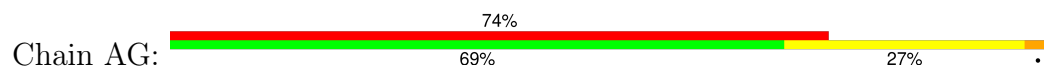
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A1322	A1323	S1324	F1325	Q1326	E1327	T1328	T1329	R1330	V1331	L1332	T1333	E1334	A1335	A1336	V1337	A1338	G1339	K1340	R1341	D1342	E1343	L1344	R1345	G1346	L1347	K1348	E1349	M1350	V1351	I1352	V1353	G1354	R1355	L1356	I1357	P1358	A1359	G1360	T1361	G1362	Y1363	A1364	Y1365	H1366	Q1367	D1368	R1369	M1370	R1371	R1372	R1373	ALA	ALA	GLY	GLY	ALA	PRO	PRO	ALA	ALA
R1262	K1263	A1264	T1265	V1266	V1267	N1268	A1269	G1270	S1271	S1272	D1273	P1274	L1275	E1276	G1277	E1278	Q1279	V1280	E1281	Y1282	S1283	R1284	V1285	K1286	I1287	A1288	R1289	R1290	E1291	L1292	E1293	A1294	N1295	G1296	K1297	V1298	G1299	A1300	T1301	Y1302	S1303	R1304	L1305	L1306	L1307	G1308	I1309	T1310	K1311	A1312	S1313	L1314	A1315	T1316	E1317	S1318	F1319	I1320	S1321	
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D1082	A1083	Q1084	G1085	N1086	D1087	V1088	L1089	I1090	P1091	G1092	T1093	D1094	M1095	P1096	A1097	Q1098	T1099	F1100	L1101	P1102	G1103	K1104	A1105	I1106	V1107	Q1108	L1109	E1110	D1111	G1112	V1113	I1114	I1115	S1116	S1117	G1118	D1119	T1120	L1121	A1122	R1123	I1124	P1125	GLU	SER	GLY	GLY	THR	LYS	ASP	ILE	THR	G1136	G1137	L1138	P1139	R1140	V1141	I1080	V1081
P1022	H1023	T1024	M1025	P1026	V1027	I1028	T1029	E1030	V1031	S1032	G1033	F1034	V1035	R1036	F1037	T1038	D1039	M1040	I1041	D1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	T1050	D1051	E1052	L1053	T1054	G1055	L1056	S1057	S1058	L1059	V1060	V1061	L1062	D1063	S1064	A1065	E1066	R1067	T1068	A1069	G1070	G1071	K1072	D1073	L1074	R1075	P1076	A1077	L1078	K1079	I1080	V1081	

- Molecule 15: DNA-directed RNA polymerase subunit omega

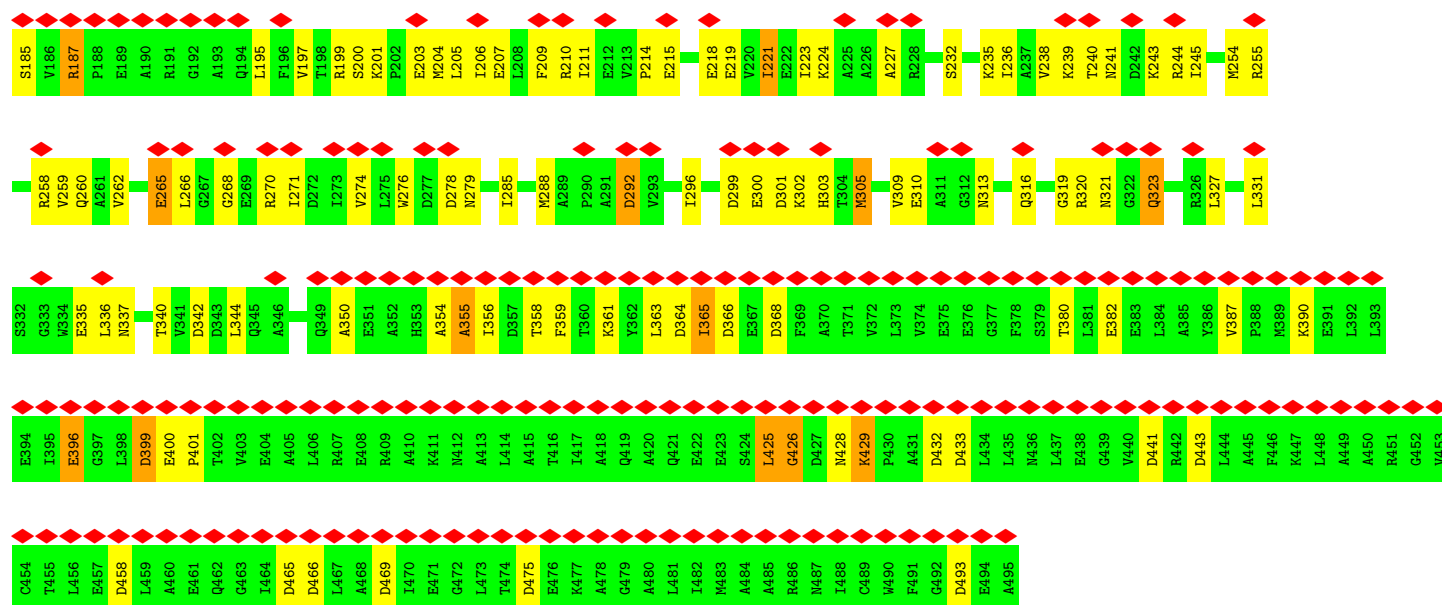


MET																																																																	
ALA		R3																																																															
V4		T5																																																															
V6		Q7																																																															
D8		A9																																																															
R9		V10																																																															
E11		K12																																																															
I13		G14																																																															
N15		R16																																																															
F17		D18																																																															
L19		V20																																																															
L21		V22																																																															
A23		A24																																																															
R25		R26																																																															
A27		R28																																																															
Q29		M30																																																															
Q31		V32																																																															
G33		G34																																																															
K35		D36																																																															
P37		L38																																																															
V39		P40																																																															
E41		E42																																																															
M43		D44																																																															
K45		T46																																																															
T47		V48																																																															
I49		A50																																																															
L51		R52																																																															
E53		I54																																																															
E55		G56																																																															
G57		L58																																																															
N59		N60																																																															
N61	Q62	I63	L64	D65	V66	R67	E68	R69	R70	E71	Q72	Q73	E74	Q75	E76	A77	A78	E79	L80	Q81	A82	V83	T84	ALA	ILE	GLU	GLY	ARG	ARG																																				

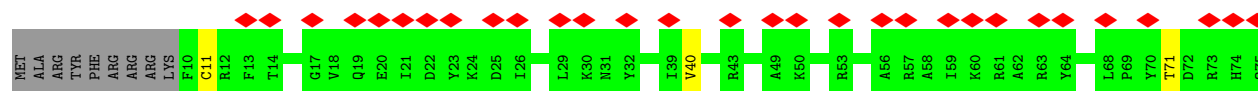
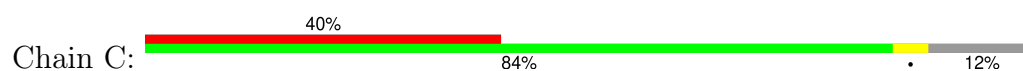
- Molecule 16: Transcription termination/antitermination protein NusA



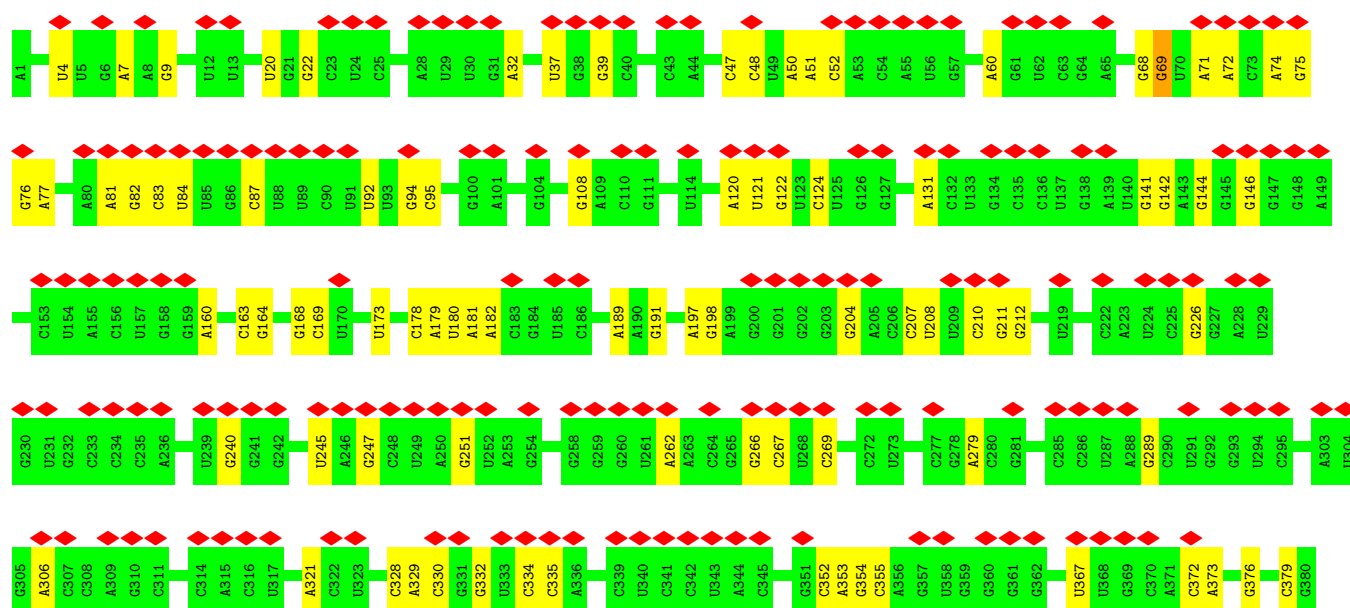
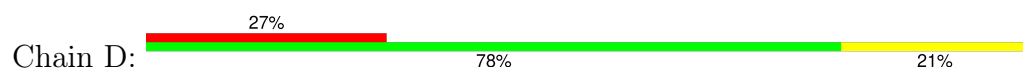
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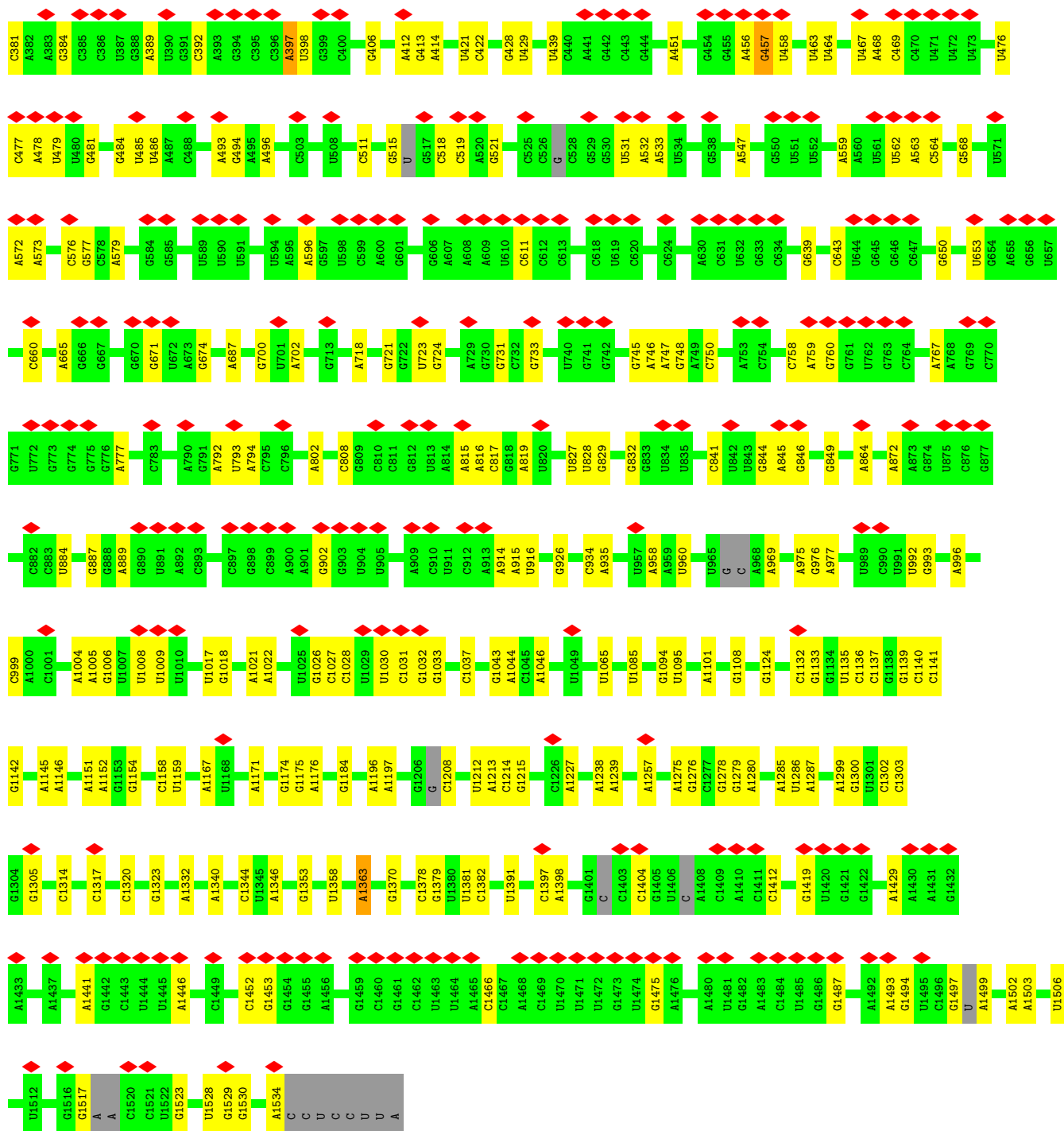


• Molecule 17: 30S ribosomal protein S18

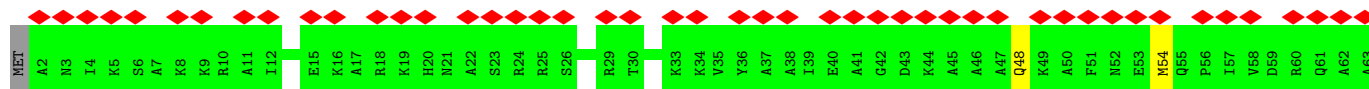
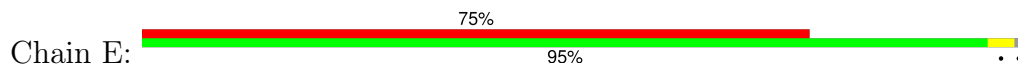


• Molecule 18: 16S rRNA



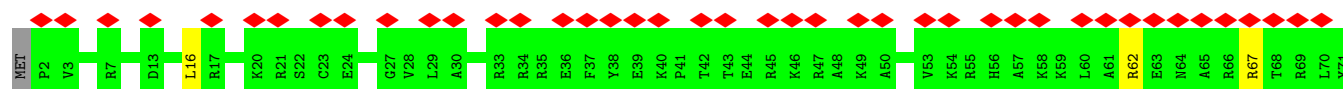


- Molecule 19: 30S ribosomal protein S20

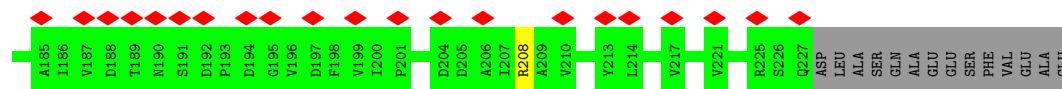
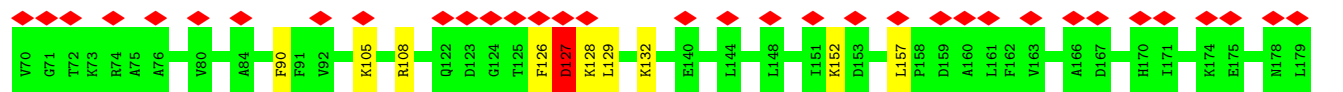
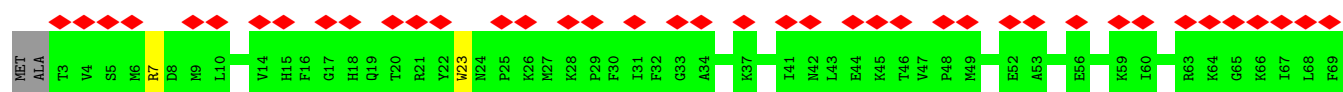
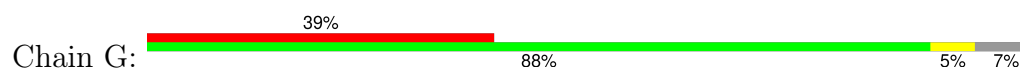




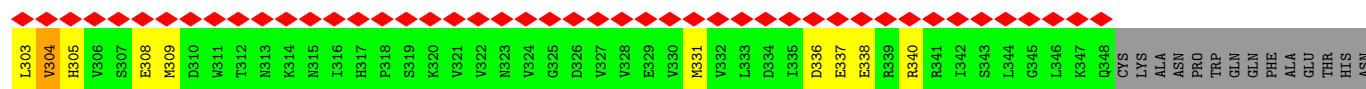
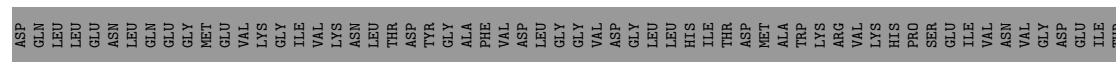
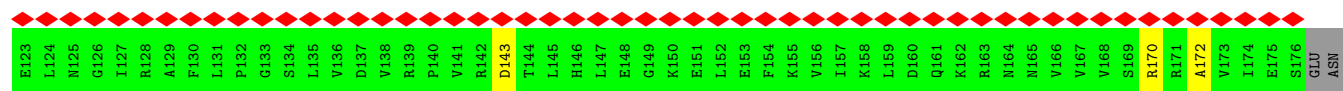
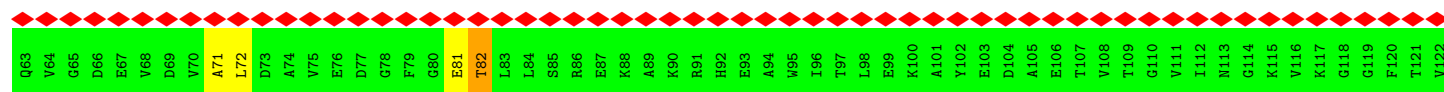
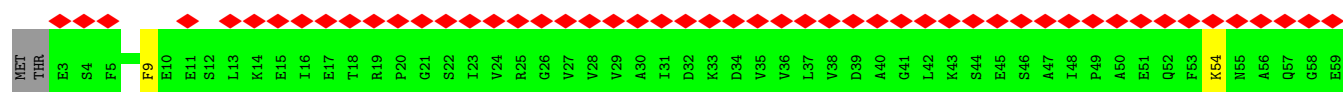
• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S2

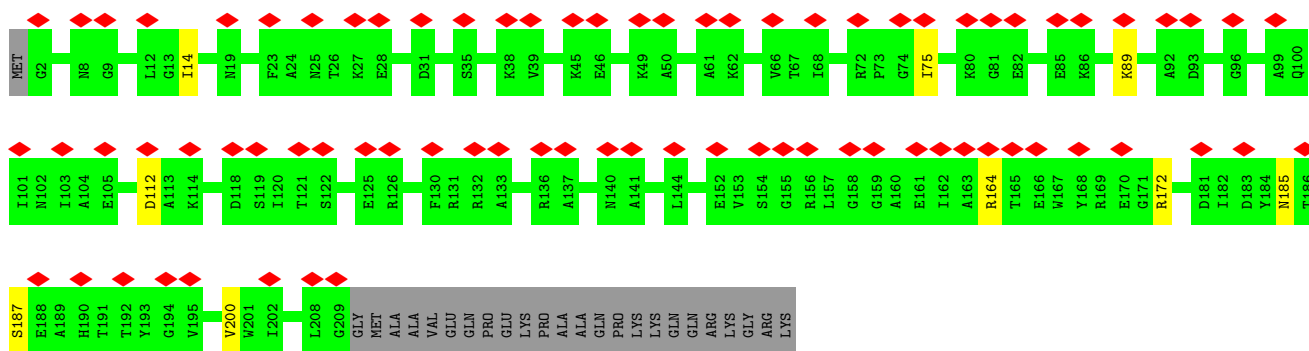
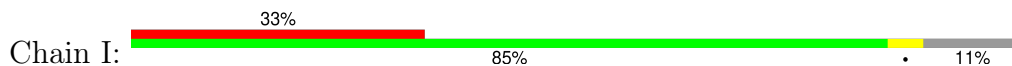


• Molecule 22: 30S ribosomal protein S1

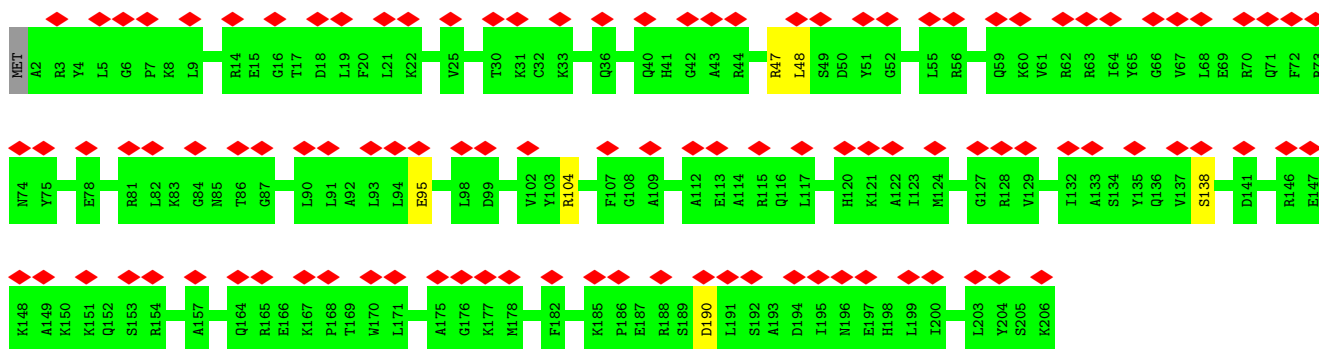


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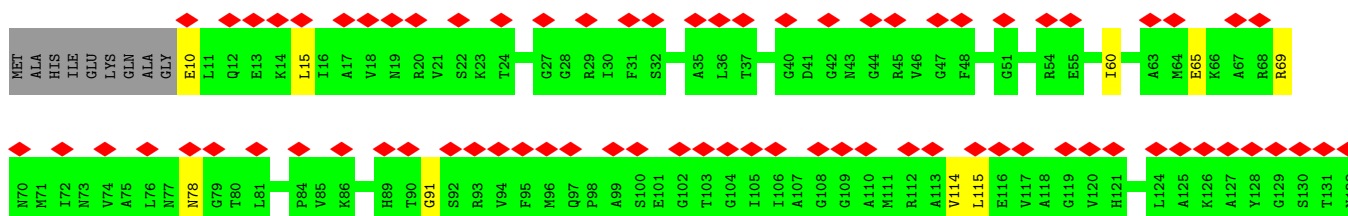
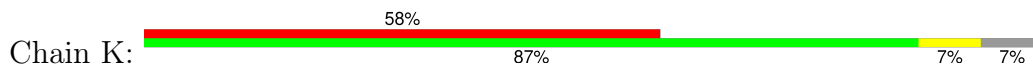
- Molecule 23: 30S ribosomal protein S3

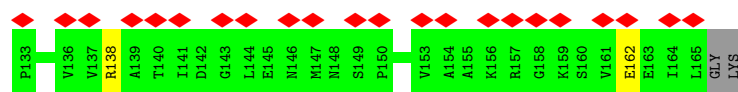


- Molecule 24: 30S ribosomal protein S4

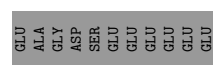
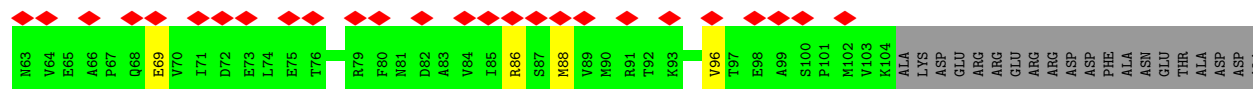
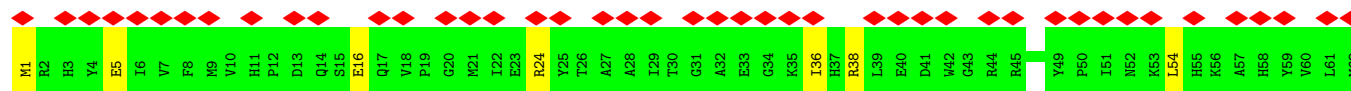


- Molecule 25: 30S ribosomal protein S5

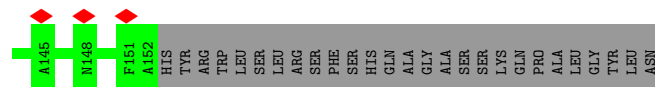
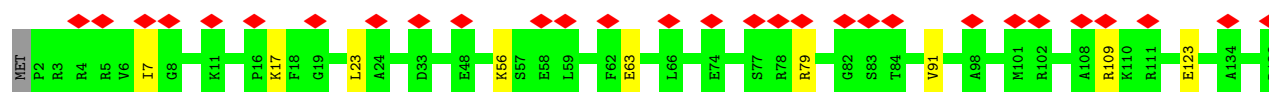
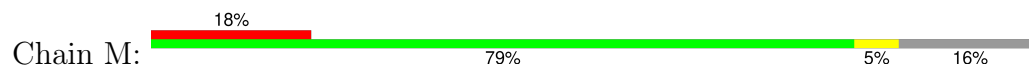




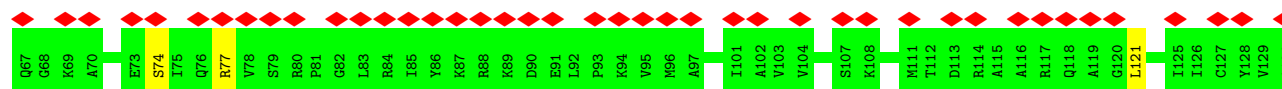
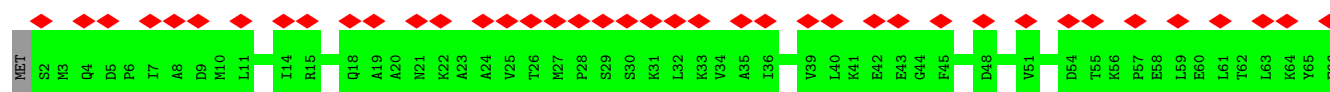
- Molecule 26: 30S ribosomal protein S6



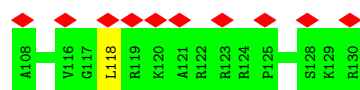
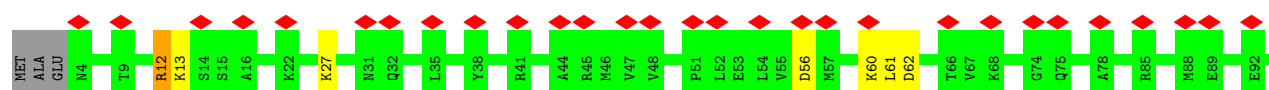
- Molecule 27: 30S ribosomal protein S7



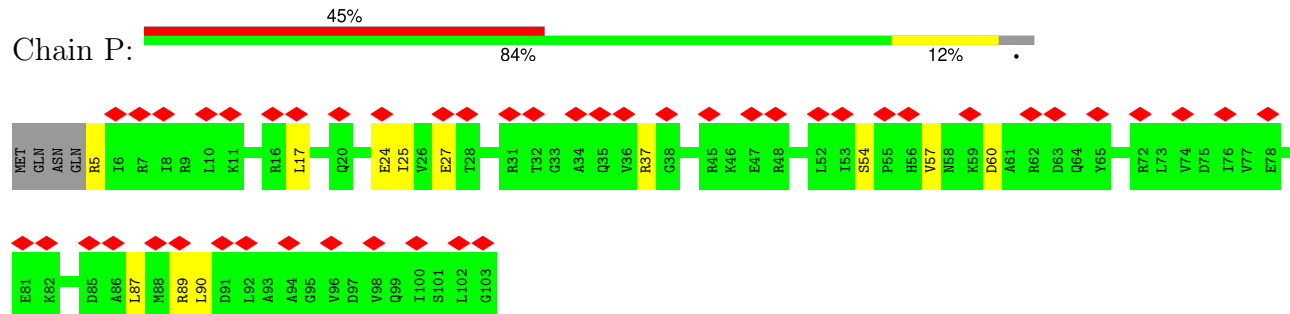
- Molecule 28: 30S ribosomal protein S8



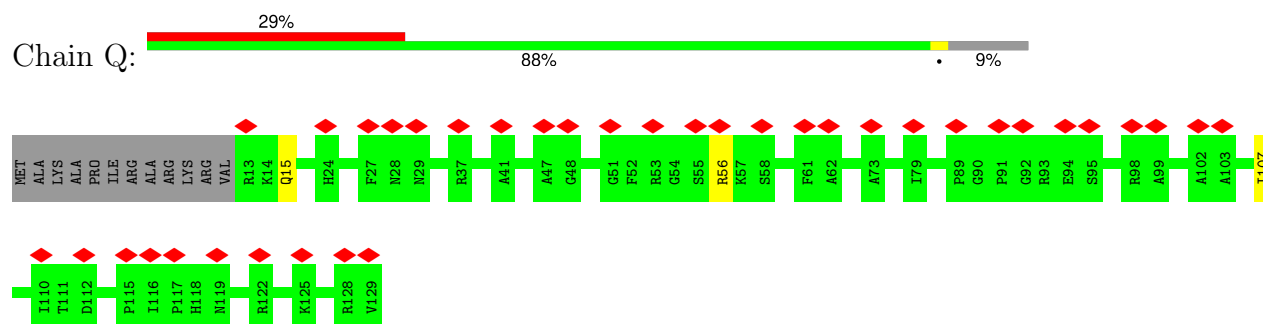
- Molecule 29: 30S ribosomal protein S9



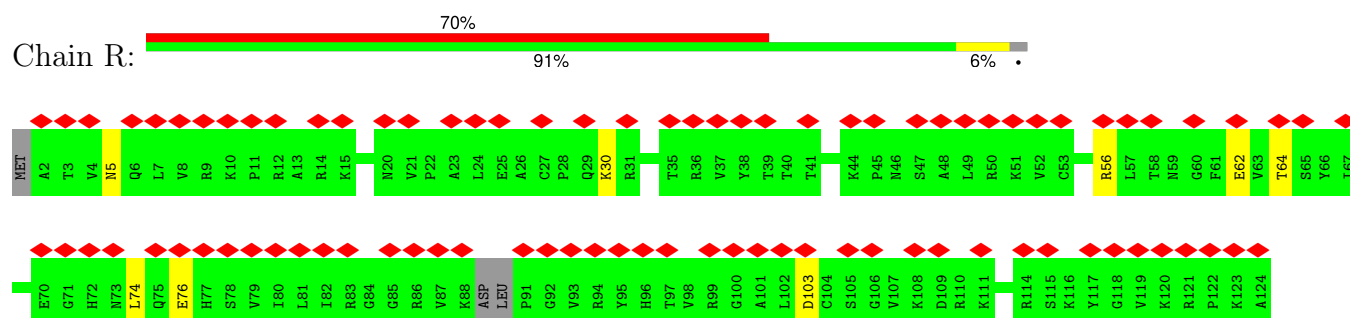
- Molecule 30: 30S ribosomal protein S10



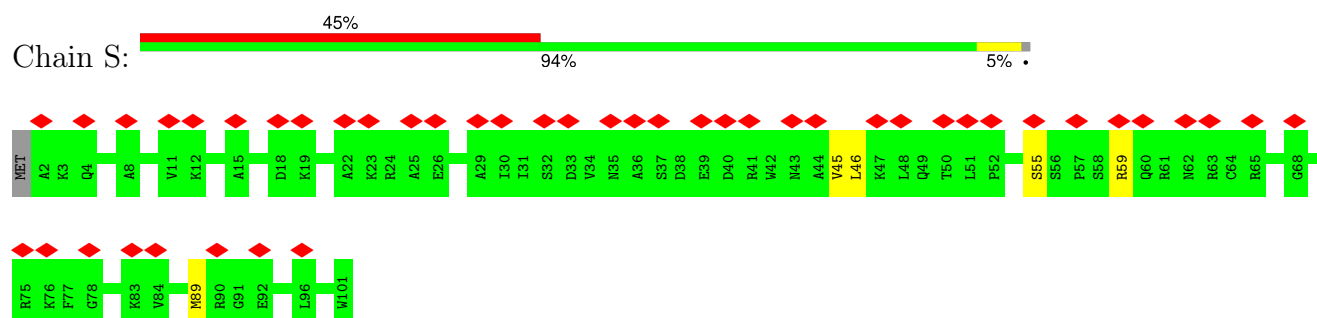
- Molecule 31: 30S ribosomal protein S11



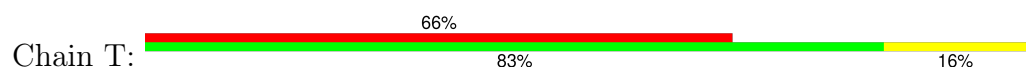
- Molecule 32: 30S ribosomal protein S12

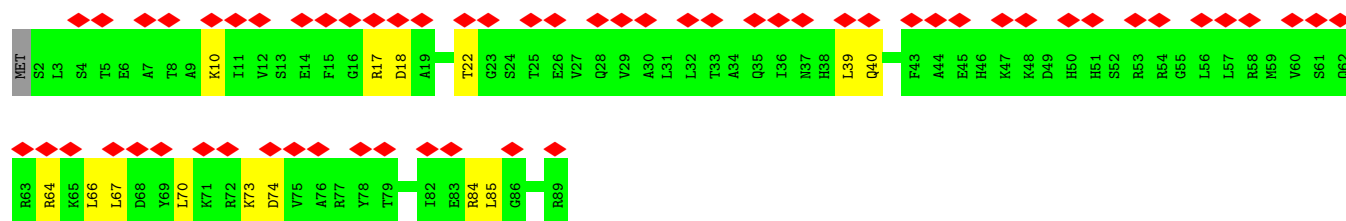


- Molecule 33: 30S ribosomal protein S14

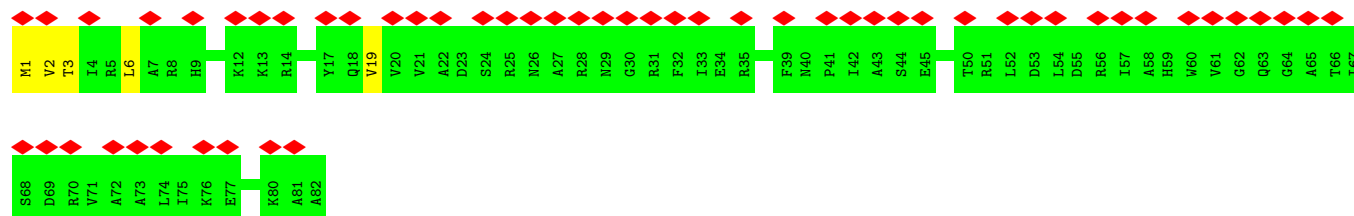


- Molecule 34: 30S ribosomal protein S15

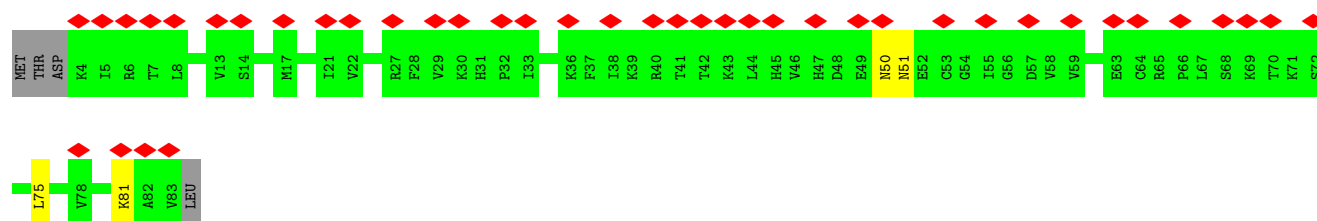
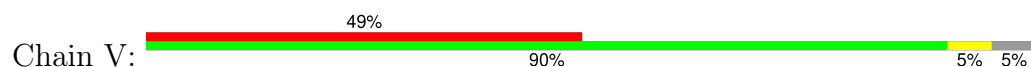




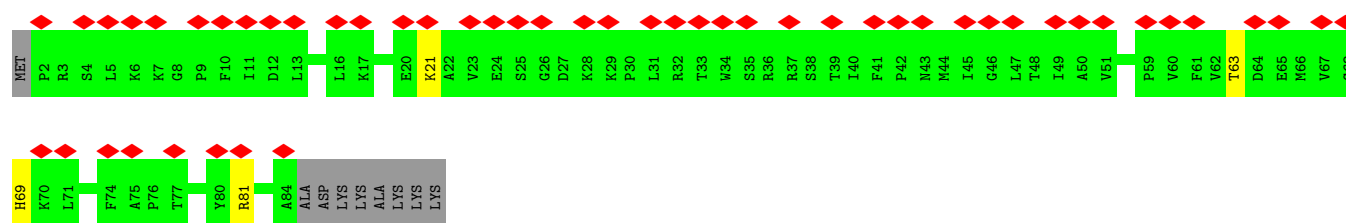
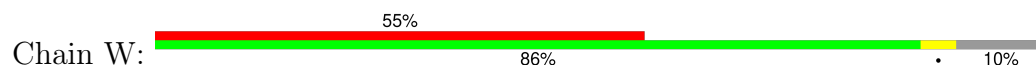
• Molecule 35: 30S ribosomal protein S16



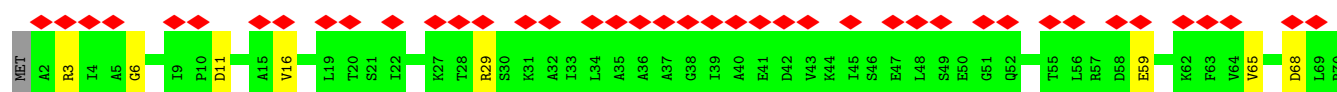
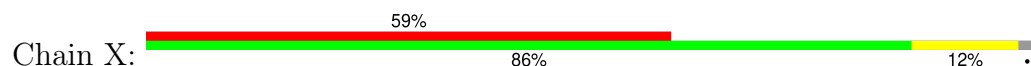
• Molecule 36: 30S ribosomal protein S17

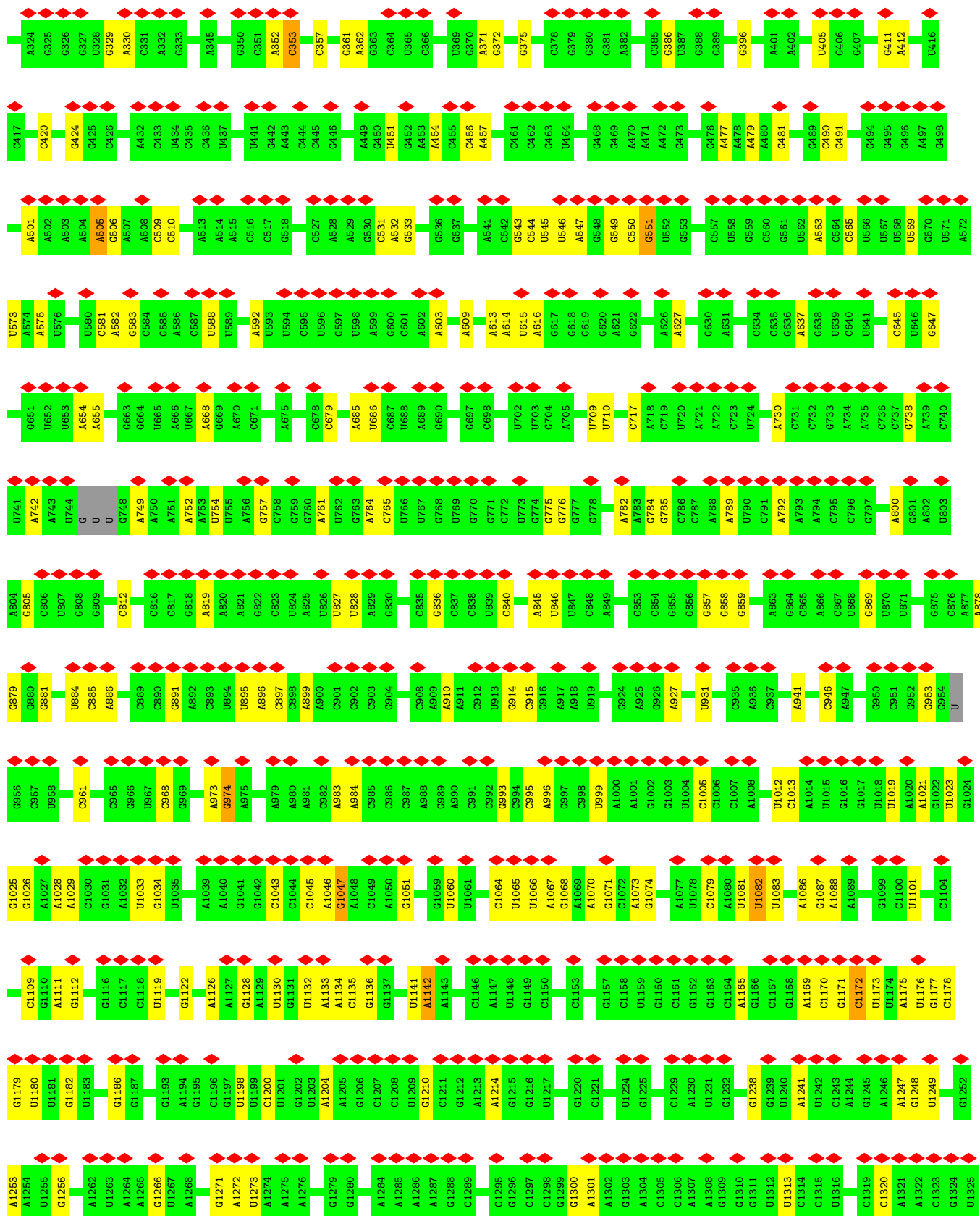


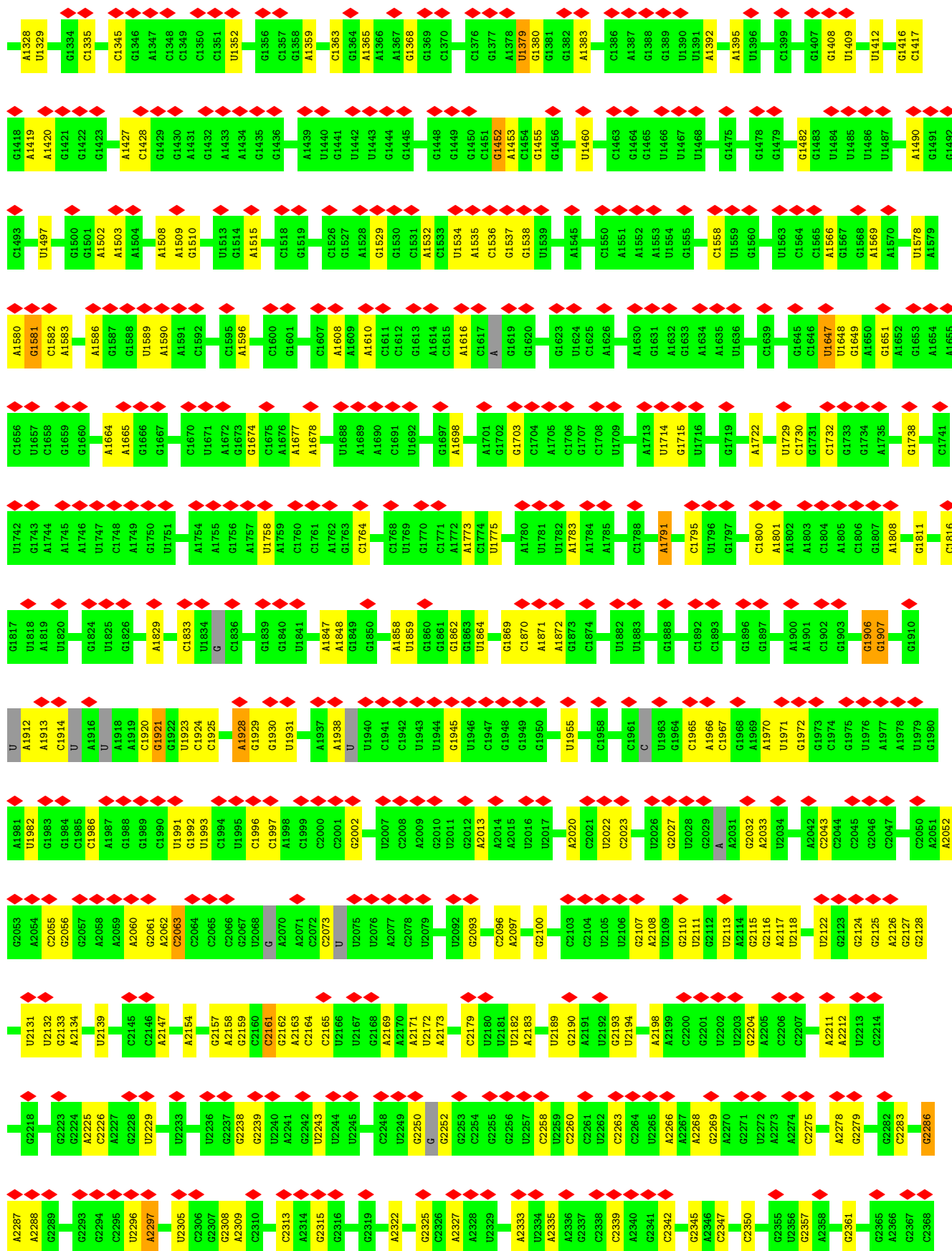
• Molecule 37: 30S ribosomal protein S19

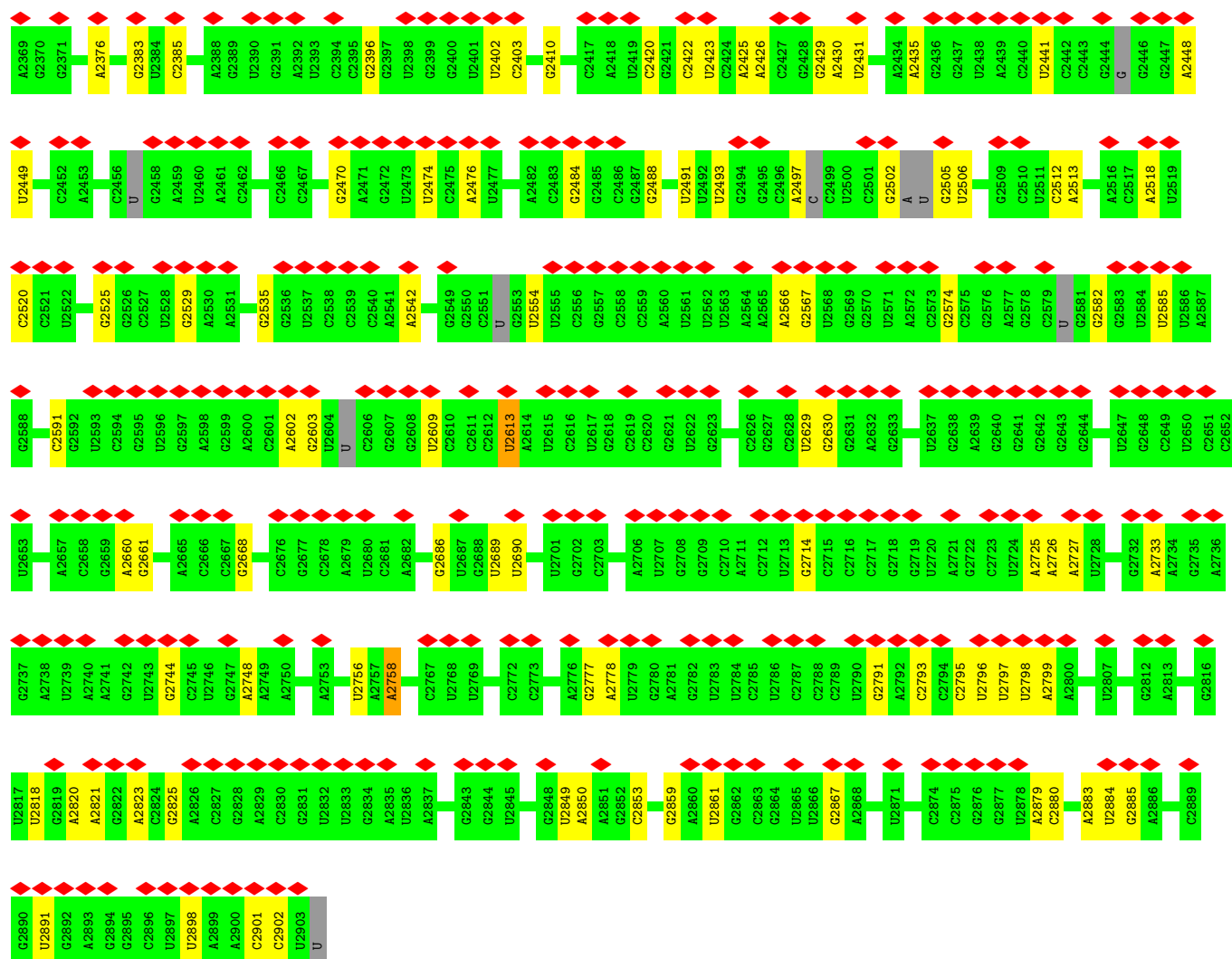


• Molecule 38: 30S ribosomal protein S13

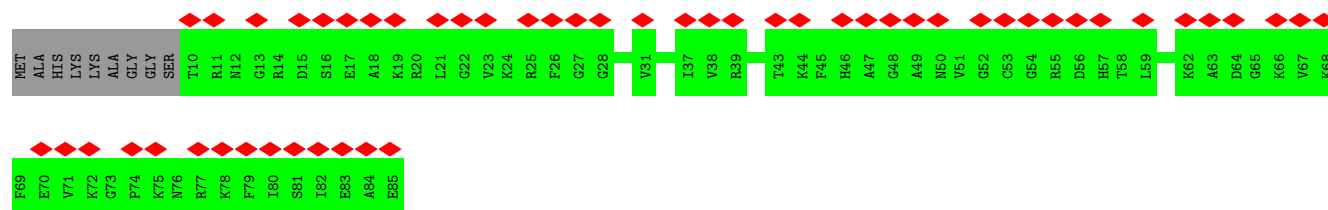
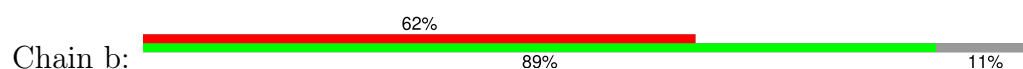




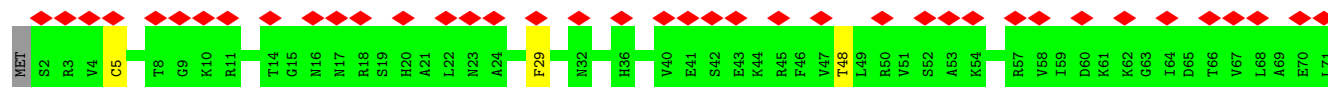


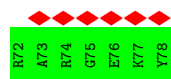


• Molecule 42: 50S ribosomal protein L27

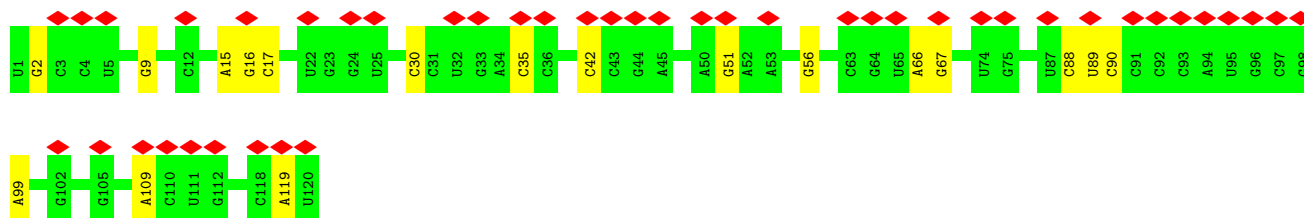
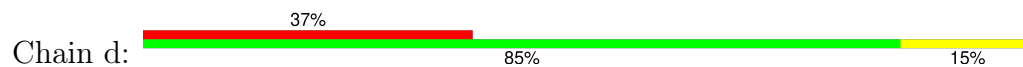


• Molecule 43: 50S ribosomal protein L28

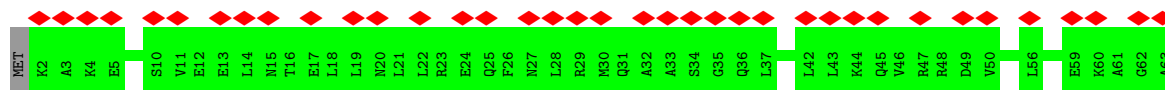




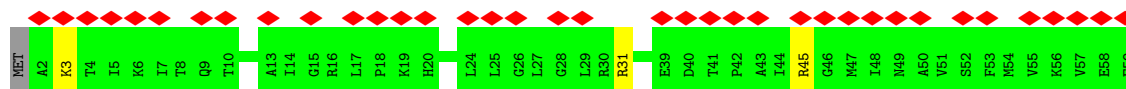
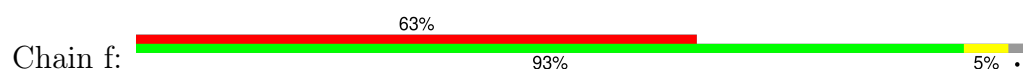
• Molecule 44: 5S rRNA



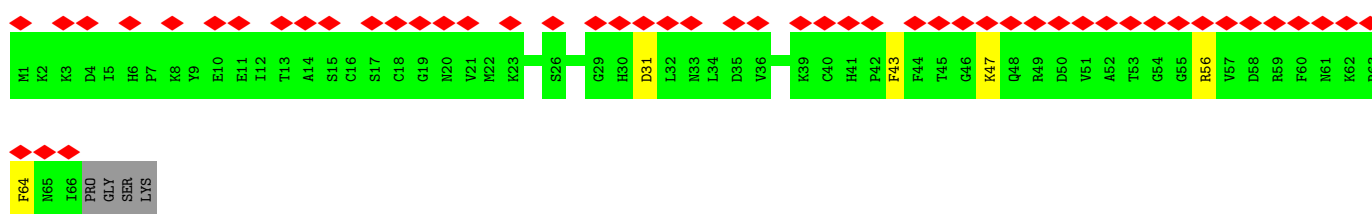
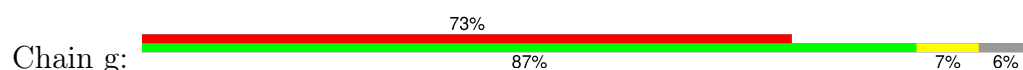
• Molecule 45: 50S ribosomal protein L29



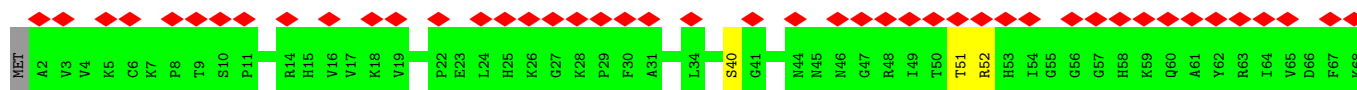
• Molecule 46: 50S ribosomal protein L30

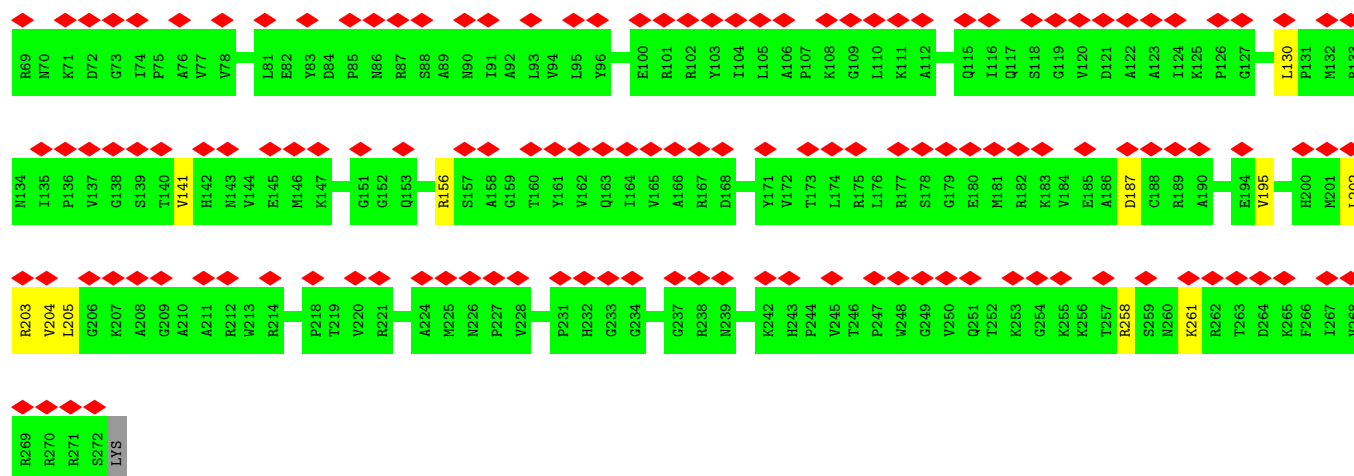


• Molecule 47: 50S ribosomal protein L31

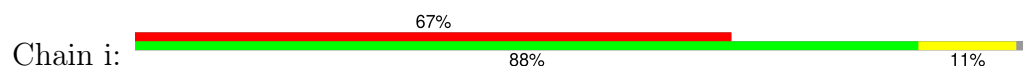


• Molecule 48: 50S ribosomal protein L2

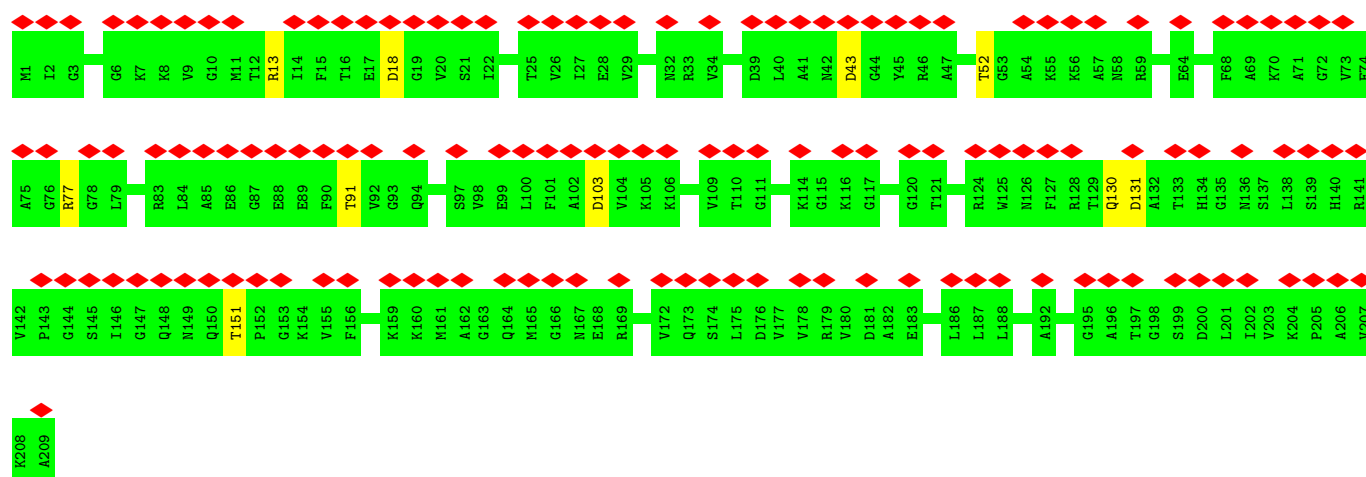




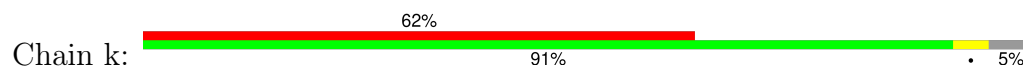
- Molecule 49: 50S ribosomal protein L32



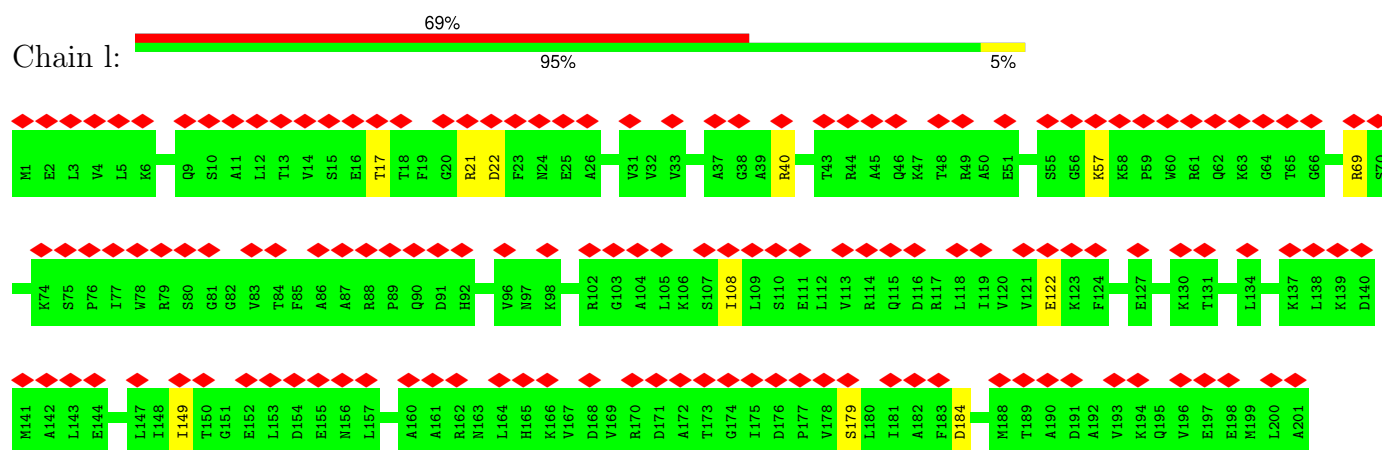
- Molecule 50: 50S ribosomal protein L3



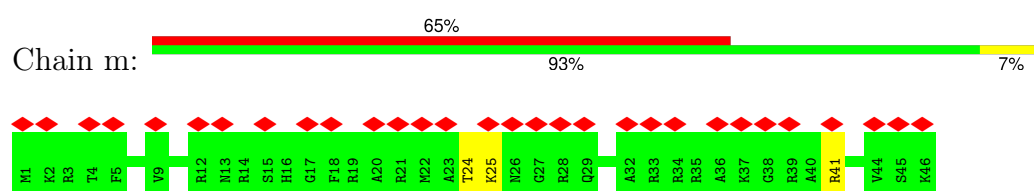
- Molecule 51: 50S ribosomal protein L33



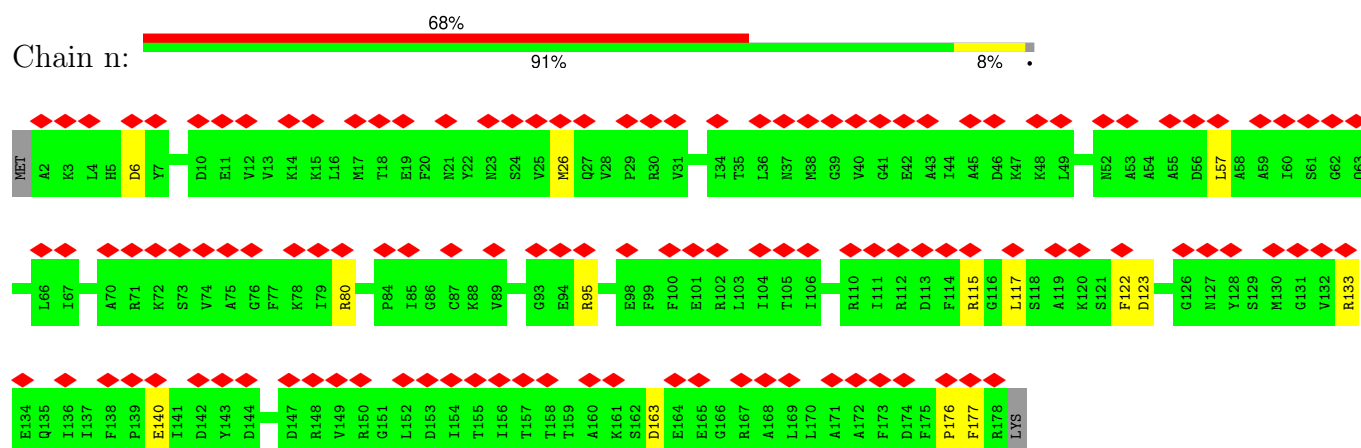
- Molecule 52: 50S ribosomal protein L4



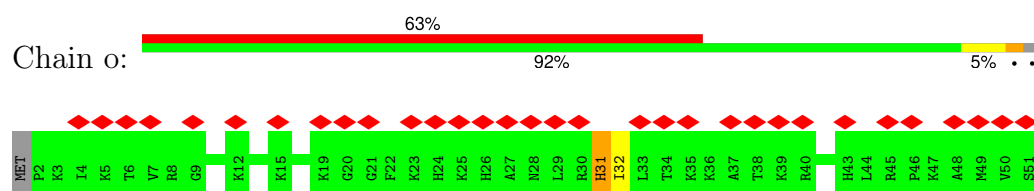
- Molecule 53: 50S ribosomal protein L34



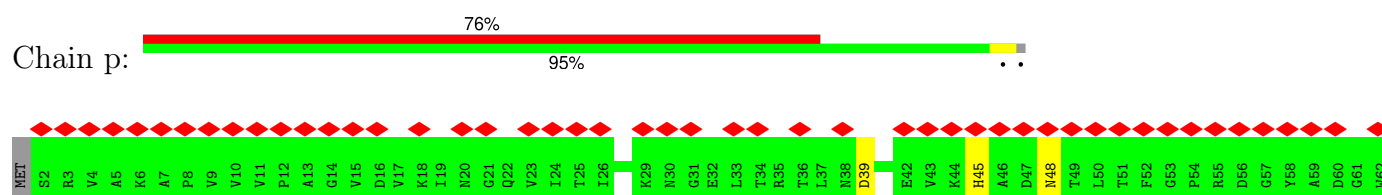
- Molecule 54: 50S ribosomal protein L5

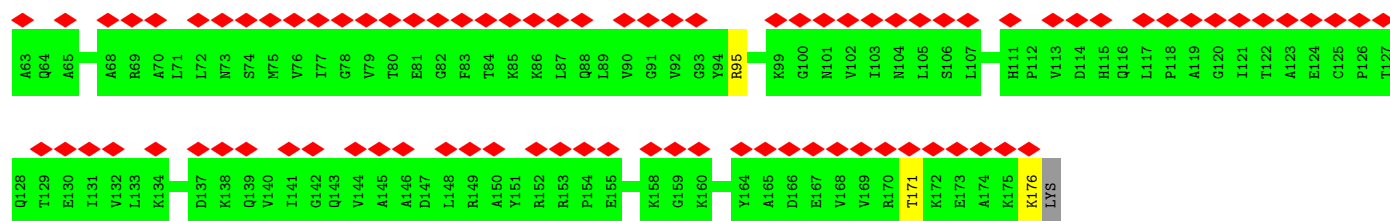


- Molecule 55: 50S ribosomal protein L35

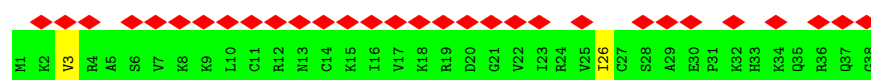
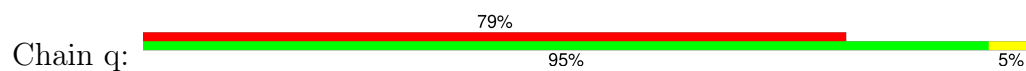


- Molecule 56: 50S ribosomal protein L6

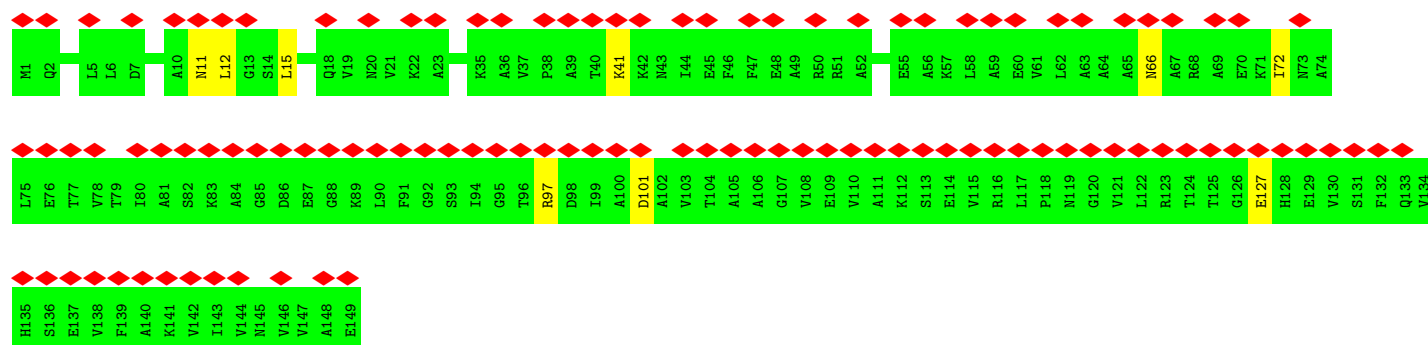
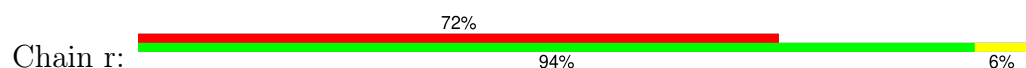




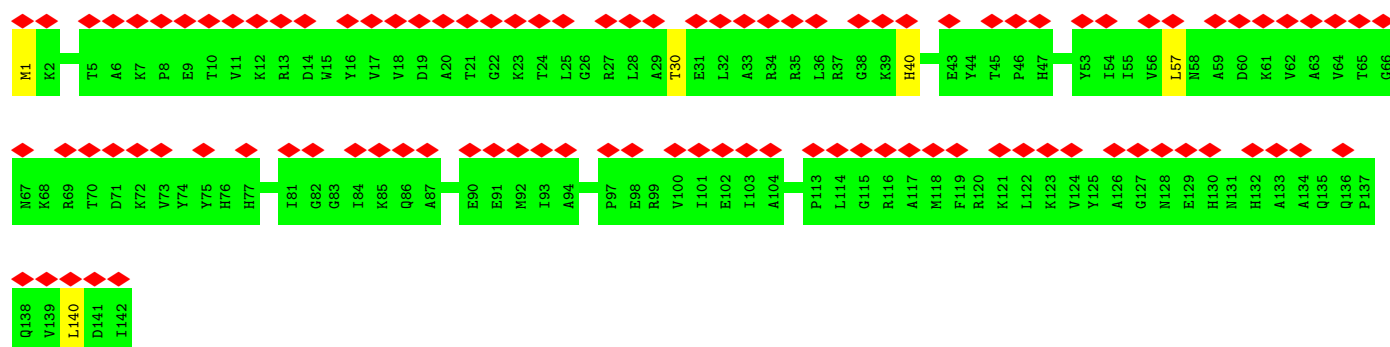
• Molecule 57: 50S ribosomal protein L36



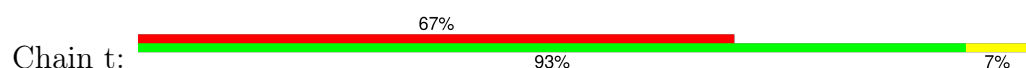
• Molecule 58: 50S ribosomal protein L9

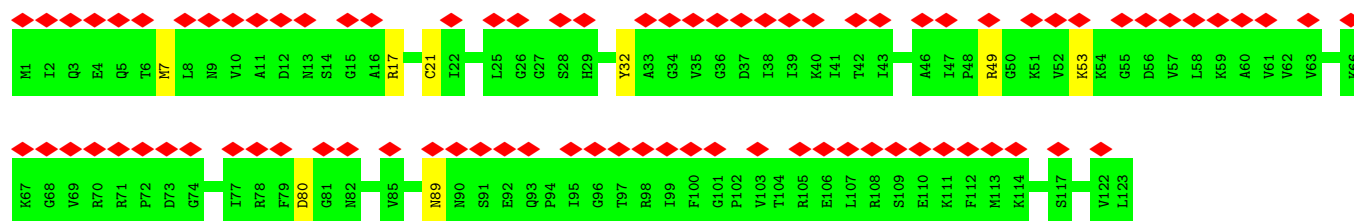


• Molecule 59: 50S ribosomal protein L13

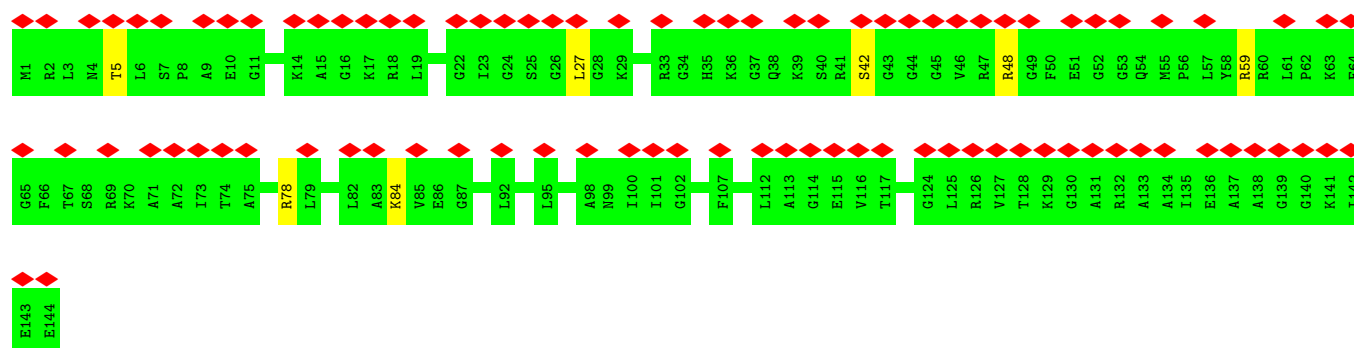


• Molecule 60: 50S ribosomal protein L14

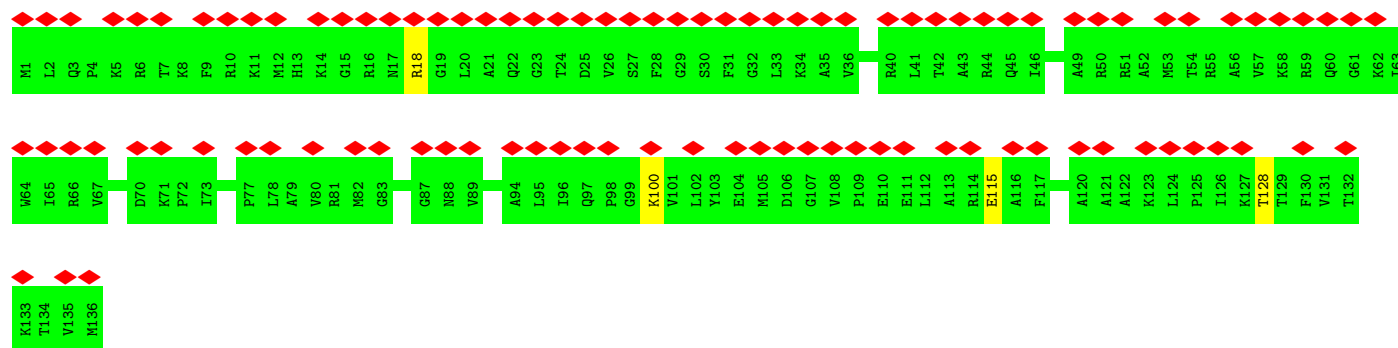




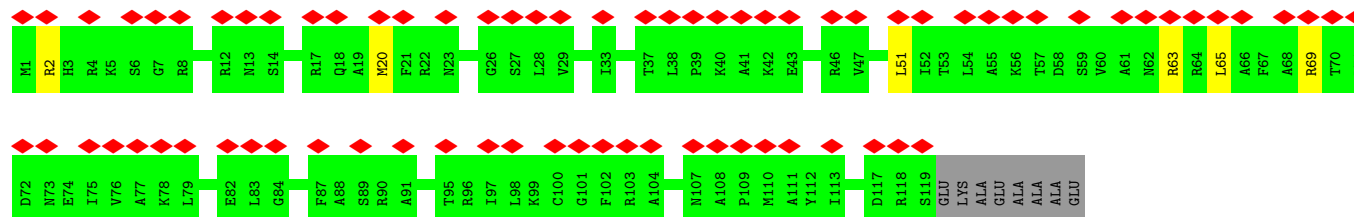
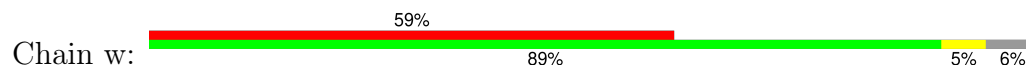
• Molecule 61: 50S ribosomal protein L15



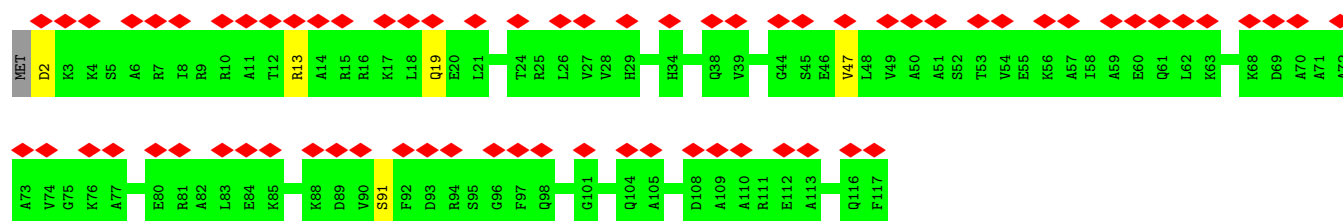
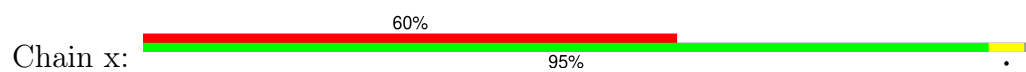
• Molecule 62: 50S ribosomal protein L16



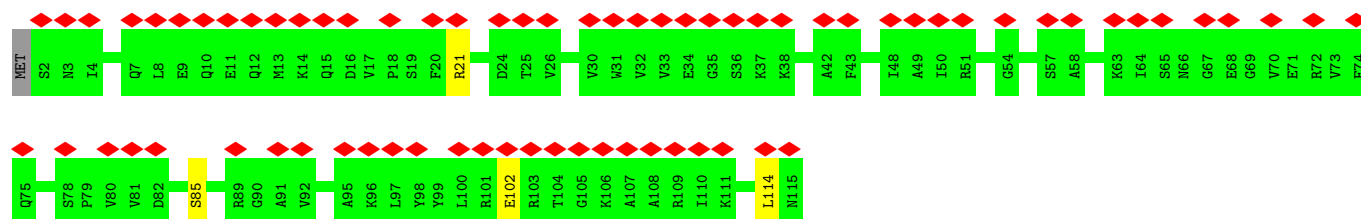
• Molecule 63: 50S ribosomal protein L17



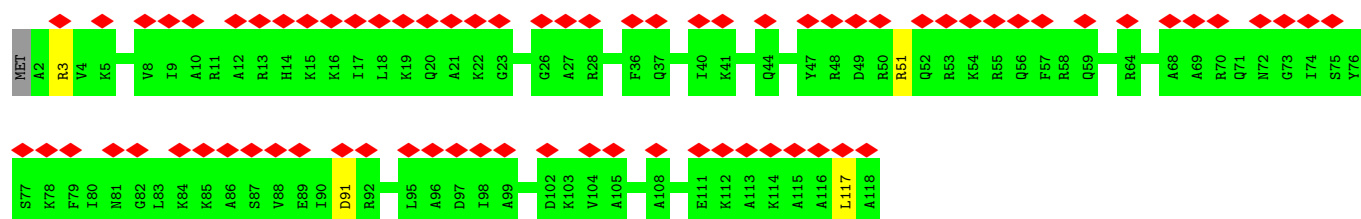
• Molecule 64: 50S ribosomal protein L18



- Molecule 65: 50S ribosomal protein L19



- Molecule 66: 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	38957	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	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	0.065	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.61	0/829	0.54	0/1107
2	1	0.59	0/864	0.55	0/1156
3	2	0.55	0/752	0.52	0/1005
4	3	0.53	0/796	0.53	0/1062
5	4	0.51	0/766	0.49	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.96	0/926
8	7	0.72	1/761 (0.1%)	1.80	23/1178 (2.0%)
9	9	0.35	0/1131	0.60	0/1524
10	A	0.71	2/1810 (0.1%)	1.25	18/2821 (0.6%)
10	B	0.95	1/1810 (0.1%)	1.50	25/2821 (0.9%)
11	AA	0.44	1/10736 (0.0%)	0.61	2/14487 (0.0%)
12	AB	0.68	2/1310 (0.2%)	0.67	2/1766 (0.1%)
13	AC	0.38	0/2113	0.58	0/2877
13	AD	0.34	0/2096	0.59	0/2854
14	AE	0.52	4/10545 (0.0%)	0.66	6/14236 (0.0%)
15	AF	0.33	0/652	0.57	0/879
16	AG	0.64	1/3897 (0.0%)	0.89	30/5273 (0.6%)
17	C	0.61	1/553 (0.2%)	0.62	0/743
18	D	1.35	22/36610 (0.1%)	1.18	99/57091 (0.2%)
19	E	0.46	0/675	0.46	0/895
20	F	0.50	0/597	0.47	0/792
21	G	0.58	1/1791 (0.1%)	0.57	1/2413 (0.0%)
22	H	0.31	0/1746	0.58	0/2382
23	I	0.53	0/1663	0.51	0/2241
24	J	0.53	0/1665	0.49	0/2227
25	K	0.60	0/1165	0.57	0/1568
26	L	0.54	0/867	0.49	0/1171
27	M	0.47	0/1195	0.53	0/1602
28	N	0.57	0/989	0.51	0/1326
29	O	0.51	0/1034	0.53	0/1375
30	P	0.46	0/800	0.54	0/1082

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Q	0.52	0/893	0.50	0/1205
32	R	0.60	0/952	0.55	0/1274
33	S	0.53	0/817	0.50	0/1088
34	T	0.52	0/722	0.51	0/964
35	U	0.54	0/659	0.52	0/884
36	V	0.55	0/657	0.51	0/881
37	W	0.47	0/680	0.51	0/915
38	X	0.45	0/909	0.51	0/1215
39	Y	0.51	2/1046 (0.2%)	0.62	0/1410
40	Z	0.24	0/227	0.40	0/304
41	a	1.45	45/69247 (0.1%)	1.12	140/107985 (0.1%)
42	b	0.59	0/589	0.51	0/779
43	c	0.57	0/635	0.55	0/848
44	d	1.23	0/2872	1.00	0/4478
45	e	0.48	0/502	0.50	0/667
46	f	0.52	0/452	0.51	0/605
47	g	0.39	0/531	0.52	0/709
48	h	0.64	0/2121	0.54	0/2852
49	i	0.57	0/450	0.55	0/599
50	j	0.63	0/1586	0.55	0/2134
51	k	0.60	0/433	0.54	0/576
52	l	0.54	0/1571	0.52	0/2113
53	m	0.63	0/380	0.54	0/498
54	n	0.47	0/1434	0.52	0/1926
55	o	0.58	0/513	0.55	0/676
56	p	0.49	0/1333	0.52	0/1805
57	q	0.58	0/303	0.55	0/397
58	r	0.40	0/1122	0.50	0/1515
59	s	0.64	0/1152	0.51	0/1551
60	t	0.63	0/955	0.52	0/1279
61	u	0.55	0/1062	0.56	0/1413
62	v	0.60	0/1093	0.53	0/1460
63	w	0.60	0/964	0.52	0/1289
64	x	0.49	0/902	0.49	0/1209
65	y	0.63	0/929	0.52	0/1242
66	z	0.68	0/960	0.50	0/1278
All	All	1.12	93/195002 (0.0%)	0.97	347/286738 (0.1%)

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
9	9	0	3
13	AC	0	3
13	AD	0	1
14	AE	0	5
16	AG	0	7
21	G	0	2
22	H	0	5
29	O	0	1
54	n	0	1
55	o	0	1
All	All	0	29

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AB	124	PRO	N-CA	13.13	1.69	1.47
21	G	157	LEU	C-N	10.81	1.54	1.34
14	AE	88	CYS	CB-SG	-10.21	1.64	1.82
41	a	74	A	C6-N1	-9.21	1.29	1.35
16	AG	429	LYS	C-N	8.82	1.51	1.34
41	a	1142	A	C6-N1	-8.75	1.29	1.35
18	D	872	A	C6-N1	-8.70	1.29	1.35
6	5	109	DT	O3'-P	8.67	1.71	1.61
41	a	1021	A	C6-N1	-8.56	1.29	1.35
41	a	2613	U	N3-C4	-8.41	1.30	1.38
11	AA	920	VAL	C-N	8.39	1.50	1.34
18	D	563	A	C6-N1	-8.37	1.29	1.35
18	D	37	U	N3-C4	-8.35	1.30	1.38
18	D	1363	A	C6-N1	-8.23	1.29	1.35
7	6	10	DG	C1'-N9	-8.20	1.35	1.47
18	D	827	U	N3-C4	-7.98	1.31	1.38
18	D	1358	U	N3-C4	-7.93	1.31	1.38
41	a	1019	U	N3-C4	-7.88	1.31	1.38
18	D	397	A	C6-N1	-7.76	1.30	1.35
41	a	1141	U	N3-C4	-7.73	1.31	1.38
6	5	121	DG	C1'-N9	-7.26	1.37	1.47
8	7	19	G	C1'-N9	-7.19	1.36	1.46
18	D	884	U	N3-C4	-6.95	1.32	1.38
41	a	2013	A	C6-N1	-6.90	1.30	1.35
41	a	1791	A	N9-C4	-6.82	1.33	1.37
18	D	37	U	C2-N3	-6.79	1.32	1.37
18	D	335	C	N1-C6	-6.71	1.33	1.37
6	5	112	DG	C1'-N9	-6.69	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	5	GLN	CA-C	6.59	1.70	1.52
6	5	100	DA	C1'-N9	-6.51	1.38	1.47
7	6	21	DA	C1'-N9	-6.46	1.38	1.47
41	a	1791	A	N3-C4	-6.41	1.31	1.34
14	AE	93	THR	CA-C	6.23	1.69	1.52
39	Y	4	VAL	CB-CG2	6.13	1.65	1.52
6	5	116	DG	C1'-N9	-6.13	1.38	1.47
12	AB	123	ARG	C-N	6.03	1.45	1.34
41	a	761	A	N9-C4	-6.03	1.34	1.37
41	a	582	A	N7-C5	-5.97	1.35	1.39
6	5	115	DA	C1'-N9	-5.97	1.38	1.47
10	A	76	A	C5-C4	-5.95	1.34	1.38
41	a	2263	C	N1-C6	-5.91	1.33	1.37
41	a	2013	A	C6-N6	-5.90	1.29	1.33
41	a	2758	A	C6-N1	-5.89	1.31	1.35
18	D	124	C	N1-C6	-5.88	1.33	1.37
14	AE	70	CYS	CA-CB	-5.83	1.41	1.53
41	a	581	C	N1-C6	-5.80	1.33	1.37
7	6	28	DA	C1'-N9	-5.73	1.39	1.47
41	a	2591	C	N1-C6	-5.64	1.33	1.37
41	a	1082	U	N3-C4	-5.63	1.33	1.38
18	D	915	A	C6-N1	-5.58	1.31	1.35
18	D	1358	U	C2-N3	-5.55	1.33	1.37
41	a	190	A	N9-C4	-5.51	1.34	1.37
41	a	1247	A	N9-C4	-5.51	1.34	1.37
10	A	76	A	C6-N6	-5.46	1.29	1.33
41	a	1086	A	C6-N1	-5.45	1.31	1.35
18	D	20	U	C2-N3	-5.43	1.33	1.37
18	D	60	A	N7-C5	-5.41	1.36	1.39
41	a	1912	A	N9-C4	-5.38	1.34	1.37
41	a	2542	A	N9-C4	-5.36	1.34	1.37
41	a	1141	U	C2-N3	-5.34	1.34	1.37
41	a	1783	A	N9-C4	-5.33	1.34	1.37
41	a	454	A	N9-C4	-5.32	1.34	1.37
41	a	836	G	N3-C4	-5.31	1.31	1.35
7	6	24	DT	C1'-N1	5.31	1.56	1.49
18	D	674	G	N9-C8	-5.31	1.34	1.37
41	a	1678	A	N9-C4	-5.30	1.34	1.37
41	a	505	A	N9-C4	-5.29	1.34	1.37
18	D	397	A	C6-N6	-5.27	1.29	1.33
41	a	764	A	N9-C4	-5.26	1.34	1.37
41	a	565	C	N1-C6	-5.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	752	A	N9-C4	-5.23	1.34	1.37
41	a	1928	A	N3-C4	-5.23	1.31	1.34
41	a	1795	C	N1-C6	-5.21	1.34	1.37
41	a	1928	A	N7-C5	-5.20	1.36	1.39
18	D	767	A	N9-C4	-5.17	1.34	1.37
41	a	2342	C	N1-C6	-5.17	1.34	1.37
41	a	1165	A	N9-C4	-5.15	1.34	1.37
41	a	2260	C	N1-C6	-5.14	1.34	1.37
41	a	1791	A	N9-C8	-5.12	1.33	1.37
41	a	2613	U	C2-N3	-5.12	1.34	1.37
17	C	40	VAL	CB-CG1	-5.11	1.42	1.52
41	a	749	A	N9-C4	-5.10	1.34	1.37
18	D	884	U	C2-N3	-5.08	1.34	1.37
18	D	334	C	N1-C6	-5.08	1.34	1.37
10	B	38	A	N9-C4	-5.08	1.34	1.37
18	D	816	A	N9-C4	-5.05	1.34	1.37
41	a	583	G	N7-C5	-5.05	1.36	1.39
41	a	679	C	N1-C6	-5.05	1.34	1.37
41	a	44	A	N9-C4	-5.04	1.34	1.37
14	AE	801	VAL	CB-CG2	-5.04	1.42	1.52
41	a	1214	A	N9-C4	-5.04	1.34	1.37
18	D	872	A	C6-N6	-5.02	1.29	1.33
41	a	592	A	N9-C4	-5.02	1.34	1.37

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	37	U	C5-C4-O4	35.68	147.31	125.90
18	D	884	U	C5-C4-O4	35.09	146.95	125.90
41	a	1019	U	C5-C4-O4	34.63	146.68	125.90
18	D	827	U	C5-C4-O4	34.07	146.34	125.90
41	a	1141	U	C5-C4-O4	33.77	146.16	125.90
41	a	2613	U	C5-C4-O4	33.62	146.07	125.90
18	D	37	U	N3-C4-O4	-33.11	96.22	119.40
18	D	884	U	N3-C4-O4	-32.96	96.33	119.40
18	D	1358	U	C5-C4-O4	32.80	145.58	125.90
41	a	1141	U	N3-C4-O4	-31.78	97.15	119.40
18	D	1358	U	N3-C4-O4	-31.56	97.31	119.40
41	a	1019	U	N3-C4-O4	-31.28	97.50	119.40
41	a	2613	U	N3-C4-O4	-30.71	97.91	119.40
41	a	1082	U	C5-C4-O4	30.45	144.17	125.90
18	D	827	U	N3-C4-O4	-30.16	98.28	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	1082	U	N3-C4-O4	-28.41	99.51	119.40
8	7	1	U	O5'-P-OP2	-23.74	82.21	110.70
18	D	397	A	N1-C6-N6	-21.15	105.91	118.60
8	7	1	U	O5'-P-OP1	-19.80	86.94	110.70
18	D	1363	A	N1-C6-N6	-17.64	108.02	118.60
41	a	1021	A	N1-C6-N6	-17.23	108.27	118.60
41	a	74	A	N1-C6-N6	-16.50	108.70	118.60
41	a	1142	A	N1-C6-N6	-16.47	108.72	118.60
41	a	1086	A	N1-C6-N6	-15.76	109.14	118.60
8	7	0	U	OP2-P-O3'	-14.86	72.50	105.20
18	D	872	A	N1-C6-N6	-14.73	109.76	118.60
41	a	2013	A	N1-C6-N6	-13.99	110.20	118.60
8	7	0	U	OP1-P-O3'	-13.94	74.54	105.20
8	7	1	U	OP1-P-OP2	13.77	140.26	119.60
41	a	74	A	C5-C6-N6	13.27	134.31	123.70
16	AG	104	ARG	C-N-CA	13.00	154.21	121.70
18	D	397	A	C5-C6-N6	12.74	133.89	123.70
18	D	1358	U	N1-C2-N3	-12.66	107.30	114.90
41	a	1021	A	C5-C6-N6	12.36	133.59	123.70
41	a	1142	A	C5-C6-N6	12.27	133.51	123.70
41	a	1019	U	C2-N3-C4	12.13	134.28	127.00
41	a	1141	U	C2-N3-C4	11.95	134.17	127.00
18	D	1358	U	C2-N3-C4	11.68	134.00	127.00
41	a	1141	U	N1-C2-N3	-11.61	107.94	114.90
18	D	563	A	N1-C6-N6	-11.56	111.66	118.60
18	D	1363	A	C5-C6-N6	11.52	132.91	123.70
18	D	827	U	C2-N3-C4	11.40	133.84	127.00
41	a	67	U	N3-C4-O4	-11.12	111.61	119.40
41	a	2613	U	C2-N3-C4	11.11	133.67	127.00
41	a	2756	U	N3-C4-O4	-10.96	111.73	119.40
41	a	1141	U	C4-C5-C6	-10.77	113.24	119.70
12	AB	124	PRO	CA-N-CD	-10.70	96.53	111.50
18	D	1358	U	C4-C5-C6	-10.55	113.37	119.70
18	D	611	C	C6-N1-C2	-10.26	116.20	120.30
8	7	-17	U	N1-C2-N3	-10.12	108.83	114.90
18	D	872	A	C5-C6-N6	9.83	131.57	123.70
41	a	1019	U	N1-C2-N3	-9.77	109.04	114.90
41	a	1086	A	C5-C6-N6	9.67	131.43	123.70
16	AG	354	ALA	O-C-N	-9.62	107.30	122.70
16	AG	292	ASP	O-C-N	-9.57	107.39	122.70
41	a	974	G	O4'-C1'-N9	9.49	115.79	108.20
14	AE	271	ARG	NE-CZ-NH2	-9.27	115.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	-18	G	N9-C4-C5	-9.17	101.73	105.40
41	a	968	C	N3-C2-O2	-9.14	115.50	121.90
18	D	884	U	C4-C5-C6	-9.13	114.22	119.70
41	a	1019	U	C4-C5-C6	-9.06	114.26	119.70
8	7	-17	U	C4-C5-C6	-9.05	114.27	119.70
21	G	90	PHE	CB-CA-C	9.05	128.50	110.40
8	7	-17	U	C6-N1-C1'	-9.02	108.57	121.20
18	D	178	C	N3-C2-O2	-9.00	115.60	121.90
18	D	37	U	C2-N3-C4	8.99	132.40	127.00
18	D	915	A	N9-C4-C5	-8.96	102.21	105.80
18	D	563	A	N1-C2-N3	-8.81	124.89	129.30
8	7	-18	G	C8-N9-C4	8.81	109.92	106.40
16	AG	355	ALA	CB-CA-C	8.70	123.16	110.10
41	a	2613	U	C4-C5-C6	-8.68	114.49	119.70
18	D	1344	C	N3-C2-O2	-8.66	115.84	121.90
8	7	-18	G	N3-C4-N9	8.61	131.17	126.00
10	B	30	G	C8-N9-C4	8.49	109.80	106.40
10	B	23	C	C6-N1-C2	8.43	123.67	120.30
10	B	30	G	N9-C4-C5	-8.35	102.06	105.40
41	a	1021	A	N1-C2-N3	-8.34	125.13	129.30
41	a	2613	U	N1-C2-N3	-8.30	109.92	114.90
8	7	-18	G	C8-N9-C1'	-8.27	116.25	127.00
18	D	334	C	C6-N1-C2	-8.24	117.00	120.30
41	a	2758	A	N1-C6-N6	-8.23	113.66	118.60
41	a	2758	A	C5-C6-N6	8.22	130.28	123.70
41	a	2901	C	N3-C2-O2	-8.21	116.15	121.90
18	D	884	U	C2-N3-C4	8.12	131.88	127.00
8	7	-17	U	C2-N1-C1'	8.02	127.33	117.70
18	D	37	U	C4-C5-C6	-7.97	114.92	119.70
10	B	36	U	C4-C5-C6	7.97	124.48	119.70
41	a	67	U	C5-C4-O4	7.94	130.66	125.90
41	a	1582	C	N1-C2-O2	7.81	123.58	118.90
18	D	1466	C	N3-C2-O2	-7.75	116.47	121.90
18	D	808	C	N3-C2-O2	-7.68	116.52	121.90
41	a	2179	C	C6-N1-C2	-7.61	117.26	120.30
18	D	178	C	N1-C2-O2	7.60	123.46	118.90
18	D	872	A	N1-C2-N3	-7.59	125.51	129.30
41	a	1142	A	N1-C2-N3	-7.57	125.52	129.30
10	A	61	C	N1-C2-O2	7.54	123.43	118.90
18	D	1314	C	N3-C2-O2	-7.51	116.64	121.90
18	D	827	U	C4-C5-C6	-7.42	115.25	119.70
41	a	1581	G	C6-C5-N7	-7.21	126.07	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	1142	A	C6-N1-C2	7.18	122.91	118.60
18	D	397	A	N1-C2-N3	-7.15	125.72	129.30
41	a	2161	C	N3-C2-O2	-7.13	116.91	121.90
16	AG	108	GLN	N-CA-CB	7.12	123.42	110.60
41	a	1060	U	C5-C4-O4	-7.11	121.63	125.90
41	a	1082	U	C2-N3-C4	7.08	131.25	127.00
10	B	71	C	C2-N1-C1'	7.06	126.56	118.80
18	D	563	A	C5-C6-N6	7.04	129.33	123.70
41	a	968	C	N1-C2-O2	7.04	123.12	118.90
41	a	2179	C	C2-N1-C1'	7.02	126.52	118.80
41	a	742	A	C6-N1-C2	-6.96	114.42	118.60
41	a	2013	A	C5-C6-N6	6.94	129.25	123.70
41	a	2073	C	N1-C2-O2	-6.92	114.75	118.90
18	D	1006	G	C8-N9-C4	-6.91	103.64	106.40
41	a	1582	C	N3-C2-O2	-6.89	117.08	121.90
18	D	20	U	C2-N1-C1'	-6.83	109.50	117.70
41	a	1907	G	N3-C2-N2	-6.82	115.12	119.90
41	a	1928	A	C8-N9-C4	-6.82	103.07	105.80
18	D	827	U	N1-C2-N3	-6.80	110.82	114.90
41	a	2756	U	C5-C4-O4	6.79	129.98	125.90
16	AG	355	ALA	N-CA-CB	6.78	119.59	110.10
10	B	22	G	C2-N3-C4	-6.77	108.52	111.90
41	a	1021	A	C6-N1-C2	6.72	122.63	118.60
18	D	915	A	C4-C5-N7	6.70	114.05	110.70
8	7	-17	U	C5-C6-N1	6.67	126.03	122.70
18	D	884	U	N1-C2-N3	-6.65	110.91	114.90
41	a	1141	U	N3-C2-O2	6.61	126.83	122.20
16	AG	108	GLN	CB-CA-C	-6.61	97.19	110.40
10	A	76	A	C5-C6-N1	6.59	121.00	117.70
10	B	42	G	N3-C4-N9	-6.58	122.05	126.00
16	AG	354	ALA	CA-C-N	6.58	131.68	117.20
10	A	2	G	N9-C4-C5	-6.57	102.77	105.40
18	D	1499	A	N1-C6-N6	6.54	122.53	118.60
18	D	1358	U	N3-C2-O2	6.54	126.78	122.20
41	a	1060	U	N3-C4-O4	6.53	123.97	119.40
18	D	1363	A	N1-C2-N3	-6.51	126.05	129.30
10	B	76	A	C8-N9-C4	-6.49	103.20	105.80
18	D	37	U	N1-C2-N3	-6.47	111.02	114.90
41	a	2853	C	N3-C2-O2	-6.45	117.39	121.90
41	a	221	A	O4'-C1'-N9	6.41	113.33	108.20
10	B	11	A	N1-C6-N6	6.38	122.43	118.60
6	5	109	DT	P-O3'-C3'	6.37	127.35	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	611	C	N3-C4-C5	-6.35	119.36	121.90
41	a	742	A	C5-C6-N6	-6.35	118.62	123.70
10	B	2	G	N9-C4-C5	-6.34	102.86	105.40
41	a	2013	A	N1-C2-N3	-6.29	126.15	129.30
18	D	563	A	N9-C4-C5	-6.28	103.29	105.80
41	a	1906	G	N3-C4-N9	6.28	129.77	126.00
41	a	62	U	N3-C2-O2	-6.23	117.84	122.20
41	a	1775	U	C5-C4-O4	-6.20	122.18	125.90
10	A	61	C	N3-C2-O2	-6.20	117.56	121.90
10	B	36	U	N1-C2-N3	6.19	118.61	114.90
18	D	1314	C	N1-C2-O2	6.19	122.61	118.90
16	AG	105	ILE	C-N-CA	6.09	136.93	121.70
18	D	20	U	C2-N3-C4	-6.09	123.35	127.00
41	a	836	G	N9-C4-C5	6.08	107.83	105.40
41	a	1082	U	N1-C2-N3	-6.08	111.25	114.90
41	a	1363	C	N1-C2-O2	-6.06	115.27	118.90
41	a	836	G	C8-N9-C4	-6.05	103.98	106.40
18	D	674	G	C4-N9-C1'	6.03	134.34	126.50
41	a	742	A	C5-C6-N1	6.01	120.70	117.70
41	a	1	G	C6-C5-N7	-6.00	126.80	130.40
10	A	2	G	C4-C5-N7	5.99	113.20	110.80
41	a	1907	G	C8-N9-C4	-5.99	104.00	106.40
18	D	269	C	N3-C2-O2	-5.98	117.71	121.90
18	D	864	A	C6-N1-C2	-5.96	115.03	118.60
16	AG	33	THR	CA-CB-CG2	5.95	120.73	112.40
18	D	915	A	C6-C5-N7	-5.94	128.14	132.30
16	AG	106	THR	OG1-CB-CG2	-5.93	96.36	110.00
41	a	45	G	C4-N9-C1'	-5.91	118.81	126.50
10	B	71	C	C6-N1-C1'	-5.90	113.72	120.80
41	a	2252	G	N1-C2-N2	-5.90	110.89	116.20
16	AG	426	GLY	O-C-N	-5.89	113.28	122.70
41	a	1921	G	C2-N3-C4	-5.89	108.96	111.90
18	D	1006	G	N7-C8-N9	5.88	116.04	113.10
41	a	1086	A	N1-C2-N3	-5.88	126.36	129.30
18	D	1340	A	C5'-C4'-O4'	5.86	116.13	109.10
12	AB	122	PRO	N-CA-CB	5.83	110.29	103.30
41	a	1	G	N3-C4-N9	5.83	129.50	126.00
18	D	745	G	C6-C5-N7	-5.82	126.91	130.40
18	D	808	C	N1-C2-O2	5.81	122.39	118.90
8	7	-11	U	O4'-C1'-N1	-5.81	103.55	108.20
41	a	1581	G	N3-C4-N9	5.80	129.48	126.00
18	D	563	A	C4-C5-N7	5.80	113.60	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	30	G	C8-N9-C1'	-5.79	119.47	127.00
10	A	22	G	N1-C2-N2	-5.79	110.99	116.20
18	D	746	A	N9-C4-C5	-5.78	103.49	105.80
14	AE	903	LEU	C-N-CA	5.77	136.12	121.70
18	D	1344	C	N1-C2-O2	5.77	122.36	118.90
41	a	2420	C	N3-C2-O2	-5.76	117.87	121.90
18	D	611	C	C5-C4-N4	5.76	124.23	120.20
41	a	2161	C	N1-C2-O2	5.76	122.35	118.90
8	7	-17	U	N1-C2-O2	5.75	126.83	122.80
18	D	20	U	N3-C4-C5	5.74	118.04	114.60
41	a	357	C	N3-C2-O2	-5.74	117.88	121.90
18	D	745	G	C4-C5-N7	5.74	113.09	110.80
18	D	1523	G	C8-N9-C4	-5.72	104.11	106.40
41	a	1581	G	C4-N9-C1'	5.72	133.93	126.50
10	B	22	G	N1-C2-N2	-5.70	111.07	116.20
18	D	179	A	N1-C6-N6	5.68	122.01	118.60
41	a	2013	A	C5-C6-N1	5.67	120.53	117.70
18	D	69	G	C4-N9-C1'	5.66	133.86	126.50
10	B	22	G	N7-C8-N9	5.64	115.92	113.10
16	AG	102	PHE	C-N-CA	5.64	135.80	121.70
41	a	1945	G	C6-C5-N7	-5.63	127.02	130.40
18	D	1303	C	N1-C2-O2	-5.63	115.52	118.90
16	AG	33	THR	C-N-CA	5.63	135.78	121.70
18	D	60	A	C4-C5-C6	5.63	119.81	117.00
41	a	551	G	C6-C5-N7	-5.63	127.02	130.40
18	D	384	G	N3-C2-N2	5.62	123.83	119.90
41	a	2263	C	C6-N1-C2	-5.61	118.06	120.30
16	AG	35	THR	CA-CB-OG1	-5.60	97.24	109.00
18	D	864	A	N3-C4-N9	5.60	131.88	127.40
14	AE	363	LEU	CA-CB-CG	5.59	128.15	115.30
10	B	24	U	N3-C2-O2	-5.56	118.31	122.20
41	a	190	A	N1-C6-N6	5.55	121.93	118.60
41	a	742	A	N3-C4-N9	5.55	131.84	127.40
41	a	2853	C	N1-C2-O2	5.55	122.23	118.90
41	a	927	A	N3-C4-N9	5.54	131.84	127.40
11	AA	920	VAL	C-N-CD	-5.54	108.42	120.60
8	7	-17	U	N1-C1'-C2'	5.54	121.20	114.00
18	D	1499	A	C5-C6-N6	-5.54	119.27	123.70
10	A	13	C	N3-C2-O2	-5.53	118.03	121.90
41	a	1200	C	N1-C2-O2	-5.53	115.58	118.90
41	a	1047	G	C8-N9-C4	5.52	108.61	106.40
41	a	1	G	N9-C4-C5	-5.49	103.21	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	191	G	C4-C5-N7	5.48	112.99	110.80
41	a	2902	C	N3-C2-O2	-5.47	118.07	121.90
18	D	872	A	C6-N1-C2	5.46	121.88	118.60
41	a	30	G	C4-N9-C1'	5.46	133.60	126.50
10	B	36	U	O4'-C1'-N1	5.45	112.56	108.20
10	B	61	C	N1-C2-O2	5.45	122.17	118.90
41	a	2686	G	C4-N9-C1'	5.44	133.57	126.50
10	A	22	G	C2-N3-C4	-5.44	109.18	111.90
16	AG	104	ARG	O-C-N	5.42	131.37	122.70
41	a	1906	G	C6-C5-N7	-5.42	127.15	130.40
8	7	-18	G	C4-N9-C1'	5.41	133.54	126.50
10	B	54	U	C2-N3-C4	5.41	130.25	127.00
10	B	11	A	C4-C5-N7	5.41	113.40	110.70
41	a	581	C	C2-N1-C1'	5.41	124.75	118.80
41	a	1	G	C4-C5-N7	5.40	112.96	110.80
10	A	71	C	C6-N1-C1'	-5.40	114.32	120.80
41	a	27	G	O4'-C1'-N9	5.40	112.52	108.20
16	AG	104	ARG	CA-C-N	-5.39	105.34	117.20
10	A	15	G	O4'-C1'-N9	-5.38	103.89	108.20
41	a	1907	G	N9-C4-C5	5.37	107.55	105.40
18	D	563	A	C6-N1-C2	5.37	121.82	118.60
18	D	750	C	N3-C2-O2	-5.36	118.15	121.90
41	a	62	U	N1-C2-O2	5.36	126.55	122.80
41	a	1335	C	N3-C2-O2	-5.36	118.15	121.90
41	a	271	G	P-O3'-C3'	5.35	126.12	119.70
41	a	2252	G	N3-C2-N2	5.34	123.64	119.90
18	D	384	G	N1-C2-N2	-5.34	111.39	116.20
10	A	2	G	N1-C6-O6	5.33	123.10	119.90
41	a	1647	U	C2-N3-C4	-5.33	123.80	127.00
41	a	1019	U	N3-C2-O2	5.33	125.93	122.20
16	AG	458	ASP	CB-CG-OD2	5.33	123.10	118.30
18	D	1412	C	C2-N1-C1'	5.33	124.66	118.80
41	a	271	G	N3-C4-N9	5.33	129.20	126.00
8	7	-16	U	O4'-C1'-N1	-5.32	103.95	108.20
10	B	30	G	N3-C2-N2	5.31	123.62	119.90
18	D	379	C	N3-C2-O2	-5.31	118.19	121.90
8	7	-18	G	C6-C5-N7	-5.29	127.23	130.40
18	D	643	C	N1-C2-O2	-5.28	115.73	118.90
18	D	69	G	C8-N9-C1'	-5.28	120.13	127.00
41	a	1328	A	C5-C6-N6	-5.27	119.48	123.70
18	D	611	C	N1-C2-N3	5.27	122.89	119.20
16	AG	469	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AG	102	PHE	N-CA-C	5.26	125.21	111.00
16	AG	465	ASP	CB-CG-OD2	5.26	123.03	118.30
41	a	353	C	C2-N1-C1'	5.26	124.58	118.80
18	D	191	G	N9-C4-C5	-5.25	103.30	105.40
18	D	457	G	C6-C5-N7	-5.25	127.25	130.40
18	D	1382	C	C5-C4-N4	5.24	123.87	120.20
16	AG	443	ASP	CB-CG-OD2	5.24	123.02	118.30
16	AG	475	ASP	CB-CG-OD2	5.24	123.02	118.30
18	D	335	C	C4-C5-C6	5.23	120.02	117.40
41	a	1931	U	N3-C2-O2	-5.23	118.54	122.20
16	AG	432	ASP	CB-CG-OD2	5.23	123.00	118.30
16	AG	368	ASP	CB-CG-OD2	5.22	123.00	118.30
41	a	582	A	N7-C8-N9	5.22	116.41	113.80
41	a	1452	G	N3-C4-C5	5.22	131.21	128.60
16	AG	433	ASP	CB-CG-OD2	5.22	123.00	118.30
11	AA	516	ASP	CB-CG-OD2	5.22	123.00	118.30
16	AG	466	ASP	CB-CG-OD2	5.22	123.00	118.30
10	B	11	A	C5-N7-C8	-5.22	101.29	103.90
41	a	927	A	C6-C5-N7	-5.21	128.65	132.30
16	AG	366	ASP	CB-CG-OD2	5.21	122.99	118.30
41	a	2286	G	C4-C5-N7	5.21	112.88	110.80
10	A	75	C	C2-N1-C1'	-5.19	113.09	118.80
18	D	1022	A	N1-C2-N3	5.19	131.90	129.30
41	a	993	G	N3-C4-N9	-5.19	122.89	126.00
41	a	754	U	C2-N1-C1'	5.19	123.93	117.70
18	D	745	G	N9-C4-C5	-5.18	103.33	105.40
41	a	45	G	C8-N9-C1'	5.18	133.74	127.00
18	D	1208	C	C6-N1-C2	5.18	122.37	120.30
41	a	1172	C	N1-C2-O2	-5.18	115.80	118.90
41	a	45	G	N3-C4-C5	5.17	131.19	128.60
10	B	10	G	N3-C4-N9	-5.17	122.90	126.00
41	a	1109	C	C6-N1-C2	5.17	122.37	120.30
41	a	1924	C	N3-C4-N4	5.16	121.61	118.00
41	a	1379	U	C5-C4-O4	5.16	129.00	125.90
16	AG	493	ASP	CB-CG-OD2	5.15	122.94	118.30
18	D	477	C	C2-N1-C1'	5.15	124.47	118.80
18	D	384	G	C6-C5-N7	-5.15	127.31	130.40
16	AG	441	ASP	CB-CG-OD2	5.15	122.93	118.30
10	A	71	C	C2-N1-C1'	5.14	124.45	118.80
41	a	1906	G	N3-C4-C5	-5.13	126.03	128.60
8	7	-17	U	N3-C4-C5	5.12	117.67	114.60
10	A	51	C	N1-C2-O2	-5.12	115.83	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	62	U	C2-N1-C1'	5.10	123.82	117.70
41	a	271	G	C6-C5-N7	-5.10	127.34	130.40
10	A	22	G	N3-C2-N2	5.09	123.46	119.90
18	D	179	A	C5-C6-N6	-5.09	119.63	123.70
41	a	2063	C	C5-C4-N4	5.09	123.76	120.20
18	D	439	U	N1-C2-N3	5.09	117.95	114.90
41	a	2297	A	C6-N1-C2	-5.09	115.55	118.60
41	a	1945	G	C4-N9-C1'	5.08	133.11	126.50
10	B	42	G	C8-N9-C1'	5.08	133.60	127.00
41	a	1986	C	N3-C2-O2	-5.08	118.35	121.90
8	7	-19	U	N1-C2-O2	-5.08	119.25	122.80
41	a	1082	U	C4-C5-C6	-5.07	116.66	119.70
18	D	439	U	C6-N1-C2	-5.07	117.96	121.00
41	a	2488	G	C6-C5-N7	-5.07	127.36	130.40
10	A	72	A	N7-C8-N9	5.06	116.33	113.80
14	AE	807	LEU	CB-CG-CD2	-5.06	102.40	111.00
18	D	334	C	N3-C2-O2	-5.06	118.36	121.90
41	a	836	G	N1-C2-N3	5.05	126.93	123.90
41	a	1596	A	N1-C6-N6	5.05	121.63	118.60
10	B	23	C	N3-C4-C5	5.04	123.92	121.90
10	A	76	A	C5-C6-N6	-5.04	119.67	123.70
41	a	1198	U	N3-C2-O2	-5.04	118.67	122.20
41	a	2505	G	N1-C2-N2	-5.04	111.66	116.20
18	D	864	A	C4-N9-C1'	5.03	135.36	126.30
41	a	2668	G	N3-C4-N9	-5.03	122.98	126.00
14	AE	73	GLY	N-CA-C	5.03	125.67	113.10
41	a	2313	C	N3-C2-O2	-5.02	118.38	121.90
41	a	2901	C	N1-C2-O2	5.02	121.91	118.90
41	a	2013	A	C4-C5-C6	-5.02	114.49	117.00
18	D	864	A	C8-N9-C1'	-5.02	118.67	127.70
10	A	2	G	C5-C6-O6	-5.02	125.59	128.60
18	D	674	G	C8-N9-C1'	-5.02	120.48	127.00
41	a	2275	C	N1-C2-O2	5.01	121.91	118.90
41	a	190	A	C5-C6-N6	-5.01	119.69	123.70
8	7	-16	U	C5-C6-N1	-5.01	120.20	122.70
14	AE	90	VAL	CA-C-N	5.01	128.22	117.20
18	D	37	U	C2-N1-C1'	-5.00	111.69	117.70
41	a	840	C	N1-C2-O2	-5.00	115.90	118.90

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	117	LEU	Peptide
9	9	49	GLY	Peptide
13	AC	192	VAL	Peptide
13	AC	319	GLU	Peptide
13	AC	321	TRP	Peptide
13	AD	20	SER	Peptide
14	AE	1184	ASP	Peptide
14	AE	1326	GLN	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
14	AE	804	ALA	Peptide
16	AG	102	PHE	Peptide
16	AG	104	ARG	Peptide,Mainchain
16	AG	11	ALA	Peptide
16	AG	214	PRO	Mainchain
16	AG	292	ASP	Mainchain
16	AG	426	GLY	Mainchain
21	G	126	PHE	Peptide
21	G	127	ASP	Peptide
22	H	274	TYR	Peptide
22	H	303	LEU	Peptide
22	H	304	VAL	Peptide
22	H	81	GLU	Peptide
22	H	82	THR	Peptide
29	O	12	ARG	Peptide
54	n	176	PRO	Peptide
55	o	31	HIS	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 [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%)	92 (91%)	9 (9%)	0	100	100
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	89 (97%)	3 (3%)	0	100	100
4	3	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
9	9	146/165 (88%)	107 (73%)	37 (25%)	2 (1%)	9	40
11	AA	1338/1342 (100%)	1206 (90%)	126 (9%)	6 (0%)	30	64
12	AB	158/181 (87%)	119 (75%)	26 (16%)	13 (8%)	1	4
13	AC	295/329 (90%)	274 (93%)	19 (6%)	2 (1%)	19	54
13	AD	293/329 (89%)	269 (92%)	24 (8%)	0	100	100
14	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	19	54
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	AG	493/495 (100%)	377 (76%)	85 (17%)	31 (6%)	1	8
17	C	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
19	E	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
20	F	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
21	G	223/241 (92%)	209 (94%)	13 (6%)	1 (0%)	30	64
22	H	255/557 (46%)	201 (79%)	45 (18%)	9 (4%)	3	20
23	I	206/233 (88%)	200 (97%)	6 (3%)	0	100	100
24	J	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
25	K	154/167 (92%)	146 (95%)	6 (4%)	2 (1%)	10	41
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	47
27	M	149/179 (83%)	139 (93%)	9 (6%)	1 (1%)	19	54
28	N	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
29	O	125/130 (96%)	118 (94%)	6 (5%)	1 (1%)	16	51
30	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	13	47
31	Q	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
32	R	117/124 (94%)	112 (96%)	4 (3%)	1 (1%)	14	49
33	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
34	T	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
35	U	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
38	X	114/118 (97%)	104 (91%)	8 (7%)	2 (2%)	7	35
39	Y	139/142 (98%)	113 (81%)	25 (18%)	1 (1%)	19	54
40	Z	28/121 (23%)	24 (86%)	4 (14%)	0	100	100
42	b	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
45	e	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
46	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	g	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
48	h	269/273 (98%)	254 (94%)	15 (6%)	0	100	100
49	i	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
52	l	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
53	m	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
54	n	175/179 (98%)	168 (96%)	6 (3%)	1 (1%)	22	57
55	o	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	37
56	p	173/177 (98%)	165 (95%)	7 (4%)	1 (1%)	22	57
57	q	36/38 (95%)	36 (100%)	0	0	100	100
58	r	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
59	s	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
60	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
61	u	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
62	v	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
63	w	117/127 (92%)	111 (95%)	6 (5%)	0	100	100
64	x	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
65	y	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
66	z	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
All	All	10159/11072 (92%)	9310 (92%)	763 (8%)	86 (1%)	19	51

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	79	PRO
11	AA	888	THR
12	AB	121	LYS
12	AB	122	PRO
12	AB	123	ARG
12	AB	175	PHE
16	AG	34	ALA
16	AG	105	ILE
16	AG	187	ARG
16	AG	221	ILE
16	AG	227	ALA
21	G	127	ASP
22	H	170	ARG
22	H	304	VAL
22	H	305	HIS
22	H	309	MET
11	AA	905	ILE
11	AA	913	VAL
11	AA	918	LEU
12	AB	125	LYS
12	AB	126	THR
14	AE	175	GLU
16	AG	63	LEU
16	AG	104	ARG
16	AG	268	GLY
16	AG	279	ASN
16	AG	350	ALA
16	AG	365	ILE
22	H	71	ALA
22	H	172	ALA
27	M	56	LYS
12	AB	124	PRO
14	AE	51	PRO
14	AE	805	GLN
16	AG	33	THR
16	AG	102	PHE
16	AG	200	SER
16	AG	305	MET
16	AG	319	GLY
16	AG	355	ALA
16	AG	396	GLU
16	AG	425	LEU
22	H	143	ASP

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Mol	Chain	Res	Type
25	K	91	GLY
29	O	13	LYS
54	n	177	PHE
56	p	48	ASN
11	AA	921	PRO
12	AB	105	ASP
12	AB	180	LYS
13	AC	193	GLU
14	AE	174	ASP
14	AE	193	ASP
16	AG	48	GLN
16	AG	265	GLU
16	AG	363	LEU
16	AG	401	PRO
22	H	340	ARG
25	K	78	ASN
38	X	6	GLY
55	o	32	ILE
12	AB	167	ARG
12	AB	178	VAL
12	AB	179	GLU
14	AE	91	GLU
16	AG	224	LYS
16	AG	399	ASP
32	R	103	ASP
13	AC	192	VAL
14	AE	49	PHE
14	AE	73	GLY
14	AE	904	ALA
16	AG	43	ILE
16	AG	70	GLN
16	AG	169	PRO
16	AG	323	GLN
16	AG	364	ASP
16	AG	382	GLU
12	AB	170	PRO
22	H	275	PRO
30	P	57	VAL
38	X	65	VAL
9	9	130	PRO
11	AA	1317	PRO
39	Y	21	PRO

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Mol	Chain	Res	Type
26	L	96	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	80 (95%)	4 (5%)	21	55
2	1	93/93 (100%)	84 (90%)	9 (10%)	6	27
3	2	81/84 (96%)	77 (95%)	4 (5%)	21	54
4	3	84/85 (99%)	78 (93%)	6 (7%)	12	42
5	4	78/78 (100%)	75 (96%)	3 (4%)	28	60
9	9	112/123 (91%)	79 (70%)	33 (30%)	0	1
11	AA	1155/1157 (100%)	1142 (99%)	13 (1%)	70	86
12	AB	138/158 (87%)	105 (76%)	33 (24%)	0	2
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	15	47
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	AG	409/409 (100%)	296 (72%)	113 (28%)	0	1
17	C	57/65 (88%)	55 (96%)	2 (4%)	31	63
19	E	65/66 (98%)	62 (95%)	3 (5%)	23	56
20	F	60/61 (98%)	57 (95%)	3 (5%)	20	54
21	G	187/199 (94%)	177 (95%)	10 (5%)	19	52
22	H	137/461 (30%)	125 (91%)	12 (9%)	8	32
23	I	171/190 (90%)	162 (95%)	9 (5%)	19	52
24	J	172/173 (99%)	166 (96%)	6 (4%)	31	63
25	K	119/126 (94%)	110 (92%)	9 (8%)	11	39
26	L	91/116 (78%)	81 (89%)	10 (11%)	5	23
27	M	124/147 (84%)	116 (94%)	8 (6%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	N	104/105 (99%)	101 (97%)	3 (3%)	37	67
29	O	105/107 (98%)	98 (93%)	7 (7%)	13	44
30	P	86/90 (96%)	75 (87%)	11 (13%)	3	17
31	Q	90/99 (91%)	87 (97%)	3 (3%)	33	64
32	R	101/104 (97%)	94 (93%)	7 (7%)	13	43
33	S	83/84 (99%)	78 (94%)	5 (6%)	16	48
34	T	76/77 (99%)	62 (82%)	14 (18%)	1	7
35	U	65/65 (100%)	60 (92%)	5 (8%)	10	39
36	V	74/78 (95%)	70 (95%)	4 (5%)	18	51
37	W	72/79 (91%)	68 (94%)	4 (6%)	17	50
38	X	94/96 (98%)	82 (87%)	12 (13%)	3	17
39	Y	109/110 (99%)	89 (82%)	20 (18%)	1	7
40	Z	26/85 (31%)	17 (65%)	9 (35%)	0	0
42	b	58/63 (92%)	58 (100%)	0	100	100
43	c	67/68 (98%)	64 (96%)	3 (4%)	23	56
45	e	54/55 (98%)	54 (100%)	0	100	100
46	f	48/49 (98%)	45 (94%)	3 (6%)	15	46
47	g	59/62 (95%)	54 (92%)	5 (8%)	8	34
48	h	216/218 (99%)	202 (94%)	14 (6%)	14	45
49	i	47/48 (98%)	41 (87%)	6 (13%)	3	17
50	j	164/164 (100%)	154 (94%)	10 (6%)	15	47
51	k	47/49 (96%)	45 (96%)	2 (4%)	25	57
52	l	165/165 (100%)	154 (93%)	11 (7%)	13	44
53	m	38/38 (100%)	35 (92%)	3 (8%)	10	38
54	n	148/150 (99%)	136 (92%)	12 (8%)	9	36
55	o	51/52 (98%)	48 (94%)	3 (6%)	16	48
56	p	136/138 (99%)	131 (96%)	5 (4%)	29	62
57	q	34/34 (100%)	32 (94%)	2 (6%)	16	48
58	r	114/114 (100%)	105 (92%)	9 (8%)	10	38
59	s	116/116 (100%)	111 (96%)	5 (4%)	25	57
60	t	104/104 (100%)	96 (92%)	8 (8%)	10	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	u	103/103 (100%)	96 (93%)	7 (7%)	13	43
62	v	109/109 (100%)	105 (96%)	4 (4%)	29	62
63	w	99/103 (96%)	93 (94%)	6 (6%)	15	47
64	x	86/87 (99%)	81 (94%)	5 (6%)	17	49
65	y	99/100 (99%)	95 (96%)	4 (4%)	27	59
66	z	89/90 (99%)	85 (96%)	4 (4%)	23	56
All	All	8314/9148 (91%)	7720 (93%)	594 (7%)	15	42

All (594) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	38	VAL
1	0	48	LYS
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	108	SER
2	1	110	ARG
3	2	1	MET
3	2	17	SER
3	2	24	MET
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	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN

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Mol	Chain	Res	Type
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	42	ARG
9	9	43	LYS
9	9	46	ARG
9	9	50	VAL
9	9	51	TYR
9	9	53	ARG
9	9	56	ARG
9	9	59	LEU
9	9	61	ARG
9	9	65	GLU
9	9	69	PHE
9	9	72	LEU
9	9	81	LEU
9	9	87	GLU
9	9	96	PHE
9	9	106	PHE
9	9	107	GLU
9	9	108	VAL
9	9	109	LYS
9	9	113	PHE
9	9	116	GLU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	129	LEU
9	9	132	TYR
9	9	134	GLU
11	AA	888	THR
11	AA	890	LYS
11	AA	892	GLU
11	AA	893	THR
11	AA	894	GLN
11	AA	895	LEU
11	AA	896	THR
11	AA	902	LEU
11	AA	903	ARG
11	AA	906	PHE
11	AA	915	ASP
11	AA	918	LEU

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Mol	Chain	Res	Type
11	AA	920	VAL
12	AB	21	ARG
12	AB	104	SER
12	AB	105	ASP
12	AB	106	LYS
12	AB	114	ARG
12	AB	123	ARG
12	AB	125	LYS
12	AB	127	LEU
12	AB	129	GLU
12	AB	135	ARG
12	AB	136	VAL
12	AB	138	ASP
12	AB	141	PHE
12	AB	143	ASP
12	AB	145	ASN
12	AB	150	GLU
12	AB	153	TYR
12	AB	154	GLU
12	AB	155	LYS
12	AB	157	ARG
12	AB	159	LYS
12	AB	161	SER
12	AB	163	SER
12	AB	164	ILE
12	AB	167	ARG
12	AB	169	THR
12	AB	171	VAL
12	AB	172	GLU
12	AB	174	ASP
12	AB	176	SER
12	AB	177	GLN
12	AB	179	GLU
12	AB	180	LYS
14	AE	40	LYS
14	AE	42	GLU
14	AE	44	ILE
14	AE	46	TYR
14	AE	47	ARG
14	AE	49	PHE
14	AE	50	LYS
14	AE	52	GLU

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Mol	Chain	Res	Type
14	AE	53	ARG
14	AE	54	ASP
14	AE	60	ARG
14	AE	67	ASP
14	AE	70	CYS
14	AE	72	CYS
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	81	ARG
14	AE	87	LYS
14	AE	88	CYS
14	AE	91	GLU
14	AE	94	GLN
14	AE	95	THR
14	AE	99	ARG
14	AE	100	GLU
14	AE	117	LEU
14	AE	119	SER
14	AE	123	ARG
14	AE	132	LEU
14	AE	135	ILE
14	AE	142	GLU
14	AE	144	TYR
14	AE	145	VAL
14	AE	147	ILE
14	AE	152	THR
14	AE	154	LEU
14	AE	157	GLN
14	AE	159	ILE
14	AE	175	GLU
14	AE	180	MET
14	AE	190	LYS
14	AE	193	ASP
14	AE	196	GLN
14	AE	210	SER
14	AE	215	LYS
14	AE	216	LYS
14	AE	222	LYS
14	AE	223	LEU
14	AE	227	PHE

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Mol	Chain	Res	Type
14	AE	232	ASN
14	AE	233	LYS
14	AE	237	MET
14	AE	238	ILE
14	AE	239	LEU
14	AE	240	THR
14	AE	244	VAL
14	AE	271	ARG
14	AE	385	LEU
14	AE	386	GLU
14	AE	390	LEU
14	AE	393	THR
14	AE	394	ILE
14	AE	395	LYS
14	AE	514	THR
14	AE	709	ARG
14	AE	836	ARG
14	AE	1172	LYS
14	AE	1373	ARG
16	AG	5	ILE
16	AG	12	VAL
16	AG	36	LYS
16	AG	37	LYS
16	AG	38	LYS
16	AG	40	GLU
16	AG	43	ILE
16	AG	49	ILE
16	AG	50	ASP
16	AG	56	PHE
16	AG	57	ASP
16	AG	61	ARG
16	AG	75	ILE
16	AG	97	ILE
16	AG	103	ASP
16	AG	104	ARG
16	AG	114	ILE
16	AG	117	LYS
16	AG	123	ARG
16	AG	125	MET
16	AG	126	VAL
16	AG	131	ARG
16	AG	139	THR

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Mol	Chain	Res	Type
16	AG	144	LYS
16	AG	150	ILE
16	AG	154	LEU
16	AG	157	ASN
16	AG	162	ILE
16	AG	167	MET
16	AG	173	PHE
16	AG	179	VAL
16	AG	180	ARG
16	AG	182	VAL
16	AG	185	SER
16	AG	187	ARG
16	AG	195	LEU
16	AG	197	VAL
16	AG	199	ARG
16	AG	201	LYS
16	AG	203	GLU
16	AG	204	MET
16	AG	205	LEU
16	AG	206	ILE
16	AG	207	GLU
16	AG	209	PHE
16	AG	210	ARG
16	AG	211	ILE
16	AG	215	GLU
16	AG	218	GLU
16	AG	219	GLU
16	AG	221	ILE
16	AG	223	ILE
16	AG	232	SER
16	AG	235	LYS
16	AG	236	ILE
16	AG	238	VAL
16	AG	239	LYS
16	AG	240	THR
16	AG	241	ASN
16	AG	243	LYS
16	AG	244	ARG
16	AG	245	ILE
16	AG	254	MET
16	AG	255	ARG
16	AG	258	ARG

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Mol	Chain	Res	Type
16	AG	259	VAL
16	AG	260	GLN
16	AG	262	VAL
16	AG	265	GLU
16	AG	266	LEU
16	AG	270	ARG
16	AG	271	ILE
16	AG	274	VAL
16	AG	276	TRP
16	AG	278	ASP
16	AG	285	ILE
16	AG	288	MET
16	AG	296	ILE
16	AG	299	ASP
16	AG	300	GLU
16	AG	301	ASP
16	AG	302	LYS
16	AG	303	HIS
16	AG	305	MET
16	AG	309	VAL
16	AG	310	GLU
16	AG	313	ASN
16	AG	316	GLN
16	AG	320	ARG
16	AG	321	ASN
16	AG	323	GLN
16	AG	327	LEU
16	AG	331	LEU
16	AG	335	GLU
16	AG	336	LEU
16	AG	337	ASN
16	AG	340	THR
16	AG	342	ASP
16	AG	344	LEU
16	AG	356	ILE
16	AG	358	THR
16	AG	359	PHE
16	AG	361	LYS
16	AG	365	ILE
16	AG	380	THR
16	AG	387	VAL
16	AG	390	LYS

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Mol	Chain	Res	Type
16	AG	396	GLU
16	AG	399	ASP
16	AG	400	GLU
16	AG	425	LEU
16	AG	428	ASN
16	AG	429	LYS
17	C	11	CYS
17	C	71	THR
19	E	48	GLN
19	E	54	MET
19	E	70	ASN
20	F	16	LEU
20	F	62	ARG
20	F	67	ARG
21	G	7	ARG
21	G	23	TRP
21	G	105	LYS
21	G	108	ARG
21	G	127	ASP
21	G	128	LYS
21	G	129	LEU
21	G	132	LYS
21	G	152	LYS
21	G	208	ARG
22	H	9	PHE
22	H	54	LYS
22	H	62	ILE
22	H	72	LEU
22	H	82	THR
22	H	273	ARG
22	H	288	THR
22	H	308	GLU
22	H	331	MET
22	H	336	ASP
22	H	337	GLU
22	H	338	GLU
23	I	14	ILE
23	I	75	ILE
23	I	89	LYS
23	I	112	ASP
23	I	164	ARG
23	I	172	ARG

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Mol	Chain	Res	Type
23	I	185	ASN
23	I	187	SER
23	I	200	VAL
24	J	47	ARG
24	J	48	LEU
24	J	95	GLU
24	J	104	ARG
24	J	138	SER
24	J	190	ASP
25	K	10	GLU
25	K	15	LEU
25	K	60	ILE
25	K	65	GLU
25	K	69	ARG
25	K	114	VAL
25	K	115	LEU
25	K	138	ARG
25	K	162	GLU
26	L	1	MET
26	L	5	GLU
26	L	16	GLU
26	L	24	ARG
26	L	36	ILE
26	L	38	ARG
26	L	54	LEU
26	L	69	GLU
26	L	86	ARG
26	L	88	MET
27	M	7	ILE
27	M	17	LYS
27	M	23	LEU
27	M	63	GLU
27	M	79	ARG
27	M	91	VAL
27	M	109	ARG
27	M	123	GLU
28	N	74	SER
28	N	77	ARG
28	N	121	LEU
29	O	12	ARG
29	O	27	LYS
29	O	56	ASP

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Mol	Chain	Res	Type
29	O	60	LYS
29	O	61	LEU
29	O	62	ASP
29	O	118	LEU
30	P	5	ARG
30	P	17	LEU
30	P	24	GLU
30	P	25	ILE
30	P	27	GLU
30	P	37	ARG
30	P	54	SER
30	P	60	ASP
30	P	87	LEU
30	P	89	ARG
30	P	90	LEU
31	Q	15	GLN
31	Q	56	ARG
31	Q	107	ILE
32	R	5	ASN
32	R	30	LYS
32	R	56	ARG
32	R	62	GLU
32	R	64	THR
32	R	74	LEU
32	R	76	GLU
33	S	45	VAL
33	S	46	LEU
33	S	55	SER
33	S	59	ARG
33	S	89	MET
34	T	10	LYS
34	T	17	ARG
34	T	18	ASP
34	T	22	THR
34	T	39	LEU
34	T	40	GLN
34	T	64	ARG
34	T	66	LEU
34	T	67	LEU
34	T	70	LEU
34	T	73	LYS
34	T	74	ASP

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Mol	Chain	Res	Type
34	T	84	ARG
34	T	85	LEU
35	U	1	MET
35	U	2	VAL
35	U	3	THR
35	U	6	LEU
35	U	19	VAL
36	V	50	ASN
36	V	51	ASN
36	V	75	LEU
36	V	81	LYS
37	W	21	LYS
37	W	63	THR
37	W	69	HIS
37	W	81	ARG
38	X	3	ARG
38	X	11	ASP
38	X	16	VAL
38	X	29	ARG
38	X	59	GLU
38	X	68	ASP
38	X	81	MET
38	X	92	ARG
38	X	93	ARG
38	X	101	ARG
38	X	104	THR
38	X	117	LYS
39	Y	5	GLN
39	Y	10	LEU
39	Y	23	VAL
39	Y	27	LEU
39	Y	30	GLN
39	Y	50	LYS
39	Y	60	VAL
39	Y	61	TYR
39	Y	91	LYS
39	Y	95	ASP
39	Y	99	LYS
39	Y	100	ILE
39	Y	102	ARG
39	Y	104	GLN
39	Y	105	LEU

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Mol	Chain	Res	Type
39	Y	112	LYS
39	Y	116	MET
39	Y	124	MET
39	Y	131	THR
39	Y	135	MET
40	Z	4	LYS
40	Z	6	GLN
40	Z	8	ILE
40	Z	16	VAL
40	Z	23	ILE
40	Z	26	MET
40	Z	28	GLU
40	Z	29	LYS
40	Z	30	PHE
43	c	5	CYS
43	c	29	PHE
43	c	48	THR
46	f	3	LYS
46	f	31	ARG
46	f	45	ARG
47	g	31	ASP
47	g	43	PHE
47	g	47	LYS
47	g	56	ARG
47	g	64	PHE
48	h	40	SER
48	h	51	THR
48	h	52	ARG
48	h	130	LEU
48	h	141	VAL
48	h	156	ARG
48	h	187	ASP
48	h	195	VAL
48	h	202	LEU
48	h	203	ARG
48	h	204	VAL
48	h	205	LEU
48	h	258	ARG
48	h	261	LYS
49	i	9	THR
49	i	26	THR
49	i	29	SER

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Mol	Chain	Res	Type
49	i	31	ASP
49	i	40	ARG
49	i	42	HIS
50	j	13	ARG
50	j	18	ASP
50	j	43	ASP
50	j	52	THR
50	j	77	ARG
50	j	91	THR
50	j	103	ASP
50	j	130	GLN
50	j	131	ASP
50	j	151	THR
51	k	5	ILE
51	k	26	ASN
52	l	17	THR
52	l	21	ARG
52	l	22	ASP
52	l	40	ARG
52	l	57	LYS
52	l	69	ARG
52	l	108	ILE
52	l	122	GLU
52	l	149	ILE
52	l	179	SER
52	l	184	ASP
53	m	24	THR
53	m	25	LYS
53	m	41	ARG
54	n	6	ASP
54	n	26	MET
54	n	57	LEU
54	n	80	ARG
54	n	95	ARG
54	n	115	ARG
54	n	117	LEU
54	n	122	PHE
54	n	123	ASP
54	n	133	ARG
54	n	140	GLU
54	n	163	ASP
55	o	31	HIS

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Mol	Chain	Res	Type
55	o	54	ASP
55	o	55	LEU
56	p	39	ASP
56	p	45	HIS
56	p	95	ARG
56	p	171	THR
56	p	176	LYS
57	q	3	VAL
57	q	26	ILE
58	r	11	ASN
58	r	12	LEU
58	r	15	LEU
58	r	41	LYS
58	r	66	ASN
58	r	72	ILE
58	r	97	ARG
58	r	101	ASP
58	r	127	GLU
59	s	1	MET
59	s	30	THR
59	s	40	HIS
59	s	57	LEU
59	s	140	LEU
60	t	7	MET
60	t	17	ARG
60	t	21	CYS
60	t	32	TYR
60	t	49	ARG
60	t	53	LYS
60	t	80	ASP
60	t	89	ASN
61	u	5	THR
61	u	27	LEU
61	u	42	SER
61	u	48	ARG
61	u	59	ARG
61	u	78	ARG
61	u	84	LYS
62	v	18	ARG
62	v	100	LYS
62	v	115	GLU
62	v	128	THR

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Mol	Chain	Res	Type
63	w	2	ARG
63	w	20	MET
63	w	51	LEU
63	w	63	ARG
63	w	65	LEU
63	w	69	ARG
64	x	2	ASP
64	x	13	ARG
64	x	19	GLN
64	x	47	VAL
64	x	91	SER
65	y	21	ARG
65	y	85	SER
65	y	102	GLU
65	y	114	LEU
66	z	3	ARG
66	z	51	ARG
66	z	91	ASP
66	z	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	59	ASN
11	AA	69	GLN
11	AA	150	HIS
11	AA	314	ASN
11	AA	513	GLN
11	AA	554	HIS
11	AA	580	GLN
11	AA	604	HIS
11	AA	688	GLN
11	AA	1268	GLN
11	AA	1313	HIS
13	AC	147	GLN
13	AD	66	HIS
13	AD	117	HIS
13	AD	227	GLN
14	AE	294	ASN
15	AF	31	GLN
16	AG	194	GLN
16	AG	241	ASN

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Mol	Chain	Res	Type
16	AG	260	GLN
16	AG	282	GLN
16	AG	316	GLN
16	AG	323	GLN
16	AG	324	ASN
16	AG	337	ASN
16	AG	428	ASN
19	E	48	GLN
19	E	52	ASN
21	G	18	HIS
21	G	39	HIS
21	G	168	HIS
25	K	70	ASN
26	L	63	ASN
27	M	68	ASN
27	M	130	ASN
27	M	148	ASN
30	P	58	ASN
31	Q	15	GLN
36	V	45	HIS
38	X	105	ASN
39	Y	5	GLN
47	g	6	HIS
50	j	150	GLN
51	k	26	ASN
55	o	31	HIS
56	p	116	GLN
62	v	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	76/76 (100%)	33 (43%)	10 (13%)
10	B	75/76 (98%)	41 (54%)	8 (10%)
18	D	1513/1542 (98%)	282 (18%)	8 (0%)
41	a	2859/2904 (98%)	534 (18%)	0
44	d	119/120 (99%)	18 (15%)	0
8	7	32/41 (78%)	19 (59%)	4 (12%)
All	All	4674/4759 (98%)	927 (19%)	30 (0%)

All (927) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-19	U
8	7	-17	U
8	7	-16	U
8	7	-15	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
8	7	-8	U
8	7	-7	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U
8	7	1	U
8	7	12	G
8	7	13	G
10	A	2	G
10	A	4	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	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	45	G
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	54	U
10	A	57	A

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Mol	Chain	Res	Type
10	A	58	A
10	A	59	A
10	A	60	U
10	A	61	C
10	A	66	C
10	A	67	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
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
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	24	U
10	B	29	G
10	B	30	G
10	B	32	C
10	B	33	U
10	B	36	U
10	B	37	A
10	B	38	A
10	B	39	C
10	B	45	G
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	56	C
10	B	57	A
10	B	58	A

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Mol	Chain	Res	Type
10	B	59	A
10	B	60	U
10	B	61	C
10	B	66	C
10	B	67	C
10	B	69	C
10	B	71	C
10	B	73	A
18	D	4	U
18	D	7	A
18	D	9	G
18	D	22	G
18	D	32	A
18	D	39	G
18	D	47	C
18	D	48	C
18	D	50	A
18	D	51	A
18	D	52	C
18	D	68	G
18	D	69	G
18	D	71	A
18	D	72	A
18	D	74	A
18	D	75	G
18	D	76	G
18	D	77	A
18	D	81	A
18	D	82	G
18	D	83	C
18	D	84	U
18	D	87	C
18	D	92	U
18	D	94	G
18	D	95	C
18	D	108	G
18	D	120	A
18	D	121	U
18	D	122	G
18	D	131	A
18	D	141	G
18	D	142	G

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Mol	Chain	Res	Type
18	D	144	G
18	D	146	G
18	D	160	A
18	D	163	C
18	D	164	G
18	D	168	G
18	D	169	C
18	D	173	U
18	D	180	U
18	D	181	A
18	D	182	A
18	D	189	A
18	D	197	A
18	D	198	G
18	D	204	G
18	D	208	U
18	D	210	C
18	D	211	G
18	D	212	G
18	D	226	G
18	D	240	G
18	D	245	U
18	D	247	G
18	D	251	G
18	D	262	A
18	D	266	G
18	D	267	C
18	D	279	A
18	D	289	G
18	D	306	A
18	D	321	A
18	D	328	C
18	D	329	A
18	D	330	C
18	D	332	G
18	D	352	C
18	D	353	A
18	D	354	G
18	D	355	C
18	D	367	U
18	D	372	C
18	D	373	A

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Mol	Chain	Res	Type
18	D	376	G
18	D	381	C
18	D	389	A
18	D	392	C
18	D	397	A
18	D	398	U
18	D	406	G
18	D	412	A
18	D	413	G
18	D	414	A
18	D	421	U
18	D	422	C
18	D	429	U
18	D	451	A
18	D	456	A
18	D	457	G
18	D	458	U
18	D	463	U
18	D	464	U
18	D	467	U
18	D	468	A
18	D	469	C
18	D	476	U
18	D	478	A
18	D	479	U
18	D	481	G
18	D	484	G
18	D	485	U
18	D	486	U
18	D	493	A
18	D	494	G
18	D	496	A
18	D	511	C
18	D	515	G
18	D	518	C
18	D	519	C
18	D	521	G
18	D	531	U
18	D	532	A
18	D	533	A
18	D	547	A
18	D	559	A

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Mol	Chain	Res	Type
18	D	562	U
18	D	564	C
18	D	568	G
18	D	572	A
18	D	573	A
18	D	576	C
18	D	577	G
18	D	579	A
18	D	596	A
18	D	639	G
18	D	650	G
18	D	653	U
18	D	660	C
18	D	665	A
18	D	671	G
18	D	687	A
18	D	700	G
18	D	702	A
18	D	718	A
18	D	721	G
18	D	723	U
18	D	724	G
18	D	731	G
18	D	733	G
18	D	747	A
18	D	748	G
18	D	759	A
18	D	760	G
18	D	777	A
18	D	792	A
18	D	793	U
18	D	794	A
18	D	802	A
18	D	815	A
18	D	817	C
18	D	819	A
18	D	828	U
18	D	829	G
18	D	832	G
18	D	841	C
18	D	844	G
18	D	845	A

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Mol	Chain	Res	Type
18	D	846	G
18	D	849	G
18	D	887	G
18	D	889	A
18	D	902	G
18	D	914	A
18	D	916	U
18	D	926	G
18	D	934	C
18	D	935	A
18	D	958	A
18	D	960	U
18	D	969	A
18	D	975	A
18	D	976	G
18	D	977	A
18	D	992	U
18	D	993	G
18	D	996	A
18	D	999	C
18	D	1004	A
18	D	1005	A
18	D	1008	U
18	D	1009	U
18	D	1017	U
18	D	1018	G
18	D	1021	A
18	D	1026	G
18	D	1027	C
18	D	1028	C
18	D	1030	U
18	D	1031	C
18	D	1032	G
18	D	1033	G
18	D	1037	C
18	D	1043	G
18	D	1044	A
18	D	1046	A
18	D	1065	U
18	D	1085	U
18	D	1094	G
18	D	1095	U

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Mol	Chain	Res	Type
18	D	1101	A
18	D	1108	G
18	D	1124	G
18	D	1132	C
18	D	1133	G
18	D	1135	U
18	D	1136	C
18	D	1137	C
18	D	1139	G
18	D	1140	C
18	D	1141	C
18	D	1142	G
18	D	1145	A
18	D	1146	A
18	D	1151	A
18	D	1152	A
18	D	1154	G
18	D	1158	C
18	D	1159	U
18	D	1167	A
18	D	1171	A
18	D	1174	G
18	D	1175	G
18	D	1176	A
18	D	1184	G
18	D	1196	A
18	D	1197	A
18	D	1212	U
18	D	1213	A
18	D	1215	G
18	D	1227	A
18	D	1238	A
18	D	1239	A
18	D	1257	A
18	D	1275	A
18	D	1276	G
18	D	1278	G
18	D	1279	G
18	D	1280	A
18	D	1285	A
18	D	1286	U
18	D	1287	A

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Mol	Chain	Res	Type
18	D	1299	A
18	D	1300	G
18	D	1302	C
18	D	1305	G
18	D	1317	C
18	D	1320	C
18	D	1323	G
18	D	1332	A
18	D	1346	A
18	D	1353	G
18	D	1363	A
18	D	1370	G
18	D	1378	C
18	D	1379	G
18	D	1381	U
18	D	1391	U
18	D	1397	C
18	D	1398	A
18	D	1404	C
18	D	1419	G
18	D	1429	A
18	D	1441	A
18	D	1446	A
18	D	1452	C
18	D	1453	G
18	D	1475	G
18	D	1487	G
18	D	1493	A
18	D	1494	G
18	D	1497	G
18	D	1502	A
18	D	1503	A
18	D	1506	U
18	D	1517	G
18	D	1528	U
18	D	1529	G
18	D	1530	G
18	D	1534	A
41	a	10	A
41	a	15	G
41	a	23	G
41	a	34	U

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Mol	Chain	Res	Type
41	a	44	A
41	a	46	G
41	a	58	G
41	a	60	G
41	a	62	U
41	a	63	A
41	a	71	A
41	a	74	A
41	a	75	G
41	a	83	A
41	a	84	A
41	a	85	G
41	a	101	A
41	a	102	U
41	a	103	A
41	a	118	A
41	a	120	U
41	a	137	U
41	a	139	U
41	a	140	C
41	a	149	A
41	a	163	C
41	a	165	A
41	a	181	A
41	a	196	A
41	a	199	A
41	a	215	G
41	a	216	A
41	a	221	A
41	a	222	A
41	a	224	U
41	a	241	A
41	a	248	G
41	a	249	C
41	a	264	C
41	a	265	A
41	a	266	G
41	a	270	A
41	a	271	G
41	a	272	A
41	a	275	C
41	a	276	U

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Mol	Chain	Res	Type
41	a	278	A
41	a	279	A
41	a	285	G
41	a	300	A
41	a	311	A
41	a	315	G
41	a	329	G
41	a	330	A
41	a	352	A
41	a	353	C
41	a	361	G
41	a	362	A
41	a	371	A
41	a	372	G
41	a	375	G
41	a	386	G
41	a	396	G
41	a	405	U
41	a	411	G
41	a	412	A
41	a	420	C
41	a	424	G
41	a	451	U
41	a	456	C
41	a	457	A
41	a	477	A
41	a	479	A
41	a	481	G
41	a	490	C
41	a	491	G
41	a	501	A
41	a	505	A
41	a	506	G
41	a	509	C
41	a	510	C
41	a	531	C
41	a	532	A
41	a	533	G
41	a	543	G
41	a	544	C
41	a	545	U
41	a	546	U

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Mol	Chain	Res	Type
41	a	547	A
41	a	549	G
41	a	550	C
41	a	551	G
41	a	563	A
41	a	569	U
41	a	573	U
41	a	575	A
41	a	588	U
41	a	603	A
41	a	609	A
41	a	613	A
41	a	614	A
41	a	615	U
41	a	616	A
41	a	627	A
41	a	637	A
41	a	645	C
41	a	647	G
41	a	654	A
41	a	655	A
41	a	668	A
41	a	685	A
41	a	686	U
41	a	709	U
41	a	710	U
41	a	717	C
41	a	730	A
41	a	738	G
41	a	757	G
41	a	765	C
41	a	775	G
41	a	776	G
41	a	782	A
41	a	784	G
41	a	785	G
41	a	789	A
41	a	792	A
41	a	800	A
41	a	805	G
41	a	812	C
41	a	819	A

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Mol	Chain	Res	Type
41	a	827	U
41	a	828	U
41	a	845	A
41	a	846	U
41	a	857	G
41	a	858	G
41	a	859	G
41	a	869	G
41	a	878	A
41	a	879	G
41	a	881	G
41	a	884	U
41	a	885	C
41	a	886	A
41	a	891	G
41	a	895	U
41	a	896	A
41	a	897	C
41	a	899	A
41	a	910	A
41	a	914	G
41	a	915	C
41	a	931	U
41	a	941	A
41	a	946	C
41	a	953	G
41	a	961	C
41	a	973	A
41	a	974	G
41	a	983	A
41	a	984	A
41	a	995	C
41	a	996	A
41	a	999	U
41	a	1005	C
41	a	1012	U
41	a	1013	C
41	a	1023	U
41	a	1025	G
41	a	1026	G
41	a	1028	A
41	a	1029	A

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Mol	Chain	Res	Type
41	a	1033	U
41	a	1034	G
41	a	1043	C
41	a	1045	C
41	a	1046	A
41	a	1047	G
41	a	1051	G
41	a	1064	C
41	a	1065	U
41	a	1066	U
41	a	1067	A
41	a	1068	G
41	a	1070	A
41	a	1071	G
41	a	1073	A
41	a	1074	G
41	a	1079	C
41	a	1081	U
41	a	1082	U
41	a	1083	U
41	a	1087	G
41	a	1088	A
41	a	1101	U
41	a	1111	A
41	a	1112	G
41	a	1119	U
41	a	1122	G
41	a	1126	A
41	a	1128	G
41	a	1130	U
41	a	1132	U
41	a	1133	A
41	a	1134	A
41	a	1135	C
41	a	1136	G
41	a	1142	A
41	a	1169	A
41	a	1170	C
41	a	1171	G
41	a	1172	C
41	a	1173	U
41	a	1175	A

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Mol	Chain	Res	Type
41	a	1176	U
41	a	1177	G
41	a	1178	C
41	a	1179	G
41	a	1180	U
41	a	1182	G
41	a	1186	G
41	a	1204	A
41	a	1210	G
41	a	1238	G
41	a	1241	A
41	a	1248	G
41	a	1249	U
41	a	1253	A
41	a	1256	G
41	a	1266	G
41	a	1271	G
41	a	1272	A
41	a	1273	U
41	a	1300	G
41	a	1301	A
41	a	1313	U
41	a	1320	C
41	a	1329	U
41	a	1345	C
41	a	1352	U
41	a	1359	A
41	a	1365	A
41	a	1368	G
41	a	1379	U
41	a	1380	G
41	a	1383	A
41	a	1392	A
41	a	1395	A
41	a	1408	G
41	a	1409	U
41	a	1412	U
41	a	1416	G
41	a	1417	C
41	a	1419	A
41	a	1420	A
41	a	1427	A

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Mol	Chain	Res	Type
41	a	1428	C
41	a	1452	G
41	a	1453	A
41	a	1455	G
41	a	1460	U
41	a	1482	G
41	a	1490	A
41	a	1497	U
41	a	1502	A
41	a	1503	A
41	a	1508	A
41	a	1509	A
41	a	1510	G
41	a	1515	A
41	a	1529	G
41	a	1532	A
41	a	1534	U
41	a	1535	A
41	a	1536	C
41	a	1537	G
41	a	1538	G
41	a	1558	C
41	a	1566	A
41	a	1569	A
41	a	1578	U
41	a	1580	A
41	a	1581	G
41	a	1583	A
41	a	1586	A
41	a	1589	U
41	a	1590	A
41	a	1608	A
41	a	1610	A
41	a	1616	A
41	a	1647	U
41	a	1648	U
41	a	1649	G
41	a	1651	G
41	a	1664	A
41	a	1665	A
41	a	1674	G
41	a	1677	A

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Mol	Chain	Res	Type
41	a	1698	A
41	a	1703	G
41	a	1714	U
41	a	1715	G
41	a	1722	A
41	a	1729	U
41	a	1730	C
41	a	1732	C
41	a	1738	G
41	a	1758	U
41	a	1764	C
41	a	1773	A
41	a	1791	A
41	a	1800	C
41	a	1801	A
41	a	1808	A
41	a	1811	G
41	a	1816	C
41	a	1829	A
41	a	1833	C
41	a	1847	A
41	a	1848	A
41	a	1858	A
41	a	1859	U
41	a	1862	G
41	a	1864	U
41	a	1869	G
41	a	1870	C
41	a	1871	A
41	a	1872	A
41	a	1906	G
41	a	1907	G
41	a	1913	A
41	a	1914	C
41	a	1920	C
41	a	1921	G
41	a	1923	U
41	a	1925	C
41	a	1928	A
41	a	1929	G
41	a	1930	G
41	a	1938	A

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Mol	Chain	Res	Type
41	a	1955	U
41	a	1965	C
41	a	1966	A
41	a	1967	C
41	a	1970	A
41	a	1971	U
41	a	1972	G
41	a	1982	U
41	a	1991	U
41	a	1992	G
41	a	1993	U
41	a	1996	C
41	a	1997	C
41	a	2002	G
41	a	2020	A
41	a	2022	U
41	a	2023	C
41	a	2027	G
41	a	2032	G
41	a	2033	A
41	a	2043	C
41	a	2052	A
41	a	2055	C
41	a	2056	G
41	a	2060	A
41	a	2061	G
41	a	2062	A
41	a	2063	C
41	a	2093	G
41	a	2096	C
41	a	2097	A
41	a	2100	G
41	a	2107	G
41	a	2108	A
41	a	2110	G
41	a	2111	U
41	a	2113	U
41	a	2115	G
41	a	2116	G
41	a	2117	A
41	a	2118	U
41	a	2122	U

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Mol	Chain	Res	Type
41	a	2124	G
41	a	2125	G
41	a	2126	A
41	a	2127	G
41	a	2128	G
41	a	2131	U
41	a	2132	U
41	a	2133	G
41	a	2134	A
41	a	2139	U
41	a	2147	A
41	a	2154	A
41	a	2157	G
41	a	2158	A
41	a	2159	G
41	a	2161	C
41	a	2162	G
41	a	2163	A
41	a	2164	C
41	a	2165	C
41	a	2169	A
41	a	2171	A
41	a	2172	U
41	a	2173	A
41	a	2182	U
41	a	2183	A
41	a	2189	U
41	a	2190	G
41	a	2193	G
41	a	2194	U
41	a	2198	A
41	a	2204	G
41	a	2211	A
41	a	2212	A
41	a	2225	A
41	a	2226	C
41	a	2229	U
41	a	2238	G
41	a	2239	G
41	a	2243	U
41	a	2250	G
41	a	2258	C

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Mol	Chain	Res	Type
41	a	2266	A
41	a	2268	A
41	a	2269	G
41	a	2278	A
41	a	2279	G
41	a	2283	C
41	a	2286	G
41	a	2287	A
41	a	2288	A
41	a	2296	U
41	a	2297	A
41	a	2305	U
41	a	2308	G
41	a	2309	A
41	a	2315	G
41	a	2322	A
41	a	2325	G
41	a	2327	A
41	a	2333	A
41	a	2335	A
41	a	2339	C
41	a	2345	G
41	a	2347	C
41	a	2350	C
41	a	2357	G
41	a	2361	G
41	a	2376	A
41	a	2383	G
41	a	2385	C
41	a	2396	G
41	a	2402	U
41	a	2403	C
41	a	2410	G
41	a	2422	C
41	a	2423	U
41	a	2425	A
41	a	2426	A
41	a	2429	G
41	a	2430	A
41	a	2431	U
41	a	2435	A
41	a	2441	U

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Mol	Chain	Res	Type
41	a	2448	A
41	a	2449	U
41	a	2470	G
41	a	2474	U
41	a	2476	A
41	a	2484	G
41	a	2491	U
41	a	2493	U
41	a	2497	A
41	a	2502	G
41	a	2506	U
41	a	2512	C
41	a	2513	A
41	a	2518	A
41	a	2520	C
41	a	2525	G
41	a	2529	G
41	a	2535	G
41	a	2554	U
41	a	2566	A
41	a	2567	G
41	a	2574	G
41	a	2582	G
41	a	2585	U
41	a	2602	A
41	a	2603	G
41	a	2609	U
41	a	2613	U
41	a	2629	U
41	a	2630	G
41	a	2660	A
41	a	2661	G
41	a	2689	U
41	a	2690	U
41	a	2714	G
41	a	2725	A
41	a	2726	A
41	a	2727	A
41	a	2733	A
41	a	2744	G
41	a	2748	A
41	a	2758	A

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Mol	Chain	Res	Type
41	a	2777	G
41	a	2778	A
41	a	2791	G
41	a	2793	C
41	a	2795	C
41	a	2796	U
41	a	2797	U
41	a	2798	U
41	a	2799	A
41	a	2818	U
41	a	2820	A
41	a	2821	A
41	a	2823	A
41	a	2825	G
41	a	2849	U
41	a	2850	A
41	a	2859	G
41	a	2861	U
41	a	2867	G
41	a	2879	A
41	a	2880	C
41	a	2883	A
41	a	2884	U
41	a	2885	G
41	a	2891	U
41	a	2898	U
44	d	2	G
44	d	9	G
44	d	15	A
44	d	16	G
44	d	17	C
44	d	30	C
44	d	35	C
44	d	42	C
44	d	51	G
44	d	56	G
44	d	66	A
44	d	67	G
44	d	88	C
44	d	89	U
44	d	90	C
44	d	99	A

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Mol	Chain	Res	Type
44	d	109	A
44	d	119	A

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-17	U
8	7	-11	U
8	7	0	U
8	7	11	U
10	A	1	C
10	A	6	G
10	A	9	G
10	A	12	G
10	A	21	A
10	A	22	G
10	A	48	C
10	A	57	A
10	A	58	A
10	A	60	U
10	B	6	G
10	B	9	G
10	B	12	G
10	B	21	A
10	B	22	G
10	B	57	A
10	B	58	A
10	B	60	U
18	D	197	A
18	D	207	C
18	D	428	G
18	D	496	A
18	D	758	C
18	D	1145	A
18	D	1214	C
18	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

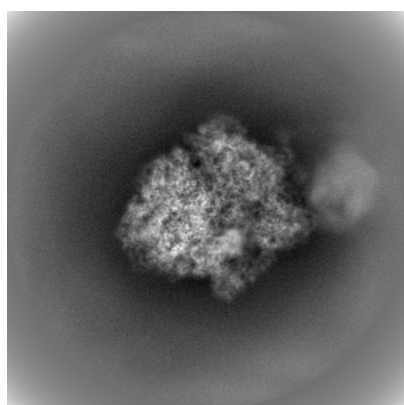
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22082. These allow visual inspection of the internal detail of the map and identification of artifacts.

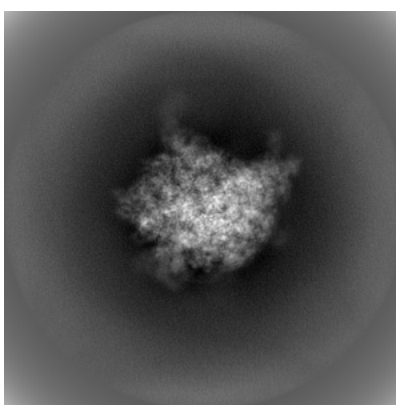
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

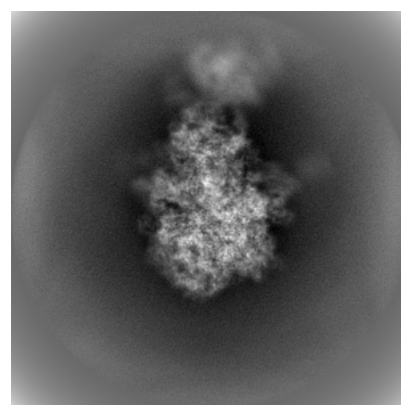
6.1.1 Primary map



X



Y

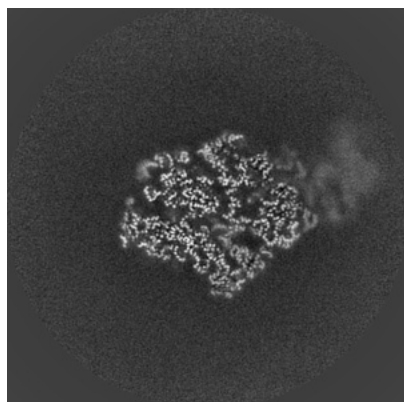


Z

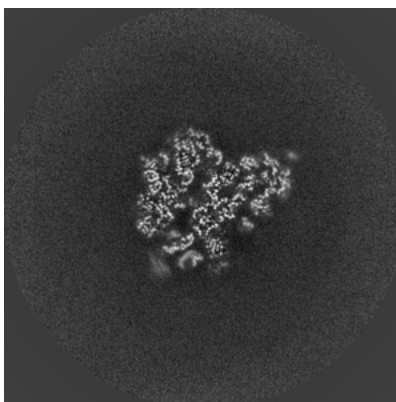
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

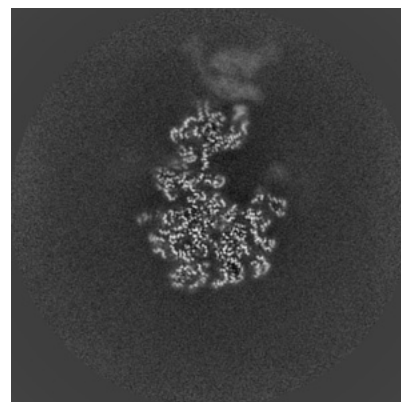
6.2.1 Primary map



X Index: 256



Y Index: 256

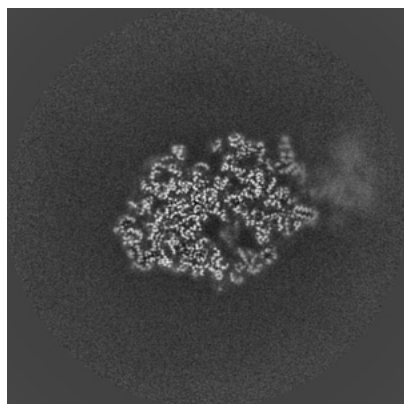


Z Index: 256

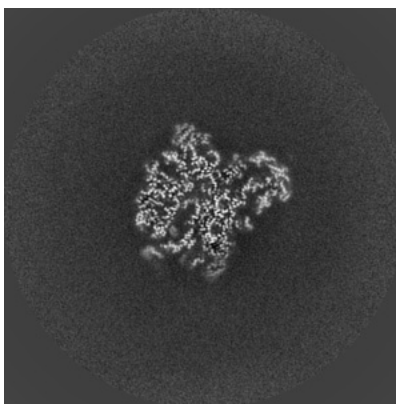
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

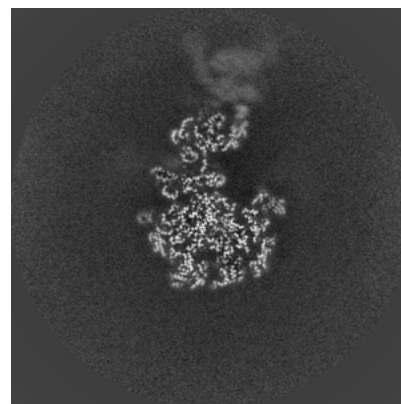
6.3.1 Primary map



X Index: 242



Y Index: 250

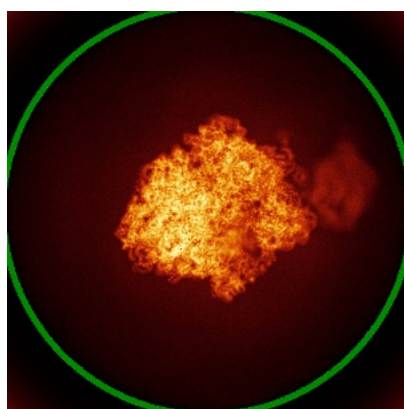


Z Index: 259

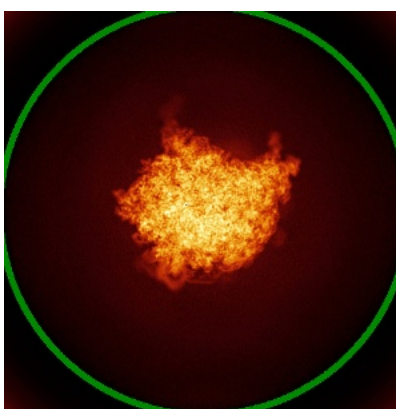
The images above show the largest variance slices of the map in three orthogonal directions.

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

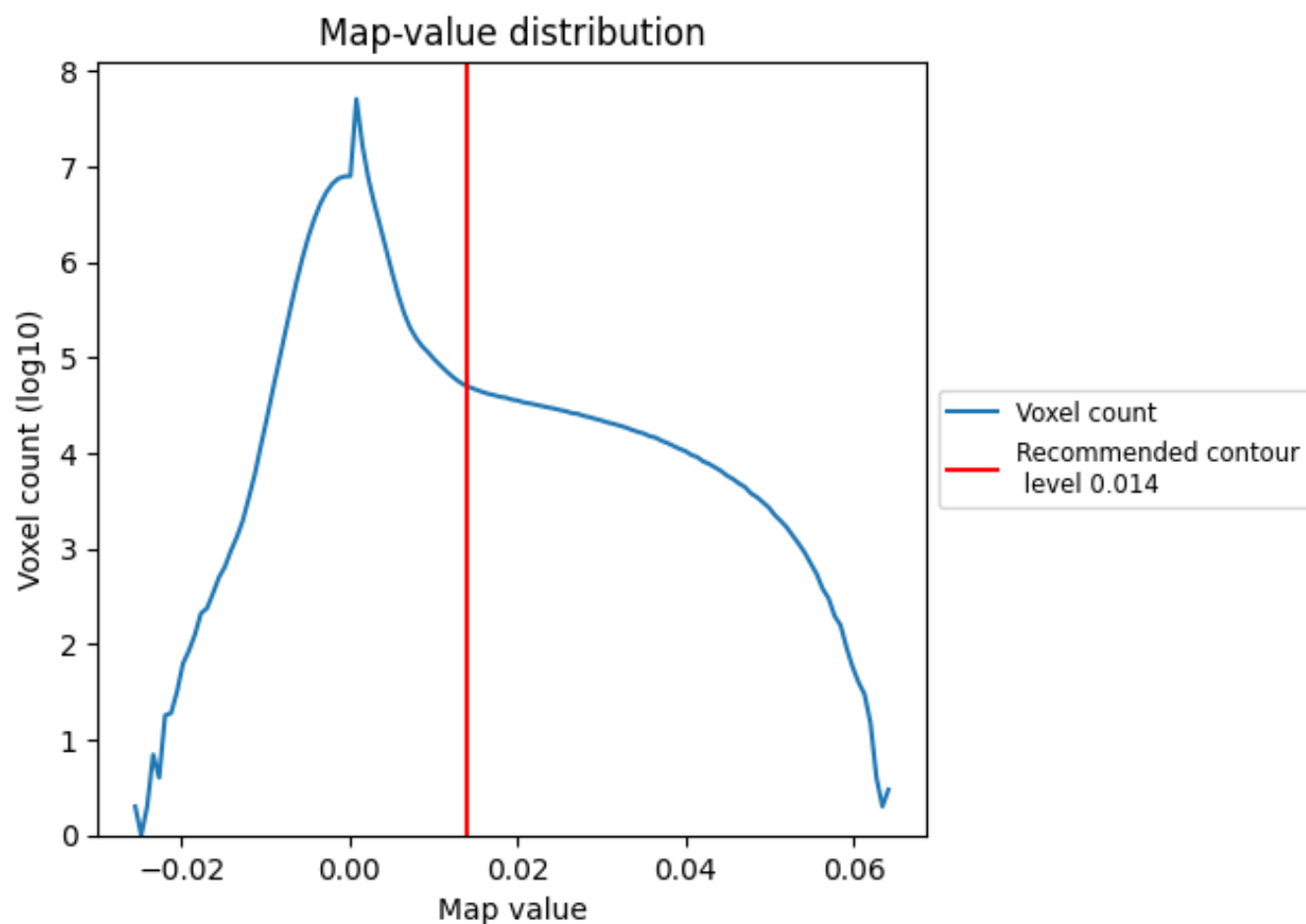
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

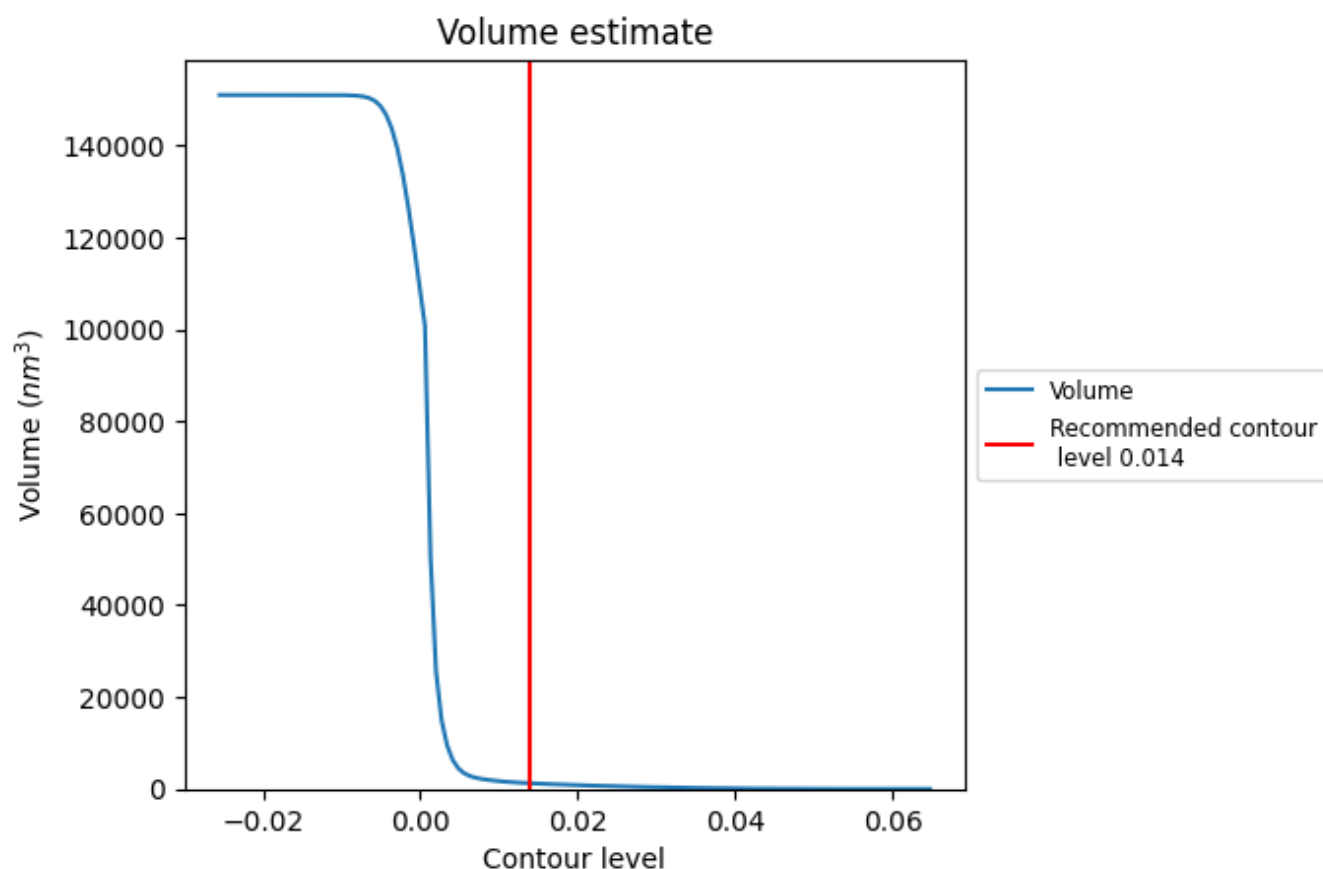
This section contains the results of statistical analysis of the map.

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.

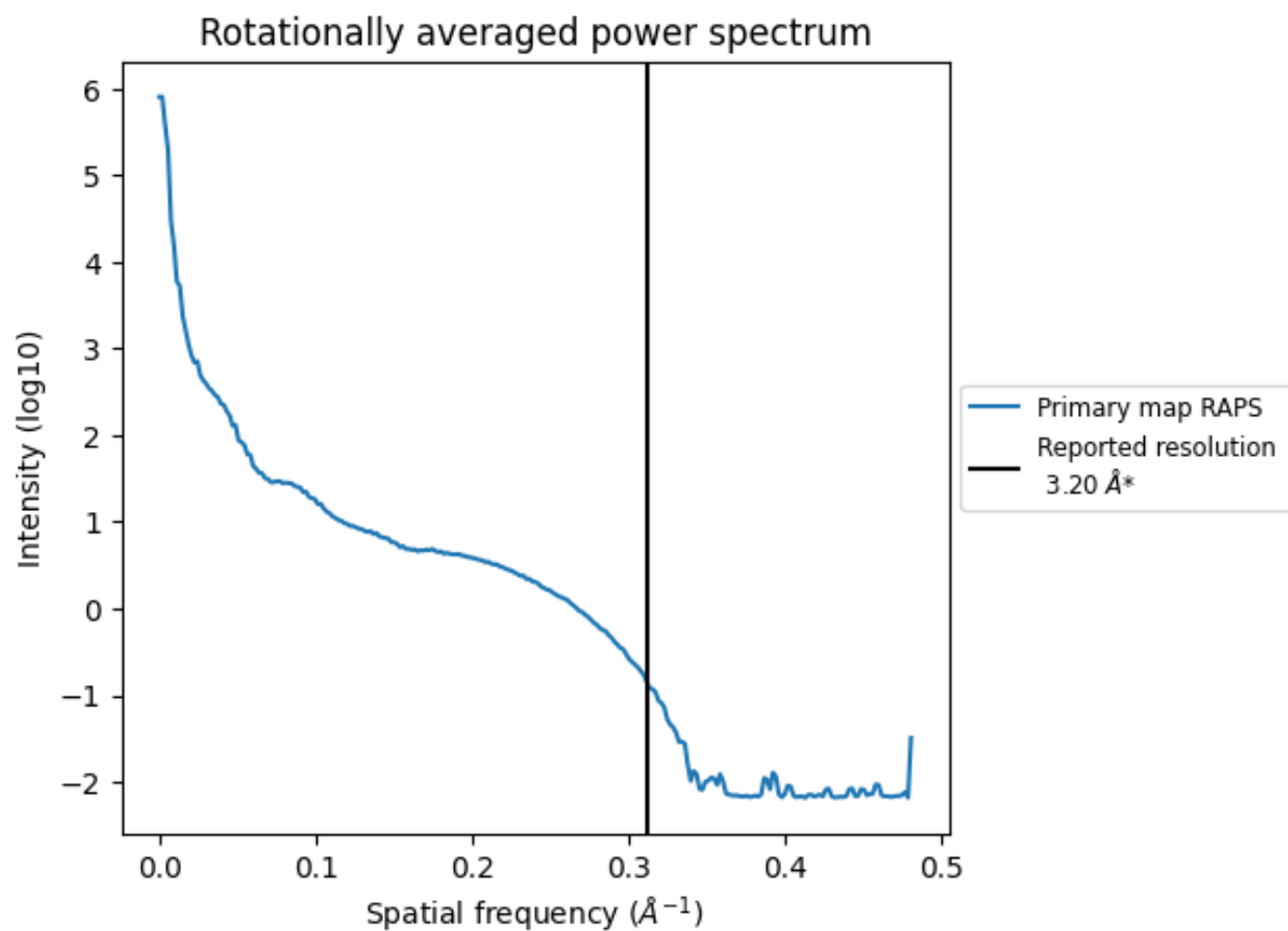
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1238 nm^3 ; this corresponds to an approximate mass of 1118 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 0.312 Å⁻¹

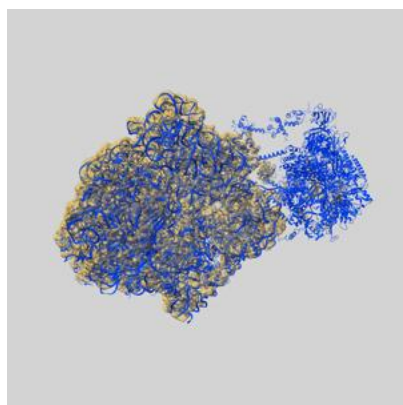
8 Fourier-Shell correlation

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

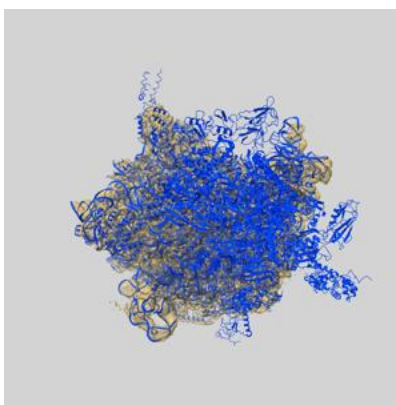
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22082 and PDB model 6X6T. Per-residue inclusion information can be found in section 3 on page 17.

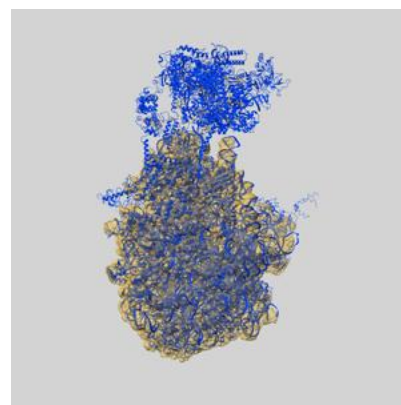
9.1 Map-model overlay [i](#)



X



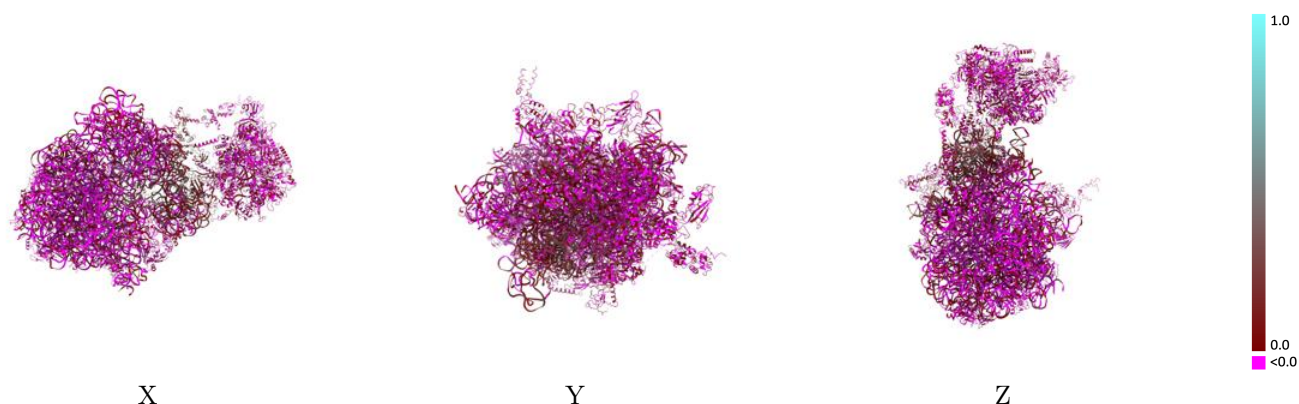
Y



Z

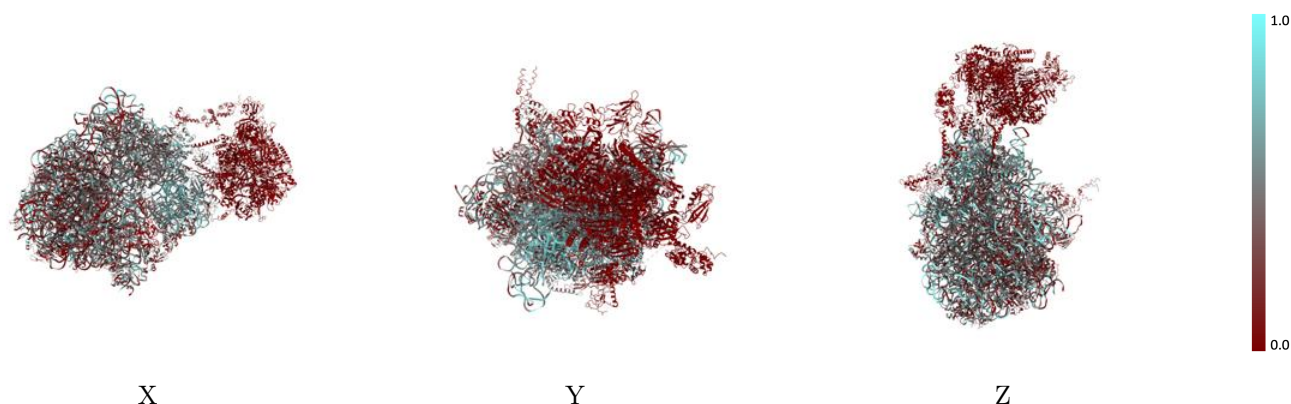
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



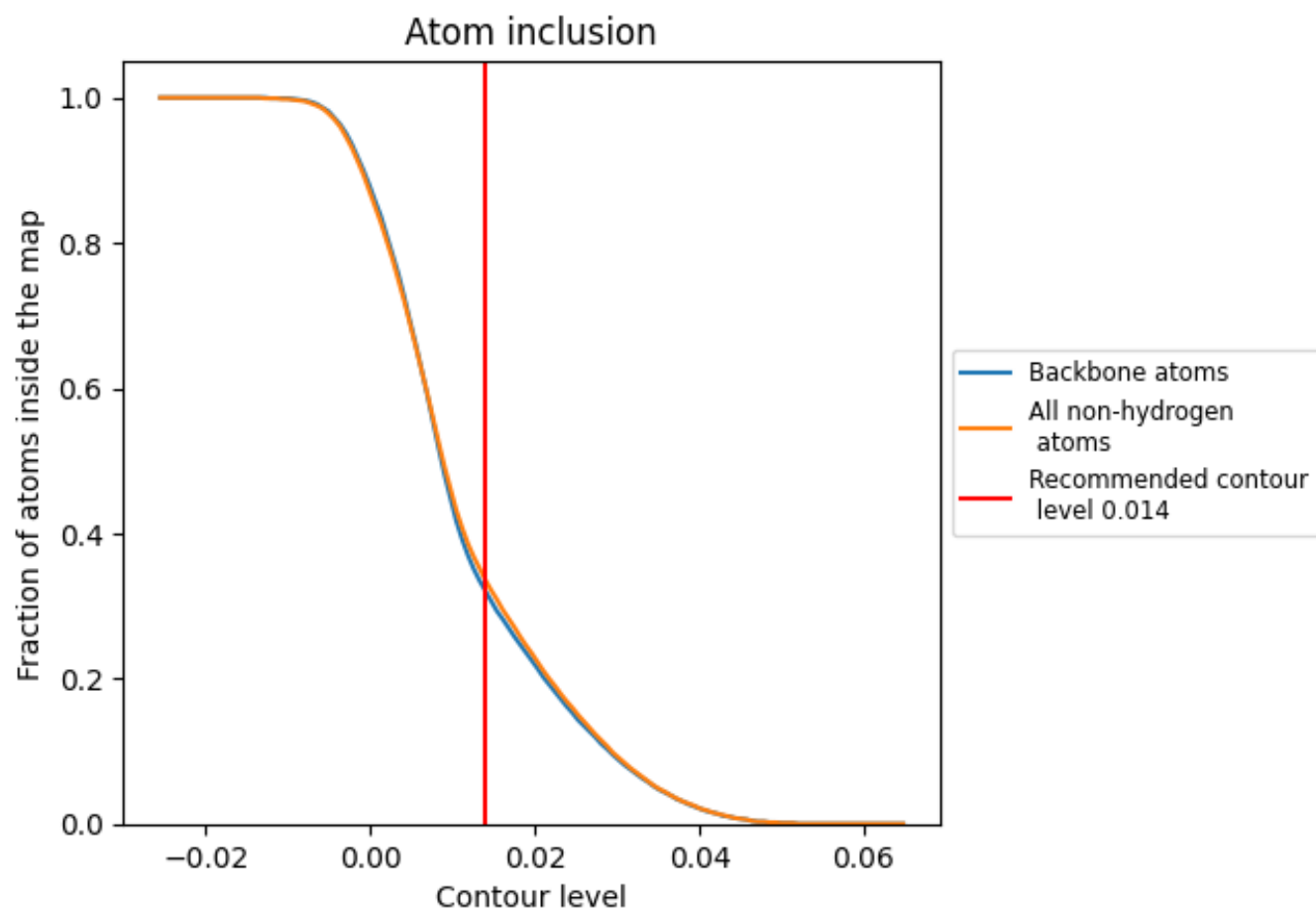
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 34% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3360	 0.0150
0	 0.2720	 -0.0410
1	 0.2300	 -0.0340
2	 0.2890	 0.0050
3	 0.4240	 0.0080
4	 0.3270	 0.0250
5	 0.0250	 0.0380
6	 0.0760	 0.0390
7	 0.1340	 0.0770
9	 0.1540	 0.0020
A	 0.4380	 0.0920
AA	 0.0070	 0.0250
AB	 0.1210	 0.1110
AC	 0.0010	 0.0090
AD	 0.0010	 0.0120
AE	 0.0030	 0.0160
AF	 0.0000	 0.0220
AG	 0.1970	 0.1380
B	 0.4330	 0.0350
C	 0.4020	 0.0440
D	 0.5580	 0.0510
E	 0.2630	 -0.0470
F	 0.3720	 0.1300
G	 0.4710	 0.1440
H	 0.0300	 0.0480
I	 0.5160	 0.2070
J	 0.4130	 0.0240
K	 0.3480	 0.0120
L	 0.3170	 -0.0540
M	 0.5520	 0.2370
N	 0.2880	 -0.0650
O	 0.5360	 0.1620
P	 0.4380	 0.1200
Q	 0.5270	 0.1840
R	 0.2590	 -0.0640



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Chain	Atom inclusion	Q-score
S	 0.4380	 0.1180
T	 0.3040	 -0.0380
U	 0.3090	 -0.0520
V	 0.3730	 -0.0230
W	 0.3460	 -0.0050
X	 0.3550	 0.0100
Y	 0.0340	 -0.0050
Z	 0.0000	 0.0130
a	 0.4330	 -0.0200
b	 0.2620	 -0.0670
c	 0.3560	 -0.0570
d	 0.4860	 -0.0050
e	 0.3520	 -0.0330
f	 0.2960	 0.0030
g	 0.2430	 0.0390
h	 0.2920	 -0.0770
i	 0.3530	 -0.0260
j	 0.2900	 -0.0160
k	 0.3090	 -0.0500
l	 0.2990	 -0.0110
m	 0.3380	 -0.0130
n	 0.2830	 -0.0430
o	 0.3180	 -0.0230
p	 0.2090	 -0.0260
q	 0.2330	 -0.0190
r	 0.2470	 0.0160
s	 0.2660	 -0.0210
t	 0.2770	 0.0020
u	 0.3100	 -0.0260
v	 0.2800	 -0.0150
w	 0.3380	 -0.0330
x	 0.3560	 -0.0420
y	 0.3130	 -0.0130
z	 0.3030	 -0.0140